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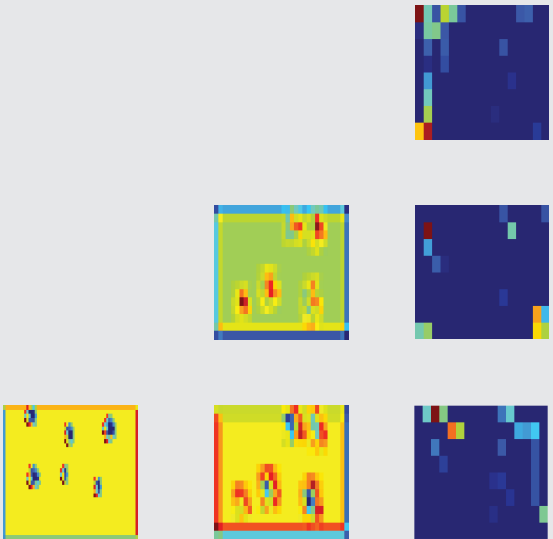

Editor

Xiaoying Zhuang

Preface

In this age of big data, machine learning techniques have been successfully applied in image processing, genomics, financial problems and even medical diagnosis. The emerging application of machine learning and big data analysis has fundamentally influenced and changed our way of how we think, plan, solve and analyze in engineering. Nevertheless, we are faced with many issues and unsolved problems when applying data drive computing and machine learning in engineering analysis.

I have conceived the organization of this conference about two years ago with Timon Rabczuk and Hehua Zhu, the presidents of the conference. Now with the financial support of HORIZON-2020-RISE BESTOFRAC project, the International Conference on Data Driven Computing and Machine Learning in Engineering (DACOMA-19) conference is made possible to take place in Shanghai in September 2019. The conference is co-organized by Tongji University, Leibniz University Hanover, Chinese Society of Computational Mechanics, International Chinese Society of Computational Mechanics, The German Association of Computational Mechanics. This proceeding collects over 100 abstracts from participants of DACOMA-19 presenting research and application in big data technology, data driving computing and artificial intelligence in engineering as well as promoting interdisciplinary topics.

I hope readers will enjoy reading this proceeding and be inspired from this book in their research in this area. I would like to acknowledge Qimin Wang, Minjing Cai, Bin Li and Wei Peng for their help in collecting and organization of DACOMA.

Xiaoying Zhuang
in Shanghai August 2019

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Machine learning based solution of Partial Differential Equations in Computational Mechanics: concepts, implementation and applications

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Abstract: Partial Differential Equations (PDE) are fundamental to model different phenomena in science and engineering mathematically. Solving them is a crucial step towards a precise knowledge of the behaviour of natural and engineered systems. In general, in order to solve PDEs that represent real systems to an acceptable degree, analytical methods are usually not enough. One has to resort to discretization methods. For engineering problems, probably the best known option is the Finite Element Method (FEM). The fundamental idea is to approximate the solution of the PDE by means of functions specifically built to have some desirable properties. In this contribution, we explore Deep Neural Networks (DNNs) as an option for approximation. They have shown impressive results in areas such as visual recognition. DNNs are regarded here as function approximation machines. There is great flexibility to define their structure and important advances in the architecture and the efficiency of the algorithms to implement them make DNNs a very interesting alternative to approximate the solution of a PDE. We concentrate in applications that have an interest for Computational Mechanics. Most contributions that have decided to explore this possibility have adopted a collocation strategy. In this contribution, we concentrate in mechanical problems and analyze the energetic format of the PDE. The energy of a mechanical system seems to be the natural loss function for a machine learning method to approach a mechanical problem. As proofs of concept, we deal with several problems and explore the capabilities of the method for applications in engineering.

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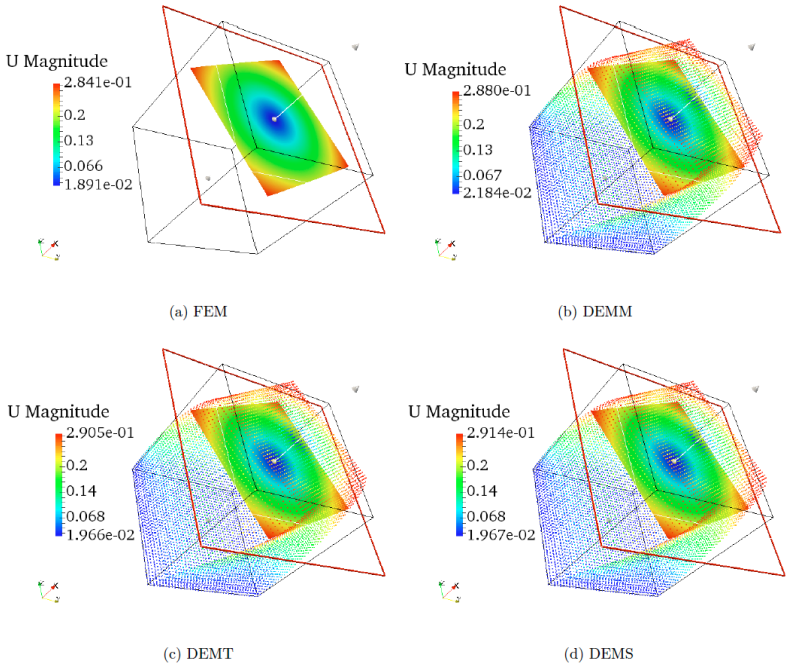

Figure 1. A comparison of displacement magnitude at the CDEF plane between reference solution and deep energy method of a twisted Neo-Hookean 3D Cuboid.

Keywords: Deep energy method; Energy approach; Physics informed; Machine learning; Partial differential equations; Hyperelastic model;

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Machine Learning for Seawall Structures Under Flooding and Erosion

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Abstract: Climate change has been changing in a harmful way to human life for recent years. Especially, the global average surface temperature has been highly increasing with a disturbing trend. It causes negative effects on our planet such as frequently occurring flood and hurricane with very high intensity in some area, but others had a long period of drought. Additionally, the most dangerous effect of global warming is the high rate of melting a glacier and sea ice at both the Earth's North and South poles leading to the sea level risen dramatically threatening to many countries located near coastlines. There are many fatal effects of increasing sea level. For example, the vanishing of various lands on the world map or a lot of infrastructures close to shorelines have been destroying because of the erosion. Therefore, researching and developing advanced methods for the resistance of flood and erosion is an urgent task. Especially, the monitoring heath structure field can help to control the safety of a complex structure to estimate any severe collapses. In this study, a hollow concrete block (HCB) used to prevent coastal erosion has been designed [1, 2]. Furthermore, machine learning has been applied to this design to predict an existed damage inside the model with a variety of fiber concrete material properties considered. Due to the lack of experiment data, the numerical simulations were employed to generate many datasets from the HCB model (see Figure 1).

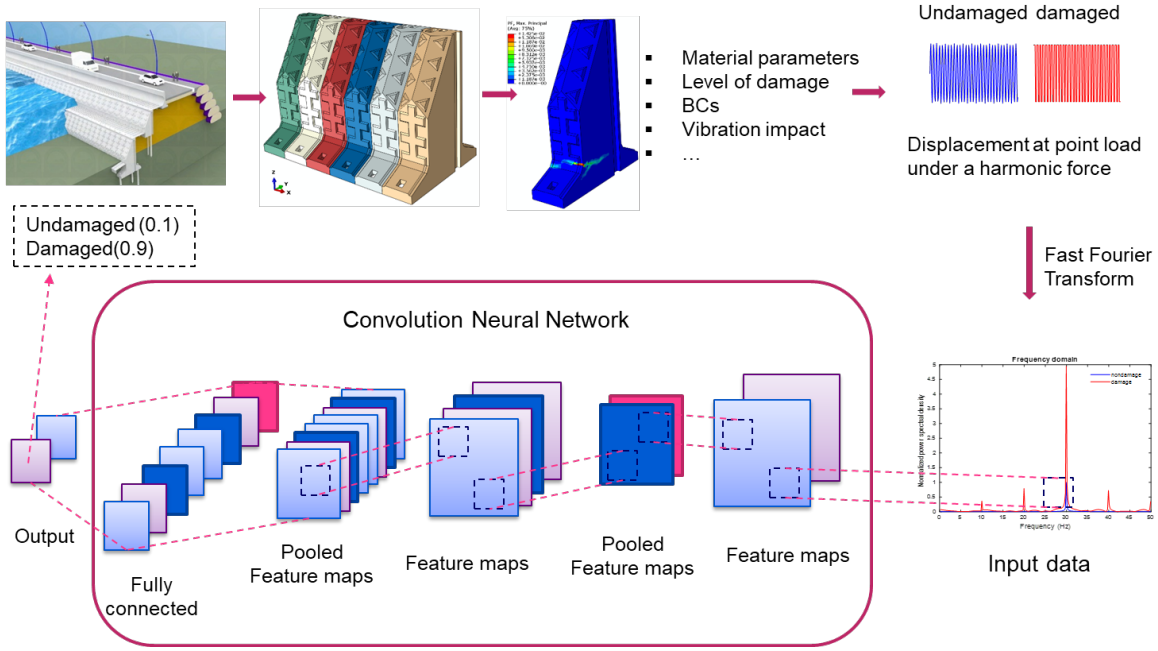

Figure 1. Framework of CNN for predicting damage of a hollow seawall block.

By changing many cases of boundary conditions and load directions on the HCB model to cover all situations can exist in a real seawall structure. Each dataset was obtained from two HCB models, one of them was acquired from an undamaged structure, while the other was obtained from a damaged one by applying a static load enough to make a random failure inside it. A harmonic load was applied to these models. Then a load point displacement with respect to time was collected as an output signal. This signal was switched to the frequency domain by employing Fast Fourier Transform [3]. Prior to putting the treated signal into Convolution Neural Networks (CNNs) [4], the

signal was normalized and extracted a two-dimensional matrix which contains values one and zeros where the value one presents a curved of the output signal. The dataset then was trained by CNNs to classify which signal is come from a damaged or undamaged model. The result shows that this method can predict accurately an existed failure inside the HCB model. By applying this method to the real seawall structures, we can predict which HCB should be fixed or replaced before all structure may be collapsed as shown in Figure 1.

Keywords: seawall structure, fibre reinforced concrete, damage modelling, vibration-based damage detection, machine learning, convolution neural network.

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Data-driven Construction and Maintenance of Urban Tunnels

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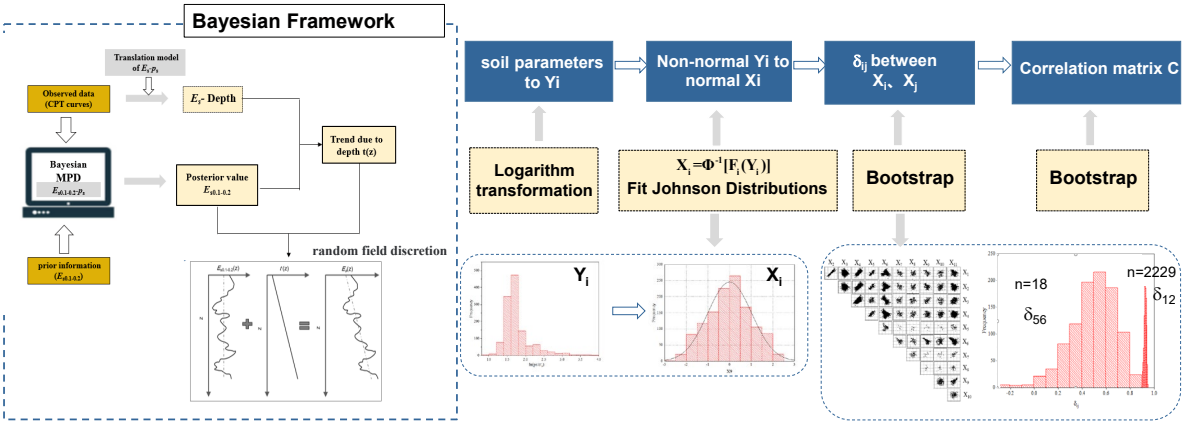
Abstract: With the development of structure health monitoring (SHM) and geotechnical testing techniques, huge amounts of data are collected from the design, construction and maintenance period of urban tunnels. To face the challenge of data explosion and data effective utilization, quite a number of data analysis methods from the grey system, time series to modern machine learning based algorithms have been paid much attentions to. 3 major cases are taken to illustrate the application effect of machine learning approach in the lifetime of urban tunnels:

(1) Shanghai clay database is compiled and learned for characterization of spatial variability and transformation uncertainty. It could help for the reliability-based design of tunnel structures.



(a) (b)

Fig. 1 Machine learning based estimation of soil properties: a) soil compressive modulus; b) multi-variate distribution of soil parameters.

(2) ML algorithms (ANN, SVP, GBR) are employed to predict the shield machine posture during the construction period. Based on the trained prediction models, construction parameters are optimized to make a better control of tunnel settlement.

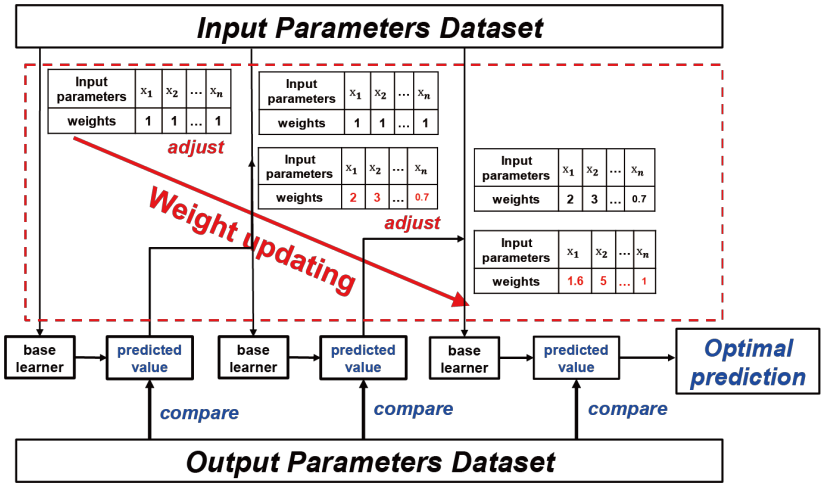


Fig. 2 Gradient boosting regression based shield tunnel posture prediction

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(3) Multi sensor data are fused using the extended Kalman filter (EKF) method for a better understanding of unknown parameters. Then an integral safety assessment is conducted based on the predicted parameters.

The study shows ML has a great prospect and can solve complicated issues in Geostructural system field.

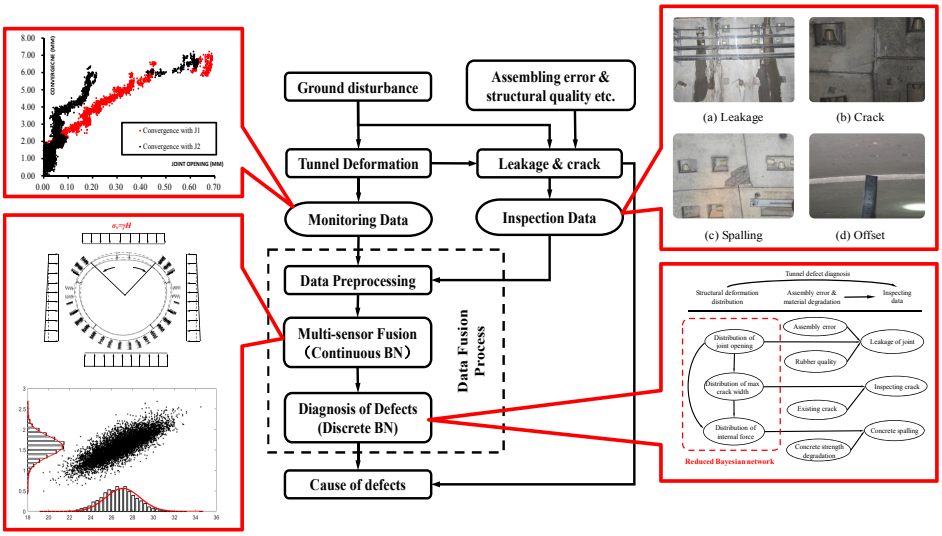

Fig. 3 Framework of dynamic tunnel structual safety assessment based on Bayesian network

Keywords: Structure Health Monitoring, Data driven construction and maintenance; Data fusion process; Machine Learning.

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Solving direct and inverse computational engineering problem through a deep learning based data-driven method

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Abstract: With the steady development of computer science, machine learning and data science have made significant progress in recent decades. These techniques generally rely on a substantial amount of data samples to extract the abstract mapping hidden within the data. Hence, these technologies have gradually attracted the attention of researchers in the field of computational mechanics and computational engineering. This paper aims to interpret several forms of applications that integrate machine learning and data science with computational mechanics and computational engineering problems. In the first application, the core algorithm of the convolutional neural network is implemented to solve the linear elastic finite element problem. A standard finite element equation is transformed into an optimization problem in this method. The method is verified by a plane strain linear elastic finite element problem. The method demonstrates promising accuracy by comparing the results obtained by traditional finite element solver. In the second application, a method is proposed to establish the implicit mapping between the effective mechanical property and the mesoscale structure of heterogeneous materials. Shale is employed in this paper as an example to illustrate the method. At the mesoscale, a shale sample is a complex heterogeneous composite that consists of multiple mineral constituents. The mechanical properties of each mineral constituent vary significantly, and mineral constituents are distributed in an utterly random manner within shale samples. Large quantities of shale samples are generated based on mesoscale scanning electron microscopy images using a stochastic reconstruction algorithm. Image processing techniques are employed to transform the shale sample images to finite element models. Finite element analysis is utilized to evaluate the effective mechanical properties of the shale samples. A convolutional neural network is trained based on the images of stochastic shale samples and their effective moduli. The trained network is validated to be able to predict the effective moduli of real shale samples accurately and efficiently. Not limited to shale, the proposed method can be further extended to predict effective mechanical properties of various heterogeneous materials. In the third application, assisted by image-based finite element analysis and deep learning, a data-driven approach is proposed for designing phononic crystals. An auto-encoder is trained to extract the topological features from sample images. Finite element analysis is employed to study the band gaps of samples. A multi-layer perceptron is trained to establish the inherent relation between band gaps and topological features. The trained models are ultimately employed to design phononic crystals with anticipated band gaps. Not limited to this material, the proposed method could be further extended to design various structured mechanical materials with specific functionalities.

Keywords: Computational engineering, computational mechanics, deep learning, finite element analysis, inverse problem.

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An investigation of deep learning in predicting shield tunnel excavation parameters

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Abstract: Shield tunneling construction method in a popular technology in building urban infrastructures. For practitioners, optimizing shield tunnel driving parameters and reducing ground settlement induced by construction is a major objective, especially in highly populated urban areas. Traditionally, calibrating shield tunnel driving parameters is a try-and-error process with high cost, and it depends largely on past experiences. In this study, we investigated the adoption of deep learning model, LSTM, in predicting shield tunnel construction parameters. The investigation data is collected from the construction of a shield tunnel in shanghai urban areas, and totally 1,387 rings of construction parameters are recorded. The construction parameter is first treated as one-dimensional time series data, and LSTM is used to predict each construction parameter separately. The LSTM prediction is compared with autoregressive integrate moving average model (ARIMA). Results show the maximum errors of LSTM and ARIMA prediction are 12% and 23%, respectively. Then, for construction under normal circumstances, the curvature, slope and depth of the tunnel are taken as input of the deep learning model to predict the driving parameters. For construction which crosses existing buildings, foundation types, building structure types, current building conditions, and ground conditions are taken as additional input to predict the driving parameters. Results show that the maximum prediction errors for normal circumstances and crossing situation are 9% and 12%, respectively. This study shows that deep learning is a very promising method in predicting shield tunnel construction parameters. The predicting accuracy could be very high even in very complicated situations such as crossing existing buildings.

Keywords: Shield tunnel, construction parameters, deep learning, LSTM.

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The application of a deep energy method in the bending and eigenvalue analysis of Kirchhoff plate

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Abstract: In this article, a deep energy method is proposed for the bending and eigenvalue analysis of Kirchhoff plate. As is known to all, deep learning has recently become a central and popular branch in research and applications, such as image processing, object detection, finance and even engineering [1], due to its potential in nonlinear processing of data with multiple hidden layers in supervised or unsupervised learning. As for the application of deep learning in civil engineering [2], there are three major approaches including the solving of PDEs with deep learning [3, 4], the surrogate of FEM by deep learning [5], and the studying of data-driven problems in engineering such as liquefaction with deep learning [6-8]. And in this article, we further broaden the scope of solving PDEs with deep learning. Instead of focusing on a dataset of targeted solutions, we directly deploy a deep feedforward neural network to discover those physical patterns involved in a certain mechanical phenomenon. Virtually, many engineering problems and natural science are governed by partial differential equations, revolving engineering mechanics [9-13], rock and soil engineering [14-22] et al.. Many classic analytical and numerical methods have been proposed and discussed to solve those problems, especially after the blossoming of computer technology, such as separation of variables, lie group method, semi-analytical methods, numerical methods, et al. After the birth of artificial neural network method, it was also applied in solving those PDEs, but did not show excellent performance until recently. With improved algorithms in computer science, advanced computer hardware, and more accessible data from Internet, deep learning, which is based on a deep neural network set, has shown favorable features that can be applied in solving partial differential equation. Moreover, our research group has observed that the deep neural networks can be further applied to unveil those physical patterns laying behind some physical problems by placing a deep neural network prior on field variables. A neural network severs as universal function approximators here [23], including computational graphs and backpropagation algorithms involved in deep learning. Unlike previous applications in directly dealing with governing equations, the deep energy method, which combines a deep learning technique with the energy minimum principle, has been established in a unified framework for solving this higher-order problem. The whole procedure begins with generating randomly distributed collocation points in the physical domain, as a result of which this method turns out to be truly "Meshfree". Then a loss function is built with the aim that the total potential energy is minimized at those collocation points. The L-BFGS optimizer is adopted to backpropagate the loss function and train the whole model. It needs to be emphasized here that, to better reveal its physical patterns, an autoencoder is added to the deep feedforward neural network and a premium layer and neuron configuration is discussed in this article. As for the activation function choice, different schemes indeed have an impact on the accuracy and efficiency of this deep energy method. Accordingly, a tailored activation function based on analytical solution is adopted here and compared with classical tanh activation function, which is proven to be a better choice. In this way, the constructed deep neural network can approximate deflection in Kirchhoff bending problems, where the C^1 continuity requirement has posed significant difficulties in traditional mesh-based methods. However, this can be solved in the framework of DEM, where the deep neural network can be deployed to approximate the transversal deflection. The DEM can be also suitable for the eigenvalue analysis of structures, where a different formulation of loss function is adopted. Once the neural network is trained, it can be efficient and accurate implemented to predicted deflection and stress in the whole physical domain. Numerical examples have demonstrated that the proposed DEM can be suitable for the bending and eigenvalue analysis of Kirchhoff plate, which ushers in a new scheme for the mechanical analysis of structural components in engineering.

Keywords: Deep learning, Deep energy method, Autoencoder layer, Activation function, Kirchhoff plate.

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Isogeometric analysis of a phase field model for simulating electromechanical behavior and morphological evolution of vesicles

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Abstract: In this paper, we develop a phase field model for a vesicle in an electrical field. We aim to obtain the morphological evolution of the system by solving it using Isogeometric analysis. Both mechanical and electrical aspects have been considered, such as elastic bending energy, flexoelectricity, dielectricity, osmotic pressure and surface tension. An energy functional represents the system is reformulated using a phase field variable, which produces a fourth-order PDE. This PDE is highly nonlinear with moving boundaries. Solving fourth-order PDEs without the need to introduce additional degrees of freedom or using mixed-formulation necessitate basis functions that are piecewise smooth and globally C1 continuous. Isogeometric analysis possesses the capability of introducing smooth C1 globally-continuous basis functions using B-splines. The primal variation of the energy functional is obtained from which a weak form of two primary variables is formulated. The model has axisymmetric configurations for which the morphological evolution of the vesicle is obtained. The results demonstrate the robustness of the phase-field model in conjunction with IGA to solve fourth-order PDEs without the need to introduce additional mathematical complexities. The effect of the mechanical-electrical coupling, electrolytes within the vesicle and outside, the flexoelectricity and the dielectricity are examined in details.

Keywords: Isogeometric Analysis, Phase-Field, Helmholtz Free Energy, Mechanical-Electrical coupling, Vesicles, Cell membrane.

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Exploration signals from higher dimensions base on machine learning

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Abstract: New technologies have enabled measurements on additional levels of the gene expression processes.The use of high-throughput technologies for finding reliable combinations poses new challenges [1]. First, in contrast to standard blood values,patient data based on high-throughput technologies are not commonly available in hospitals. This means, they have to be generated separately. Secondly, although the prices for generating data from high-throughput technologies are constantly decreasing, it is still quite expensive and time-consuming to carry out these experiments. This implies high costs for such data. The advantage and the curse at the same time is that such experiments easily yield thousands or even far beyond 10,000 possible candidates for signal. The sample size in expensive pilot studies is usually very limited, sometimes less than 20. From a machine learning or classification point of view one then tries to derive a classifier from a data set with more than 1000 candidates and perhaps only around 20 or 30 instances. Finding random associations and overfitting is therefore difficult to avoid. An essential step for the construction of a classifier is feature selection (selecting a subset from the candidates) and sometimes feature extraction (defining new scores based on the given candidates) [2,3]. A large number of methods for feature selection and extraction has been developed within machine learning. However, these techniques are usually not tailored to the typical setting of signals, where the number of features is usually very large and the number of cases (donors, mice…) is often very limited. The study aims at adjusting state-of-the-art and developing new feature selection and extraction methods.

Keywords: Machine learning, High-throughput technologies, Gene, Feature selection.

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Volumetric parametrization using convolution neural networks

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Abstract: Currently, the usage of convolution neural networks (CNNs) for image processing has gained wide-spread attention. The advantage of CNN is that it is capable to handle all the details, including the fine details of given images [1]. Here, we present an approach for using a CNN for converting a given voxel-based images to analysis suitable volumetric meshes. There is rich a literature on approaches for volumetric meshes generation. The results are, however, highly dependent on the expertise of user. Therefore, it would be appealing to use machine learning for volumetric mesh generation. For a given voxelized image, we propose to use the B-Spline filters as the convolution layer of CNN for geometry features identification. The advantage of using B-Spline filters is that the obtained volumetric parametrization is described in a standard CAD format and can be directly used for analysis using an isoparametric approach [2]. We validate the creation of volumetric meshes using simple models such as square and sphere, and further use it for robust learning of other shapes. We show the efficiency of our approach through the implementation of volumetric parametrization and analysis on benchmark and real-world problems.

Keywords: Convolution neural networks, Volumetric parametrization, B-Spline filters.

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Boundary Shape Identification of the Heat Conduction Problem Based on Machine Learning

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Abstract: The development of machine learning has been highly motivated with the advancement of computer science [1,2]. In this paper, machine learning is proposed to solve the boundary shape identification of the heat conduction problem by the measured temperature on the surface. The heat conduction problem with irregular boundary shape and constant thermal conductivity is transformed to the regular boundary shape with variable thermal conductivity by the modified one-dimensional correction method [3]. Then the problem is transformed to identify the thermal conductivity. Compared to the traditional methods, the proposed method can avoid remeshing the domain. The relationship between the measurement temperature and the thermal conductivity is established through the finite element calculations and machine learning. The thermal conductivity of the heat conduction problem is successfully identified by a convolutional neural network based on the measured temperature. After that the unknown boundary shape is evaluated. The influences of measurement point numbers and measurement errors upon the inverse results are also investigated [4,5]. Numerical examples show that the proposed method can reconstitute the unknown boundary geometry shapes effectively. With the increase of measurement point numbers and the decrease of measurement errors, the inverse results are more accurate.

Keywords: Inverse problem, Identification of the boundary geometry shape, Finite element method, Deep learning, Modified one-dimensional correction method.

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Free vibration analysis of Timoshenko nanobeam using differential transform method and general nonlocal theory

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Abstract: Most scientific problems in science and engineering fields can be defined by the partial differential equations. A diversity of analytical and numerical approaches has been established to achieve precise estimated solutions for the problems in the literature. The Differential Transform Method (DTM) is one of the semi-analytical techniques to many problems. This approach is expedient to attain the solutions of linear and nonlinear differential equations. There is no requirement to linearization or discretization. Large computational work and round-off errors are evaded. The exact solution cannot be found or is hard to find for problems of complex nature. In such cases, approximation approach is used. But, the exact solution can be attained by employing DTM, even for the complex problems.

Application of nanomaterials have been extended and induce interest among the scientific communities in the area of physics, engineering and nanotechnology. Nanomaterials play very important roles in numerous nanoelectromechanical systems. Among these, beam kind structures show a vital role in the field of nanotechnology. Beam type structures are generally exploited in mechanical, aerospace and civil engineering. Continuum mechanics are classified into classical and nonclassical continuum mechanics. Wang and Hu [1] stated that the classical theory are not able to expect the decrease in phase velocities of wave propagation in a carbon nanotube when the wavenumber is so large. Hence several nonclassical continuum theories such as strain gradient theory, couple stress theory, micropolar theory and nonlocal elasticity theory have been neestablished to integrate size effect by introducing an intrinsic length scale. Among these theories, nonlocal elasticity theory suggested by Eringen [2] has been extensively used in the vibration and static response of nanobeams. Reddy [3] examined analytical solutions for numerous beam theories like Euler–Bernoulli, Timoshenko, Reddy and Levinson in case of simply supported boundary condition. Shaat and Abdelkefi [4] showed that Eringen's nonlocal theory is useless to fit the dispersion curves of some materials. In order to remove this problem of Eringen's nonlocal theory, a general form of the nonlocal theory was suggested [4]. In this work we use this theory for modeling of nonlocal Timoshenko beam. This general nonlocal theory is recognized with considering different attenuation functions for the existing material moduli.

This work serves a semi analytical-numerical approach called DTM is used to study static and free vibration of nanobeams corresponding on nonlocal-Timoshenko beam theory. The governing equations of motion a Timoshenko beam is transformed to a set of simpler algebraic revolving equations by means of DTM. Then solving the transformed equations and employing a procedure of inverse transformation to attain precise mode frequency and displacement

Keywords: Differential Transform Method**,** Nonlocal Timoshenko beam, Free vibration analysis, General nonlocal theory.

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Data-Driven Simulation of History-Dependent Materials Using Structured Data Sets and Transition Rules

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Abstract: Data-driven computational mechanics replaces phenomenological constitutive functions by data sets in stress-strain space. The distance of modeling values, e.g. stresses and strains in Gauss-points of a finite elements calculation, from the data set is then minimized with respect to an appropriate metric, subject to equilibrium and compatibility constraints, see [1]. While this approach works well for nonlinear elasticity, there are problems when dealing with history-dependent materials, because the same point in stress-strain space might correspond to different material behavior. In [2], this issue is treated by including local histories into the data set. There however, it is still necessary to include models for the evolution of internal variables. Thus, we speak about a mixed formulation consisting of a combination of classical and data-driven modeling.

In the approach presented here, we solve this issue by augmenting the data set by directions in the tangent space of the specific points in stress-strain space. Moreover, we divide the data set into subsets corresponding to different material behavior, e.g. elastic versus inelastic or loading versus unloading. Based on this subdivision, we introduce transition rules mapping the modeling points to the various subsets. We demonstrate the operability of the proposed approach by applying it to a model of small strain elastoplasticity with isotropic hardening.

Keywords: Data-driven, History-dependence, Structured data sets.

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Artificial neural networks for solving coupled PDEs in flexoelectricity

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Abstract: In this study, a neural network is introduced to approximate solutions for a coupled model of flexoelectric materials. Flexoelectricity is an electromechanical model of piezoelectric structures [1, 2] associated with strain gradients typically involved with the effect of micro-structures, reported in Refs. [3, 4, 5, 6, 7, 8]. Therefore, computation of such models does not only solve the coupled problem of mechanical and electrical behaviors but also deals with high-order differentiation. The concept of using neural networks for integrated models of flexoelectricity is based on the algorithm of meshless method which the computational domain is discretized by collocation points instead of using meshes. The energy function is accordingly constructed from mathematical definition of equilibrium equations as well as kinematic equations. The deep neural network is applied to minimize the total energy function to find the approximation solution. This technique, discussed in [9, 10, 11] is also called by *Deep Energy Method* (DEM). The DEM has provided remarkable advantages of modeling coupled models with high computational accuracy and efficiency in comparison with conventional finite element approaches.

The implementation of DEM is based on the built-in library of *Tensorflow*. A 2D flexoelectric cantilever beam is taken into the modeling of electromechanical behaviors, subjected by mechanical and electrical loading. The energy function of the flexoelectric model is reported in Refs. [3, 12]. A neural network is established with two inputs represented for coordinates of collocation points and three outputs represented for mechanical deformations in x and y-direction and the electric potential ϕ. The architecture of the neural network is also illustrated in Figure. 1. In this deep neural network, the hyperbolic tangent function (*Tanh*) is chosen to be the activation function for hidden layers.

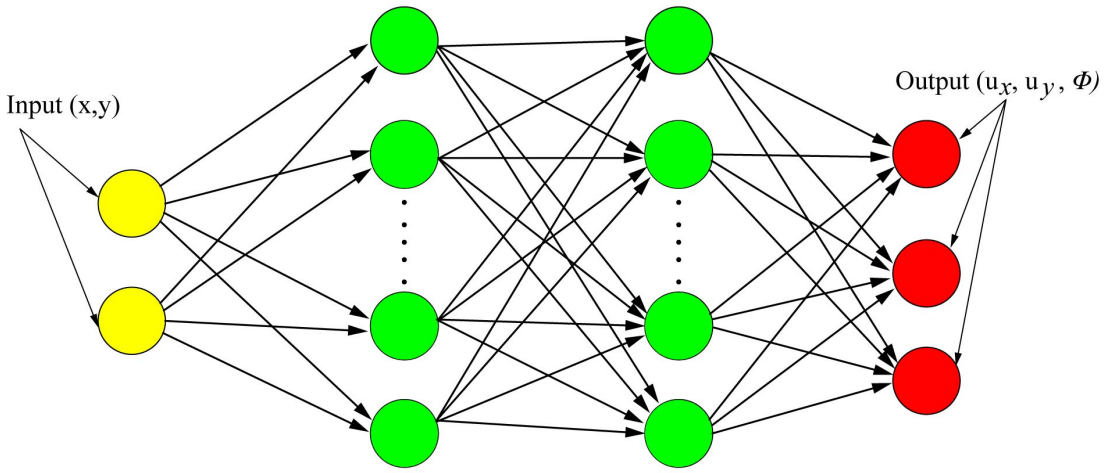

Figure 1: The architecture of the neural network for flexoelectric model

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The process of seeking solution is to learn a network, or in other words to learn iteratively by updating parameters of the neural network $\boldsymbol{\theta}$ such that the sum of the energy function and the squared error of boundary conditions is minimized. Minimizing the energy function is involved in derivatives of outputs with respect to their inputs, and therefore the gradient of the neural network's parameters is also defined by using gradient techniques. The LBFGS is applied for training purpose in this study.

Keywords: Neural networks, Deep energy, Finite elements, Partial differential equations, Collocation method.

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Nonlinear mechanical behavior and failure mechanism of three-dimensional complex carbon nanotube networks

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Abstract: The coarse-grained (CG) potentials of single-walled carbon nanotubes (SWCNTs) were developed in our previous work [1]. However, these CG potentials can only be used to exactly obtain the linear mechanical properties of the carbon nanotube networks (CNNs) without crosslinked CNTs but not the nonlinear mechanical properties of CNNs with crosslinked CNTs, because the quadratic CG stretching and bending potentials are only considered in the CG bonded potentials, where the full-atom harmonic potentials of CNTs are only considered. To design and assemble CNT-based flexible nanodevices in practical applications, the nonlinear mechanical behavior and failure mechanism of CNNs are extremely important and necessary. In this study [2], the explicit expressions of the chirality-dependent high-order nonlinear CG stretching and bending potentials in the CG bonded potentials are systematically established based on the full-atom Morse potential and the Reactive Empirical Bond-Order (REBO) interatomic potential of second generation, respectively. In particular, the CG non-bonded potentials are improved by using the 18-24 Lennard-Jones (LJ) potentials. By comparison with the full-atom molecular dynamics (MD) simulations and our analytical results, the present nonlinear CG potentials have high accuracy. The obtained nonlinear CG potentials can be used to efficiently characterize the nonlinear mechanical behaviors of CNNs with crosslinked CNTs under different loading conditions at minor computational cost.

Keywords: Nonlinear, Coarse-grained potentials, REBO potential, Carbon nanotube networks.

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Designing phononic crystal with anticipated band gap through a deep learning based data-driven method

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Abstract: Phononic crystal is a type of artificial heterogeneous material constituted by a periodic repetition of cells. This characteristic of phononic crystals provides a possible solution to the accurate manipulation of acoustic and elastic waves. For this reason, phononic crystal is of application potentials in vibration and noise reduction, filtering, acoustic lens, acoustic imaging, acoustic stealth, etc. It is thus of significance in the fields of information, communication, medical, and military applications. To design phononic crystal with anticipated manipulation characteristic has become a research hotspot in recent years. Though, to accurately manipulate acoustic and mechanical wave is still a major challenge for existing designing approaches. Hence, assisted by image-based finite element analysis and deep learning, a data-driven approach is proposed in this study for designing phononic crystals. In this approach, a generative deep learning model is trained to establish the inherent relation between frequency bands and phononic crystal topologies; a stochastic modeling method is investigated to generate stochastic samples with novel topologies. Image-based finite element analysis is developed to study the frequency bands of stochastic samples. The topologies and frequency bands of the stochastic samples are employed to expand the knowledge database of the deep learning model. The model is ultimately employed to design novel phononic crystals with designated frequency band features. Not limited to phononic crystals, the proposed method can be further extended to design various structured mechanical materials with specific functionalities.

Keywords: Material design; phononic crystal; band gap; deep learning; finite element analysis.

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A comparative study of machine learning methods applied to the singular integrals in the boundary element method

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Abstract: Accurate and efficient evaluation of singular integrals and nearly singular integrals is of crucial importance for successful implementation of the boundary element method (BEM) [1]. The singular integrals arise when the source point is located on the element of integration. In this case, the value of the integrand is infinite when the source point and the field point coincide. Some methods, such as coordinate transformation [2], have to be adopted to remove singularities. The nearly singular integrals arise when the source point is close to but not on the element of integration. They are difficult to be evaluated using the traditional Gaussian quadrature rules because the value of the integrand varies dramatically as the source point approaches the element. Element subdivision [3] is one of the most widely used methods for evaluating nearly singular integral. Compared with regular integrals, these two kinds of integrals require a large number of Gauss points to obtain accurate integral results. The computational time is considerable when there are many singular integrals and nearly singular integrals in the computational model.

This paper describes a method to evaluate the singular integrals and nearly singular integrals by using machine learning methods. In the data preparation phase, a large number of integration samples are collected in the local coordinate system. The element shapes and the source point positions of these samples are varies. It should be demonstrated that the original integrand can't be used directly for computing the training samples, because the value of the fundamental solutions in the integrand is related to the coordinates of the points in the global coordinate system. However, the samples can only be calculated in the hypothetical local coordinate system in the data preparation phase. In this paper, the formulas of the fundamental solutions are divided into several sub-formulas. The integral value of each sub-formula can be converted from the local coordinate system to the global coordinate system, as long as the coordinate transformation matrix is obtained. In the training phase, the coordinates of the element nodes and the source points are treated as input variables. The element integral matrices computed are treated as output variables. Some classical machine learning methods [4] for regression problems including Extreme Learning Machine (ELM) [5], Gaussian Process Regression(GPR), K-Nearest Neighbor (KNN), Support Vector Regression(SVR) and Regression Tree(RT) are adopted to training the samples and their performances are compared. In the application phase, the predictive model produced in the training phase is implemented on the numerical quadrature process of the boundary element analysis code. For nearly singular integrals and singular integrals, the element integral results are obtained directly by the predictive model. Traditional Gaussian quadrature process is omitted. For the regular integrals, accurate results can be obtained using traditional Gaussian quadrature.

The fundamental solutions of elastostatics are taken as example to derive the sub-formulas and compute the integral samples. Linear quadrilateral elements are used as integral element. Other types of element can be trained using the same method. The results of one of the test sets are shown in Fig. 1. The Fig. 1(a) and Fig. 1(b) represent the test results of singular integrals and nearly singular integrals respectively. The mean relative errors(MRE) of the results of the machine learning methods are listed in the Table 1. It can be observed that the predictive results of all of the methods are in good agreement with the test results. For the singular integral, ELM and GPR are more outstanding than other methods. For the nearly singular integral, SVR and ELM are better than other methods.

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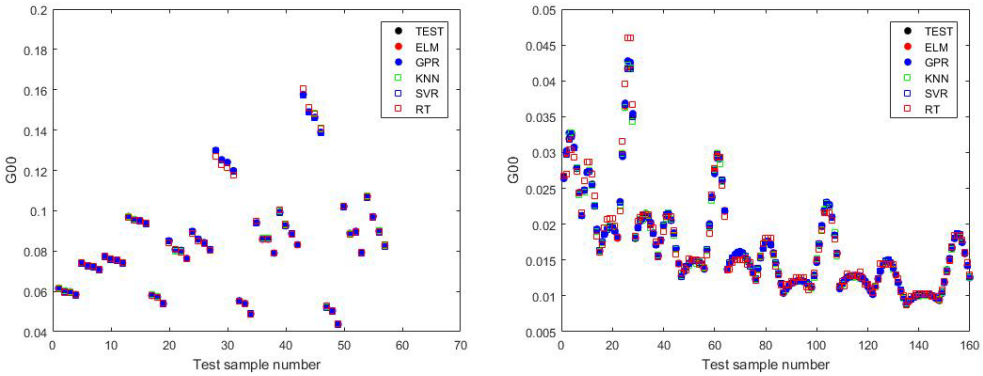

(a) results of the singular integral (b) results of the nearly singular integral

Figure 1. Comparison of the results of some classical machine learning methods

Table 1. The mean relative errors of the results of the machine learning methods

	ELM	GPR	KNN	SVR	RT
MRE of the singular integral	4.4569e-5	3.5646e-5	0.0052	0.0036	0.0106
MRE of the nearly singular integral	0.0040	0.0066	0.0081	0.0019	0.0398

Keywords: Boundary element method, Singular element integral, Nearly singular element integral, Machine learning.

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Data driven thermo-mechanical calculation during additive manufacturing process

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Abstract: Additive manufacturing (AM), commonly known as 3D printing has developed rapidly in recent years. This technology opened up a range of new perspectives on complex geometries which until then were considered laborious. Its contribution to lightweighting is a profound asset for aerospace industry where AM gained significant popularity. However, thermally induced residual deformations and residual stresses in AM parts must be effectively predicted to guarantee wide industrial adoption of AM technology. In this work, a numerical modelling based on the finite element and level-set methods is implemented to study direct material deposition (DMD) of metal alloys. Metal deposition is followed up by updating the level-set layer by layer. Nevertheless, conventional thermo-mechanical calculation for AM simulation is time consuming, especially for large parts. In order to increase the computational efficiency and maintain the precision, the data driven thermo-mechanical model is proposed. In the model based on the inherent strain theory, the plastic strain rate is extracted from first layer depositions and is considered as inherent strain rate, thus non-linear calculation becomes linear problem. The model validation is carried out with a single wall produced by depositing multiple single tracks on top of each other, and its application is successfully extended to a rectangular wall contour geometry. The simplified method reduces noteworthy the computational cost and it is in good agreement with the conventional calculation for predicting residual distortions.

Keywords: Data driven thermo-mechanical calculation, Inherent strain rate method, Direct material deposition.

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Residual-based Goal-oriented *A Posteriori* Error Estimation and Adaptive Mesh Refinement in Thermoelastic Problems

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Abstract: In recent years, substantial attention has been devoted to thermoelastic multifield problems and their numerical analysis. Thermoelasticity is one of the important categories of multifield problems which deals with the effect of mechanical and thermal disturbances on an elastic body. In other words, thermoelasticity encompasses the phenomena that describe the elastic and thermal behavior of solids and their interactions under thermo-mechanical loadings. Since providing an analytical solution for general coupled thermoelasticity problems is mathematically complicated, the development of alternative numerical solution techniques seems essential [1-5].

Due to the nature of numerical analysis methods, presence of error in results is inevitable, therefore in any numerical simulation, the main concern is the accuracy of the approximation. There are different error estimation (EE) methods to assess the overall quality of numerical approximation. In many real-life numerical simulations, not only the overall error, but also the local error or error in a particular quantity of interest is of main interest. The error estimation techniques which are developed to evaluate the error in the quantity of interest are known as "goal-oriented" error estimation (GOEE) methods [6-9].

In this research, the goal-oriented *a posteriori* error estimation in thermoelasticity problems is investigated. Generally, the *a posteriori* error estimation techniques can be categorized into two major branches of recovery-based [10-12] and residual-based [13-15] error estimators. This article focuses on the application of the residual-based error estimator in thermoelasticity. Moreover, in order to reduce the error in the quantity of interest efficiently and optimally in two-/three-dimensional (2D/3D) thermo-mechanical multifield problems, goal-oriented adaptive mesh refinement is performed.

To investigate the goal-oriented error estimation in thermoelastic problems, a new dual weighted residual (DWR) [16,17] method for *a posteriori* error estimation and mesh adaptation is developed and implemented in thermoelasticity. The developed method, which relies on the duality principles, consists of an adjoint problem solution. The mesh adaptivity procedure based on the DWR method is performed by adaptive local *h*-refinement/coarsening with allowed hanging nodes. According to the proposed DWR method, the error contribution of each element is evaluated. In the refinement process, the contribution of each element to the goal error is considered as the mesh refinement criterion.

In order to substantiate the accuracy and performance of the developed methods, they are applied to several numerical problems with analytical solutions and the estimated errors are compared with the exact errors. Here, 2D and 3D problems under thermo-mechanical loadings are considered as benchmark problems. In these examples, several singular functions are considered as the quantity of interest. To show the accuracy of the developed estimator, in all examples, the goal error effectivity index as a standard measure of the quality of an estimator is calculated. In all examples, after few initial coarse meshes, the goal error effectivity index lies in the acceptable range and by further refinements approaches to the ideal value of 1.

Moreover, in order to demonstrate the efficiency of the proposed method and show the optimal behavior of the employed refinement method, the results of different conventional error estimators and refinement techniques (e.g., global uniform refinement, Kelly, and weighted Kelly techniques) are used for comparison. This comparison shows that among the selected error estimation and refinement techniques, the employed DWR method is the most optimum and efficient one and the global uniform refinement has the least convergence rate. On average, in the studied examples, the DWR, Kelly, and W-Kelly methods show, respectively, 0.68%, 0.42%, and 0.26% higher convergence rates compared to the global uniform refinement. This efficiency enhancement leads to the considerable computational time saving.

Keywords: Thermoelasticity, Finite element method (FEM), Residual-based error estimation, Goal-oriented error estimation (GOEE), Mesh adaptivity.

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Theoretical and experimental study of long-term creep in multilayered composites

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Abstract: In most industries, composite materials have dominated the market compared with traditional materials and structures, due to their unique properties. Composite structures, in addition to their proper weights, have a good corrosion resistance and have a relatively high life span. Due to their long operational time, composite structures are usually subjected to long-term loading and experience creep phenomenon. The occurrence of creep leads to reduction in mechanical properties and makes the composite structure more susceptible to failure. Therefore, studying the behavior of these structures in long-term periods requires the analysis of the creep phenomenon as one of the most important factors of their life-time and durability.

There have been very few studies conducted to investigate the long-term creep behavior of cylindrical composite [1-10]. Most studies in this field are experimental and theoretical which have been done on a limited basis. Prediction for any composite lamination requires repeated testing, and long-term behavior cannot be modeled without costly and time-consuming experiments.

The main objective of this article is developing an integrated modeling for evaluating long-term creep phenomenon in cylindrical composite structures under constant loading for a period of one year. In this model, the creep caused by constant load on the composite structure is simulated and investigated using the long-term data of pure resin. This data can be obtained from the Time Temperature Superposition [11]. This model can be used as a suitable tool for predicting long-term creep behavior of composite structures and reduce the costs of long-term test programs. The model is validated and improved on the basis of an empirical study. Experimental program consists of suitable equipment for monitoring and collecting long-term creep data on a cylindrical composite structure subjected to compressive transverse loading as a case study. Also, Theoretical model for simulating long-term creep is acquired by numerical methods based on linear viscoelasticity [12-13] and with implementing UMAT subroutine into ABAQUS.

Keywords: Composite, Creep, Cylindrical composite structures, FEM, UMAT.

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Deep learning Approach to Analysis and Prediction of Infrastructure Disaster

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Abstract: Natural disasters have capable of disastrous consequences impacts on the functionality of infrastructure systems and able intense systemic and socio-economic losses. According to budget restrictions, it is crucial to optimize decisions regarding mitigation, preparedness, response, and recovery practices for these systems. This requires accurate and efficient means to evaluate the infrastructure system reliability. Machine learning is a hot subject in the recent decade, and the influence of Artificial Neural Network (ANN) is especially notable, which is the most extensively used models of machine learning in assessment of infrastructure. This study provides damage detection assessment of seismic performance of reinforced concrete (RC) bridges, by using machine learning methods. This study developed a deep learning (DL) model for estimating of seismic vibration on railway RC bridges. A multi-layered perceptron (MLP) with a back-propagation (BP) algorithm neural network was implemented to predict the seismic performances of the designated bridges. ANN models were developed, trained and tested in a based MATLAB and Python program. A training set and a validation set of bridges were produced from dynamic response of different RC bridges. Finite Element Analysis (FEA) was used to generate training and testing set of ANN models. A training and a validation data set of RC bridges will produced from FEA analysis results of the dynamic response of RC bridges by shifting parameters (the input parameters of ANN) including accelerations and axle loads ,concrete compressive strength, reinforcement ratio, Size of column, column shape, width of the slab, effective depth of tension reinforcement, slab shape Peak acceleration, Shear wall, Story height, max width of bay in X, Y direction and etc., Under the near-fault earthquakes. On the other hand, Output will be dimensional dynamic response in terms of the roof displacement, base shear forces and base bending moments, accurately when compared with the results of conventional methods like FEA[1][2]. The method performs on the collected feature measurements on a railway RC bridge during dynamic response of bridges structures, which for this study were gathered in a numerical experiment using a three dimensional finite element model. Thus, the next step consists in the design and unsupervised training of Artificial Neural Networks that used as mentioned input data [3]. The results demonstration that the proposed method is robust and capable of capturing the physical complexities for the dynamic damage detection force on RC bridge prediction task. Therefore results will compared with analytical and exact deflection[4]. The results showed that an appropriately trained neural network could consistently predict permanent earthquake-induced seismic deformation of the RC bridges. Bridges fragility analysis to calculate failure probability was another achieved that were created by using nonlinear analysis (NA) and artificial neural networks (ANNs). Nonlinear response history analyses were achieved, in order to calculate the seismic performances of the bridges. To this end, 306 bridge-earthquake cases were considered. The MLP neural networks considered herein consist of an input layers vectors, hidden layers and an output vector. In order to train ANNs, 70% of the numerical results were selected, and the remained 30% were employed for testing the reliability and validation of ANNs. Numerous structures of MLP neural networks were analyzed in order to obtain efficient and effective neural networks. After achieving the best structure of neural network, it was used for generating new data. A total number of 600 new bridge-earthquake cases were generated based on neural simulation. Finally, probabilistic seismic safety analyses were conducted. Therefore bridges fragility analysis were developed using numerical results, neural predictions and the combination of numerical and neural data. Consequences of this study demonstrate that ANNs are suitable tools for predicting damage detection of seismic performances of RC bridges. It was also shown that efficiency stresses of the reinforcements is one of the important sources of uncertainty in fragility analysis of RC bridges [5]. It is evident from this evaluation that ANNs have been successfully applied to many Infrastructure engineering areas like prediction, risk analysis, decision-making, resources optimization, classification, and selection etc. It was demonstrated that the neural network based approach is highly successful to determine response of bridges and buildings subjected to Seismic evaluation. Based on the results of case studies, it is evident that ANNs perform better than as similarity to the conventional methods[6].

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Keywords: Seismic evaluation, Dynamic analysis, RC bridge, Artificial Neural Network, FEM, Deep Learning, Damage detection

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Inverse design of phononic Topological insulators using Machine learning

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Abstract: Topological insulators (TIs) are a new state of matter the behavior of which depends on its topology rather than geometry. The TIs act as insulator in the bulk and allows wave propagation along the surface. These surface states are topologically protected which makes them immune to backscattering and remain robust even in the presence of defects. Quantum Hall effect (QHE) is a phenomenon in which the presence of magnetic field enable electrons to travel along the edge of a semi-conductor under external voltage. Quantum Spin Hall effect (QSHE) [1,2,3] is a phenomenon discovered later, in which the edge protected electron movement is achieved even in the absence of an external magnetic field. The edge state due to QSHE is helical while due to QHE is chiral. The helical edge state leads to propagation of opposite spin states, so an electron can backscatter if the spin is flipped.

The acoustic and elastic analogue of QSHE has been achieved, while majority of them are in discrete lattice. Though there are works available on inverse design of phononic metamaterial (MM) for band gaps, there have been only very few works on inverse design of phononic TI for topological band gaps [4,5]. A band gap prevents wave propagation in the bulk while topological band gap prevents wave propagation in the bulk but allows waves along the edge. The inverse design procedures adopted utilize a level set based optimization method or SIMP. The emergence of QSHE in a phononic metamaterial necessitates the unit cell topology to offer a double Dirac cone in its band structure. In [4], objective function based on unit cell band structure is formulated to determine the topologies of different topological phase.

While in [5], the objective function is formulated directly based on the amplitude of wave intensity such that the intensity is zero in the bulk and maximum in the interface. As an alternative, it is possible to construct an objective function based on the supercell made of two different unit cells. The band structure determined for the supercell need to have interface modes lying in a bulk band gap. The topology can be represented by pseudo density of elements or using level set function. The Convolution Neural Network (CNN) can be trained with supercell topology as input and band structure determined by finite element method as output. The frame work for designing a phononic TI based on QSHE is shown in Figure 1. The results are obtained for solving forward problem by FEM and inverse design of supercell using Genetic algorithms such that the band structure has intersecting interface modes in a bulk band gap. Future work includes training the CNN to solve both the forward problem and inverse design of phononic topological insulators.

Keywords: QSHE, Topological insulators, Phononic MMs, Topology optimization, CNN

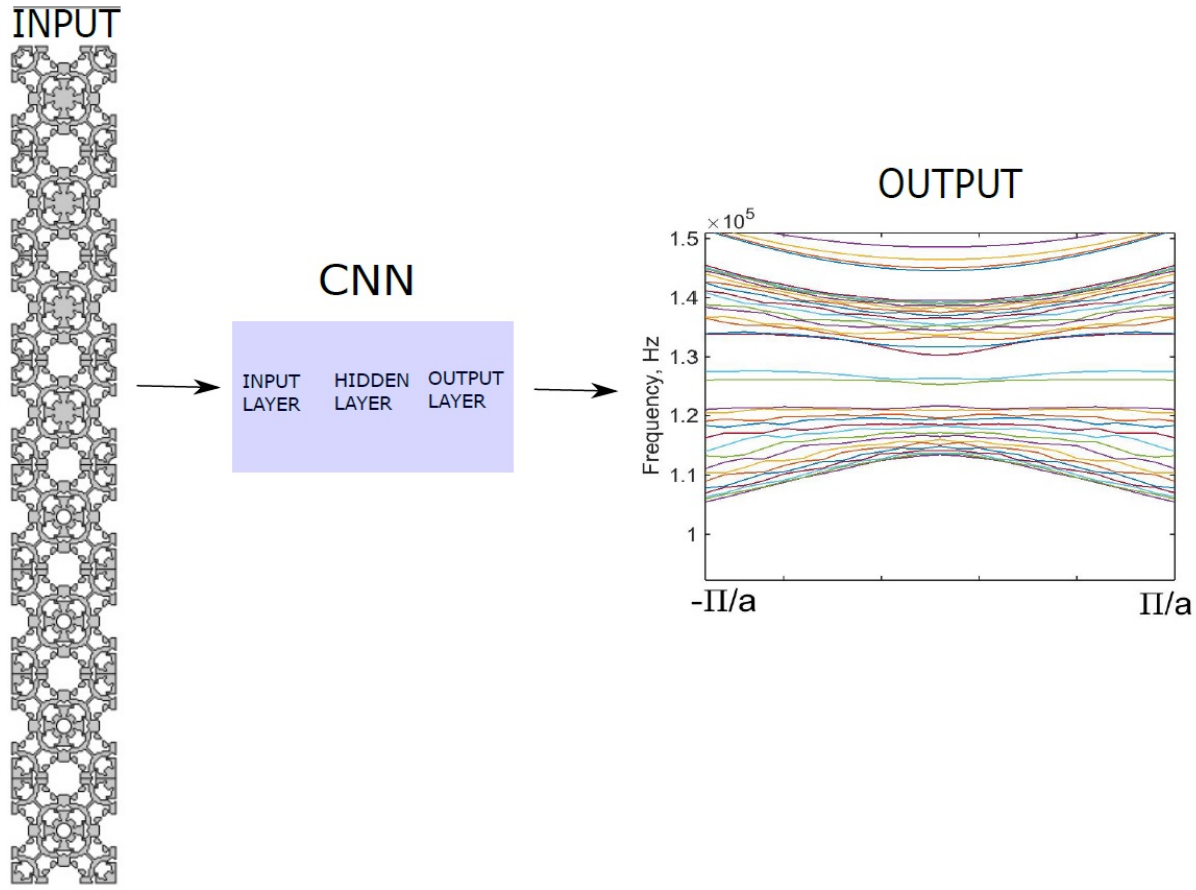

Figure 1 : The Framework for designing of a phononic topological insulator based on QSHE.

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A Deep Learning Method for a Fully Coupled Thermomechanical Model

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Abstract: This study presents a robust method used to solve fully coupled thermomechanical model. The proposed method is based on computational graphs and backward stochastic differential equations to solve coupled partial differential equations (PDEs). In this way, solution of a coupled system between a transient heat conduction and linear elastic mechanical model thus can be obtained. To validate the method numerical results using Pytorch are implemented. The numerical solutions are compared with exact solution and good agreement is obtained illustrating robust and accuracy of the method. The method provides a great tool that opens a new door for solving complex multiphysics problems in industrial application.

At first the computational domain is filled by randomly generated collocation points. Kinematical quantities are computed that are inserted into the constitutive equations. A loss function including the governing partial differential equations and boundary conditions is then constructed and minimized at the collocation points via a combination of optimizers adopted in the back propagation process. By doing so, a set of hyperparameters can be obtained [1-3]. Figure 1 shows an example of a deep neural network including 2 hidden layers [4].

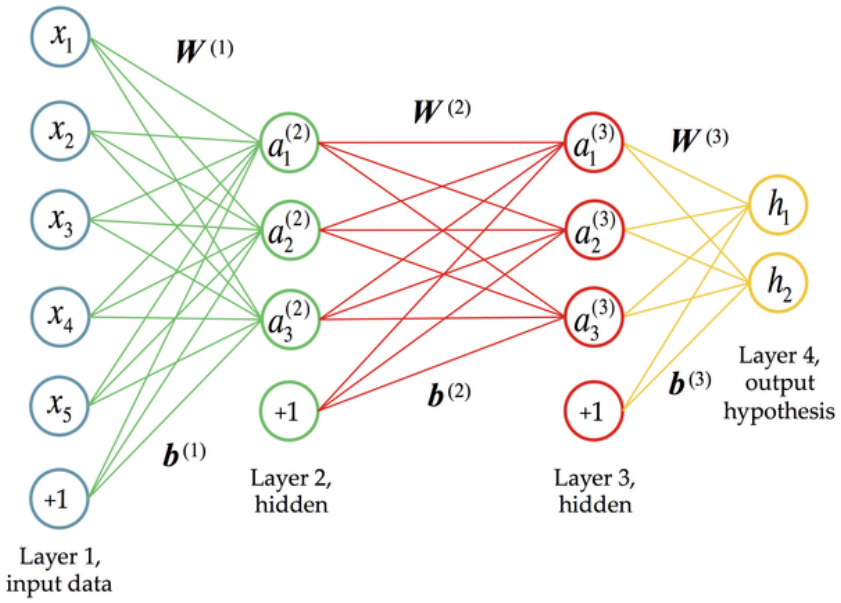

Figure 1: A schematic diagram of a deep neural network with two hidden layers [4]

Let consider the strong forms of the coupled partial differential equations [5,6]

Balance of momentum

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$$\begin{cases} \mathrm{div}\boldsymbol{\sigma} + \boldsymbol{b} = \boldsymbol{0} & \text{in } \Omega \\ \boldsymbol{u} = \bar{\boldsymbol{u}} & \text{on } \partial\Omega_u \\ \boldsymbol{\sigma} \cdot \boldsymbol{n} = \bar{\boldsymbol{t}} & \text{on } \partial\Omega_t \end{cases}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{b}$ is the respective Cauchy stress and the body force; $\bar{\boldsymbol{u}}$, $\bar{\boldsymbol{t}}$ and denotes the Dirichlet and Neumann boundaries, respectively.

Balance for the temperature

$$\begin{cases} c_F\, \dot{\theta} + \mathrm{div}\boldsymbol{q} = Q & \text{in } \Omega \\ \boldsymbol{\theta} = \bar{\boldsymbol{\theta}} & \text{on } \partial\Omega_\theta \\ -\boldsymbol{q} \cdot \boldsymbol{n} = \bar{\boldsymbol{q}} & \text{on } \partial\Omega_q \end{cases}$$

where $\boldsymbol{\theta}$ and $\boldsymbol{q}$ is the respective temperature and heat flux; $\boldsymbol{\theta}$, $\bar{\boldsymbol{q}}$ and denotes the Dirichlet and Neumann boundaries, respectively.

Keywords: Deep energy method (DEM), Thermomechanical model, Artificial neural network (ANN).

Acknowledgement

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A Date Driven Framework to Design Seismic Metamaterial

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Abstract: Earthquakes are one of the most harmful natural disasters to humans. When an earthquake occurs, the source area is undergoing rapid rupture and movement, which constitutes an oscillation source. The oscillation propagates through the Earth's medium, forming elastic waves in the continuum, namely seismic waves. Waves can be elastic, acoustic or electromagnetic, but there is one phenomenon in the same: for certain frequency range, periodic materials or structures, i.e., the so-called metamaterial, can be constructed to hinder wave propagation of the corresponding frequencies. This phenomenon is the bandgap. To actively prevent structures from potential seismic damage, design of seismic metamaterial has become an aroused research topic [1]. A seismic metamaterial is a periodic structure made of different elastic materials, which creates the exact bandgap, mainly for controlling the propagation of low-frequency seismic surface waves. Although the basic principle of elastic wave propagation has been established by Brillouin [2], recent research in this field has focused on theory [3, 4] and experimental proofs [5, 6] of the bandgap. Nevertheless, the design process of seismic metamaterials so far has been quite limited, mainly by trial-and-error, leaving multitudinous potential optimal design space unexplored.

Machine learning has been applied as an alternative to discover optimal materials such as mechanical metamaterials with unprecedented properties, such as the accelerated searching of graphene origami [7] and the self-learning-based hierarchical composite design [8, 9]. The numerical simulation of phononic crystals is a complex eigenvalue problem. However, due to structural periodicity, the wave vector can be reduced to the Irreducible Brillouin zone (IBZ) of the solution dimension. With COMSOL and COMSOL Live Link for MATLAB, we simulated the bandgap of two-dimensional simple periodic structures using the parameter sweeping of IBZ boundaries, and proved that simple periodic structures can be effective as the prospective seismic material. With Python and PyTorch, we realized the data driven framework to build a surrogate model for the eigenvalue analysis and the bandgap prediction, as shown in Figure 1. Under the same training conditions, we compared the performance of the linear regression, the shallow feedforward NN (neural network) and the deep CNN (Convolutional neural network).

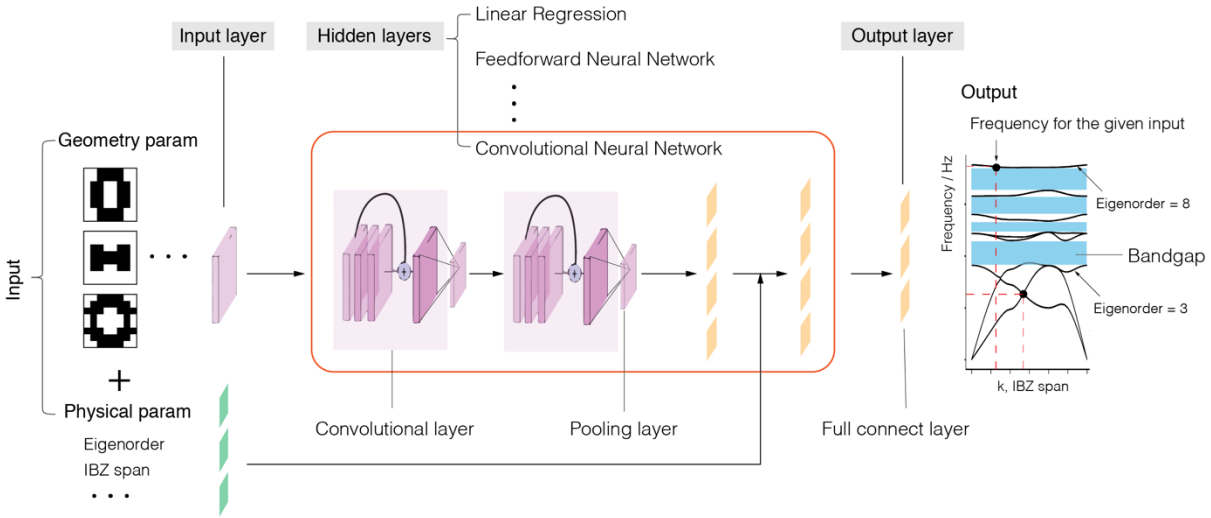

Figure 1: Our data driven framework for seismic metamaterial design.

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Results show when taking the MSE (Mean square error) as the model accuracy criterion, the MSE of the NN could be merely 10% of that of the linear regression. Moreover, after introducing the convolutional layers into the neural network, the MSE of CNN is only 50% of that of NN. This finding proves the intrinsic difference among the classic data driven method like linear regression and the neural network, as well as the function of convolutional layers to learn deep features. Our study also shows that in terms of optimizers, the Stochastic Gradient Descent performs better under relatively the smaller batch size (256) and the smaller learning rate (0.02), whereas Adam instead performs better under the larger batch size (1480) and the larger learning rate (0.001), which might be helpful for similar data driven problems.

Keywords: Seismic Metamaterial, Bandgap, Data Driven, Neural Network, Convolutional Neural Network.

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Simulation of nonlinear propagating waves in hysteresis media via higher-order central-WENO high resolution schemes

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Abstract: In this study, higher-order (third and fourth-order) central-WENO high resolution schemes [1-3] are integrated with different hysteresis models to simulate non-linear wave propagation problems in hysteresis media. In this regard, both discontinuous solutions and nonlinear waves due hysteresis media can be simulated properly. The discontinuous solutions can be developed either to abrupt changing in media properties (e.g., density) or nonlinear responses. For this end, wave equations will be re-expressed as first-order hyperbolic partial differential equations, the so called strain-velocity or stress-velocity representation. The importance of using the higher-order schemes is capturing high frequency waves with small wave numbers which is challenging problem in numerical simulations due to numerical dissipation of different schemes [4] (for instance, the second order Kurganov-Tadmor (KT) central high resolution method, and common finite element and finite difference methods). Media with the elasto-plastic [5] and Duhem [6] hysteresis models were integrated with second order central schemes. Here, the higher-order central-WENO schemes are incorporated with hysteresis models especially those developed for soil-dynamic problems (such as, the (modified) hyperbolic hysteresis model). This is important for different projects; for example: effects of soil-nonlinearity on high-speed railway tracks and the site-effects for important projects located near earthquake sources which emitting wide-range of frequencies (even up to 30 Hz). Finally, it should be mentioned that the common equivalent linear method, used in different commercial codes, can considerably underestimate the responses in the high frequency range.

Keywords: Central-WENO, nonlinear wave, hysteresis media, higher-order schemes.

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Numerical Simulation of Stability Analysis of Jointed Rock Slope Based on SPH Method

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Abstract: In recent years, there are more and more large-scale jointed slope projects. the stability of slopes is becoming more and more complicated and important. The anisotropic characteristic of rock mass complicates the problems of rock mechanics. The traditional numerical simulation analysis methods are difficult to analyze the stability coefficient and potential slip surface of the slope, and it is also difficult to analyze the large deformation process of the slope after instability, thus, it brings hidden dangers to the safety of the slope engineering. Based on the smooth particle dynamics (SPH) method described by Lagrange, the SPH program for simulating the stability of jointed slopes and the large deformation of landslides after instability is compiled in Fortran language, and the elastic-plastic constitutive equation of rock mass is introduced. The numerical simulation of the stability of jointed slopes is carried out based on the elastoplastic constitutive model and the Mohr-coulomb yield criterion. This study makes up for the shortcomings of current numerical simulation methods, and has theoretical and practical significance for revealing the failure mechanism of jointed slope and optimum design of slope engineering.

Keywords: Smoothed Particle Hydrodynamics (SPH), Rock slope, Joints and fracture, Stability analysis, Numerical Simulation.

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Effect of size of microcapsules on the self-healing concrete

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Abstract: The microcapsule-enabled self-healing materials are appealing since they can heal the cracks automatically. Although much research has been carried out, the influence of the radius of microcapsules on the self-healing effect is still not well investigated. This research uses the two-dimensional discrete element method (DEM) to investigate the cracking behavior of specimens containing one microcapsule and one microcrack. The influence of the size of microcapsules is considered. The potential healing time and the influence of the initial damage are studied. A large amount of simulation have been conducted and analyzed. The results indicate that the crack coalescence type between the pre-existing crack and the hole is influenced by the size of holes. The elastic modulus, the compressive strength and the coalescence stress decrease with the rise of the radius of holes. The initial damage in experiments should be greater than 95% of the compressive strength to enhance the self-healing effect. The larger microcapsules require less initial damage. A new type of displacement field near the crack and a new type of coalescence crack are observed. The research enhances the understanding of the influence of sizes of holes on the cracking behavior of concrete containing a circular hole and a pre-existing crack.

Keywords: Microcapsule, size, cracking processes, DEM.

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Application of a deep learning method for solving PDEs for compressed air energy storage

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Abstract: Compressed air energy storage (CAES) is an energy-storage and power generation technology that has numerous potential applications. Compared with other energy-storage patterns, such as pumped hydroelectric storage (PHS), CAES has lower capital investment and maintenance costs [1, 2]. A CAES plant utilizes compressed air as an energy storage and power generation carrier. When the electricity supply exceeds demand, surplus electrical power is used to drive air compressors and store compressed air into underground caverns. Meanwhile, during peak hours, the stored compressed air is expelled and mixed with gas fuels. The mixed gas is then fired and driven to facilitate gas turbine expansion, which in turn runs the electrical power generators.

An underground reservoir is the main component of a CAES plant, and excavations of new hard rock caverns could provide additional possible site selections although no existing commercial CAES plant is using this kind of caverns. So researchers have explored possibilities of air storage in hard rock caverns. In unlined rock caverns, the air is normally prevented from leaking by natural groundwater or artificial water curtain. Thus the stored air pressure is balanced by the ambient hydrostatic water pressure within the host rock. However, these groundwater control methods are unsuitable for regions where water is scare. Thus, an alternative method, CAES in lined rock caverns, is studied in the current study and was found to have has a better applicability. Two types of the underground cavern for CAES are shown in Fig. 1.

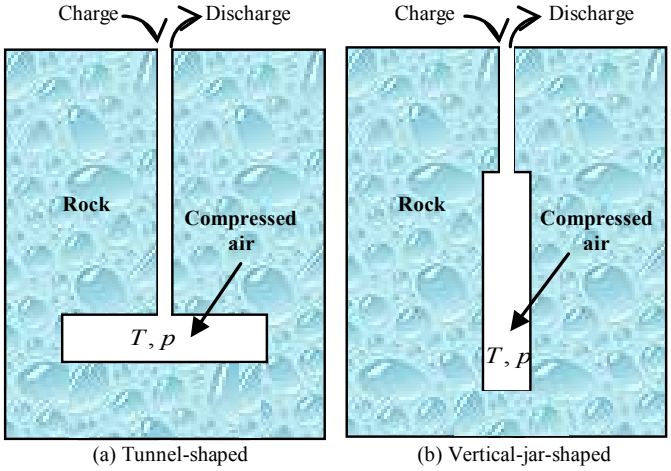

Figure 1: Two types of underground caverns for CAES

It is a great challenge to predict air temperature and pressure in an underground cavern for compressed-air energy storage (CAES) owing to huge operational cycles and multiple field interaction [3, 4]. The deep-learning approach is proved an effective tool for solving this [5]. We applied a deep-learning method to solve the corresponding equation set after the strong form is established, while the solution is approximated with a deep neural network [6, 7]. Necessary train processes are required to adjust the differential operator, initial condition, and boundary conditions. Meshfree implementation is used and we also constitute a simple analytical solution for the purpose of comparison. The neural network is trained on batches of randomly sampled time and space points, while the deep learning method provides the general solution to the mass conservation equation, energy conservation equation, and air state equation. The used method has a similar spirit to Galerkin methods, with the solution approximated by a neural

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network instead of a linear combination of basis functions. The compassion of the results solved by the deep learning method and the analytical solution shows a significant agreement.

Keywords: Deep learning, PDEs, Compressed air energy storage, Neural network, Air state.

Acknowledgement

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Machine Learning based Crack Growth Prediction: Application to a Helicopter Component Digital Twin

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Abstract: Digital Twin is an integrated multiphysics, multiscale, probabilistic simulation of an as-built vehicle or system that uses the best available physical models, sensor updates, fleet history, etc., to mirror the life of its corresponding physical twin [1]. In the digital twin application, the load data from onboard sensors is used to predict the crack growth and remaining life in real time. However, traditional fracture mechanics simulation methods are time-consuming. In this article, we propose a machine learning based approach, combining with high performance fracture mechanics simulation, to perform real-time fatigue crack growth prediction for structures with complex geometry. High-fidelity simulations are carried out, by using the SGBEM-FEM alternating method [2] to generate the training data. The mapping between various loads /crack geometry and stress intensity factor (SIF) of crack fronts is established as a surrogate model by machine learning method such as gaussian progress regression (GPR) and support vector regression (SVR). With the real-time load and current crack geometry as input, the surrogate model can quickly export the SIF to the fatigue crack growth model to analyze the crack growth and update the crack geometry step by step. Here an example of a flawed helicopter lift frame [3] is presented to demonstrate the analysis procedure and capabilities of the method. The crack configuration is a small corner defect at the edge of a large central hole in a flanged plate made of 7010 aluminum alloy, and the component is subjected to the ASTERIX spectrum load. To reduce the variables representing the complex crack shapes, the principle component analysis (PCA) were used to parameterize the crack fronts. The generalized Frost–Dugdale law [4] and NASGRO equation [5] were used to predict the fatigue crack growth. The crack growth history and remaining life obtained by our approach coincide well with simulation and experiment results presented in other papers [6-8]. Results show that the proposed approach can accurately predict the evolution of the crack growth over entire load histories and substantially reduce the computing time, which can be used for real-time health monitoring in digital twin applications.

Keywords: Fatigue crack growth, Surrogate model, Machine learning, SGBEM-FEAM, Digital twin.

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Numerical implementation of data-driven computational mechanics

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Abstract: Data-driven computational mechanics emerges as a new methodology in computational mechanics, which directly uses raw material data instead of empirical material models in calculation [1,2]. The solution of data-driven solver is to find the optimal material states ($\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$) minimizing the distances between the material data sets and equilibrium & compatibility constraints. The distance is defined in the metric of strain energy of a pseudo linear-elastic material. In this paper, we thoroughly investigate the effects of the pseudo linear-elastic material on data-driven computing solver. The data-driven solver is decomposed into two sub-problems. The inner sub-problem finds the optimal material states ($\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$) in the equilibrium & compatibility constraints closest to prescribed material state in the material data set. This process is independent of the pseudo linear-elastic material. The outer sub-problem finds the nearest neighbor of the calculated material states ($\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$) in the material data sets. The nearest neighbor search space can be regarded as a super-ellipsoid centered at ($\boldsymbol{\varepsilon}$, $\boldsymbol{\sigma}$). Some issues in numerical implementation are discussed and several key parameters are investigated. It is found that the construction of super-elliptical search space along the direction of the equilibrium & compatibility constraints will improve the efficiency and accuracy of the iteratively data-driven computing process.

Keywords: Data-driven computational mechanics, Material data set, Nearest neighbor search.

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A Real-Time Structural Topology Optimization Method using Conditional Generative Adversarial Networks

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Abstract: Traditional topology optimization methods such SIMP method [1] or level set method rely on time-consuming iterative algorithms, and with the increase of the degrees of freedom of the background grid, the computation time increases exponentially, that is, the so-called "dimension curse" problem. To solve this problem, this paper proposes a real-time topology optimization method based on Conditional Generative Adversarial Networks (CGAN) [2], which can almost real-time predict accurate optimization results according to input displacement and load boundary conditions. First, we establish a data set using the simulation data generated by SIMP method, and then train the dataset by using Conditional Generative Adversarial Networks with Gradient Penalty (CGAN-GP) to generate optimized structures (see Fig. 1). To improve quality of optimized structures generated by CGAN-GP, we use Pix2pix GAN to enhance the sharpness of these topologies, and get the structure with high clarity. Comparing the traditional topology optimization, numerical examples illustrate that computational time can be reduced dramatically while the accuracy rate is up to 85%.

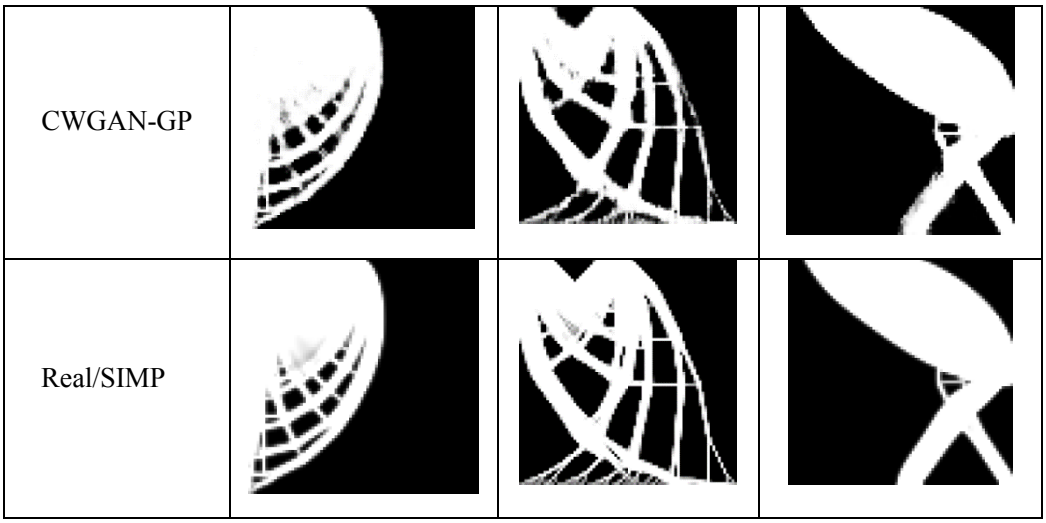

Figure 1: Comparison of optimized structures obtained by the presented method and traditional SIMP algorithm.

Keywords: Real-Time Structural Topology Optimization, Conditional Generative Adversarial Networks, Deep learning, Artificial intelligence.

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Analysis of discontinuous evolutions in phase-field fracture modelling

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Abstract: Phase field modelling of fracture has revitalized the study of failure phenomena in the scientific community during the last two decades. Multiple applications in multi-field frameworks [1-3] have been attempted to exploit the advantages of the approach. Complex crack behaviors like nucleation, merging and branching, which used to rely on intricate numerical techniques, are naturally handled by an additional partial differential equation. From a theoretical point of view, a phase-field crack evolution is dictated by three energetical principles [4] namely, energy conservation, irreversibility and global stability. While irreversibility and energy conservation are grounded on thermodynamic principles and are widely accepted, the third one is still under debate. As pointed out by [5], a global stability criterion results in unphysical results in nonconvex variational problems since a jumps over energy barriers would be necessary in order to reach a global minimum. In terms of fracture modelling, numerical results show cracks propagating instantaneously through the domain when a continuously evolving crack is expected. A local stability criterion would be more suitable, however as shown by [5], even in this scenario the formulation allows jumps during crack growth, breaking the causality principle [5]. Modifications to the theoretical framework have been proposed by [5] and [6] pointing out the necessity of capturing rate dependent effects during fast crack propagation to obtain physically meaningful solutions. However the implementation of a numerical scheme capable of representing viscous and inertial effects in a rate independent framework has not been tackled yet. Here, an algorithm based on a Machine Learning algorithm is proposed in order to study the space of admissible solutions during the optimization process.

Machine learning has been successfully applied in other contexts to define the optimization domain in problems with non-convex objective functions in material science [7]. In [8] a classification of learning algorithm was used to define an optimization domain based on data from experiments and numerical simulations. In [9] an adaptive algorithm is defined in order to modify the definition of the space of interest during the optimization process. Following the same line of idea, a multilayered feed-forward neural network is used to explore the effect of inertial effects on crack propagation during fast transitions. The finite element method is used to discretize the partial differential equations resulting from the minimization of the total energy functional. Crack propagation in the quasi-static and dynamic cases is considered. The Alternating Minimization Algorithm (AMA) is adopted here to solve the quasi-static problem and implicit generalized alpha integration method for the dynamic case. By feeding pairs of simulations of the quasi-static and dynamic crack propagation examples a multilayer neural network is trained to calculate a relaxation ratio of a sequence of solutions of the evolution problem. Afterwards, the relaxation ratio is used along with the quasi-static scheme to obtain improved solutions that better reflect the rate dependent phenomena that are expected during jumps in the system evolution.

The results show that the total energy of the system is not conserved during fast crack growth, however the energy imbalance obtained with the calculated relaxation ratio agrees well, within a certain range of crack propagation velocities, with the energy associated to inertial effects in the dynamic case. For crack tip velocities beyond this threshold the quasi-static solution becomes inadequate to model crack propagation since phenomena like branching and crack propagation promoted by wave reflection take on a dominating roll during the evolution.

Keywords: Phase-fields, variational formulation, fracture, rate independent.

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Robust topology optimization using an improved adaptive Gaussian process

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Abstract: Topology optimization is a mathematical tool that optimizes the geometry of an object, within a given space and for a given set of loads and constraints. The goal remains to maximize the performance of a part of the system by reducing its mass and the cost of manufacturing. Out of various optimization procedures, topology optimization yields the optimum configuration. Over the years, the concept has gained huge popularity among both researchers and practicing engineers. Popular topology optimization methods are based on density, level set, topological derivative, phase field, evolutionary approaches and several others [1]. Further advanced methods by coupling two or more of the above-mentioned methods can also be found in literature [2]. However, all the methods discussed above conveniently neglect the presence of uncertainties in the system. In this context, it is to be noted that all physical systems have inherent uncertainties associated. Ignoring these uncertainties can lead to systems that exhibit poor performance, or even fail. Therefore, it is of utter importance to consider the effect of uncertainties while optimizing a system.

In this work, a novel approach for topology optimization under uncertainty has been proposed. Out of two available options for optimization under uncertainty [3], namely robust design optimization (RDO) and reliability-based design optimization, the former has been pursued in this study. In order to reduce the computational effort associated with robust topology optimization, an improved version of Gaussian process, referred to as hybrid polynomial correlated function expansion (H-PCFE) [4] has been integrated within the topology optimization framework. H-PCFE is used for computing the moments associated with the objective function in robust topology optimization (RTO). It is argued that re-training the H-PCFE at every iteration will make the overall algorithm computationally expensive and time consuming. To alleviate this issue, an adaptive algorithm that automatically decides whether to retrain the H-PCFE or to use the available H-PCFE model, is proposed. The proposed approach is highly flexible and can be integrated with already available deterministic topology optimization codes from literature.

Mathematically, RTO can be represented as:

$$d^* = \text{argmin } c_{RTO}\left(\text{E}(c(d,X)), \text{var}(c(d,X))\right)$$
$$\text{subject to } \begin{cases} \dfrac{V(d)}{V_0} = f \\ KU = F \\ 0 < d_{i,\min} \le d_i, i = 1,...,N_d \end{cases}, \tag{1}$$

where ***d*** represents the design variables, $d_{i,\min}$ is the minimum relative density for the i^{th} design variable, and N_d is the total number of design variables. X represents the variables with uncertainty. E(•) and var(•) denote the mean and the variance operator, respectively. **F**, **K** and **U** in equation (1) represent the force vector, stiffness matrix and the displacement vector of the global system respectively. $V(d)$ and V_0 represent the material volume and design domain volume, respectively, f indicates the prescribed volume fraction and $c(d,X)$ denotes the compliance of the system.

Performance of the proposed approach has been investigated on the well-known MBB beam. The geometrical domain and the boundary conditions are shown in Figure 1(a). Due to symmetrical boundary conditions, only half on the structure, shown in Figure 1(b), is analyzed. Among the material properties, Poisson's ratio, $\upsilon = 0.3$ and young's modulus, E is uncertain with spatial variability and is modelled as a Gaussian random field. The overall domain is discretized into 60x40 four noded unit square element. Like [1], the mean of the random field is

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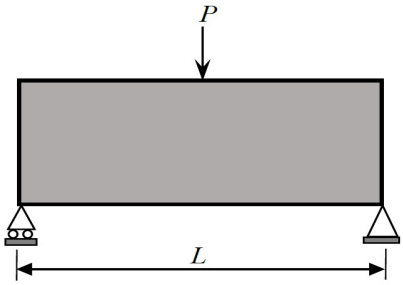
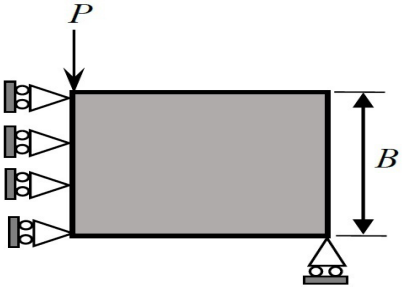
considered as unity. The random field is discretized into 16 random variables by using Karhunen- Loève expansion. The objective of the problem is to compute the optimum topology of the system. The RTO problem has 2400 design variables. Figure 1(d) shows the results obtained using the proposed approach. The results obtained using the deterministic optimization is shown in Figure 1(c). We can see that considering uncertainty results in a more conservative design (additional limbs). This is expected and is consistent with results in RDO literature. This, in turn, provides insurance against structural failure due to uncertainties in the system.



(a) Complete design domain for topology optimization



(b) Symmetrical boundary conditions

(c) Deterministic topology optimization

(d) Robust topology optimization

Figure 1

Keywords: RDO, Topology optimization, Uncertainty, H-PCFE.

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An intelligent detection model based on fully convolutional neural network for pavement crack

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Abstract: Crack is an often appearing pavement disease, if not timely treatment, will result in the pavement damage deepening, and affect the normal use of the road. Therefore, it is of great significance to establish an efficient intelligent identification model for pavement cracks. Neural network is a method of simulating animal nervous system using gradient descent [1] to predict results by learning weight matrix, which has been widely used in geotechnical engineering [2], computer vision [3-5], medicine [6] and other fields. However, there are three major problems in the application of neural network method for crack identification: Too few layers; Extracted crack features are not complete; Low efficiency to calculate the whole picture. In this paper, a fully convolutional neural network [7] based on resnet-101[8] is used to establish an intelligent identification model of pavement crack region. This method using convolutional layer instead of fully connected layer realizes full convolution and speeds up calculation. The sub-region comes from the feature map at the end of the base network, which avoids multiple computations of the same picture. In order to improve the recognition accuracy of the model, OHEM and data-augmentation techniques are adopted. Concrete Crack Images for Classification (CCIC) which is a public data set collected by using smart phone and the Crack Image Database (CIDB) automatically collected by vehicle-mounted CCD camera are trained and tested, the identification accuracy reaches 91.4% and 86.4%, respectively. Comparing with Faster RCNN and different depth models, the proposed model has higher recognition accuracy and recall rate as shown in fig.1, and can extract more complete and accurate crack features in CIDB. Furthermore, rotation, translation and scaling images are analyzed. The proposed model has strong robustness and stability, and can automatically identify image cracks of different forms. The proposed model has broad application prospects in practical engineering problems.

Keywords: Fully convolutional neural network, Pavement crack, Intelligent detection, Crack Image Database.

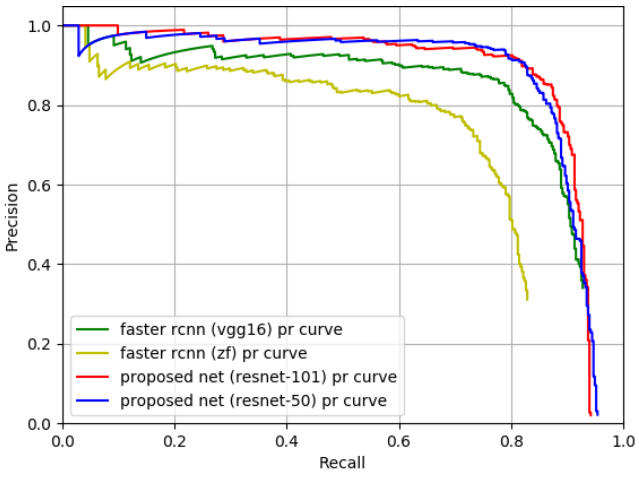

Figure 1

Acknowledgement

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Bayesian solution for inverse elasticity problems with hybrid uncertainties using Polynomial Chaos Surrogate dictionaries

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Abstract: A method is proposed for inferring the presence of an inclusion/void inside an elastic domain under both material and geometric uncertainties. Marzouk.et.al [2] tried, for the first time, to accelerate the Bayesian inference by using Polynomial Chaos Expansions (PCE) to represent random variables. Advantage of such a method is that the evaluation of integrals over the unknown parametric space gets recast into random variable space that underlies the PCE. Conteras.et.a [1] extended this approach to develop PCE based offline dictionaries for one single inclusion case of different shapes and sizes within an elastic domain. During the online stage, a model selection approach based on the evidence provided by the Bayes factor for each of the offline dictionaries were determined and the most suitable dictionary was chosen that had the highest evidence. Yan.et.al [3] proposed a guided Bayesian inference approach for detecting multiple flaws in structures using the extended finite element method. Clearly, there exists a gap in literature where a Bayesian inversion is carried out on elasticity problems were uncertainties in both geometric and material properties do exist. In this work, a novel method is proposed to address this gap wherein, in the offline stage, a few PCE surrogates are developed for different combinations of material uncertainties and inclusion/void geometry. Both the material and geometric uncertainties are taken into account in PCE surrogate construction using a novel stochastic XFEM method developed in our lab. Thereafter, under the assumption that there exist only one inclusion/void in the elastic domain, the uncertain material parameters and geometric features are inferred using the Bayesian evidence estimation with the help of some synthetic data and model averaging. The proposed novel method is exemplified using a simple 2D elastic domain under static loading case.

Keywords: Bayesian evidence, Model selection, Stochastic XFEM, Material uncertainty, Geometric uncertainty.

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Adaptive grid refinement in a 3D peridynamic model

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Abstract: The differentiability of displacement field is a rudimentary assumption in the classical continuum mechanics. In this theory the equations of motion are derived based on partial differential equations. Therefore, this assumption breaks downs when solution of problems containing discontinuities, such as crack propagation, is of concern [1]. In fact, the situation becomes more complicated when real life problems, such as 3D propagation of cracks, come into the picture [2-5].

More recently, peridynamics is receiving a great amount of attention by many researchers in the computational mechanics community. It is considered to be as an alternative and promising theory appropriately formulated for discontinuous problems [6-10]. Peridynamic is well designed to describe failure in structures as the theory makes use of integral equations rather than partial differential equations. In fact, in peridynamics, the equation of motion is described by a nonlocal integral operator rather than the divergence of the stress tensor involved in the classical theory [6,7].

The most common way of implementing and discretizing peridynamics is a meshfree approach which uses a uniform grid of nodes [7, 11]. The peridynamic models most often are much more expensive that methods based on the classical theory. This lies in the fact that, in peridynamic models, each computational node interacts with many neighboring nodes over a finite region. To this end, performing realistic problems (in particular 3D problems) with peridynamic models requires a vast amount of computational resources. In addition, the restriction of the discretization to uniform grid of nodes leads to inefficiency of the method when a very dense grid for a localized area is required [11, 12].

Based on the aforementioned issue, in this study a new adaptive refinement technique for 3D peridynamic models is developed. We shall show that the method can be applied to crack propagation problems in both brittle and ductile materials; moreover, it permits to increase the resolution of the analysis only in critical zones. The proposed method is based on a new technique that couples two peridynamic grids (with different grid sizes) using a morphing strategy. The performance of the method in solution of some 3D real life problems including quasi static propagation of cracks in composite plates, impact loading conditions on fragile industrial structures is investigated. We compare the solutions of the present method with those of a conventional peridynamic model, which employs uniform discretization, and show that the same solution is obtained at a much smaller computational cost.

Keywords: Peridynamic, Meshfree, Nonlocal theory, Adaptive grid refinement, failure, 3D problems.

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Feasibility of machine learning methods for the prediction of roadheader performance in underground excavation project-A case study

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Abstract: Estimation of roadheader performance is one of the main subjects in determining the economics of the underground excavation projects. The poor performance estimation of the roadheaders can lead to costly contractual claims. In this paper, the application of machine learning methods for data analysis named artificial neural network (ANN) optimized by hybrid ant colony optimization (ACO) to estimate of roadheader performance is demonstrated. The estimation abilities offered using ANN-ACO were presented by using field data of achieved from tunnels for Istanbul's sewerage system, Turkey. In this model, Schmidt hammer rebound values and rock quality designation (RQD) were utilized as the input parameters, while net cutting rates was the output parameter. Various statistical performance indexes were used to compare the performance of those estimation model. The results achieved indicate that the ANN-ACO model has strong potential to estimation of roadheader performance with high degree of accuracy and robustness.

Keywords: Machine learning, Roadheader performance, ant colony optimization, Artificial neural network.

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Applying adaptive neuro fuzzy inference system to predict surface settlement caused by mechanized tunneling-A case study

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Abstract: Surface settlement (SS) is an important parameter for the design and operation of earth pressure balance (EPB) shields that should be determined before tunneling. Machine learning methods are accepted as a technology that offers an alternative way to tackle highly complex problems that can't be modeled in mathematics. They can learn from examples and they are able to handle incomplete data and noisy data. The adaptive network–based fuzzy inference system (ANFIS) is kind of machine learning methods that was used in this study to build a prediction model for the SS caused by tunneling. The estimation abilities offered using model was presented by using field data from the Bangkok Subway Project in Thailand. In this model, depth, distance from shaft, ground water level from tunnel invert, average face pressure, average penetrate rate, pitching angle, tail void grouting pressure and percent tail void grout filling were utilized as the input parameters, while the SS was the output parameter. The results achieved indicate that the ANFIS model has strong potential to prediction of SS with high degree of accuracy and robustness.

Keywords: Surface settlement, Machine learning, Mechanized tunneling, Adaptive neuro fuzzy inference system.

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Classification of surrounding rock of highway tunnel based on migration learning

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Abstract: At present, the main construction method of domestic mountain tunnels still adopts the new Austrian method. The initial flexible support must be applied immediately after the tunnel is excavated, and the strength of the support method depends on the real-time classification of the surrounding rock of the tunnel surface. Existing methods of surrounding rock classification need to use complex equipment to extract the surrounding rock classification parameters. In fact, relying on the subjective experience of engineers and technicians in the construction phase is still the main way of surrounding rock classification. The reason is due to cost and efficiency. However, without rich professional knowledge and experience in surrounding rock classification, there are often cases of misjudgment. Therefore, it is an inevitable trend to find a new method for classify tunnel surrounding rock that overcomes the traditional drawbacks.

Based on the image and mechanical parameters of the collected highway tunnel surface, using edge calculation, deep learning and image recognition technology[see Fig.1], the Python language is used to integrate the above functions to develop a set of surrounding rock image integrity recognition system for auxiliary surrounding rock classification. The edge calculation and deep learning technology upgrades the traditional surrounding rock classification to the level of artificial intelligence. The accumulated experience of machine learning can lead to the classification result automatically, which reduces the dependence on the subjective experience of engineers. The main advantage of this method is that with the advantage of artificial intelligence in data storage and analysis, the machine language can quickly classify and judge the integrity of surrounding rock. It is expected to change the present situation of surrounding rock classification that relies too much on professional knowledge and experience, and the accuracy and timeliness of surrounding rock classification can be improved.

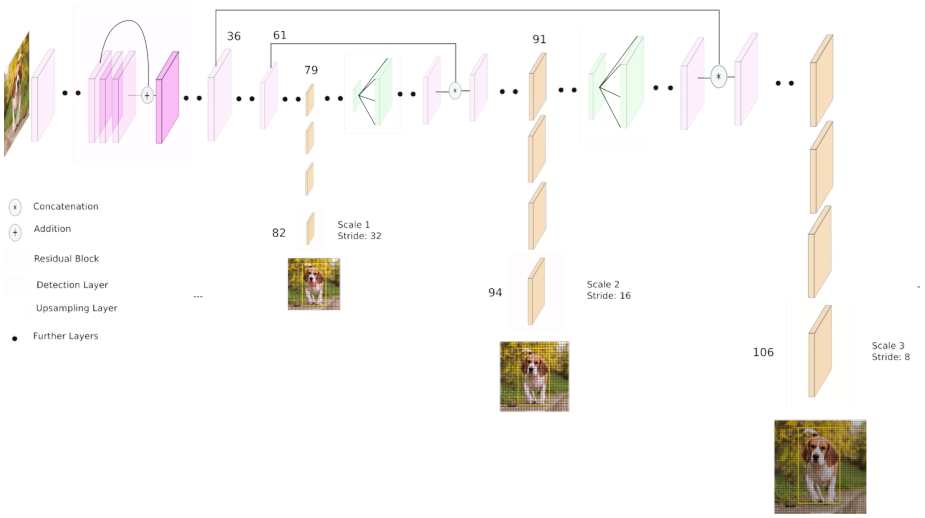

Figure 1: YOLO 3 Integral Structure of Depth Neural Network Used in Pre-research

By collecting more than 800 surface rock images, a deep convolutional neural network model was established to identify the distributed features of surrounding rock, such as joints, fissures fracture degree, integrity, mud and groundwater, and to identify the surrounding rock classification parameters. The discriminating factors of the surrounding rock classification are converted into the modified BQ values for classification, and then combined with the measured rock mechanical parameters for quantitative classification, and finally used to assist in judging the surrounding rock level of the site.

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The following results were obtained through research:

(1) The grading result is automatically generated by relying on surface rock images, and the surrounding rock integrity grading can be quickly and automatically performed after the image of the face is uploaded to the application. The upload process also updates and integrates the data, and gradually judges and corrects the results. □□

(2) Factors affecting the integrity of rock mass in traditional surrounding rock classification- Groundwater impact correction coefficient (K1 value), main soft rock structural surface correction coefficient (K2 value), initial stress state correction coefficient (K3 value) is reclassified by machine learning, and the hardness of the rock (Kv value) is manually intervened in combination with the measured mechanical parameters. Finally, the corrected BQ value is obtained. This method is suitable for tunnel excavation. Fast grading with high quantitative grading characteristics.

(3) Successfully developed the highway tunnel surrounding rock image integrity identification system, and applied it to the actual projects such as the Dongxiang Tunnel of Xingyi Huancheng highway and the No. 1 and No. 2 tunnels of Dadongpo, and compared and verified with the original design surrounding rock grade. It proves that the system is suitable for the classification of surrounding rock of highway tunnels.

Keywords: Highway tunnel, Edge calculation, Deep learning, Image recognition.

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Automatic lithology identification based on machine learning: A case study of TZ4 well

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Abstract: Lithology identification of hydrocarbon reservoir based on well logging curve is significant for drilling planning and reservoir development. The conventional stratigraphic identification methods usually require large amount of labour work. The machine learning is able to deal with the data-intensive tasks and enhancing the lithology/formation recognition, and make it easier to build a lithotype profile. Four typical algorithms, i.e. Adaboost, decision tree, random forest and linear support vector machine are introduced in present study. By comparing the prediction accuracy of each algorithm on TZ4 well logging data, an optimal algorithm is chosen for further study. Then, the sensitivity analysis of data dimensionality reduction and training set adjustment is carried out, so as to explore the main factors affecting the accuracy of formation identification. The results show that decision tree algorithm has higher accuracy in the selected four algorithms and when the training ratio reaches 50% and the number of logging parameters is at least four, the accuracy can reach 90%.

Keywords: Lithology identification, Machine learning, Sensitivity analysis, Prediction accuracy.

Lithology identification is an indispensable part of oil and gas exploration and development. The recognition results allow better understanding on the stratigraphic profile and oil and gas distribution, providing reference for oil and gas field development. The efficiency of formation identification technology is required to improve to deal with the data intensive tasks. Machine learning methods are introduced to meet this requirement and to build the lithotypes profile efficiently and accurately.

In 1991, Ruiz first proposed the use of artificial neural networks to divide the strata, which laid the foundation for stratigraphic intelligent identification [1]. Many scholars began to use neural network methods. After nearly two decades of development, the intelligent recognition technology of the formation has become more and more developed. Roy used the linear PCA reduction method for classification of seismic facies [2]. T. Zhao used SVM to classify 3D seismic data by lithology [3]. Tang applied artificial neural networks for the automated lithotyping [4]. John uses the Bayesian approach to estimate the distribution of facies [5]. Al-Anazi and Gates attempted to use the SVM method for lithology prediction [6]. Zazoun R.S used neural networks to predict fractured reservoirs [7]. The above research proves that the intelligent identification of formation has important application value and wide application prospects. However，although the existing stratigraphic intelligent identification method improves the work efficiency, there are still some problems such as difficulty in data collection and insufficient accuracy. Therefore, it is necessary to propose a stratigraphic intelligent identification method that can widely identify the well logging data and has high precision and applicability.

The intelligent recognition method of formation is based on the machine learning classification algorithm, which can classify and identify the logging data, effectively learn and remember the characteristics of the rock formation in the reservoir. This method can compare the four algorithms of Adaboost, decision tree, random forest and SVM, and select the highest accuracy for lithology identification. The TZ4 well is located in the Tarim Basin. The location is the Devonian Donghetang Formation, which contains three lithologies such as fine sandstone. In order to explore the impact of different algorithms on accuracy, the TZ4 well was tested with 50% training ratio and eight logging data. The test results are shown in Fig.1. The left column stands for lithology from real core sample, which is the ground truth of the lithology/formation recognition. Prediction results of four different methods e.g. Adaboost, Decision tree, Random forests and SVM are shown in the middle column.

The results from Fig. 1 show that the decision tree algorithm has the highest accuracy of 91.32%, The accuracy of

Adaboost, random forest, and SVM algorithms are 82.96%, 70.42%, and 54.98%, respectively. Therefore, the decision tree algorithm is used to analyze the sensitivity of training data volume and data dimension.

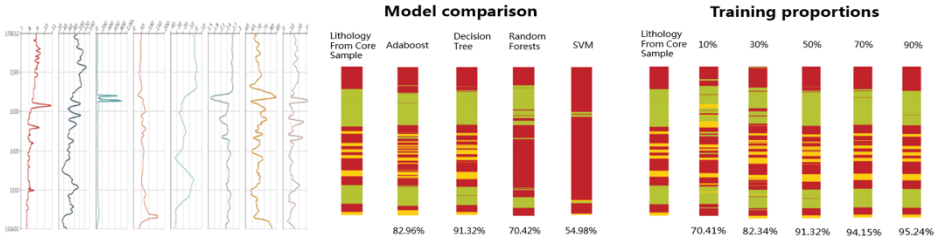

Figure 1: Model comparison and training proportions based on well logging data

The accuracy can be greatly influenced by training data volume in total data set. Five groups of scenarios are conducted using the decision tree algorithm to investigate the impact of different training proportions on the prediction result. Typical results for different training set volume are shown in the right column of Fig. 1. It is found that by training only 30% of the total data set, the accuracy can reach above 80%. And the accuracy is positively correlated with the training data ratio, the accuracy increases as the training ratio rises.

In order to explore the impact of different logging parameters on accuracy, several groups of scenarios are conducted, using decision tree algorithm and 50% training proportion. By adding the number of logging parameters, the test results are presented in Tab. 1.

Table 1: Data dimension based on lithology labels

Case#	Parameters	Accuracy, %
1	ILD	60.25
2	ILD, SP	79.81
3	ILD, SP, CN	87.78
4	ILD, SP, CN, ILM	88.42
5	ILD, SP, CN, ILM, GR	91.27
6	ILD, SP, CN, ILM, GR, CAL	91.32
7	ILD, SP, CN, ILM, GR, CAL, AC	91.36
8	ILD, SP, CN, ILM, GR, CAL, AC, DEN	91.61

Tab. 1 shows that the accuracy gradually increases from 60% by adding number of parameters. Using the same training ratio and algorithm, the combinations of the most accurate parameters are shown. The ILD is the most influential factor and contributes most on the accuracy. It is found that accuracy can reach 90% by using four or more logging parameters. When the number parameters are greater than four, the accuracy tends to stay steady.

Acknowledgement

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Automatic identification of gas hydrate formation using machine learning algorithms

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Abstract: Ensemble learning integrates the results of multiple weak learners through certain rules, so it has better learning effect than single weak learner. As a method of machine learning, it has been widely used in various fields. Existing hydrate recognition methods are highly empirical and lack of efficiency. Gas hydrate has the characteristics of high resistivity, abnormal potential and low gamma parameters, so it can be considered to be identified by using machine learning method with well logging parameters. Ensemble learning has the characteristics of fast speed and high accuracy, and has a wide application prospect. In this paper, a complete data analysis process and corresponding data analysis algorithm are used to analyze and process logging data, and the accuracy of integrated learning in hydrate recognition is verified by comparing with the real formation conditions. Comparing different ensemble learning algorithms for the accuracy of final prediction results, the ensemble learning algorithm presents the highest accuracy, which can be applied for further analysis, e.g. dimension reduction and data training, thus reducing the workload of data processing.

Keywords: Ensemble learning, Well logging data, Hydrate recognition, Machine learning.

Natural gas hydrate is a non-stoichiometric cage-like crystalline compound formed by natural gas and water at high pressure and low temperature. The main components are methane, including ethane, propane and other substances. How to improve the accuracy and timeliness of hydrate recognition has become the primary problem.

Current hydrate identification methods are divided into direct identification method and indirect identification method. Direct identification is judged by the visual observation of formation sampling. The cost of this method is high, and hydrate is easy to decompose in this process, resulting in deviation of judgement. Indirect identification method is realized by physical and chemical properties of hydrate and logging and seismic parameters [1]. Gas hydrate has the characteristics of high resistivity, increasing P-wave time difference and negative potential anomaly [2]. At present, Archie formula is commonly used to estimate hydrate saturation by resistivity [3]. Schlumberger explores formation hydrate by Carbon-Oxygen Ratio Method [4]. The principle of seismic method is to use the difference of seismic reflection velocity in different strata to detect target strata [5]. The methods of identifying hydrate by seismic parameters include BSR, blank seismic reflection zone, AVO inversion technology, polarity inversion and so on, etc. [6].

At present, there are still some problems in hydrate identification methods, such as poor timeliness and accuracy. For example, BSR does not correspond to hydrate one by one. BSR does not exist in all hydrates [7]. Inks et al. found that the interpretation results of acoustic logging on the northern slope of Alaska are inconsistent with those of three-dimensional seismic prediction [8].

In this paper, the integrated learning algorithm is used to program, and four integrated learning algorithms, Adaboost, SVM, random forest and decision tree, are used to predict whether the formation contains hydrate. Logging data are from Northwest Eileen State-2 well. Strata are marked separately according to whether hydrates are present or not. Then the program is written with Python, and the formation data and labels are divided into training set and testing set respectively. The model is trained with training set and the stratum is predicted with test set. The results of prediction and the actual stratum situation are compared. The test results show that the AdaBoost algorithm has the highest prediction result for formation. As shown in Fig.1, the test results illustrate that the method based on

ensemble learning has higher accuracy and application value for formation hydrate recognition.

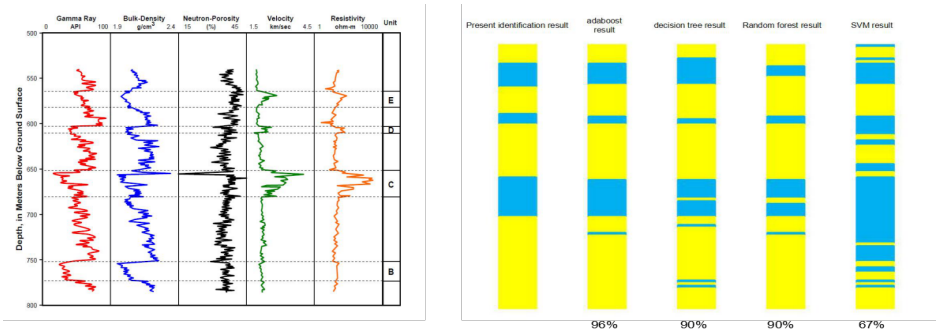

Figure 1: Model comparison based on logging data

Precision rate and recall rate are two indicators to measure the prediction results. Precision rate is the proportion of the correct prediction in the predicted sample, while recall rate is the proportion of the correct prediction in the actual sample. And F1 score is an index used to synthesize the two.

The binary average of F1 fraction predicted by AdaBoost algorithm is 0.89, while that predicted by SVM algorithm is only 0.628. The low value of F1 indicates that there is a big difference between precision and recall rate. The fact proves that the strata predicted by SVM algorithm are not in good agreement with the actual strata. The following table lists the F1 scores, precision and recall rates calculated by various methods.

Table 1: Performance metrics comparison between different algorithms

Algorithm	F1 score	precision	recall rate
Adaboost	0.890	0.962	0.862
SVM	0.628	0.474	0.931
Decision tree	0.807	0.821	0.793
Random forest	0.766	0.950	0.655

Acknowledgement

The present research is supported by the Strategic Priority Research Program of the Chinese Academy of Sciences, Grant No. XDA14040401 and Grant No. XDA14040402.

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Automatic damage analysis of cracked concrete specimens using deep learning-based crack detection techniques

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Abstract: During their service life, civil engineering materials such as concrete have a strong possibility of cracking which causes a reduction in ultimate load bearing capacity and stiffness. To correctly predict the remaining load bearing capacity of cracked engineering structures is of great importance for not only the safety concern but also economic considerations. However, one of the big challenges is the accurate and efficient detection of existing cracks in civil infrastructures. As a substitution of the traditional human-based inspection methods and image processing techniques, machine learning, which has been extensively studied worldwide in the field of computer science in past decades and shown strong ability in image recognition, has been applied for damage detection in concrete structures, among which, the deep learning method using convolutional neural networks shows very robust and accurate performance in image analysis. In this work, an indoor experiment of damaged reinforced concrete box is analyzed. At first a deep learning model using convolutional neural networks is trained using other sources of cracked and intact concrete images. Then the pictures taken in the indoor experiment once the crack forms during loading are split into smaller equal-sized square pictures and these pictures are analyzed using the developed deep leaning model to detect whether the squares are cracked or not. Afterwards a numerical model using mixed cover meshless interpolation and the continuum damage mechanics are automatically established taking these generated squares as meshes, in which those detected cracked elements are given a large damage factor while the others not. The subsequent loading analysis is carried out using the concept of a continuum damage model regularized by fracture mechanics. The obtained force displacement curve and final crack patterns are then compared to the experimental results. This method can be served as an application to the safety assessment of real damaged reinforced concrete structures.

Keywords: Image recognition, Deep learning, Cracks, Reinforced concrete.

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A new method of tunnel leakage water identification based on terrestrial laser scanning

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Abstract: Terrestrial laser scanning is widely used to obtain point cloud data and describe the deformation and surface geometric conditions of tunnels. In particular, the reflection intensity values of point cloud can be used to identify tunnel leakage water. In this paper, a new method based on laser reflection intensity and coordinates of point clouds is proposed to identify the leakage water location in tunnels and remove the geometric interference of tunnel facilities such as ventilation ducts, cables and bolt holes. The method is performed in the following steps: (1) use machine learning to fit the relationship between distance, incidence angle, roughness and laser reflection intensity values of point clouds, (2) compare the fitting laser reflection intensity value with the real laser reflection intensity value of each point in the area to be measured and identify the possible leakage points, (3) use piecewise parabola to fit the cross section curve of tunnel and exclude geometric interference points, and (4) the remaining possible leakage points represent the real leakage water location. The proposed method have been applied to a highway tunnel project in Sichuan province, China. The results show that the leakage water location can be well identified and the geometric interference of tunnel facilities can be removed effectively.

Keywords: Tunnel, Leakage Water, Terrestrial Laser Scanning, Machine Learning.

Acknowledgement

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Dynamic Classification of Surrounding Rock Mass in Tunneling Boring Process Based on Big Operational Data

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Abstract: Tunnel Boring Machine (TBM) has become an essential part in long infrastructural tunneling excavation since 19th century, because of its high safety, less effect on surroundings and rapid excavation speed [1, 2]. However, TBMs are more sensitive to geological conditions (i.e. rock bursts, water bursts and other geological hazards) than other tunneling method [3]. Considering that the actual geological conditions are nearly unknowable before excavation because observation and measurement cannot be conducted during tunneling nowadays [4-6]. The high-speed excavation capability of TBMs cannot be fully utilized, especially in rock-soil mixed-face ground or other unfavorable geological conditions [7]. To depict the real-time profile of the geological conditions of tunnel face, a series of studies have been conducted based on the operational data of TBMs via state-of-the-art machine learning methods [3, 4]. But when they conducted the machine learning methods to predict the accordingly surroundings, they ignored one problem that in many cases, the rock mass types are imbalanced. Contrarily, traditional machine learning methods are based on the balanced data hypothesis, which will perform bad in imbalanced data [8]. To solve this problem and obtain a better view of the tunnel face's conditions, cost-sensitive AdaCost algorithm was proposed. The database of this study composed by more than 5×10^6 data collects from the Songhua River Water Conveyance project in Jilin province, China. The typical rock mass information including rock mass types and their corresponding length recorded by in-situ survey before the tunneling was presented in Tab. 1. The proportion of granite in the rock mass types is 45.21%, while that of diorite in the rock mass types is 10.81%, showing the characteristic of slight imbalanced.

Table 1: Rock mass information

Rock mass types	Length (m)	Percentage of length (%)
Diorite	2096	10.81
Granite	8766	45.21
Sandstone	3448	17.78
Tuff	5081	26.20
Summary	19391	100.00

There are 199 kinds of available TBM operational data generated each second during excavating process. Thus, efficient preprocessing is significant for reducing redundant and improving computational efficiency. In this study, data preprocessing was conducted as shown in Fig. 1. Ten operational variables related to cutterhead rotational speed and boot pressure were selected by feature engineering as input variables, and their relative importance are shown in Fig. 2.

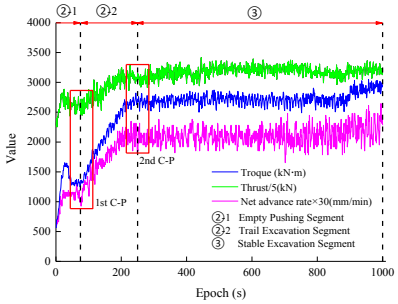

Figure 1: The evolution of advancing speed, thrust force and cutterhead torque in a certain tunneling cycle.

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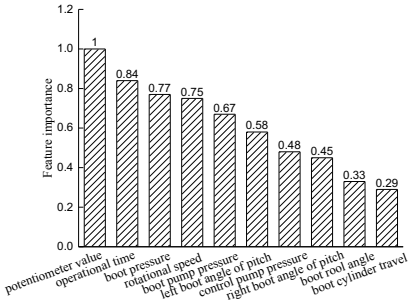

Figure 2: The relative importance of tunneling parameters to the class of surrounding rock

By dividing the database into 90% training sets and 10% test sets, the accuracy of traditional machine learning methods and cost-sensitive AdaCost methods was calculated and compared in Table 2. Although the total accuracy of traditional methods is 91%, its performance in the minority class, i.e., Rank IV and Rank V, is relatively poor. However, the accuracy of classification rises 16% and 50% in Rank IV and Rank V respectively by conducting cost-sensitive algorithm, which indicated that the proposed AdaCost algorithm has strong applicability to imbalanced data than traditional machine learning methods.

Table 2: The class of surrounding rock obtained by RF model and AdaCost model respectively

Accuracy	Rock mass rank				
	Rank II	Rank III	Rank IV	Rank V	Total
Traditional methods	0.88	0.97	0.50	0.00	0.91
AdaCost	0.88	0.98	0.66	0.50	0.94

Keywords: Rock mass classification, Tunneling Boring Machine, Imbalanced big data, AdaCost.

Acknowledgement

This study was funded by the National Natural Science Foundation (4182780021) ("Basic research on scientific instruments of the national natural science foundation of China").

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Prediction of Strength of Foamed Concrete under Cyclic Loading Using Artificial Neural Network

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Abstract: Foamed concrete fill has been increasingly used as backfill material in geotechnical engineering. Sometimes, foamed concrete fill is subjected to cyclic loading, such as traffic loading and machine vibration. Thus, using unconfined compressive stress of foamed concrete could be unsafe as dynamic loading has potential for degradation of material properties. This study conducted a series of unconfined compressive test of foamed concrete under static and cyclic loading to explore the influence of loading type on the strength of foamed concrete. The results show that the cyclic loading yielded lower strength of foamed concrete than static loading, as its internal structure is easier to fail under cyclic loading. In an affect to predict the unconfined strength of foamed concrete under cyclic loading based on its strength under static loading, artificial neural network (ANN) was used. Good agreements between predictions and the real values were obtained after training the model using the test results.

Keywords: Foamed concrete, Unconfined compressive strength, Cyclic loading, Artificial neural network, Data training.

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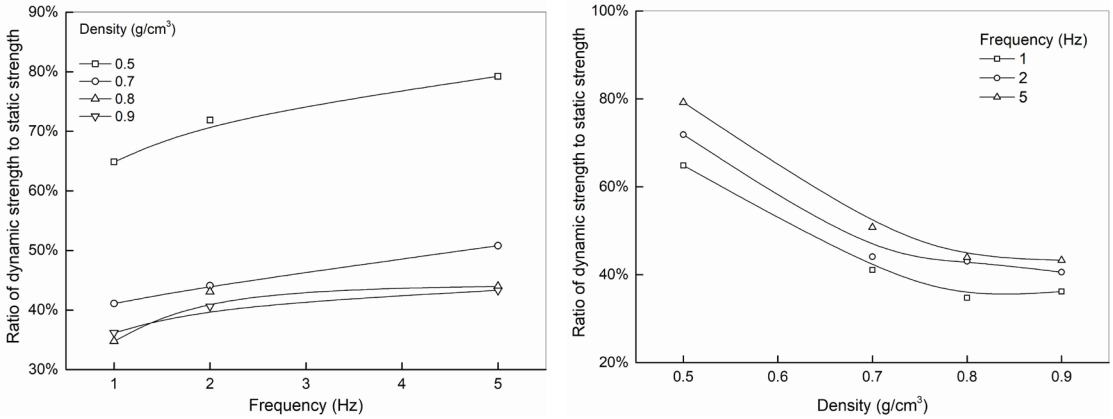
Key pictures

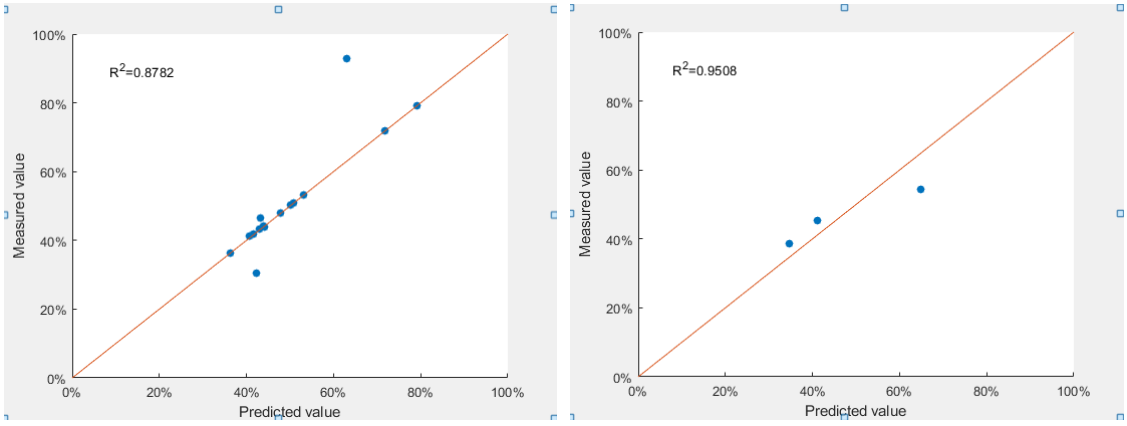
(a) Low density (b) High density

Figure 1: Failure mode of foamed concrete with different density



(a) With frequency (b) With density

Figure 2: Variation of ratio of dynamic strength to static strength



(a) Training (b) Testing

Figure 3: A comparison between measured value and value predicted by ANN

A coarse-grained model for carbon nanotube/polymer nanocomposites

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Abstract: Although molecular simulations have been widely used in the modeling of nanocomposites, the huge computational effort required by the simulations severely limits their applicability to small molecular systems over a limited time scale. One approach to overcome this drawback is the development of coarse-grained (CG) models [1-4]. The principle of CG models is to map a set of atoms to a CG bead, which enables to extend the accessible time and length-scales while maintaining the molecular details of an atomistic system (see Fig. 3). The mapping scheme relates the atomistic coordinates of a structure to the bead positions in the CG model. The CG models provide a reduced picture and interpretation of complex molecular phenomena by averaging over unessential atomic details. It facilitates the study of molecular systems since (1) the total number of particles is reduced, (2) the interaction potentials are simplified and (3) the potential energy surface on which the molecules move is smoothed, leading to an acceleration of molecular simulations. The main challenge is therefore to develop a CG model that reproduces the same physical behavior as the atomistic reference system.

In this study, a CG model for carbon nanotube (CNT) reinforced polymer matrix composites is developed. The CG force fields for nanotubes and polymer chains are calibrated using the strain energy conservation between CG and all-atom systems. The ability of the CG model in predicting the material properties of CNT/polymer composites are evaluated through verification processes with atomistic simulations. The simulation results reveal that the CG model is able to estimate the elastic properties of the nanocomposites with high accuracy and low computational cost. The effect of the volume fraction of CNT reinforcements on the Young's modulus of the nanocomposites is investigated. The application of the method in the modeling of large unit cells with randomly distributed CNT reinforcements is examined. The proposed CG model will enable the simulation of reinforced polymer matrix composites across a wide range of length scales from nano to mesoscale. In the future, the CG model can also be utilized and developed to predict the mechanical properties of polymer composites reinforced by functionalized SWCNs and multi-walled CNTs subjected to static and dynamic loading.

Keywords: Polymer nanocomposite, Carbon nanotube, Material properties, Coarse-grained model, Molecular simulations.

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Analysis of discontinuous evolutions in phase-field fracture modelling

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Abstract: Phase field modelling of fracture has revitalized the study of failure phenomena in the scientific community during the last two decades. Multiple applications in multi-field frameworks [1-3] have been attempted to exploit the advantages of the approach. Complex crack behaviors like nucleation, merging and branching, which used to rely on intricate numerical techniques, are naturally handled by an additional partial differential equation. From a theoretical point of view, a phase-field crack evolution is dictated by three energetical principles [4] namely, energy conservation, irreversibility and global stability. While irreversibility and energy conservation are grounded on thermodynamic principles and are widely accepted, the third one is still under debate. As pointed out by [5], a global stability criterion results in unphysical results in nonconvex variational problems since a jumps over energy barriers would be necessary in order to reach a global minimum. In terms of fracture modelling, numerical results show cracks propagating instantaneously through the domain when a continuously evolving crack is expected. A local stability criterion would be more suitable, however as shown by [5], even in this scenario the formulation allows jumps during crack growth, breaking the causality principle [5]. Modifications to the theoretical framework have been proposed by [5] and [6] pointing out the necessity of capturing rate dependent effects during fast crack propagation to obtain physically meaningful solutions. However the implementation of a numerical scheme capable of representing viscous and inertial effects in a rate independent framework has not been tackled yet. Here, an algorithm based on a Machine Learning algorithm is proposed in order to study the space of admissible solutions during the optimization process.

Machine learning has been successfully applied in other contexts to define the optimization domain in problems with non-convex objective functions in material science [7]. In [8] a classification of learning algorithm was used to define an optimization domain based on data from experiments and numerical simulations. In [9] an adaptive algorithm is defined in order to modify the definition of the space of interest during the optimization process. Following the same line of idea, a multilayered feed-forward neural network is used to explore the effect of inertial effects on crack propagation during fast transitions. The finite element method is used to discretize the partial differential equations resulting from the minimization of the total energy functional. Crack propagation in the quasi-static and dynamic cases is considered. The Alternating Minimization Algorithm (AMA) is adopted here to solve the quasi-static problem and implicit generalized alpha integration method for the dynamic case. By feeding pairs of simulations of the quasi-static and dynamic crack propagation examples a multilayer neural network is trained to calculate a relaxation ratio of a sequence of solutions of the evolution problem. Afterwards, the relaxation ratio is used along with the quasi-static scheme to obtain improved solutions that better reflect the rate dependent phenomena that are expected during jumps in the system evolution.

The results show that the total energy of the system is not conserved during fast crack growth, however the energy imbalance obtained with the calculated relaxation ratio agrees well, within a certain range of crack propagation velocities, with the energy associated to inertial effects in the dynamic case. For crack tip velocities beyond this threshold the quasi-static solution becomes inadequate to model crack propagation since phenomena like branching and crack propagation promoted by wave reflection take on a dominating roll during the evolution.

Keywords: Phase-fields, variational formulation, fracture, rate independent.

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A finite element framework for vibration problem of hybrid nanocomposite beams reinforced with graphene platelet and carbon fiber

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Abstract: Dispersion of nanosize reinforcements in an initial matrix has attracted the researchers' attention in the last two decades. The main reason for the widespread implementation of nanofibers and nanoparticles in a matrix to generate nanocomposites is enhanced material properties of nanomaterials in comparison with their bulk specimen. Through this fact, nanomaterials like carbon nanotube (CNT), graphene, and graphene platelet (GPL) were highly employed by designers to improve the material properties of an initial resin. For instance, [Ke, Yang and Kitipornchai (2010)] analyzed the nonlinear vibrational characteristics of CNT-reinforced (CNTR) nanocomposite beams. The thermo-mechanical postbuckling problem of nanocomposite cylindrical panels reinforced with CNTs was solved by [Shen and Xiang (2014)] once the structure is subjected to an axial compression. In another investigation, the large deformation behaviors of CNTR nanocomposite skew plates were monitored by [Zhang, Liew (2015)] based on the finite element method (FEM). The issue of investigating the impacts of nanofibers' agglomeration on the natural frequency of CNTR nanocomposite doubly-curved shells was probed by [Tornabene, Fantuzzi, Bacciocchi et al. (2016)]. On the other hand, [Barati and Zenkour (2017)] carried out a postbuckling study dealing with stability responses of GPL-reinforced (GPLR) nanocomposite beams regarding for the geometrical imperfection of the structure. The thermal stability problem of graphene-reinforced (GR) nanocomposite plates was solved by [Shen, Xiang, Lin et al. (2017)]. Both free and forced frequency characteristics of GPLR nanocomposite plates were surveyed by [Song, Kitipornchai and Yang (2017)] in the framework of the first-order shear deformation theory (FSDT) of plates. The dependency of material properties of GR nanocomposites are included in a nonlinear thermal buckling analysis conducted by [Kiani and Mirzaei (2018)] to investigate the stability behaviors of nanocomposite beams.

Recently, a novel type of nanocomposites has been developed, fabricated from three phases, in particular an initial matrix strengthened via both macro- and nano-scale reinforcements. Due to the nature of such newly developed nanocomposites, they are called multi-scale hybrid nanocomposites. [Ebrahimi and Habibi (2018)] enriched a numerical answer for the low-velocity impact problem of multi-scale hybrid nanocomposites reinforced with carbon fibers (CFs) and CNTs. The vibrational characteristics of multi-scale hybrid nanocomposite plates reinforced with CFs and CNTs were investigated by [Ebrahimi and Dabbagh (2019)] in the framework of the classical theory of plates in association with the micromechanical homogenization methods. The major objective of this manuscript is to present a powerful FE-based framework founded on the basis of the Rayleigh-Ritz method for the purpose of solving the natural frequency problem of multi-scale hybrid nanocomposite structures strengthened by dispersion of nanosize GPLs and macroscale CFs in a polymeric matrix. The under observation geometry is a beam with rectangular cross-section which is assumed to be modeled implementing a refined shear deformable beam hypothesis. The strain-displacement relations will be achieved using the definition of the infinitesimal strain tensor in the continuum mechanics. Afterward, dependent expressions will be developed for both kinetic and strain energies of the nanocomposite beam. The next step belongs to achievement of the maximum amounts of the abovementioned energies by the means of the Rayleigh-Ritz method. Finally, the partial differentiations of the Rayleigh parameter with respect to the unknown coefficients will be calculated to obtain the final eigenvalue of the problem. It is worth mentioning that the presented methodology will be able to consider for various edge supports at the ends of the structure. The results of this work indicate on the unbelievable role of the nanoscale reinforcements on the natural frequency of the nanocomposite structure as well as the volume fraction of the utilized macroscale CFs.

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Keywords: Free vibration, finite element (FE), multi-scale hybrid nanocomposites, Graphene platelet (GPL), Refined shear deformable beam model.

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Modeling effect of thin film's surface roughness on nanoindentation test using random forest

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Abstract: Nanoindentation test is one of the tests to measure the mechanical properties of materials, especially macro-composites, which have been used since the mid-1970s. This test was carried out by a device of the same name that during this test, the tip-shaped of the device penetrates on the surface of the specimen to a size of a few nanometers, and the force-displacement curve is obtained as a direct output from this test. Experimental results indicate that this test is dependent on the roughness of the tested part [1]. In the study of mechanical properties using nanoindentation test, the perfect surface finish on the test specimen is often required [2]. Reaching to a perfect surface finish is also depends on the limitation of the cutting tool devices [3]. Greenwood and Williamson defined one of the firsts elastic contact models [4]. However this model can predict the mechanical properties in too many cases without coatings, this model is not an efficient one in some cases with coatings [5]. In addition to these cases, access to this device, as well as performing this test in special circumstances, such as high-temperature nanoindentation test, is one of the instrumental limitations of this test. Also, the production of samples that have coatings due to the availability of the required devices, is also a timely process to achieve the desired mechanical properties for the users. In this study, this test defined with a 3D finite element model in Abaqus CAE and the validity was proved by experimental cases like coating materials. Although this simulation has taken an effective step in speeding up this process, as well as the ability to carry out this test on a wide range of materials defined by the user, this study attempts to even allow the user to not to perform simulations and also let the user to achieved the parameters like stiffness and surface hardness in a fraction of a second. This part of the research is carried out by the machine learning process. Due to the wide variety of base materials and various coatings that exist, because of the conventional use of steel in the industry, the specimens like steel base materials with commercial coatings become the purpose of this research is to continue the process by using machine learning process. After all this, for achieving to the parameters like stiffness and surface hardness, The user even does not need to simulate this test on steel base materials with conventional industrial coatings, and only uses the properties that are defined to machine learning process input, and get stiffness and hardness values in fractions of a second to desired surface.

Keywords: Nanoindentation, Surface roughness, Stiffness, Hardness, Machine learning.

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Assessing the spalling risk of fire-loaded tunnel linings by multifield model and machine learning strategy

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Abstract: Concrete structures may experience spalling when subjected to fire loading. Spalling is the violent splitting of concrete pieces from the surface of the structure, greatly jeopardizing the durability of the structure. Spalling is closely related to various chemical and physical processes such as dehydration of heated concrete, phase change of pore water, formation of moisture clog, and consequent fast increasing of pore pressure. Different concrete mixtures, ambient humidity, and fire scenarios provide different spalling risks. The strongly coupled multi-field model can take into account a single working condition and need considerable computing efforts, which is unable to consider the uncertainty of concrete materials and environments.

Aiming at solving these problems, this work proposes a fast spalling risk evaluation method, combining the multi-field model and the machine learning method. Firstly, a large number of material parameters, humidity and fire scenarios are considered as input parameters for simulations by means of the coupled multi-field model [1-3], providing the data samples for machine learning. Then the machine learning method is used to study the correlations between the input parameters and the obtained results such as maximum pore pressure of concrete, see Figure 1. Finally, by comparing six different algorithms: 1) Logistic Regression, 2) Support Vector Machine, 3) Gaussian Naive Bayes, 4) Random Forest, 5) Decision Tree, 6) K-Nearest Neighbor, we found that regarding the maximum pore pressure the prediction accuracies of all algorithms are between 84% and 100% in which the decision tree algorithm can reach up to 99.18%. The method presented in this study can very quickly predict key factors affecting spalling risks such as the maximum pore pressure and the temperature at the same depth based on different material properties and environmental conditions.

Keywords: Tunnel fire, spalling risk, multifield model, machine learning.

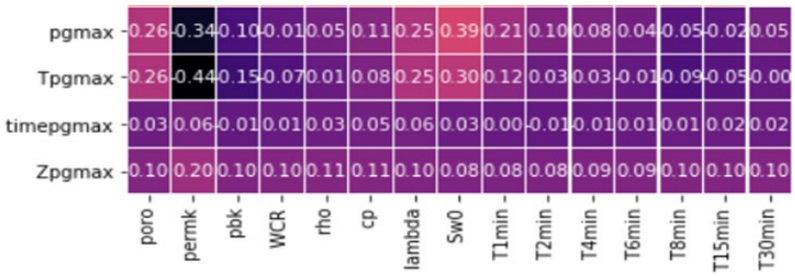

Figure 1: Correlation analysis of the spalling factors

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Computational Modeling for Effect of Crack Healing Pattern in Self-Healing Concrete

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Abstract: Concrete is the most widely used construction material in the world, therefore, is considered the second-most consumed materials on earth, after water. But the weakest point that it subjected to cracking and deterioration with the time, and the renovation of the buildings made of it costs a lot especially for infrastructure maintenance which is not easily accessible. Recently, the biological systems become the inspiration for the material scientists. This fundamental change in material design philosophy has resulted in the creation of 'smart' materials, like self-healing materials. The development of self-healing concrete (SHC) has recently attracted a lot of attention due to its inherent ability of automatic crack detection and crack repair with the goal of significantly prolong the service life and reduce the cost of maintenance [1]. The aim of this research is to study the healing efficiency, life expectancy of the concrete for the given design of micro-capsules and distribution, as well as material degradation over time. In fact, studies on crack healing pattern are more important when incorporated in research on design of self-healing structure because different positioning of healing capsules can lead to different crack healing pattern. However, if the applied load is sustainable or the crack propagation is fast, partial healing at crack mouth will appear because the capillary force might not be large enough to suck healing agent to fulfill the space above the self-healing capsule. In addition there are possibilities where fully bonding is not established in the healing zone because chemical properties of healing agent can be changed during storing or manufacturing process. There are a lot of laboratories studies and experiments were done to study either the fracture interaction between the capsules and the concrete matrix or the healing efficiency and healing performance such as [2]. Recently a lot of computational modeling in SHC is done to study the fracture interaction between the capsules and the concrete matrix with different modeling techniques; using cohesive elements [3] and using XFEM with cohesive surface which showed high accuracy [4]. But the computational modeling of the healing efficiency or healing performance of SHC is still in its infancy. In this study, numerical simulations with XFEM, where properties of elements represent for healing agent are randomly assigned, adopted to simulate the reliability of healing effect.

Keywords: Self-healing concrete, Healing efficiency, Healing pattern, XFEM.

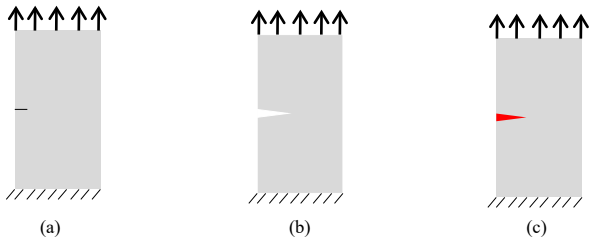

Figure 1: Schematic sketch of modeling direct tension test: (a) Notched virgin material; (b) Crack propagation; (c) Healed material

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A data-driven solution for the governing equation of flexoelectricity

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Abstract: Electromechanical coupling effect has been widely utilized in various applications ranging from building structures [1,2], sensors [4,5] to biomedical devices [6,7]. Flexoelectricity, a type of electromechanical coupling effect, has shown great potential for the electromechanical device at small length-scale thanks to its size-dependent effect [7]. However, the involvement of the strain gradient term in the governing equation of flexoelectricity imposes C^1 continuity for solving the partial differential equation. Meshfree method [8] and Mixed finite element method (MFEM) [9] overcomes this obstacle by applying higher-order shape function and imposing extra degree of freedoms, respectively, which largely increase the computational load. This makes the simulation of the electromechanical response of the complex 3D flexoelectric device by the Meshfree or MFEM computational expensive and ineffective.

A data-driven technique for solving nonlinear partial differential equation has been successfully implemented in [10]. The physics-informed neural network in [10] is trained to solve supervised learning tasks with respecting to the given law of physics. In this study, we implement the mixed finite element method model for flexoelectricity in AceGen [11] to generate the training data for the physics informed neural network in [10]. With TensorFlow, we implement the data-driven framework to build the physics-informed surrogate model for analyzing the electromechanical response of certain flexoelectric devices. Our results show that the physics-informed neural network captures the electromechanical response of the studied flexoelectric devices with marginal errors. It's also found that the learning speed and accuracy of the physics-informed neural network depends on the given batch size.

Keywords: Flexoelectricity, Data-driven computing, Strain gradient, Neural network, Coupled problem

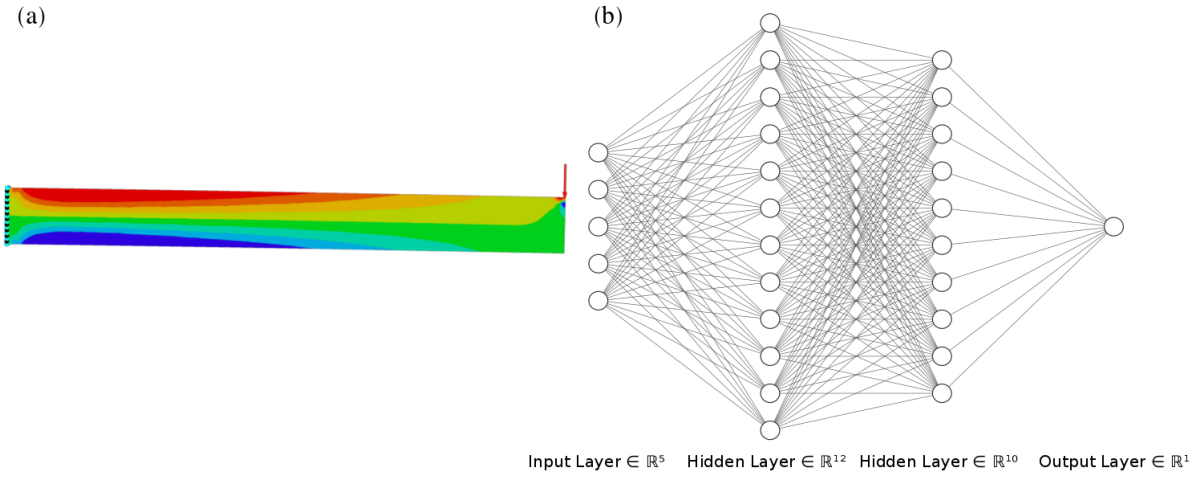

Figure 1: (a) Electromechanical response of a cantilever beam due to flexoelectric effect by MFEM; (b) The schematic illustration of the physics-informed neural network applied in this work

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Synthesis and study of copper ferrite-copper oxide nanocomposites

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Abstract: In this research copper ferrite as a core magnetic nanostructure were fabricate by a simple precipitation method using green capping. Some fruits like lemon and orange were applied as biocompatible surface active agents. Regarding their biocompatibility, low toxicity and adjustable magnetic properties, magnetic copper ferrite nanoparticles have special physical and chemical properties because of their super-paramagnetism, quantum size effect and surface-boundary effect [1-4]. Then copper oxide nanoparticles and copper ferrite-copper oxide nanocomposites were synthesis by a fast chemical procedure. The X-ray diffraction pattern has suitable agreement with standards and confirms purity of the nanocomposites. Scherrer equation was estimated of crystallite size under 100nm. The SEM image for various $CuFe_2O_4$, CuO and $CuFe_2O_4$/ CuO indicate mono- disperse particles with mediocre size under 100 nm. FT-IR spectrum of nanoparticles indicate the absorption peak of $CuFe_2O_4$/ CuO. The hysteresis loop of $CuFe_2O_4$and $CuFe_2O_4$/ CuO exhibits super paramagnetic behaviour. The photocatalytic activity of the $CuFe_2O_4$/ CuO nanocomposites were degradation Acid black and methyl orange azo dyes above 90% at 60 min. Due to their unique optical properties it possess various applications in lasers, light-emitting diodes, multi-exciton generation solar cell detectors, nonlinear optics, single electron devices and biological imaging [5-10].

Keywords: Nanostructures, Photocatalyst, Copper ferrite, Copper oxide.

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Comprehensive Study of Crack Propagation of different Percentage of Doping of Boron Atoms on the Mechanical Properties of Polycrystalline Graphene

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Abstract: This article investigates the effect of different initial crack sizes on the mechanical response of single-layer boron doped polycrystalline graphene nanosheets by Molecular Dynamics (MD) simulations. We study 1%, 3%, 6% and 10% of boron doped polycrystalline graphene nanosheets with grain sizes of 10 and 15 nm for eight different initial crack lengths of 0.02L, 0.04L, 0.08L, 0.12L, 0.16L, 0.2L, 0.24L, and 0.32L, where L is the initial length of the nanosheet. We found that 1. brittle fracture for boron doped polycrystalline graphene as the failure occurs without any sign of plastic deformation and low energy absorption and 2. the ultimate tensile strength is independent of the initial crack size. For identical grain sizes and doping of boron atoms, the ultimate tensile stress and strain decrease as the crack lengths increases. In contrast, a clear trend was not observed in the ultimate tensile strength for the same crack length and doping of boron atoms as the grain size increases. The highest difference of 13.4% in the ultimate tensile strength was observed between grain sizes of 10 and 15 nm for 3% of boron doped nanosheets with an initial crack size of 20 Å.

Keywords: Boron nanosheet, doped polycrystalline graphene, fracture behavior, molecular dynamic simulation, Initial crack.

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Phase field modelling of microstructural length scale effects on stressed grain growth in polycrystalline copper thin films

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Abstract: The phase field modeling approach has recently emerged as a powerful simulation tool for microstructure evolution applications [1-8]. In this approach, the microstructure is represented by a set of non-conserved phase field variables which are continuous in space and time. Each variable represents the local volume fraction of its corresponding phase i.e. it takes unity in its corresponding grain and zero elsewhere. Grain boundaries are modeled as diffuse interfaces across which the phase field variables have a smooth transition. Evolution of the phase field variables under the effect of thermodynamic driving forces implicitly represents grain boundary migration and microstructure evolution. In the present research, phase field simulations are employed to investigate the effect of microstructural length scale on the evolution of microstructure and texture in a polycrystalline copper thin films. It is generally demonstrated that increasing the microstructural length scale results in a transition from normal to abnormal grain growth [2]. Such a transition is attributed to the relative magnitude of the two interacting driving forces i.e. the strain energy minimizing driving force and the curvature driving force. The strain energy minimizing driving force is kept constant under a fixed applied strain and acts in favor of the texture component with lower strain energy. On the other hand, the curvature driving force is inversely proportional to the microstructural length scale and is impartial to grain orientations. As a result, the relative magnitude of the two driving forces is sensitive to the microstructural length scale and hence the evolution of microstructure and texture is significantly affected by the microstructural length scale. For the case of small microstructural length scale, computer simulations have revealed that (i) the dominance of curvature driving force results in the evolution of microstructure by normal grain growth, (ii) Stressed grain growth is impartial to different texture components i.e. no change in texture occurs, (iii) The final microstructure contains equiaxed grains with log-normal grain size distribution, and (iv) the overall stiffness of the polycrystalline aggregate is unchanged during stressed grain growth. On the other hand, for the case of large microstructural length scale we have observed that (i) the dominance of strain energy minimizing driving force results in the evolution of microstructure by abnormal grain growth, (ii) stressed grain growth results in the rapid abnormal growth of the texture component with lower strain energy, (iii) the final microstructure contains abnormal-shaped grains with bimodal grain size distribution, (iv) the overall stiffness of the polycrystalline aggregate decreases by stressed grain growth. For intermediate values of the microstructural length scale, a transitional behavior between the two extreme regimes was observed.

Keywords: Stressed grain growth, Phase field modelling, Polycrystalline microstructure, Microstructural length scale

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Parametric Investigation of Large Stretchability of Graphene Nanoribbon Springs

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Abstract: Graphene has several interesting electronic, thermal and mechanical properties [1,2]. The very high tensile modulus (1 TPa) and tensile strength (130 Gpa) [3] are useful in various structural applications. However, graphene is also known to be quite brittle, where tensile fracture strain does not exceed a few percents [4], which restricts the use of graphene when dealing with large deformation strains. A periodic cutting pattern has been used to enhance the fracture strain of graphene (graphene kirigami) [5]. The distance between cuts and cut orientations strongly define the stretchability of graphene kirigami [6]. For straight cuts, the increase in longitudinal spacing between cuts decreases the out-of-plane deflection and decrease the fracture strain. The shorter distance between curved cuts decreases the fracture strain [7]. The larger stretchability requires a careful design of cut length and cut orientations. Hence, in search of a set of optimal parameters which produce higher stretchability require a large number of simulations or experiments. Machine learning (ML) is an optimal choice for dealing with these large data sets. A recent study employed ML to accelerate the search of these parameters for graphene kirigami [8]. In a similar direction of graphene kirigami, a periodic undulating graphene nanoribbon is a promising choice for better stretchability. There are different types of possibilities of undulations such as sinus, U shape, half-circles, elliptical and, horseshoe shape [9]. The graphene ribbons with the periodic modifications are similar to a two-dimensional spring, known as graphene nanoribbon springs (GNRS). A recent experimental report demonstrates the lithography technique to reliable manufacturing of GNRS [10]. The effect of structural parameters on the mechanical properties of GNRS is unknown.

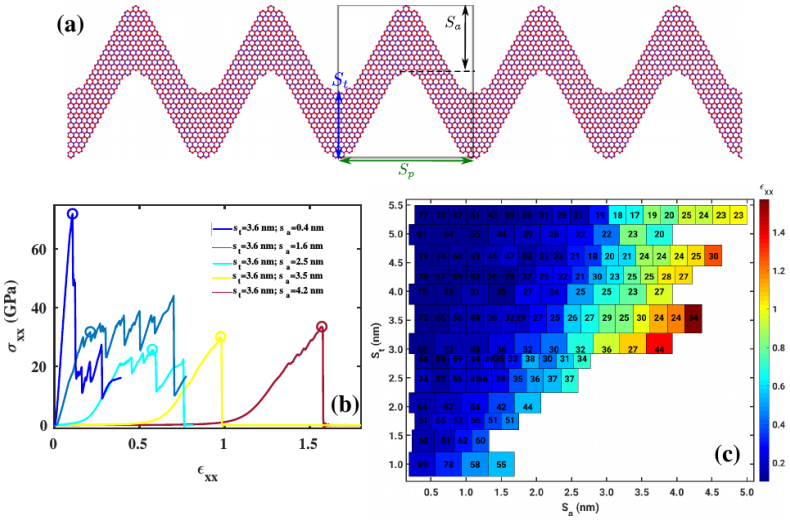

Figure 1: (a) GNRS atomic configuraiton. (b) Stress-strain response for GNRS. Markers indicate the fracture stress and fracture strain. (c) Fracture stress and fracture strain values for different St and Sa. Color indicates the strain and value denote the stress.

In this work, we consider studying the mechanical properties of GNRS in sinus shape and the effect of structural parameters. Fig. 1(a) represent the GNRS model. The structural parameters for GNRS are spring pitch (S_p), spring thickness (S_t) and spring amplitude (S_a). These three parameters strongly define the mechanical response of GNRS

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in sinus shape. To study the mechanical properties of GNRS, we employed classical molecular dynamics (MD) simulations. The atomic interaction between carbon atoms was modeled using the Tersoff potential. We consider S_p as 6 nm and vary S_t and S_a. We consider the lower bound of S_t in a way that it can accommodate at least two hexagonal carbon rings. Similarly, S_a varies from 0.2 nm to 6 nm. Overall about 200 structures of GNRS are simulated within in the given range of S_t and S_a. We evaluate the virial stress and strain at equal intervals of time under tensile loading with periodic boundary conditions.

Fig. 1(b) shows the stress-strain curves for a selected set of S_t and S_a. The fracture stress for GNRS with S_a smaller than S_t is very high and the fracture strain is lower than pristine graphene (~0.2). When S_a is 0.5 times S_t, the fracture strain is nearly equal to pristine graphene with 25% of graphene fracture stress. In this GNRS, we observe many structural defects, which avoids the brittle failure by coalescence of defects. The ultimate failure is at 0.6 strain. The response of GNRS with S_a 0.7 times S_t is similar to the previous case. The fracture strain is very much enhanced (about 1) when S_a is nearly equal to S_t. The GNRS is going to out-of-plane deflections with tensile deformation, which helps to increase the strain with very low-stress values. For $S_a = 1.6S_t$, the fracture strain is even more (about 1.6) with nearly 30 GPa fracture stress. Fig. 1(c) reports the fracture stress and fracture strain for different combinations of S_t and S_a. From these results, it is clear that a good choice of S_t and S_a yields a GNRS system with very large stretchability.

The present results only focused on varying the S_t and S_a parameters. The effect of S_p and shape are other factors that also need to be considered. Therefore, a very large data set has to be analyzed and obtain the fracture properties. As the number of possible configurations between these structural parameters increases, it is impractical to find the optimal set with good stretchability. ML represents an alternative and promising approach for this type of problems. Systematic production of training data for ML process using MD simulations to find the fracture stress and fracture strain is considered as a future aspect in this research.

Keywords: Graphene nanoribbon springs, tensile strength, tensile strain, molecular dynamics.

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Multiscale computation based on FNN and RNN

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Abstract: Computational homogenization method offers high accuracy at the expense of high computational cost. The neural networks can be used to construct fully decoupled approaches in nonlinear multiscale methods by mapping macroscopic loading and microscopic response. Computational homogenization method for nonlinear material and implementation of offline multiscale computation are studied to generate data set. This article intends to model the multiscale constitution using feedforward neural network (FNN) and recurrent neural network(RNN), and proper loading paths are selected to effectively generalized to unknown paths. Finally, applications to 2-dimensional multiscale analysis are addressed in detail.

Data-driven methods were thus developed to compute the response of heterogeneous microstructures using an interpolation technique in a higher dimensional space from a prior set of databases computed from offline nonlinear calculations on the representative volume element (RVE) [1]. Artificial neural networks (ANNs) have also been used to approximate various constitutive models because of the capability to learn complex nonlinear relationships. In the early 90s, Ghaboussi et al. [2] proposed to model the material behavior with neural network.

The use of ANN for direct representation macroscopic mechanical properties has been studied by many researchers [3-5]. However, choosing the loading case for adequate training of multiscale constitutive model is a challenging task, which is not precisely known at this time. Most neural networks for multiscale constitutive model are based on feedforward neural network (FNN) and BP algorithm. Recurrent neural network (RNN) is a type of neural network where the output from previous step are fed as input to the current step, so that it may be used to model the nonlinear multiscale constitutive model considering material history dependency. However, only limited papers have adopted RNN for constitutive modeling. This article intends to model the multiscale constitution using FNN and RNN, and proper loading paths are selected to effectively generalize to unknown paths.

In the nonlinear computational homogenization scheme, the macroscale incremental strain is applied on RVE, while the homogenized incremental effective stress and homogenized tangent constitutiove tensor are return back to macroscale model. For offline multiscale calculation, the macroscopic strain, obtained prior from a given loading path without calculated from macroscale model, is applied on a single RVE with constrain equations. The microscale model is simulated incrementally by the restart analysis in ABAQUS until the final step of the loading path is reached. To calculate the macroscopic stress and tangent tensor, one general three perturbation steps for plane-stress problems will be carried out on the microscale model. For restart analysis, the analysis results from the last step are used for the analysis of the current step and are overwritten for the next step, which greatly reduces the calculation file storage.

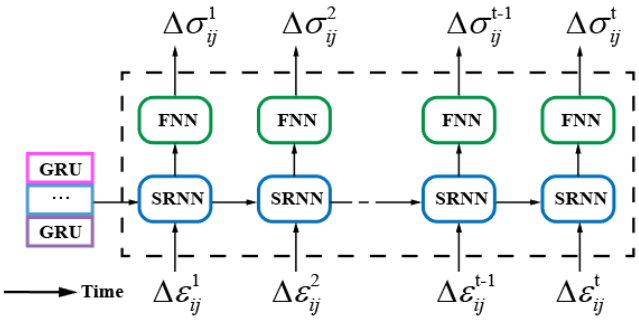

Figure 1: The stacked GRU neural networks unrolled through time

As the nonlinear response of macroscale model is depend on the loading history and current load increment, the macroscopic stress and strain of the previous step and the current incremental strain are used as the input parameters for FNN. The motivation to use RNN for multiscale nonlinear computation is that the loading history information can be

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retained. Different from training discrete data points for each path in FNN, a loading path is used as a time-dependent data chain in RNN, and the previous data will affect the later outputs. Within this paper, a stacked GRU neural network (SRNN) connected with fully connected layers at each time step is adopted, which is illustrated in Fig. 1.

The question of what constitutes sufficient data sets for adequate training of neural network material model is not precisely known at this time, and a well-trained neural network model doesn't guarantee a good generalization to other paths. Within this paper, macroscopic strain tensor increment is set to be cosine function and total macroscopic strain tensor component is given as

$$\varepsilon_i^t = \varepsilon_i^{t-1} + \frac{k}{n} R\cos(\theta_i^t) \quad k = 1, \cdots n \tag{1}$$

where $\varepsilon_i^0 = 0$, R and θ are the loading radius and angle. The applied macroscopic strain tensor components are increased with independent constant increments until k=n, then the loading angles will change randomly within the set $\{0^\circ, 1^\circ \cdots, 180^\circ\}$. Therefore, the training data can reflect the characteristics of different loading direction. The procedure for applying the strain component is illustrated in Fig.2.

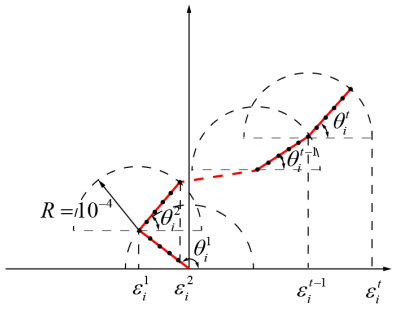

Figure 2: The procedure for applying the strain component

In neural network, hyperparameters refer to prior parameters that need to be tuned to optimize it, including the network structure, optimized parameters and regularization coefficient. Grid search and manual search are the most widely used strategies for hyperparameter optimization. Within this paper, grid search with orthogonal experimental design (OED) is used to obtain optimal result in a short time. Finally, applications to 2-dimensional multiscale analysis are addressed in detail. It's found that the trained FNN and RNN model both have good generalization ability on test set, and the stacked RNN model is more capable of mapping a given path, but also more sensitive to hyperparameters and initial parameters.

Keywords: Multiscale method, constitutive model, FNN, RNN.

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A Manifold Learning Approach for Multiscale Phase Field Evolution for Fracture

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Abstract: The multi-scale fracture simulation of heterogeneous materials is a popular and important subject in solid mechanics and materials science due to the wide application of composite materials. In this paper we propose a new computational strategy for solving multiscale fracture problem efficiently through homogenization in a FE^2-like [1] framework. To take into account the phase field induced by fracture at the microstructure level, the Representative Volume Element (RVE), which consists of an elastic matrix and inclusions (fiber), is endowed. We randomly place an initial crack in the RVE in order to represent the possible microscopic crack paths. The crack is described by the regularized variational theory of fracture, or so-called phase field approach, which is able to predict crack nucleation, propagation and branching without extra criteria [3]. Then the RVE response is homogenized and upscaled to the macroscale as a phase field constitutive model previously developed by the authors [2], which is then used in a framework of a phase field modeling of propagating fracture.

This computational scheme for solving multiscale fracture problems can be inefficient and inflexible because the phase field method requires an unpredictable number of iterations. In this paper we consider an alternative route that adopts techniques well known in the machine learning community in order to extract the manifold that contains the inputs to the RVE, namely the initial crack path and the load. Then output data, which is the evolved phase fields, can be interpolated accurately with minimum online computation. In particular, the locally linear embedding is chosen in this work for the local phase field evolution for fracture of heterogeneous microstructures. We construct a manifold which can efficiently and accurately interpolate micro crack evolution laws with given microstructures. In this paper, we perform a manifold learning approach based on the use of LLE technique [6]. Locally linear embedding (LLE) [6], a particular example of kernel principal component analysis (kernel PCA) [4,5,7], is an unsupervised learning algorithm that computes low-dimensional, topology-preserving embeddings of high-dimensional data points. The offline procedure consists of two stages: (1) dataset construction with the phase field analysis for the RVE. (2) data manifold construction with the LLE. The online interpolation procedure then readily delivers the phase field evolution. In the presentation, an accuracy check between FEM results and manifold interpolation is provided.

Keywords: Multiscale simulation, Manifold learning, Locally linear embedding, Phase field for fracture, Computational homogenization

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Numerical simulations on the material point method of impact damage problems

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Abstract: The impact damage problems was studied based on the material point method (MPM). The high-energy explosive explosion calculation model is established, the underwater and air explosion calculation model is discussed, the material point method non-reflective boundary treatment method is perfected, the structural plastic dynamic response and failure model is given, and the numerical simulation of the structural damage effect of explosives in water and air media is calculated. Using pressure, density, etc. as a typical result analysis, a concrete solution for calculating the dynamic response of structural plasticity by material point method is given.

Keywords: Material Point Method, Numerical Simulation, Impact problems, Damage.

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Numerical Modeling of Crack Propagation in the Presence of Inclusion Using Extended Finite Element Method

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Abstract: The characteristic of crack propagation in the presence of inclusion is investigated numerically. In this study, the crack growth is modeled using extended finite element method (XFEM). Two-dimensional rectangular plate with single inclusion embedded off-centered is modeled. The specimen is subjected to uniaxial tension. The motion of the crack is modeled by XFEM based on traction-separation cohesive behavior for 2D mixed mode problem. In addition, enrichment procedure is used to implicitly determine predefined crack in XFEM framework. Two different inclusions, which are soft and hard inclusions, are considered on crack propagation scheme. The effects of soft and hard inclusions on crack propagation are studied and observed. It is found that the presence of inclusion plays a crucial role on the crack trajectory inside the material. The presence of inclusion in the material is proved to be one of the dominant factors which can alter the crack growth characteristics.

Keywords: Crack propagation, Extended finite element method, Traction-separation, Inclusions.

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Active Machine Learning to Design Novel Two-dimensional Carbon Nitrides

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Abstract: Two-dimensional (2D) materials are currently among the most attractive family of materials with highly promising application prospects for a wide range of advanced technologies. Graphene as the most prominent member of 2D materials family has been proven to exhibit exceptionally high mechanical and thermal conduction properties along with unique optical and electronic features. In general, for many applications in nanoelectronics and nanooptics presenting a narrow and direct band-gap is among the most important requirements, however graphene is a zero band-gap semimetal. Worthy to remind via chemical doping with nitrogen or boron atoms, mechanical straining or creation of nanomesh structures, a band-gap can be opened in the graphene. Nevertheless, these aforementioned methods require additional processing steps after the first synthesize of graphene, which question their practical application due to the increase in the fabrication time and cost as well. Such that designing novel 2D materials that are semiconductors in their pristine form has been among the most appealing approached for the employment of 2D materials in nanoelectronics and nanophotonics.

Among the various classes of 2D materials, carbon-nitride nanomembranes have been among the most successful nanomaterials with inherent semiconducting electronic characters. These 2D allotropes show a common chemical formula CxNy, where x and y represent the number of C and N atoms in the unit cell, respectively. Carbon-nitride nanomaterials offer stiff and stable components owing to the formation of strong covalent bonds between the C-C and C-N bonds. Depending on the composition of C and N atoms in various atomic lattices, carbon-nitride allotropes can exhibit diverse electronic, optical, electrochemical, mechanical and thermal conduction properties. Unlike the graphene, carbon nitride nanosheets show porous atomic lattices and more importantly are inherent semiconductors, highly promising to design novel nanoelectronics. Carbon nitride 2D structures also show good mechanical properties and have been proven as promising candidates for the employment; in energy conversion/storage, catalysis, photocatalysis and oxygen reduction systems. In this work motivated by the exceptional properties of carbon-nitride nanosheets, we predicted three novel porous lattices; C_7N_6, C_9N_4 and $C_{10}N_3$. Stability, mechanical properties and electronic/optical properties of these novel nanomembranes were explored by the first-principles density functional theory (DFT) simulations. Acquired theoretical results confirm the stability and highlight highly attractive properties of C_7N_6 and C_9N_4 nanosheets, and may hopefully motivate and guide future experimental and theoretical studies. In the following illustration the predicted nanosheets are illustrated.

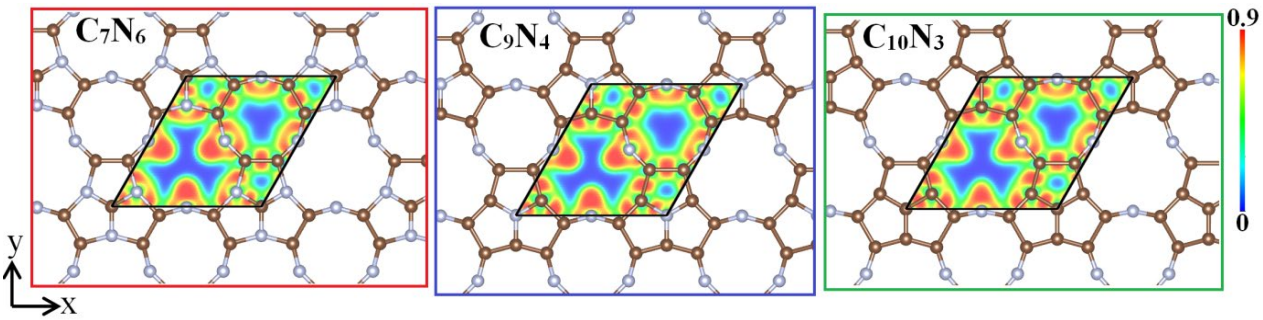

Figure 1: Atomic structure of C_7N_6, C_9N_4 and $C_{10}N_3$ monolayers. Contours illustrate the electron localization function within the unit-cell.

The acquired first-principles results confirm the thermal, dynamical and elastic stability of C_7N_6 and C_9N_4 nanosheets and also highlight that these novel 2D systems can endure under severe loading conditions, owing to their strong covalent bonding nature. Our extensive calculations confirm the stability and highlight highly attractive

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properties of C_7N_6 and C_9N_4 nanosheets, and may hopefully motivate and guide future experimental and theoretical studies. In the following illustration the predicted nanosheets are illustrated. Nonetheless, these observations cannot confirm that the predicted lattices are the global minimum structures. To address this important issue, we will conduct extensive search and prediction of various possible structures, by employing crystal structure prediction methods. In this approach, novel materials prediction will be accomplished by developing machine-learning interatomic potential to approximate quantum-mechanical energies and an active learning algorithm for the automatic selection of an optimal training dataset [1,2]. This approach substantially reduces the amount of highly demanding DFT calculations, as the DFT will be only used to produce the training data, while structural optimization is performed using the interatomic potentials. In this method, we first conduct ab-initio molecular dynamics simulations for around 30 well-known carbon-nitride monolayers, in order to train a moment tensor potential for approximating the quantum-mechanical energies. Using the proposed method, we will predict novel carbon-nitride nanosheets with computational costs by around two orders of magnitude faster than the common DFT based material prediction techniques. Moreover, we will be hopefully able to plot the phase diagram of this attractive class of 2D semiconductors. These results can serve as a unique guide for the future experimental and theoretical studies.

Keywords: Carbon-nitride, 2D materials, Machine-learning, Interatomic potential, Quantum-mechanics.

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Prediction of bending angle of laser bent tailor welded blanks using artificial neural network (ANN)

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Abstract: Laser bending is a flexible forming process that needs no hard tooling or external forces [1]. It is used in some industrial applications such as shipbuilding, automobile, microelectronics and aerospace [2-4]. In this paper, artificial neural network (ANN) is used for prediction of the effects of laser and sheet parameters on bending angle of laser bent tailor welded blanks. In addition, the ANN is compared with multivariate regression in prediction of the effects of process parameters on bending angle. The input parameters are laser power, irradiating speed and laser diameter. The results show that the correlation coefficient of the neural network is 0.9999 and the average square error of the results is 0.12666 % which these results indicate the high accuracy of the predicted model by ANN. In addition, the results of predicted model by multivariate regression are 0.9961 and 0.6738% for correlation coefficient and average square error respectively. Comparison of obtained results by artificial neural network and multivariate regression show that the accuracy of the predicted model by neural network is very high and the error rate is very low in comparison with multivariate regression.

Keywords: Laser bending process, Bending angle, Artificial neural network (ANN), Multivariate regression.

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Multi-objective optimization of perforated variable-stiffness plates using NSGA-II

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Abstract: Variable stiffness composites are a new type of composite materials in which the fibers follow particular curves. As the stiffness of these structures could be controlled by changing the curves of the fibers, their strength under various types of loadings is higher than constant stiffness composites. This is more observable when the laminates contain holes since the stress concentration in the vicinity of the cutouts in variable stiffness composites is considerably smaller than constant stiffness composite structures. This paper represents the optimization of variable stiffness composite plates containing a central cutout. The fiber curves are considered as the main design variable while increasing the maximum failure load and decreasing the weight of the laminates are taken as the objective functions. The stress analysis of these plates is conducted using Layer-wise finite element method. Non-dominated Sorting Genetic Algorithm (NSGA-II) which has been proved to be a robust meta-heuristic algorithm is employed as the optimizer in this study. Several examples of rectangular variable stiffness composite plates with circular and oval cutouts are presented to show the influence of the shape of holes on their load bearing capacity.

Keywords: Variable-stiffness composite plates, NSGA-II, Layer-wise theory.

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Investigation of nonlinear self-healing theory in continuum damage-healing mechanics

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Abstract: The theoretical investigation of self-healing variables is presented here. Special focus is addressed to the nonlinear self-healing theory. New healing variables are defined based on elastic modulus, shear modulus, Poisson's ratio and bulk modulus. These variables are defined such that they fit the upper and lower limits of continuum damage-healing mechanics and the generalized nonlinear and quadratic self-healing models. The formulation is applied for both isotropic and anisotropic materials using scalar and tensor variables, respectively. The hypotheses of elastic strain equivalence and elastic energy equivalence are used to elucidate the evolution of the healing variable calculated based on cross-section as function of the healing variable calculated based on the elastic stiffness. In addition, examples of isotropic elasticity, plane stress and plane strain are applied using the nonlinear healing models along with the calculation of the components of the fourth-rank healing tensor is each example.

Keywords: Damage, Healing, Nonlinear, Quadratic, Anisotropy.

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Application of an adaptive neuro fuzzy inference system for modelling of temperature and force in robotic bone drilling process

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Abstract: The bone drilling is one of the most important, common in the field of biomedical engineering. It is also very important in dentistry and bone sampling operations. Bone is a very complex material and the process of drilling is very sensitive. Thus, bone drilling process is indispensable in orthopaedic surgeries and treating bone breakages. The bone drilling process can be promoted using automatic drilling machines and surgery-assisting robots. The problematic issue during operation is the high increase in drilling process temperature (higher than 47 ^{0}C) which leads to the so-called 'thermal necrosis' or cell death, and local burn in bone tissue. Furthermore, imposing higher forces to bone might yield to breaking or cracking, and consequently causes serious damages in bone. In this paper, the tool rotational speed, feed ratio and tool diameter were taken into account as process input parameters, and process temperature and thrust force were taken as output parameters. An adaptive neuro fuzzy inference system (ANFIS) is used for modelling of the effects of process input parameters on temperature and force in bone drilling. The ANFIS network is learned by 75% of data and 25% of data have been employed for testing the appropriateness of the models into ANFIS network models and results were compared by two statistical criterions (R , RMSE). The results show that the proposed model by ANFIS is efficient and valid and it can be used for more general states.

Keywords: Machining; orthopaedic surgery; adaptive neuro fuzzy inference system (ANFIS).

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Modelling of creep age forming of aluminum 7075 tailor machined blanks using adaptive neuro fuzzy inference system (ANFIS)

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Abstract: In this paper, an adaptive neuro fuzzy inference system (ANFIS) is used for modelling of the effects of creep age forming of aluminum 7075 tailor machined blanks parameters on characteristics of deformed blank. Creep age forming of tailor machined blanks is more difficult than monolithic plates due to presence of two different thicknesses in theses blanks [1-4]. Therefore, prediction of forming behavior of tailor machined blanks with creep age forming process with a powerful tool is important especially in the aerospace industries. In the present work, the effects of two main creep forming process parameters namely time and temperature are investigated on spring-back of both thin and thick sections of a tailor machined blank with adaptive neuro fuzzy inference system (ANFIS). The ANFIS network is instructed by 75% of data. Twenty-five percent of primary data which is considered for testing the appropriateness of the models is entered into ANFIS network models and results were compared by two statistical criterions (R, RMSE). Considering the results, it is obvious that the proposed modeling by ANFIS is efficient and valid and it can be expanded for more general states.

Keywords: Creep age forming process, Al 7075 tailor machined blank, adaptive neuro fuzzy inference system (ANFIS).

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Isogeometric Analysis for Phase-Field Models of High-Order Surface PDEs with Application to biomembrane modeling

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Abstract: We present a NURBS-based isogeometric analysis for phase-field models of high-order surface partial differential equations (PDEs) [1]. We first consider mean curvature flow and Willmore flow problems, which are prime examples of geometric PDEs, and discuss their corresponding phase-field approximations. Based on the method of manufactured solutions, we study the convergence behavior of isogeometric formulation for the phase-field models of geometric PDEs. The numerical convergence of these phase-field approximations to the sharp-interface solutions is also discussed. Next, we solve the Cahn-Hilliard equation on a unit sphere as a model problem for high-order PDEs on stationary surfaces, where we model the surface using a phase-field approach. Finally, we consider a phase-field model of multi-component biomembranes which represents a model problem for high-order coupled surface PDEs. We perform several numerical tests in 2D, 3D and axisymmetric 3D settings and make comparisons with available numerical or experimental results. Our simulation results show the robustness of IGA for solving the considered phase-field models.

Keywords: Isogeometric analysis, phase-field modeling, high-order surface PDEs, geometric PDEs, multi-component vesicles

Acknowledgement

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Influence of Thermostatting on Nonequilibrium Molecular Dynamics Simulations of Heat Transport in Solids

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Abstract: Nonequilibrium molecular dynamics (NEMD) has been extensively used to study thermal transport at various length scales in many materials. In this method, two local thermostats at different temperatures are used to generate a nonequilibrium steady state with a constant heat flux. Conventionally, the thermal conductivity of a finite system is calculated as the ratio between the heat flux and the temperature gradient extracted from the linear part of the temperature profile away from the local thermostats. Here we show that, with a proper choice of the thermostat, the nonlinear part of the temperature profile should not be excluded in thermal transport calculations [1,2]. We compare NEMD results against those from the atomistic Green's function [3,4] method in the ballistic regime, and those from the homogeneous nonequilibrium molecular dynamics method in the ballistic-to-diffusive regime. These comparisons suggest that in all the transport regimes, one should directly calculate the thermal conductance from the temperature difference between the heat source and sink and, if needed, convert it to the thermal conductivity by multiplying it with the system length. Furthermore, we find that the Langevin thermostat outperforms the Nosé-Hoover chain thermostat in NEMD simulations because of its stochastic and local nature. We show that this is particularly important for studying asymmetric carbon-based nanostructures, for which the Nosé-Hoover thermostat can produce artifacts leading to unphysical thermal rectification. Our findings are important to obtain correct results from MD simulations of nanoscale heat transport as the accuracy of the interatomic potentials is rapidly improving.

Keywords: Nonequilibrium molecular dynamics, Thermal transport, Local thermostats, Temperature gradient.

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Crack Propagation with Different Radius Local Random Damage based on peridynamic theory

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Abstract: Inheriting the advantages of traditional theories, the theory of peridynamics can well clarify the mechanism of crack propagation by the integral solution. Moreover, it is not necessary to set the initial crack and crack path in advance. In this paper, specimens with bilateral cracks are tested using the theory of peridynamics in different conditions, namely the specimen without local damage, that with small radius local damage, and that with large radius local damage. The crack propagation path under the uniaxial tension and the displacement in the Y-direction are compared and analysed, in order to figure out the influence of local stochastic damage with different radiuses on the crack propagation path and Y-direction displacement.

The calculating example 2, the crack propagation path in picture 9 as below

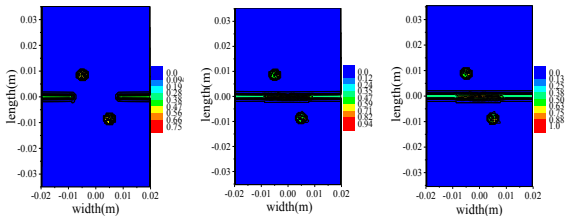

Figure 9: Crack propagation path of specimen 10-00 with r=2 mm

Keywords: Fracture mechanics, peridynamics, stochastic damage, bilateral crack.

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Topology optimization of piezoelectric materials

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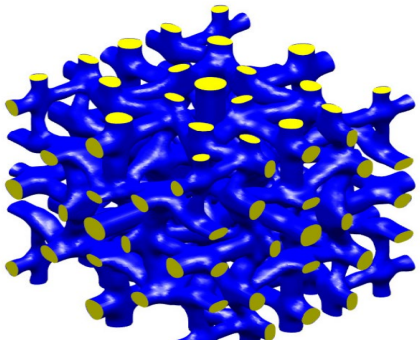
Abstract: Piezoelectric materials are characterized by the electromechanical coupling phenomenon, i.e., able to produce an electric field when being stressed, and deform when subjected to an electric field. Such materials are found in various engineering application such as sensors, actuators and transducers. Auxetic materials, i.e., materials have negative Poissons ratio, have show potential applications from biomedical to defense problems. Kinematic deformation are affected by the Poissons ratio can enhance the performance of piezoelectric transducer. Under a compressive load on surface of the piezocomposites device, the auxetic polymer matrix contracts laterally and allow the ceramic rods expand, resulting in enhanced electromechanical coupling device [1].

In this work, we focus on design of piezocomposites by mean of topology optimization based on the parameterized level set method [2, 3]. Level set funciton implicitly represent the design boundaries as the zero level set of the one-higher-dimension level set function, directly evolves the design boundaries during the topology optimization and ensures the optimized designs have clear boundaries and avoid numerical problems such as checkerboard patterns, gray-scale elements. The charge coefficients or electromechanical coupling factor are optimized for the hydrophone application. The matrix material are optimized in order to have auxetic behavior. Figure 1 shows the three dimensional unit cell which are optimized with the level set method. The next steps is to embed the material structure in to classes of 1-3 and 2-2 piezocomposites, we expect the performance piezoelectric devices are improved.



Keywords: Piezoelectric materials, Auxetic materials, Topology optimization

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A prediction model of debris flow susceptibility in Southwest China based on a quantitative data processing method

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Abstract: Southwest China is charactered by steep mountains and deep valleys, and is strongly affected by the uplift activity of the Qinghai-Tibet Plateau. Furthermore, there is an abundance of loose material and rainfall, making it a severe disaster zone in terms of debris flow. Evaluation on the debris flow susceptibility requires the quantitative assessment of the factors leading to the initiation, propagation and deposition of debris flows. In the existing literatures [1-3], however, the debris flow susceptibility is mainly determined using a qualitative method with relevant specifications, and little reliable quantitative prediction models were presented. To evaluate the susceptibility to the debris flow in this area, in total of 70 typical debris flows distributed in five water catchments (the Brahmaputra River, Nujiang River, Yalong River, Dadu River, and Ming River) were investigated in the past three years.

In the five water catchments, a detailed field work was carried out from the valley outlet to the valley watershed, including the investigation of watershed terrain, geological structure, outbreak scale, loose material distribution, processes of occurrence and movement, frequency of debris flows. A bulk density test (specimen size 50 cm × 50 cm × 50 cm) and screening test of the loose material were conducted in the deposit zone of the debris flow. According to the superelevation and flow depth of the curved gully zone, the speed of the debris flow was calculated to provide the basic data for the dynamic parameter calculation. For the active debris flow gullies, the geologic condition in the source areas was invested in drilling and geophysical prospecting, so that the source material volume, soil composition, structure, and content of the fine-grained soil could be determined precisely. In addition, the precipitation data before the outbreak of debris flows were collected from local meteorological bureaus. The impulse force, the sediment discharge, and other dynamic parameters were calculated.

Considering debris flow features and index-acquisition conditions, 9 indexes were selected to evaluate the susceptibility of debris flow in this work. These were the catchment area, longitudinal grade, average gradient of slope on both sides of the gully, catchment morphology, valley slope orientation, loose material reserves, loose material position, antecedent precipitation, and H_{1p} rainfall intensity. Each factor was classified into certain categories according to their values. The values of the 9 indexes of the 70 debris flows in Southwest China were obtained through the field investigation.

In Japan, the Hayashi methods of quantification are well known and widely used in various fields such as coal mine flooding risk assessment, earthquake-triggered damage assessment of tunnels, and the gas leakage prediction model of large explosions in hard rocks. According to a reasonable principle, the quantitative and qualitative variables can be mutually transformed using this method. Therefore, with respect to the processing of the quantitative and qualitative influencing factors of earthquake-induced hazards, this method has a considerable degree of flexibility and applicability.

In the quantification theory, qualitative variables are termed items and all possibilities for each item are termed categories. To express the response of an item and the category for each sample, the dummy variable $\delta_i(j, k)$ is introduced into the model; here, sample i represents the factor in category k of item j. The matrix composed of all categories $\delta_i(j, k)$ is referred to as the response matrix X:

$$X = \begin{pmatrix} \delta_1(1,1)\cdots\delta_1(1,r_1) & \delta_1(2,1)\cdots\delta_1(2,r_2)\cdots\delta_1(m,1)\cdots\delta_1(m,r_m) \\ \delta_2(1,1)\cdots\delta_2(1,r_1) & \delta_2(2,1)\cdots\delta_2(2,r_2)\cdots\delta_2(m,1)\cdots\delta_2(m,r_m) \\ \vdots \quad\quad \vdots & \vdots \quad\quad \vdots \quad\quad \vdots \quad\quad \vdots \\ \delta_n(1,1)\cdots\delta_n(1,r_1) & \delta_n(2,1)\cdots\delta_n(2,r_2)\cdots\delta_n(m,1)\cdots\delta_n(m,r_m) \end{pmatrix} \quad (1)$$

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To establish a quantitative prediction model, we use qualitative and quantitative experimental observations to fit the linear relationship between the concerned independent variable and the dependent variable affecting its variations. Quantification theory type *I* supposes that the random variable changes with the *m* variables:

$$y_i = \sum_{j=1}^{m} \sum_{k=1}^{r_j} \delta_i(j,k) b_{jk} + \varepsilon_i \quad (2)$$

where y_i denotes the susceptibility of the *i*th debris flow gully and b_{jk} is a constant coefficient that relies on category *k* in item *j*. ε_i represents a random error in the *i*th spot-check and consists of all $\delta_i(j, k)$.

Using Eq. 2 and matrix derivation regression calculation, the contribution values of each item can be obtained, and the susceptibility prediction model of debris flow is established and is represented as follows:

$$Y = 0.573x_{11} + 0.821x_{12} + 0.910x_{13} + 0.875x_{21} + 0.955x_{22} + 0.320x_{23} - 0.107x_{32} - 0.163x_{41} + 0.135x_{42} + 0.213x_{43} - 0.136x_{51} - 0.174x_{52} + 0.246x_{62} + 0.454x_{63} - 0.220x_{71} - 0.161x_{72} + 0.034x_{82} + 0.071x_{83} - 0.038x_{91} + 0.043x_{92} \quad (3)$$

In Eq. 3, *Y* is the susceptibility for the debris flow. When the predicted value (*Y*) is less than 1.5, the susceptibility is low. When *Y* is greater than or equal to 1.5 but less than 2.5, the susceptibility for the debris flow is medium. When *Y* is greater than or equal to 2.5, the susceptibility for the debris flow is high.

The values of each index are obtained from the field investigation, and the susceptibility of the 70 debris flows can be calculated using the proposed model. Fig. 1 compares the predicted susceptibilities with the actual ones. It is shown that the coincidence rate is 78.53% for low-susceptibility debris flow valleys, 92.38% for medium-susceptibility debris flow valleys, 82.01% for high-susceptibility debris flow valleys, and 86.38% for all the samples, which indicates that the regression model can predict the susceptibility well.

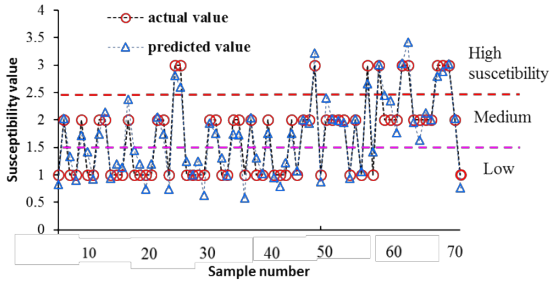

Figure 1: Comparison of measured and predicted values

Keywords: Debris flow, Susceptibility, Prediction model, Factor index system, Quantification theory type I.

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Prediction of shield moving performance during tunnelling based on optimized LSTM neural network

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Abstract: Shield moving performance prediction is of a significant importance to the safety of tunnelling construction process. The analysis of shield moving performance, such as advance rates and thrust values, can improve shield tunnelling efficiency. With a rapid development of monitoring techniques, a huge amount of data including geological and operational data can be collected during the tunnelling construction process. The analysis and mining of these complex coupled and nonlinear parameters related to shield moving performance are challenging for project managers and tunnelling engineers. To improve the accuracy of prediction and achieve the dynamic prediction of advance rates and thrust values of the shield machine, this paper proposes the improved particle swarm optimization (IPSO) and a IPSO-LSTM hybrid algorithm which integrates the particle swarm optimization (PSO) with the long-short term memory (LSTM) neural network. The IPSO is utilized to optimize parameters (geological and operational variables) since it is complex and difficult to determine the parameters of LSTM, such as the number of neurons, iterations and learning rate. Besides, a nonlinear inertia weight is provided to improve the convergence speed and global research of PSO. The case study of Shenzhen Metro project is adopted to validate the proposed model (IPSO-LSTM). Results demonstrated that the developed model achieves well prediction performance of shield machine during tunnelling when the LSTM has two hidden layers. This work provides a feasible and accurate tool for shield performance prediction in shield tunnelling projects.

Keywords: Shield tunnelling, Advance rates and thrust values prediction, Geological and operational data, IPSO-LSTM, Nonlinear inertia weight.

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Data-driven approach to Inverse Problems using Deep Learning Networks

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Abstract: Inverse source problems such as the determination of the contaminant source's locations and properties from measurement data in the field of air/water quality management are challenging and ill-posed due to sparsity information. Optimization based approaches (e.g., Levenberg–Marquardt algorithm [1]) and statistical based approaches (e.g., Bayesian inferences [2]) are normally used for such problems. However, they require the knowledge of mathematical models which govern the physical phenomenon under investigation (aka., a forward model). Furthermore, solving repeatedly the forward model in an optimization procedure is computationally expensive. This paper presents a complete framework to perform inverse source problems using deep learning networks. The framework consists of two Long Short-Term Memory (LSTM) [3] networks to perform two different tasks. The first network is an LSTM-Classifier to classify the number of contaminant source components, while the second one is an LSTM-Regressor to predict the sources' properties, namely location, width, and strength of the sources. The LSTM networks are chosen in the context of sensor measurement, where recorded data is time-variant responses in the sense of continuous or discontinuous sequences. An experimental study based on a two-dimensional water surface model is conducted and an extensive study of hyper-parameters (e.g. number of hidden layers, learning rate, etc.) is also performed. The results show that the proposed framework is very efficient in terms of computational time and prediction accuracy and expected to function as a tool of studying inverse source problems for water/air quality management as well as similar applications.

Keywords: Inverse source problems, Deep learning networks, LSTMs, Classification, Regression.

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Data-driven methods for quantifying the effects of geological variables on performance degradation of metro tunnel in operation

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Abstract: The construction speed of the urban rail transit is increasing in recent years [1, 2], leading to the problem that the long-term serviceability of shield tunnel is often ignored. In order to avoid the irreversible destruction caused by structure deterioration, it is necessary to have a study on serviceability degradation model of shield tunnel based on its performance assessment, thus providing guidance for daily maintenance. Therefore, this paper conducted clustering analysis to identify different degradation models of shield tunnel. On this basis, the influence of geological variables on degradation model was quantitatively evaluated using statistical learning methods. These data-driven methods were applied to 5 tunnel intervals of Shanghai ML 1 and 2.

Specifically, an existing assessment indicator, Tunnel Serviceability Index (TSI), was employed to evaluate the condition of shield tunnels in soft soils in this study [3]. Currently, TSI is the official index to evaluate the tunnel serviceability according to Shanghai Engineering Technical Standard. The value range of TSI is 0 to 5, where 0 indicates the best condition and 5 is the worst condition. The final formula of TSI was shown in Eq. (1).

$$\mathrm{TSI} = 0.16\sqrt{s_{ave}} + 0.01 s_{diff,ave} + 0.09 c_{ave} + 0.08 d_l + 0.05 d_c + 0.50 d_s - 0.23 \quad (1)$$

Since the cumulative settlement of ML 1 and 2 is observed twice a year while other measurable variables are not monitored as frequently as cumulative settlement, TSI_s which is merely related to settlement factors instead of TSI is calculated and adopted for further analysis. 5 metro intervals including 196 tunnel sections are investigated. Each section includes 50 segment rings and is 60 m long. The length of TSI_s time series for ML 1 and 2 is 32 and 26, separately. Fig. 1 shows the observations of TSI_s time series. It can be seen that with the increase of service age, TSI_s increases and the condition of tunnel sections becomes worse.

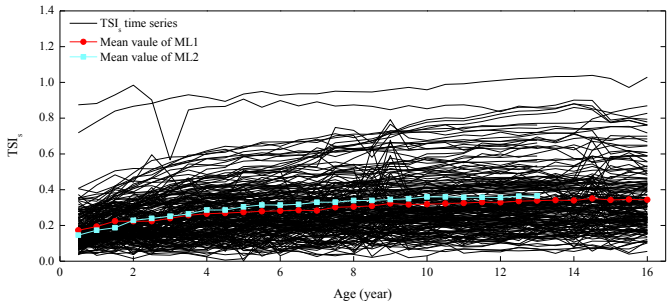

Fig. 1. The observations of TSI_s time series

Generally, TSI_s changes dynamically over time. Thus, the identification of performance degradation model should consider the change of TSI_s in the whole historical period, which can be achieved by time series clustering analysis. In view of the low dimensionality of TSI_s time series, 196 sets of TSI_s time series data are processed and analyzed by the k-means algorithm based on DTW distance. Compared to Euclidean distance, DTW can find out the distance which has the minimal warping cost under different conditions and allows time series data being compressed or stretched [4], which is suitable for modeling clustering problems when the length of time series data is different. The clustering quantity parameter K is determined and optimized by ten-fold cross method by comparing Mean Squared Distortion (MSD) (Fig. 2). Finding the "elbow" where the MSD stops decreasing significantly is one of the criteria employed to choose the optimum number of components [5]. The results show that the clustering analysis can identify 4 various clusters objectively, each of which shows similar trends and characteristics (Fig. 3).

Next, five independent variables, namely, average depth of burial DEPTH, thickness of soil passing through the third layer SOIL3, thickness of soil passing through the forth layer SOIL4, the river length RIVER and the station length STATION are selected as geological variables according to geological prospecting data. After Z-score

standardization method, the influence of these five variables on the performance degradation model of shield tunnels is studied quantitatively by using the Ordinal Logistic Regression Model. The results show that the statistical influences of these five independent variables are significant and the regression parameters are estimated to be -0.866, -0.655, -0.799, -0.594 and -0.332, respectively (Tab. 1). These parameters indicate that with the increase of DEPTH, SOIL3, SOIL4, RIVER and STATION, the probability of tunnel sections which stay in worse performance degradation model will increase. The practical significance of the five independent parameters is explained in combination with mechanical concepts and existing empirical knowledge.

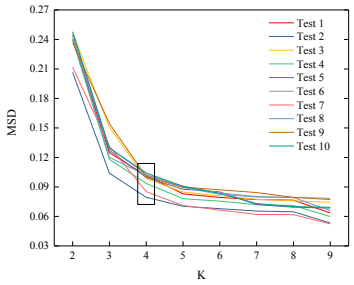

Fig. 2. Mean squared distortion of ten sets for k-means

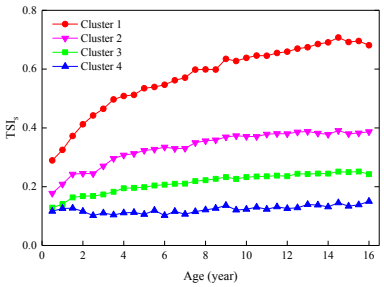

Fig. 3. Mean TSI_s time series of the finial 4 clusters

Tab. 1. Parameter estimation results of Ordinal Logistic Regression method

Variables	Parameter Estimation	Standard Error	OR	P-value	95% Confidence Interval	
					Lower	Upper
DEPTH	-0.866	0.248	0.421	0.000	-1.352	-0.379
SOIL3	-0.655	0.233	0.519	0.005	-1.112	-0.198
SOIL4	-0.799	0.253	0.450	0.002	-1.296	-0.303
RIVER	-0.594	0.193	0.552	0.002	-0.973	-0.216
STATION	-0.332	0.144	0.717	0.021	-0.613	-0.050

Besides, Tab. 2 shows the results of parallel line test. P-value equals 0.060 which is bigger than 0.05, indicating the regression equations are parallel to each other, thus validating the availability of Ordinal Logistic process.

Tab. 2. Results of parallel line test

Model	-2 Log Likelihood	Chi-square	df	P-value
Zero Hypothesis	482.164	—	—	—
Generalized	464.430	17.734	10	0.060

Keywords: Tunnel Serviceability Index (TSI), Degradation model, Clustering analysis, Ordinal Logistic Regression, Geological variables.

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Study on K-means Evaluation Method for Service Performance of Highway Tunnels

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Abstract: The service performance of highway tunnel is the comprehensive reflection and evolution of many engineering data and parameters of tunnel engineering[1,2]. In order to reflect the influence of these data on the service performance of tunnels, according to the idea of big data analysis method[3-6], a big data evaluation index system for the service performance of existing highway tunnels is constructed, and a K-means evaluation method for the service performance of existing highway tunnels is proposed by introducing K-means clustering algorithm[7-10]. The main results are as follows: (1) According to the state of tunnel engineering data in the service period of tunnel, the tunnel engineering data can be divided into static data and dynamic data. The static data include engineering prospection data, engineering design data and engineering construction data, which are basically unchanged when the tunnel project enters service period; The dynamic data are mainly the maintenance and inspection data of the tunnel in service, which are constantly changing during the service period. (2) There are more than 100 initial types of static and dynamic data in tunnel engineering. After preliminary screening by expert experience method and secondary screening by machine learning (static data adopts Spielman correlation coefficient algorithm and dynamic data adopts Apriority association rule algorithm), 19 evaluation indexes are finally screened out. Among them, there are 10 static indexes: stratum lithology, geological structure, unfavorable geology, special rock and soil, groundwater, climate characteristics, tunnel length, secondary lining concrete, pavement structure type, construction disaster accident; 9 dynamic indexes: tunnel portal level, leakage level, pavement level, maintenance road facility level, drainage facility level, ceiling level, interior decoration level and marking line level.(3) On the basis of 19 evaluation indexes, a tunnel service performance evaluation model based on K-means clustering algorithm is constructed. The best clustering effect is determined by Xie-Beni value. The clustering centers of each evaluation index are determined by 186 engineering cases with different tunnel service performance. (4) By 36 engineering case tests, it shows that the accuracy rate of the K-means tunnel service performance evaluation model is 75%, which indicates that the K-means tunnel service performance evaluation can generally reflect the tunnel service performance.

Keywords: Highway Tunnels, Big Data, Service Performance, Evaluation Model, Evaluation Index

Acknowledgement

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A LSTM framework in predicting changes in digital parameters of granite compositions under uniaxial compression load

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Abstract: Using the video images photographed during the laboratory uniaxial compression tests, the regions of various compositions in granite specimen was determined and labeled using the threshold segmentation. Digital parameters of each composition with time were then obtained. After constructing and training a LSTM (Long-Short Term Memory) framework, we estimated the changes in digital parameters of the compositions using RMSE (Root Mean Square Error) to measure the reliability. It shows that there is a good agreement between the observed and predicted digital parameters.

Existing studies. Ben-Yosef et al [1] constructed a full interpretation model to identify the semantic features of the object images. Klyuchnikov et al. [2] presented an identification technique in determining rock type at the drilling bit using machine learning classification methods. Imamverdiyev and Sukhostat [3] developed a model for geological facies classification in wells using the deep learning. Sagheer and Kotb [4] proposed a deep long-short term memory (DLSTM) architecture using the production data of two actual oilfields. Gao et al [5] used the traditional recurrent neural (RNN) networks, long-short term memory (LSTM) networks and gated recurrent unit (GRU) networks to conduct the real-time prediction of operating parameters in tunnel boring machines (TBM). Zhou et al [6] presents a predictive framework, containing a wavelet transform noise filter, convolutional neural network feature extractor, and long short-term memory predictor, for determining the attitude and position of the shield machine. Yang et al [7] used the time series theory and long and short term memory neural network (LSTM) to predict the transient landslide displacement. Zuo et al [8] reviews the state-of-the-art application of deep learning algorithms for processing geochemical exploration data and mining the geochemical patterns.

We first extract digital parameters of compositions in granite at each constant. The size of the rock specimen was around 50 mm × 50 mm × 100 mm. The video images were photographed during the laboratory uniaxial compression tests, by leveling the camera normal to the specimen surface with a distance of about 0.5m. For each frame in the test video image, the threshold segmentation was used to extract the regions including the compositions, or biotite, feldspar, quartz, and crack. The labeling was then performed for each composition. Digital features of a composition were characterized by area A, eccentricity E, and inscribed radius R_I. Figure 1 shows the area A with time of biotite in granite specimen under axial load. In the figure, the horizontal label is the second transferred from the total 732 frames with the fps of 25.

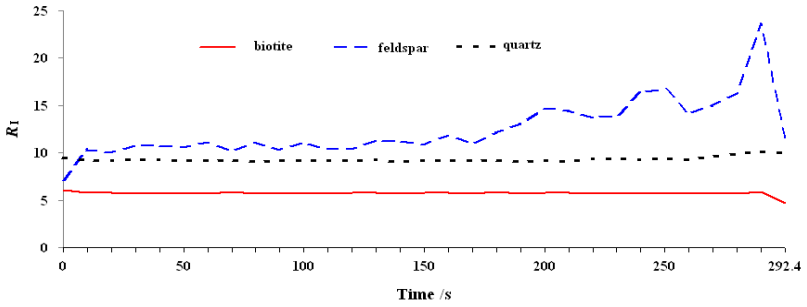

Figure 1. Inscribed radius R_I (in pixel) with time of compositions in granite specimen under axial load.

We then constructed a LSTM framework. All digital parameters of the compositions were considered as the data set, in which 90% and 10% were respectively partitioned into the training and test ones. For later convenience, these parameters were standardized with the zero mean and unit variance. A simple LSTM (Long-Short Term Memory) framework (see Figure 2) was established to predict the changes in digital parameters of compositions. In the LSTM framework, we set the parameters of input size (in Sequence Input Layer), number of hidden units (in LSTM Layer), and number of responses (in Fully Connected Layer), as 1, 1, and 200, respectively.

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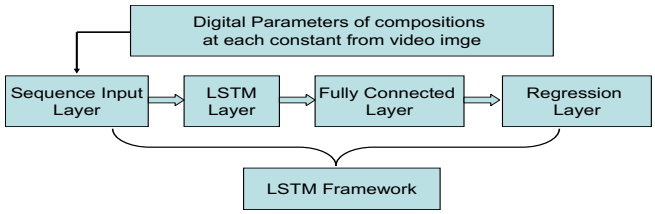

Figure 1. LSTM framework for predicting changes in digital parameters of granite compositions

We trained the LSTM framework and estimated the changes in digital parameters of compositions. To train the LSTM framework, the ADAM technique was used as the optimization algorithm, the maximum epochs, gradient threshold, initial learn rate, learn rate drop period, and learn rate drop factor were set as 250, 1, 0.005,125, 0.2, respectively. RMSE (Root Mean Square Error) was used to measure the difference between the observed and predicted values. Figure 3 shows the observed and predicted eccentricities of feldspar using the LSTM framework. It can be seen that there is a good agreement between the observed and predicted eccentricities.

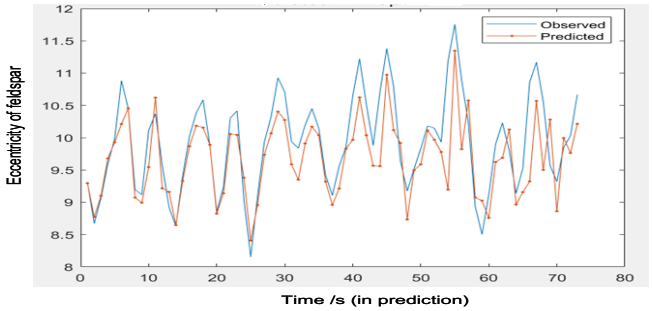

Figure 3. Observed and predicted eccentricities of feldspar using constructed LSTM framework.

The estimation of other digital parameters of other compositions, influences of LSTM parameters and composition locations, and relations between these parameter changes with mechanical features of the rock should be investigated in more detail.

Keywords: LSTM Framework, Digital Parameter, Granite Composition, Uniaxial Compression Load.

Acknowledgement

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A newly-developed alloy gas atomization process and the powder product used in selective laser melting process

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Abstract: Selective laser melting process(SLM), as a common additive manufactory (AM or 3D printing) process, has been widely used in high-end manufacturing, such as dental and bone implants for medical treatment, lightweight structure and functional components of aerospace, prototype manufacturing of automotive parts, etc. However, the high cost of powder raw materials is one of the reasons that hinder the application of this process in batch-production industries. Our group combined with the existing work foundation of atomization powder process, powder metallurgy and SLM technology. Firstly we carried out the innovation of atomization process to obtain low-cost new SLM printing powder. Subsequently, we developed matching printing process based on the performance of the printing powder. And we secondly optimized topology of lightweight lattice structures from the developed printing parameters. In this paper, the design principles and results of the new atomization process are described[1, 2]. And the case of our typical aluminum alloy powder product was used to demonstrate the characteristics of the powder product, the printing results and the secondary topology optimization example of lightweight lattice structure.

Keywords: Additive manufactory, Gas atomization, Aluminum alloy powders, Lattice structure.

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Prediction of Undrained Shear Strength of Soft Clays Using LightGBM Method Based on Bayesian Optimization

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Abstract: This study applies a novel data-driven lightGBM machine learning method [1] for capturing the relationships between the undrained shear strength and various basic soil parameters. Based on the method, a general approach is developed to predict the undrained shear strength (s_u) of soft clays by employing soil data sets from sites including Finland, Sweden and Norway [2], available in the TC304 database. The s_u is predicted in consideration of six feature variables including the preconsolidation stress, vertical effective stress, liquid limit, plastic limit, natural water content, and sensitivity [3][4].In order to reduce the dependence on the rule of thumb and bruteforce search, the Gaussian Bayesian optimization method is used to find the model hyperparameters [5]. The developed model is used as a contrastive analysis with other approaches (including traditional empirical equations and other machine learning methods) under 10-fold cross-validation for better persuasive results. It is shown that lightGBM model outperforms these approaches in terms of both accuracy and computational efficiency, which makes it a satisfactory tool in prediction of geotechnical parameters. For geotechnical engineering applications, a new lightGBM -based model can be readily obtained from the proposed approach with reasonable accuracy, provided that the new site-specific test data are available.

Keywords: Undrained Shear Strength, Computational Efficiency, LightGBM, Machine Learning Method, Bayesian Optimization.

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The authors would like to thank the members of the TC304 Committee on Engineering Practice of Risk Assessment & Management of the International Society of Soil Mechanics and Geotechnical Engineering for developing the database 304dB used in this study and making it available for scientific inquiry. We also wish to thank M. D'Ignazio, T.T. Länsivaara, J. Ching and K.K. Phoon for contributing this database to the TC304 compendium of databases. The study is partially supported by the Natural Science Foundation of Chongqing, China (cstc2018jcyjAX0632) and Venture & Innovation Support Program for Chongqing Overseas Returnees (cx2017123).

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A Review in Recent Development of 5 Axis CNC Milling Machine Tool Operations

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Abstract: To produce sophisticated parts with free form surfaces such as turbine blades, airfoils, impellers and aircraft components, 5-axis CNC machine tools are used. To increase the accuracy as well as efficiency in process of part production using 5-axis CNC machine tools, effective parameters and errors such as geometric and gouging errors are considered in the research works. Also, machining operations of sculptured surfaces by using 5-axis CNC machine tools are analyzed and modified to increase quality of part production. Feed rate scheduling and optimization systems in 5-axis CNC machine tool operations are developed in order to increase surface quality in machined parts. Cutting forces prediction and analysis are presented to provide ability of cutting force and cutting tool monitoring system along machining paths. Cutting Toolpath and cutter orientation in 5-axis CNC machine tool operations are analyzed and optimized to increase efficiency in process of part production. To create and analyze actual machined parts in virtual environments, virtual machining systems are developed. Rotary axis of 5-axis CNC machine tools are analyzed and modified in order to increase accuracy of the axis in machining operations of free form surfaces. In order to increase efficiency in process of part production, optimized cutting tool paths with regard to minimum energy consumption are generated. A review of recent development in 5-axis CNC machine tool operations is presented in this paper to develop the process of part production using machining operations.

Keywords: 5-axis CNC machine tools, Geometrical errors, Cutting forces, Process optimization.

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Mineral Segmentation from Polarized Light Microscopy Images of Rock Slices via Deep Neural Networks

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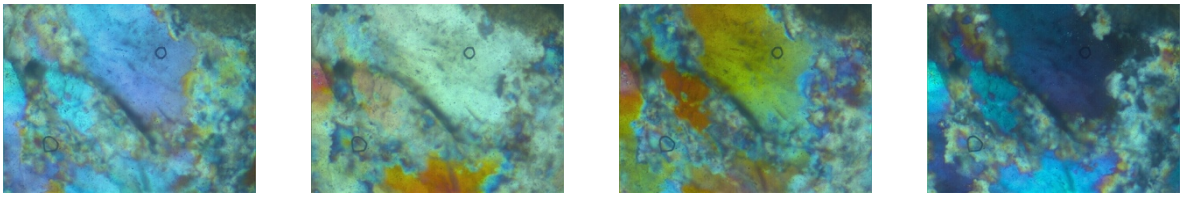
Abstract: There are about 3000 known minerals on earth. A mineral is an element or chemical compound that is normally crystalline and that has been formed as a result of geological processes [1]. All rocks are made up of 2 or more of these minerals. Different mineral bends light in different ways, which enables identifying the types of mineral by colors of the transmitted light and the reflected light, as shown in Fig. 1. Polarization microscopy is routinely applied in material sciences and geology to identify minerals on the basis of characteristic refraction properties and colors. This phenomenon is the so-called birefringence, which is the optical property of a material having a refractive index that depends on the polarization and propagation direction of light, as shown in Fig. 2. This effect was first described by the Danish scientist Rasmus Bartholin in 1669, who observed it [2] in calcite, a crystal having one of the strongest birefringence. Crystals with non-cubic crystal structures are often birefringent, as are plastics under mechanical stress. Whereas polarizing microscopes are commonly used in imaging of cellulose in cell walls of plants and starch grains in biology, polarizing microscopes are also used for identification or imaging of birefringent structures like crystals in rock slices. We operated the Leica DM750 microscope in Fig. 3 for polarized light imaging. Utilizing the image processing software Leica QWin, all the images of rock slices were generated in a similar photography condition regarding the light source, the exposure time, the focus and the gaining.



(a) 0° (b) 45° (c) 90° (d) 135°

Figure 1: Images of the same rock slice region at different relative polarized angles (magnified by 10 times)

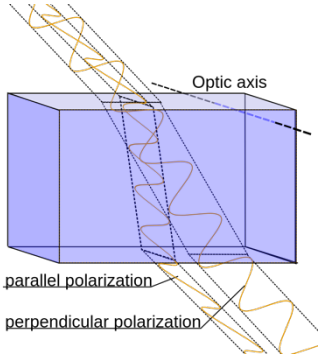


Figure 2: Explanation of birefringence

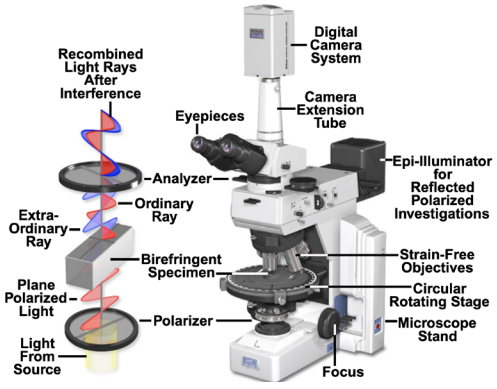


Figure 3: Polarized light microscope configuration

Using the microscopy system, we have generated a rock slice images database of about 200, where the samples are from the different location of the same site. However indistinguishable on the macro scale, the rock slices are

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unrevealed remarkably heterogeneous on the micro scale by the polarized light microscopy. By shifting the relative polarized angle of the two polarized gratings, we observed dramatic colors changing of different minerals (Fig. 4), which could be good basis for minerals classification. However, this approach is often hindered by the efficiency to rotate the gratings, and by the accuracy of polarized angle. During certain range of polarized angle , colors of minerals changes enormously. We proposed a data driven method to render the underlying features, or the semantic content of a rock slice image in different polarized angles, given only the image at 0°. Arguably, a major limiting factor for previous approaches has been the lack of image representations that explicitly represent semantic information and, thus, allow to separate image content from style [3]. Here we use rock image features derived from Convolutional Neural Networks (CNN) optimised for object recognition, which make high level rock information explicit, as shown in Fig. 4. The method allows us to produce new images of different polarized angles that requires limited prior images.

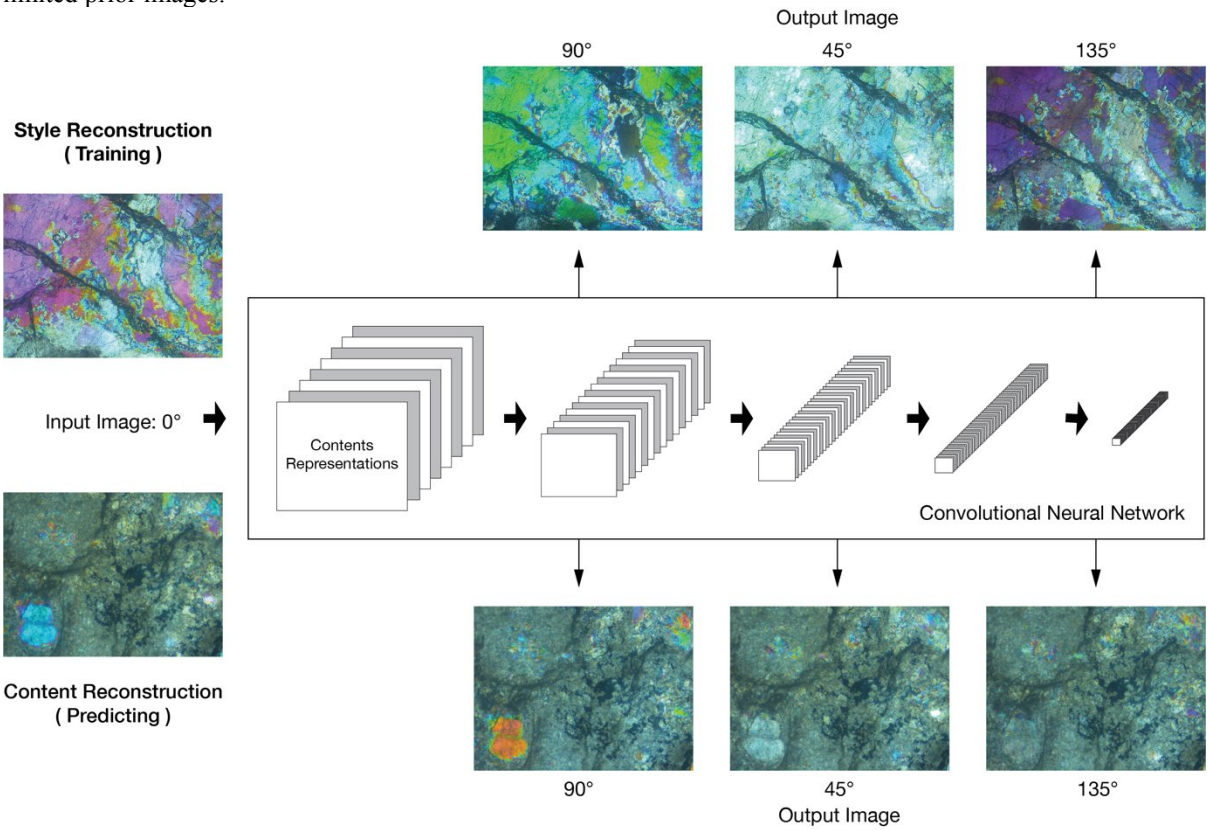

Figure 4: Rock slice image style transfer in a Convolutional Neural Network (CNN)

Keywords: Image segmentation, Polarized lighting microscopy, Rock slices, Deep neural networks.

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A Novel Method for Health Assessment of Subway Shield Tunnel Structure Based on Knowledge Graph

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Abstract: With the rapid increasing traffic pressure in large cities, Fast urban rail transit has shown more and more importance to relieve traffic, and it has gradually become the preferred travel mode. Most of the urban rail transit adopts the form of underground shield tunnel. Due to the large-scale construction of subway shield tunnels, the construction environment around the tunnel is becoming more and more complicated. As an underground structure, the subway structure is inevitably degraded with the influence of external loads and service time. In order to improve the subway service, its daily operation time is getting longer and longer, which puts forward higher requirements for the health inspection, evaluation and maintenance of tunnel structure. In order to evaluate the structural performance or health of tunnels in a timely and scientific manner, the researchers have carried out a lot of research work in testing methods, equipment and evaluation methods. At present, the commonly used health evaluation methods are indicator-based methods, including single factor, multiple factors, comprehensive evaluation and so on. However there are exist many and complicated influence factors of tunnel structure, such as construction ways, service time, structure scale, structure form, structural defects (leakage water, crack, staggered segment, segment spalling, etc.), material aging, state of bolt tightening, tunnel section shape, tunnel structure repair and reinforcement, surrounding strata, surrounding construction and so on [1]. These factors are always difficult to consider, and many factors are difficult to describe quantitatively, so the most commonly used evaluation method is only based on the tunnel structure itself, using multiple factors to carry out weighted synthetic evaluation [2]. Limited to the complexity of underground tunnel engineering, the weight of each factor is still mainly based on the experience of experts, resulting in the factor that can`t be considered completely in structural evaluation, and the degree of influence of factors is greatly affected by human experience and the assessment takes long time which is also difficult to consider the dynamic evolution characteristics of tunnel health. The concept of Knowledge Graph （KG） was proposed by Google in 2012[3]. It converts factual text content into interconnected graph structures and establishes connections between massive chaotic information. It can provide users with a concise, easy to understand and visualization data support [4]. Based on KG, the detailed information of large-scale rail transit tunnel structures can be fully constructed, which provides the basic data for the structure health assessment. This paper focuses on the shield tunnel constructed in soft ground in Shanghai. Firstly, based on the concept of subway tunnel to construct the KG [5], which mainly includes the information of shield tunnel construction (including construction contractor, construction method, construction date, construction process and acceptance, etc.), operating environment (including the surrounding environment, geological and hydrology, the adjacent construction, internal environment, train traffic load, station platform type and subways transfer, etc.), the structure characteristics (including the structure section size, tunnel section shape, the segment assembling modal, etc.), segment ring unit (per five rings or connected aisle as a unit, including internal force and deformation of the structure, defect characteristics, reinforcement and repair, etc.). Then, taking conceptual KG as the template, taking the concrete subway tunnel project as the object, using the Neo4j [6] diagram database to construct the subway KG which covers all the 16 operating subway lines in Shanghai (total 415 subway sections, 705*2 kilometers of shield tunnel). The Multi-index weighted comprehensive evaluation method is adopted to evaluate the structural health degree of each segment ring unit. To improve the reliability of the evaluation results, a Web-based Delphi method will be used. The health degree of segment ring unit then be added to the KG as new nodes. Thirdly, a Graph Neural Network (GNN) model was built with Pytorch [7,8]. Taking the KG of segment ring unit as input and the its health degree index as output, the training and testing samples were prepared. And then, the model is trained and validated. Finally, when the knowledge information of segment ring unit changed, using the trained model to evaluate its structural health degree, then update its KG. Compared with the traditional methods, the novel method of shield tunnel structure health assessment proposed in this paper, can obtain more comprehensive information that affects tunnel structure health, on the other hand, it can use the trained model to evaluate the health degree fast and automatically. With the advantages of Knowledge Graphs, it is convenient to

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manage and query information related to subway tunnels, and provide support for artificial intelligence services based on big data. Based on the subway KG, it is expected to provide intelligent support for the tunnel operation and maintenance decision-making.

Keywords: Shield tunnel, Structural health, Knowledge Graph, Graph neural network.

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An Adaptive Collocated Method for PHT Splines with Optimal Selection of Collocation Points

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Abstract: We propose an adaptive isogeometric analysis (IGA) collocation method with a recovery based error estimator. The proposed collocation method is based on a new basis for polynomial hierarchical splines over T-meshes (PHT-splines) [1]. The improved method collocates at Gauss points [2] in the interior of the domain, which are the optimal for the new PHT elements with C1 continuity. Near the boundary, the locations of the collocation points are determined by an optimization method based on machine learning algorithms.

The new PHT basis is based on local knot vectors and has improved conditioning compared to the original PHT basis [3]. Furthermore, based on the new PHT basis, the improved IGA collocation can be extended to arbitrary degree polynomials. The local refinement strategy is driven by a recovery-based error estimator by computing a higher order recovered solution. The improved IGA collocation method is also compared with the Galerkin method as well as the Greville-abscissae collocation. The improved IGA collocation has been tested on several 2D and 3D problems and results in optimal convergent rates and high accuracy and robustness of the approximation.

Keywords: isogeometric collocation, PHT splines, Gauss points, recovery-based error estimator.

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Optimal Placement of Active Members in Adaptive Cable-Strut tensile Structure Using an Optimal Combination Algorithm

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Abstract: An adaptive cable-strut tensile structure is defined as a controllable structure which can actively alter its configuration or self-stress in response to variation of the outer environment by changing the length of active members with actuators. The realization of such alteration is involved with optimization and control processes. The shape control or the internal force control of such structure had already been studied in some researches [1-3]. However, the number and placement of active members in their control were usually determined subjectively or on random search. Since the optimization of the placement active members concerns about discrete variables, intelligent optimization algorithms based on random search are often introduced to solve such problems, such as genetic algorithm, simulated annealing algorithm, particle swarm optimization, ant colony algorithm and so on [4-6].

By analyzing the coefficient matrix of the incremental calculation of the control equations, this paper reveals a mathematical relationship between the number and placement of active members and the solution of control equations. The criteria of the number and placement of active elements are proposed. A mathematic formulation for optimal placement with the objective of minimizing control efforts is established, and a solution strategy based on genetic algorithm is proposed. A simple-supported tensegrity beam has been used for the validation of the proposed strategy (Fig. 1).

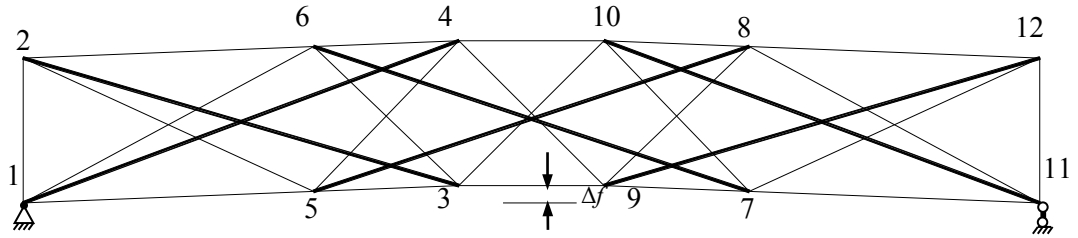

Figure 1: The target shape of a tensegrity beam

Furthermore, taking minimizing shape control errors, the length changes and the number of active members as objective functions, a hybrid variable multi-objective optimization model with active member distribution vector and the length change as variables has been established, and an optimal combination algorithm with non-dominant sorting genetic algorithm(NSGA-Ⅱ)and sequential quadratic programming(SQP) is introduced. The controlling validity is investigated via case study. The results present the contradiction relationship between the optimal solutions of each objective function, and indicate that the higher accuracy demanded the more active members needed.

Keywords: Optimal placement, Active member, NSGA-Ⅱ, SQP, Adaptivestructure.

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Two Applications of Isogeometric Boundary Element Method for Axisymmetric Singular Helmholtz Acoustic Problems

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Abstract: In this article, two applications are developed for axisymmetric singular time harmonic wave propagation (Helmholtz equation) in acoustic problems [1]. The boundary element methods (BEM) [2] is coupled with isogeometric analysis (IGA) with parameterizing the computational domain and approximating the unknown solution using non-uniform rational B-splines basis functions (NURBS) [3].

In the first application, the horn problem with cylindrical symmetry is solved. Due to the axisymmetric horn body, the three-dimensional problem is simplified in BEM from a surface integral of Helmholtz equation to a combination of line integral - similar to a two-dimensional BEM problem – with another integral over the angle of revolution. The discretization is applied only to the former integration. This leads to significant computational savings [4].
Similar to the first axisymmetric application, the muffler problem is studied. In addition, the muffler body includes internal components (the extended inlet and outlet tubes in mufflers). To model these internal components in BEM, another equation is needed in addition to the main direct integral equation (DIE). The additional equation is formulated by considering the normal derivative of DIE on the surface of the internal component [5]. Since both applications have singular kernels, special singularity treatments are utilized for the integration of these kernels [6].
Several numerical examples are considered and the results are compared against previously published numerical methods to validate the present formulation and verify the efficiency of the proposed approaches.

Keywords: BEM, Isogeometric, Acoustics, Axisymmetric, Singularity.

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Parameter Optimization in Penalty-Based Implicit Discontinuous Approach for Efficient Rock Failure Analysis

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Abstract: The penalty function method is a commonly used approach in discontinuous/contact computation methods for its simplicity in implementation. However, the choice of the penalty parameters is an important task in its application in geotechnical problems, in terms of computational accuracy and efficiency. In discontinuum-based approaches, such as discrete element method (DEM) [1,2] and discontinuous deformation analysis (DDA) [3,4], the contact models are applied in mainly two scenarios, i.e., (a) the contact of real joints/cracks and (b) the bond between particles/blocks. For contact of real joints, the contact parameter values calibrated by field measurements or lab-scale tests results are the preferred choice. In simulation cases without the realistic data, the empirical data associated with the geotechnical materials can also be applied. In addition to the explicit representation of jointed rock block systems, the bonded block/particle models are also used to represent the meso-scale rock structures (e.g., grain structure of crystalline rocks) [5]. In these applications, the contact penalty parameters (normal and tangential stiffness) and the contact strength parameters influence the computation in the following aspects: (1) the stiffness and deformation of the global model; (2) the potential failure pattern of a model; (3) the computational efficiency in solution of the global stiffness matrix in implicit DDA approach; (4) the critical time step size in explicit DEM approach.

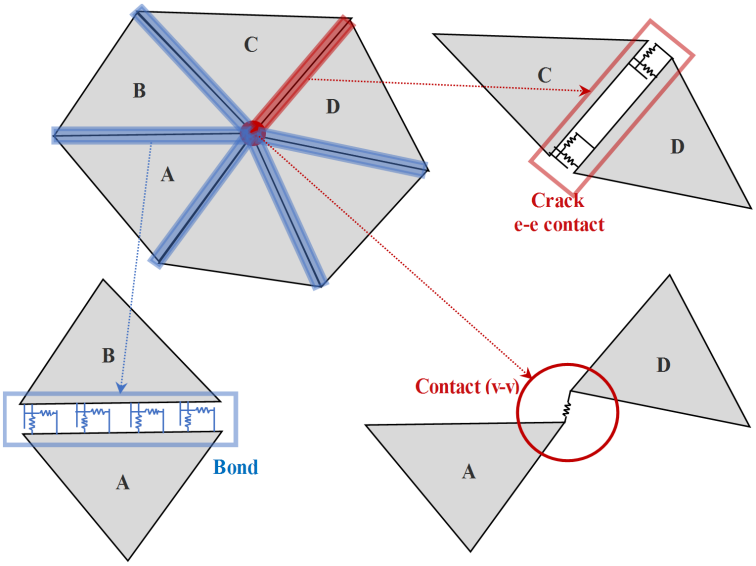

Figure 1: An illustration of the bond and contact model in discontinuum-based approach

In this work, the accuracy and efficiency of bonded block models using DDA approach are investigated. With the implicit time integration approach, DDA methods have the advantages of unconditionally stable time step and efficient algorithmic damping for quasi-static analysis of contact problems. An illustration model for the investigated bonded block model is shown in Fig. 1. In this triangular block-based representation, the edge-edge bonds, edge-edge contact and vertex-vertex contact controls the deformation and failure mechanism of the model. The key parameters, including the normal and tangential stiffness in bonds and contacts, are investigated with various combinations. The associated computational efficiency, the relationship of meso-scale contact stiffness and strength parameters with the macro-scale deformation properties and failure patterns are evaluated. A multi-level sensitivity analysis approach is used to investigated both the impact of changing input parameters and the sensitivity

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of input parameters on the computational efficiency and the macro-scale system bulk response. The strategies to select the optimized input penalty parameters are proposed in this paper.

Keywords: Parameter Optimization, Penalty function, Discontinuous approach, Rock failure analysis.

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Application of Machine Learning to the Prediction of Displacement Capacities of Non-ductile RC Beam-Columns

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Abstract: Provisions in modern design standards attempt to preclude less ductile or brittle failure modes in lateral load resisting systems, as their occurrence may lead to catastrophic failures under extreme loading events, such as earthquakes. Such modes depend on the type and characteristics of the structural element/connection. For reinforced concrete (RC) beam-column components, the most desirable failure mode is the flexural (and not the shear, or axial) mode. Observations from previous earthquakes reveal that a significant portion of existing inventories of structural frames do not necessarily satisfy modern expectations, as shear and axial failure modes were frequently recorded in post-event surveys. Given the existing vulnerabilities, there is a need to efficiently and accurately predict the seismic behavior of large numbers of buildings. Prior efforts in this realm focused on experimental characterization of brittle failure modes, data from which fed combinations of analytical and statistical studies that yielded numerous predictive formulae/models [1-3]. These prior studies have identified the key parameters that control the hierarchy of failure models, which include longitudinal/transversal reinforcement ratios, axial load level, plastic-to-nominal shear force ratio, sectional dimensions, and transverse reinforcement spacing [4-8]. The numbers of these parameters hints at the complex nature of the problem, and despite a fair number of attempts, considerable errors are still encountered in validation studies on presently available predictive models [3]. In the present study, we make use of an extensive database that contained data from 326 rectangular RC beam-columns and carry out an exhaustive training of an Artificial Neural Network (ANN) to predict the lateral displacement (drift) capacities. A variety of ANN architectures with different hidden layers and neurons are considered and the data set is randomly divided into training and testing subsets producing a large number of ANN realizations for evaluation. The accuracy of the most precise architecture is significantly higher than any of the prior predictive models considered in this study.

Keywords: ANN, RC beam-column elements, Displacement capacity prediction, Flexure-shear-axial failure, Statistical analyses.

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Damage Evolution and Energy Absorption Modeling of Laminated GFRP Plate with Weave Pattern Variation Under High Velocity Impact

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Abstract: The effectiveness design of composite structures should be understand the impact induced damage mechanism in laminates especially in military and structural applications. It starts with the development of numerous experimental and numerical analysis to study the dynamic response of the composite structures in the dynamic loading phenomena. It is considered that the numerical analysis would significantly saving the computational cost in predicting the ballistic impact as experimental work of damage evolution can be prohibitively expensive. This study aims to investigate the damage evaluation and energy absorption performance characteristics of laminated GFRP plate with weave structure as the variable under high velocity impact in numerical analysis view point. TexGen software is used to generate the weave patterns whilst ABAQUS is utilized to simulate the explicit three-dimensional finite element analysis. A series of ballistic impact simulations has been performed on proposed woven GFRP plates with a conical nose shaped projectile. Selecting a proper material models and contact definition is the major criteria to ensure the accuracy of the modeling. The damage evolution model based on Hashin's criteria has been assigned to predict the failure of the laminates. The projectile has a conical nose shaped with 6.24 mm of diameter, 10 g mass and 13.83 mm in length. The impact velocity is ranged from 200 to 450 m/s. A good correlation between the simulated composite plate with selected weave patterns has been drawn in terms of damage evolution and energy absorption criteria during impact.

Keywords: Damage evolution, Weave patterns, Energy absorption, Ballistic impact.

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An experimental study on natural frequencies measurement in steel plates/beams using PAK-Mobile MKII system

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Abstract: PAK Mobil MKII is a compact mobile multi-channel measuring system used for vibration and acoustic analysis of engineering structures. It can be universally configured for any common measurement pickups and is easy to adapt to the task. In this paper, an experimental investigation into obtaining the natural frequencies of thin plates made of steel is conducted. The experimental results are then compared with the theoretical results. Good agreement between the results is observed. The results presented in the paper can be used as a useful guideline for engineers and industries.

Keywords: PAK Mobil MKII system, Experimental study, Natural frequencies, Steel Plates/Beams.

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Assessment of pipe-pile integrity using transverse velocity signal -- Numerical simulation

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Abstract: In order to study the feasibility of transverse velocity response for the evaluation of pipe-pile integrity, 3D (a three-dimensional) finite integration model of pile-soil system is established, and the numerical analysis of low-strain integrity testing of the pipe-pile containing cracks is carried out. The vertical and transverse velocity responses of the pile-top are obtained using the EFIT (elastodynamic finite integration technique), and the accuracy of the algorithm is verified via comparing with the measured data. The characteristics of the reflected waves due to the cracks are analyzed. It is found that the transverse velocity response can be used to determine the integrity of pipe-piles and has advantages in identifying vertical cracks. The main component of reflected waves in transverse velocity signal is from the shear waves. The circumferential velocity at 180° from excitation point is not affected by 3D interference. The wider the excitation pulse is, the worse the identification effect of transverse crack becomes; however, the location of transverse crack derived from the traditional 1D theory is shallow. The proposed correction method can help to improve the performance in locating cracks. This research enriches the theory of low strain testing and provides references for low strain testing of the pipe-pile containing cracks.

Major cracks can affect the quality and reliability of pipe-piles. Cracks might be a results of poor construction, or can be a results of damages during transportation, and installation. Pile integrity can provide valuable information about the presence of such cracks. However, the inspection and evaluation of integrity problems are often challenging, mainly because these cracks are surrounded by soil and not easily accessible for visual inspection. Low strain integrity testing can shed light on this hidden part of concrete piles, which has been widely used for assessing the quality of piles in civil engineering. Generally, this method provides information about continuity, defects such as necking, soil incursions, changes in cross section.

The objective of this paper is to study the feasibility of transverse velocity response for the evaluation of pipe-pile integrity. Firstly, a pile-soil interaction model in cylindrical coordinate system is established under the low strain integrity testing conditions. By means of the appropriate treatment of boundary conditions, the numerical solution of an initial-boundary value problem for pipe-pile testing is obtained using the EFIT. Secondly, the wave propagation process in the pipe-pile containing cracks is shown, and the transverse velocity histories at pile-top are illustrated. Besides, the influences of sensor location, contact time of the hammer, sampling position, and the stiffness of surrounding soil on testing results are analyzed in order to identify cracks more accurately.

The location of the stress and the velocity components produced by the EFIT are shown in Fig. 1, in which these components are located at different positions. This “staggered-grid” arrangement outperforms conventional grids concerning the implementation of boundary conditions and numerical stability.

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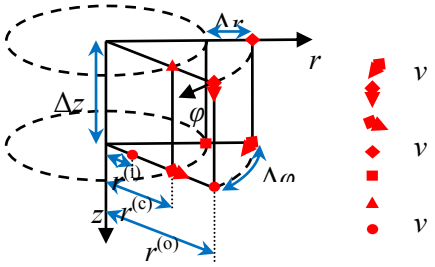


Fig. 1 Location of velocity and stress components on the EFIT cell

A pipe-pile containing an axial crack is modeled as shown in Fig. 2. The velocity histories received from both the intact pipe-pile and the defect one are plotted in Fig. 3. From Fig. 3a, it can been seen that there is little difference between the two curves, which indicates that the vertical-velocity signals cannot be used to identify axial cracks. However, it is shown that in Fig. 3b, reflected wave from crack can be clearly recognized in the circumferential-velocity curve, which shows that the circumferential-velocity has a strong advantage in crack identification. Therefore, 3D sensors are urgently needed for pipe-pile integrity testing.

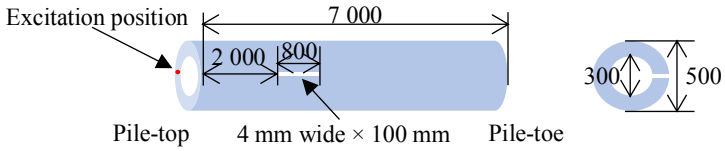
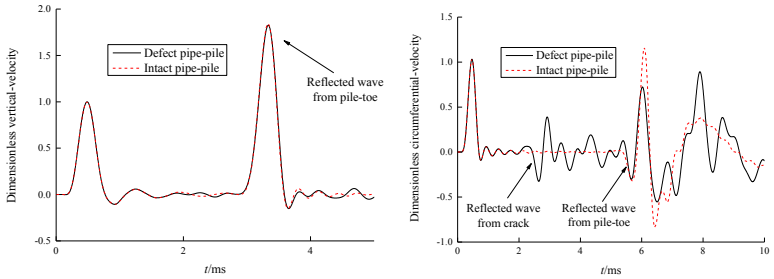


Fig. 2 Dimensions of a pipe-pile containing crack (All dimensiors are in mm)



(a) Vertical-velocity historyies (b) Circumferential-velocity histories

Fig. 3 Velocity histories received from pipe-pile top

Keywords: Transverse velocity response, Elastodynamic finite integration technique, Pipe-pile integrity, 3D interference, Low-strain integrity testing.

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Experimental and numerical analyses on mixing uniformity of water and saline in pipe flow

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Abstract: Two-phase flow is commonly observed in many industrial applications [1, 2]. In order to study the mixing process of soluble two-phase in turbulent pipeline, saline was chosen as a tracer and was injected into the pipeline [3]. In the present study, the computational fluid dynamics (CFD) software 'FLUENT' was employed to simulate flow fields in water–saline pipelines. Three variates (volumetric flow rate ratio, pipe diameter, and cross-flow flux) were considered to investigate the effects of multivariate on mixing uniformity [4, 5]. The coefficient of variation (COV) was selected as the evaluation index of mixing uniformity, effective mixing length (EML, the distance from the fertilizer inlet to the fully mixed position) was chosen to quantitatively analyze the fully mixed position of water and saline in pipelines[6, 7]. The results of this numerical model agree well with experimental measurements and it shows that this model can well predict the concentration field of water and saline in pipeline. Based on the experimental and simulated results, it was found that for the fixed flow rate ratio and cross-flow flux, the values of *EML* increased significantly with increasing pipe diameters. Furthermore, dimensional analysis (D-A) and regression analysis (R-A) were adopted to examine the influences of the three variates on *EML*, and their correlation coefficients of curve-fitting equation were calculated to be 0.997 and 0.967.

Keywords: Concentration distribution, Dimensional analysis, Effective mixing length, Numerical simulation, Pipe flow.

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On the Generation of Design Response Spectrum for Muscat Region in Oman

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Abstract: When a structure is subjected to an earthquake loading, it faces time varying loads. As a result, time-varying stresses and displacements are developed. From the design point of view, only maximum values of these quantities are of interest as the structure should withstand the maximum possible load subjected to it. To generate these results, response spectrum analysis is abundantly performed, also categorized as dynamic analysis of structures. Response spectra for a particular region is of great importance for design engineers as it is used to simulate the behaviour of the structure when subjected to earthquake loading in that region. This analysis is also performed in estimating the performance of existing structures. In order to generate the design response spectrum for Oman region, a single degree of freedom model is prepared using SAP 2000 software. The model is subjected to earthquake time histories that is generated by software program ProShake. Available earthquake records of nearby locations of Oman (GCC countries) are also utilized in order to generate 'Design Response Spectrum' for Oman region. An effort is made to generate a smooth design spectrum that can be used for the analysis. Generated 'Design Response Spectrum' is capable of providing adequate earthquake resistance design of structures for Oman region.

Keywords: Design Response Spectrum, Dynamic Analysis, Earthquake Engineering.

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Effects of Radial Charge Parameters of Liner on the Velocity of Shaped Charge Jet

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Abstract: In this paper, the explosive impulse in the detonation process of shaped charge is analyzed theoretically. Taking the shaped charge with a diameter of 56mm as an example, the influences of the ratio of the outer diameter of the charge to the liner on the velocity of shaped charge jet is investigated with the cone angles from 30 to 70 degrees. The effects of radial charge parameters and cone angles of liner on jet velocity was further studied by numerical simulation. The results of theoretical analysis and numerical simulation show that when the ratio of the outer diameter of the charge to the liner is greater than 4, the velocity of the jet formed by the liner tends to be stable, which accounts for about 17.9% of the total height of liner. The maximum velocity of jet is approximately linear with the cone angle of liner. The theory is applicable to the calculation of jet velocity under different cone angles, which provides a theoretical basis for the design of shaped charge.

Keywords: Liner, Shaped Charge jet, Velocity, Cone angle.

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Application of Multi Objective Bees Algorithm to Access the Optimal Generalization of Nonlinear Full Vehicle Model

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Abstract: A generalized nonlinear model was formulated and proposed for the dynamic analysis of nine degree of freedom (9 DOF) model road vehicle with passive and semi-active suspension systems. The model incorporates a nonlinear suspension spring and nonlinear damping force for passive and semi-active dampers, while the contribution due to biodynamic of the human operator was considered to be negligible. The semi-active damper is characterized by force generators in accordance with the control laws based on suspension mass velocity.

There is a set of optimal solutions, well-known as Pareto optimal solutions [1-3], which distinguishes significantly the inherent natures between single- objective and multi-objective optimization problems. In this paper, we used the Bees algorithm [4-5] for multi-objective optimization. Griffin et. al. [6], Rakheja [7], and Barak [8] have shown that the interior vibration of a vehicle has a significant effect in comfort and road holding capability. Bouazara and Richard [9] studied three types of suspension system (active, semi-active and passive) for an eight-degree of freedom vibration model. Gündoğdu [10] presented an optimization of a four-degree of freedom quarter car seat and suspension system using genetic algorithms. Alkhatib et. al. [11] applied genetic algorithm (GA) to the optimization problem of a linear one-degree of freedom (1-DOF) vibration isolator. The general optimization problem was stated mathematically in [12].

A systematic methodology was applied in an effort to select optimum values for the suspension damping and stiffness parameters of 9 DOF full-car nonlinear models, subjected to road excitation. First, models involving passive suspension dampers with constant or dual rate characteristics were considered. In addition, models with semi-active suspensions were also examined. Moreover, special emphasis was put in modeling possible temporary separations of the wheel from the ground. For all these models, appropriate methodologies are employed for capturing the motions of the vehicle resulting from passing with a constant horizontal speed over roads involving an isolated or a distributed geometric irregularity. The optimization process was based on three suitable performance criteria, related to ride comfort, suspension travel and road holding of the vehicle and yielding the most important suspension stiffness and damping parameters. As these criteria are conflicting, a suitable multi-objective optimization methodology is set up using the Bees Algorithm (BA) [13]. As a result, a series of diagrams with typical numerical results are presented and compared in both the corresponding objective spaces (in the form of classical Pareto fronts) and parameter spaces.

Keywords: Multi Objective Bees Algorithm, Ride Comfort, Road Holding, Linear and Nonlinear Model, Suspension System.

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Machine learning in the engineering crack identification problems

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Abstract: Machine learning (ML) method is used for the numerical solution of crack identification problems in two-dimensional piezoelectric structures under dynamic loads. The machine learning method is a flexible numerical approach to make predictions based on some pre-obtained training data without the need of any explicit functions. Fracture is modeled by the extended finite element method (XFEM), which allows the use of a single regular mesh for a large number of iterations with different crack geometries. The effects of various dynamical test loads on the crack identification are investigated. In this work, the XFEM-ML methodology is applied to two-dimensional electromechanical problems where different number of cracks is considered. The results show that this methodology can be effectively employed for detecting multiple cracks in piezoelectric materials.

Keywords: Machine learning, Crack identification, XFEM, Dynamic load.

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Road surface damage detection using neural network

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Abstract: In the road safety inspection, a road surface damage detection is a time consuming and an expensive process. In this contribution, a deep learning model based on Convolutional Neural network (CNN) algorithm is employed for prediction of presence or absence of damage in a road surface. Also for detection of damage type, the model is trained and tested for different damage types: longitudinal crack, lateral crack and alligator damage. The CNN model is implemented using the Keras library at front-end and TensorFlow at back-end and also openCV library is used for image processing. The comparison of the damage type predicted using the proposed model with the experimental data proves the fidelity of the proposed model for prediction of damage type in a road surface and its application for road safety inspection.

Keywords: Damage type detection, Image processing, Deep learning, Neural network.

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Modeling the stability of a soil-rock-mixture slope based on the digital image technology and numerical manifold method

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Abstract: As a widely distributed geotechnical material, the soil-rock mixtures (SRM), which are composed of high-strength block stones, fine-grained soil and pores, had formed since the Quaternary period. In regarding to the physical and mechanical properties, there are significant differences between the soil and rock materials. Hence the SRMs show extremely heterogeneous character. With the development of large and even giant hydropower projects in the southwest areas of China, many SRM slopes with different scales are encountered in the reservoir areas or/and near the dam areas [1-3]. The failure of these SRM slopes may result in great casualties and economic losses. Therefore, evaluating the stability and proposing reinforcing measures for the weak areas of the SRM slopes are of great importance to the safety of the project during the process of construction and operation. With the rapid development of computer hardware technology and image theory, digital image processing has provided an indispensable technical means for the development of modern science and technology. It has been applied to various subject areas, such as in the medicine, biology, aerospace and geotechnical engineering, and has achieved satisfying results. In the present paper, the digital image processing technology is employed to establish the real structure model of a soil-rock-mixture slope. The numerical manifold method (NMM) can solve the problems of continuity and discontinuity in geotechnical engineering in a unified way [4]. For the analysis of discontinuous problems, the unique and superior features of the NMM include the following [5] : (1) large displacement, sliding along joint faces and even discrete blocky movement are allowed; (2) by simply cutting mathematical patches with joints or material interfaces, discontinuity can be captured in a natural way without employing jump functions; and (3) the employed discontinuity representation algorithm is suitable for any number and any geometrical complexities such as intersections, junctions and the branching of discontinuities in one element. On this basis, the numerical manifold method is used to simulate the stability of a soil-rock mixture slope. An improved shear strength reduction technique is implemented into the numerical manifold method to evaluate the stability of the slope, as well as to obtain the factor of safety (FOS). In this technique [6], with the application of the relationship between the internal friction angle φ and the Poisson's ratio υ, υ is also adjusted for the purpose of eliminating the spurious plastic deformation that may happen in the SRM slope. The simulation results show that: (1) the improved numerical manifold method is able to accurately predict the FOSs of slopes; (2) it is very difficult to form a slipping surface passing from the toe of the SRM slope to the top of the slope; (3) the rock blocks in the SRM slope make the internal stress field of the slope became very heterogeneous; (4) the sliding zone of the soil-rock mixed slope obtained by shear strength reduction method is very zigzag.

Keywords: Soil-Rock Mixture Slope, Digital Image Processing, Shear Strength Reduction Method, Numerical Manifold Method, Slope Stability Analysis.

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DEM study of modeling method and thermal cracking of sandstone

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Abstract: Sandstone is a common sedimentary rock composed mainly of sand-sized mineral particles with some cement (clay or quartz etc.). Generally, the sandstone structure, as well as the shape of the mineral particles have a significant influence on the properties of sandstone. This paper presents a novel method to simulate sandstone with any shaped mineral particles and investigates the effects of particle shape and sandstone structure on the thermal cracking responses. A random angular bend (RAB) algorithm and overlap detection algorithm is proposed to build the numerical model of sandstone. Three representative parameters are used to quantitatively control the shape feature of mineral particles in term of three major aspects, including form, roundness and surface texture, respectively. The overlap detection algorithm is developed to address the difficulties associated with spatial allocation of irregularly shaped particles. Finally, the effect of particle shape and sandstone structure on thermal cracking of sandstone are investigated based on discrete element method. Some useful conclusions for numerical simulation on Sandstone are arrived at.

Keywords: Particle shape, Discrete element method, Sandstone structure, Overlap detection, Thermal cracking

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Hip Fracture Risk Assessment based on Different Failure Criteria using QCT-based Finite Element Modeling

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Abstract: The most common injury of the elderly during the sideways fall is hip fracture. It was reported that hip fracture may lead to a long term disability and death of individuals [1]. The total number of hip fracture is increasing over the world [2]. Therefore, a special attention must be dedicated on this important issue in order to provide appropriate plans for prevention and treatment of hip fracture. Precise evaluation of hip fracture risk leads to reduce hip fracture occurrence in individuals and assist to check the effect of a treatment. Accurate assessment of hip fracture risk in the elderly also helps us to consider proper preventing schemes such as effective design of hip protectors and or providing proper treatment plans to protect the elderly against future hip fracture.

By integrating an imaging technology such as Dual-Energy X-ray Absorptiometry (DXA) or Quantitative Computed Tomography (QCT) and a numerical method such as the Finite Element (FE) Method, a category of more reliable tools for assessing hip fracture risk has been developed which does not have the limitations of statistical models and methods which are based on measuring bone mineral density (BMD). However, in numerical and computational models such as QCT-based finite element models, choosing a proper failure criterion based on bone microstructure is very important for accurate assessment of hip fracture risk. The human femur consists of inhomogeneous (porous) cancellous bone and nearly homogenous cortical bone, so, their failure mechanism is totally different due to their different microstructures. Failure mechanism of the cancellous bone is often in the form of buckling, and the failure of denser cancellous bone and the cortical bone is mostly characterized by local cracking [3,4]. Although stress- and strain-based failure criteria are accurate for ductile materials such as metal, they may not be accurate for bones because bone is categorized as a brittle material [5]. The tensile strength of bones is smaller than their compressive strength, indicating bone should be classified as a brittle material [5]. Due to this property of bones, strain energy criterion which is a combination of both stress and strain effects may lead to more accurate assessment of hip fracture risk. In the literature, hip fracture risk was usually estimated using the von Mises stress and strain criteria [6-9], the maximum principle stress and strain criteria [10-13], the maximum shear stress criterion [14], the maximum distortion energy criterion [14], and the strain energy criterion [15,16]. To the best of our knowledge, there is no comparative study in hip fracture risk assessment by using different failure criteria. The aim of this study is to define hip fracture risk index using the strain energy, the von-Mises stress, and the von-Mises strain criteria and compare the calculated fracture risk indices using these criteria at the critical regions of femur.

A subject-specific QCT-based finite element model is introduced to evaluate hip fracture risk using the strain energy, the von-Mises stress, and the von-Mises strain criteria during the single-leg stance and the sideways fall configurations. We construct FE model of the femur from the QCT image of clinical cases and then simulate the single-leg stance and sideways fall configurations by finite element analyses, and finally fracture risk indices are assessed in the critical regions of femur, regions with high stress and strain [17, 18], using the strain energy, the von-Mises stress, and the von-Mises strain criteria, and then we evaluate and discuss about their rate of conservation and accuracy based on the bone failure mechanism.

It was found that based on these criteria, the hip fracture risk at the femoral neck and the intertrochanteric region is higher than other parts of the femur, probably due to the larger amount of cancellous bone in these regions. The results of this study also showed that the strain energy criterion gives more reasonable assessment of hip fracture risk based on the bone failure mechanism and the von-Mises strain criterion is more conservative than two other criteria and leads to higher hip fracture risk indices.

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Keywords: Hip Fracture Risk, Finite Element Model, Strain Energy, von-Mises Stress, von-Mises Strain.

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Parametric Study of Hip Fracture Risk using QCT-based Finite Element Model

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Abstract: Different parameters such as age, height, weight, and body mass index (BMI) may influence on the hip fracture risk in the elderlies which is the most common injury for them especially during the sideways fall. Hence, a study considering various parameters can be useful to prevent probable hip fracture in the elderlies and propose an appropriate treatment for the case of hip fracture occurrence. Parametric studies of hip fracture risk based on the gender, age, height, weight, and BMI of subjects lead to a precise estimation of hip fracture relation to the specifications and lifestyle of a community.

In this study, the correlations between the hip fracture risk and different parameters such as age, body height, body weight, and BMI are investigated and attained for 30 females (totally 60 right and left femurs) and 30 males (totally 60 right and left femurs). To this purpose, we construct subject-specific QCT-based finite element model of the femur using Mimics and ANSYS software based on the QCT data of subjects and then hip fracture risk index is calculated based on the strain energy criterion [1, 2] using MATLAB codes at the critical regions of the femur, locations usually receiving high stress and strain within sideways fall [3, 4]. The hip fracture risk index versus age, body height, body weight, and BMI (representative of body shape) at the three critical cross-sections of femur during the single-leg stance and the sideways fall for 30 females and 30 males are shown in the scattered plots. The correlation coefficients (r) and the corresponding statistical significance (p-value) are calculated using in-house MATLAB codes for the parameters considered in this study.

According to the obtained results, there is an increasing trend of hip fracture risk with age, body height, body weight, and BMI at the three critical regions of the femur in both women and men during the single-leg stance and the sideways fall. The correlations of hip fracture risk with age and height are not much significant ($p > 0.05$) for the clinical cases investigated in this study. It means that at least for the clinical cases investigated in this study, we cannot conclude that the hip fracture risk strongly increases with the age and it may depend on the individual's health status and lifestyle. The results of this study also show that there is a strong correlation between the hip fracture risk with the body weight and BMI ($p < 0.05$). It indicates that subjects with higher body weight and BMI, overweight and obese subjects, are more prone to the hip fracture risk.

Keywords: Hip Fracture Risk, Parametric Study, Finite Element Model, Strain Energy.

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Phase field fracture in elasto-plastic solids: a length-scale insensitive model for constitutive behaviour of quasi-brittle materials

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Abstract: The phase-field model for fracture has been coupled with continuum plasticity to capture complex constitutive behaviour. However, the length scale parameter in the existing coupled models must be interpreted as a material property to match the material strength in experiments. This may lead to overly diffuse damage and the Γ-convergence of the regularized variational model cannot be guaranteed. This study presents a coupled phase-field fracture and plasticity model for quasi-brittle materials with emphasis on the effect on the length scale. The proposed model is formulated in the variational framework using energetic principles [1]. The numerical implementation of the proposed model is introduced by using the finite element method [2]. The effective yield stress in the proposed model is calibrated to vary with the length scale parameter such that the tensile strength of the quasi-static brittle materials remains the same. The length scale parameter is not determined by the tensile strength of the material and can take any proper values. Five representative benchmark tests are considered to validate the capability of the developed model. The numerical force versus displacement curves and crack paths are both in good agreement with the corresponding experimental results. More importantly, the global response of the structures is insensitive to the length scale though it may influence the size of the failure zone.

Keywords: Phase-field modelling, Elasto-plastic mechanics, Variational formulation, Fracture, Quasi-brittle material.

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Research on the Design Construction Building Information Exchange (DCBIE) based on BIM

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Abstract: The collaborative project management method based on BIM benchmark model, will improve our efficiency of project management, because it represents the project as a multi objective dynamic optimization process from original fragmented management of investment, quality and schedule to a benchmark BIM model. The data exchange standards is fundamental and important when we talk about the exchange based on the benchmark model from one single stage to multi stages of construction projects. In this paper, one standard of design construction building information exchange based on BIM is put forward to realize the collaborative project management, which using a standard data exchange file, to solve many problems such as model reuse, information transfer and multi objective dynamic modification after design changes.

Keywords: Benchmark BIM, Design construction building information exchange, Collaborative project management.

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Optimization and Studying the Effect of Machining Parameters in the Cortical Bone Turning by Sensitivity Analysis

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Abstract: Machining and cutting of cortical bones are very common and important in the field of orthopedic surgeries. Considerable advances in bone machining are obtained by using CNC machines and automatic surgery robots but still, researches are needed to investigate the effects of machining parameters in bone machining. Surface quality is a decisive parameter and choosing the proper tool and machining parameter is vital [1]. In this paper, for the first time, the effect of machining parameters on surface quality obtained in the cortical bone turning is studied. The machining parameters included in the investigation are cutting speed, feed rate and depth of cut and the response surface methodology is used to analyze the obtained surface quality according to a second order regression model. The sensitivity of surface quality to the input parameters was measured by applying Sobol sensitivity analysis and the results are optimized by Dringer algorithm. Finally, the optimum machining condition is determined as 30 m/s cutting speed, 0.1 mm/rev feed rate, and 0.5 mm depth of cut. Furthermore, the effectiveness of the input parameters on the surface quality is determined as 19% for cutting speed, 74% for feed rate and 7% depth of cut.

Keywords: Bone machining, Cortical Bone, Machining parameters, Sensitivity Analysis, Optimization, Surface quality.

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A machine learning-based continuum damage model for predicting complex crack propagation

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Abstract: Micro damage is a complicated mechanical behavior related to fracture diffusion process. To describe the phenomena, some analytic model has been applied such as continuum damage model or phase-field fracture model. However, the most difficulty in modeling the structural failure and crack propagation is the constitutive relation between the damage variable and the stress/strain state is difficult to determine. Some fundamental modes of fracture are assumpted to simplify the analytical models however this is inadequate to capture the realistic behavior fracture where the structures are usually subjected to mixed modes fracture or multiple cracks. Constructing a reliable and high accurate model to describe the damage phenomena still a challenge due to the lack of information of the constitutive relations especially at the microscale where the initiated microdamage can finally lead to the propagation of macro cracks.

The development of machine learning has been motivated by high-speed computers which allows handling a big amount of data. The artificial neural network, a branch of machine learning, employs complicated multilayers of artificial neuron in order to construct a mapping function based on the training data as the input of the system. Artificial neural networks recently have been adopted in a wide range of engineerings including mechanics to solve to tackle the difficulties in examining the constitutive relations in solid mechanics [1, 2, 3, 4, 5, 6]. The accuracy of input data is the core that determines the success of a machine learning model. Because of that, in order to utilize machine learning as a useful tool for studying solid materials, the prepared data play an important role. Thank to the development of advanced imaging techniques such as computed tomography (CT), ultrasound imaging (UI), image scanning microscopy (ISM), optical coherence tomography (OCT), scanning electron microscope (SEM) and magnetic resonance imaging (MRI), the information of microstructure is revealed which allows a great opportunity to acquire a large amount of data of microstructure. Because of that reason, image-based machine learning has been applied to study a wide range of mechanic problems such as inverse elasticity problem [7], heterogeneous composite materials [8, 9], porous plasticity media [10], designing materials [11].

In this proposed work, the data of deflected microstructure will be obtained via an imaging technique and constructed as input parameters of the neuron network. The network will be trained in order to be able to predict the constitutive relation of damage variable for any given stress/strain state. The trained damage model, in turn, is applied into the conventional framework of an analysis tool such as FEM, IGA to simulate the fracture process and crack propagation in structures and test for practical applications where the machine learning system has to expose with some cracking situations that it has not encountered before.

Keywords: Machine learning, Damage model, Image based constitutive relation.

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Methods Based on Artificial Neural Networks for the Solution of Partial Differential Equations on Domains with Complex Geometries

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Abstract: Machine learning and methods based on artificial neural networks have become increasingly applied to a variety of topics in areas such as image processing, voice recognition, and object detection. In this work, we present a set of algorithms for solving partial differential equations using the approximation properties of deep neural networks (DNN). The proposed procedure is designed to solve partial differential equations on complex geometries, such as the ones obtained from spline description and can alleviate the problems encountered due to gaps in geometry description or other boundary parameterization issues.

We will consider and compare algorithms based on collocation (as in [1]), as well as those based on energy minimization [2] which require evaluating an interior integral from scattered points in the domain. The relation between the standard spline-based approximation spaces and DNNs with different activation functions will be examined in in detail. The method proposed has been tested on benchmark problems with known solutions, which allows for a better understanding of the approximation and convergence properties of DNNs.

Keywords: Artificial neural networks, Partial differential equations, Collocation, Energy minimization.

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Research on Application of Machine Learning and Optimization Algorithm in Transparent Soil: A Review

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Abstract: This paper reviews the application and development of machine learning in geotechnical engineering. It is found that artificial intelligence methods such as machine learning has important application value and development prospects in geotechnical engineering problems, such as flood, landslide, soil pile friction, slope displacement and shear strength. For transparent soil, a special synthetic soil, based on the characteristics of transparent soil: transparency, shear strength, oil content, liquid limit, plastic limit, a combination of machine learning and optimization algorithms is proposed to analyze and predict the Correlation coefficient of transparent soil. Finally, the application process, selected parameters, prediction methods and precautions of machine learning in the model test of transparent soil slope is discussed.

Keywords: Geotechnical engineering, Artificial intelligence, Slope, Transparent soil, Review.

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Thermal conductivity identification of nonlinear functionally graded materials via a machine learning strategy

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Abstract: A machine learning strategy based on the genetic algorithm (GA) [1] and the semi-analytical collocation solver (SACS) [2] is presented for the thermal conductivity identification of nonlinear functionally graded materials (FGMs) [3]. In this study, only the temperature or heat flow on the FGM surface can be non-invasively measured via the thermal sensors. Instead of extensive experiments, the semi-analytical collocation solver is used to construct the database of the relationship between the thermal conductivity and the temperature or heat flow on the FGM surface. Based on the aforementioned constructed database, the GA-based machine learning strategy is implemented to identify the thermal conductivity of nonlinear FGMs [4]. In addition, the Tikhonov regularization is introduced to eliminate the effect of measuring noise in the measurement data. Several benchmark examples are presented to verify the feasibility, robustness and applicability of the proposed machine learning strategy.

Keywords: Machine learning, Genetic algorithm, Semi-analytical, Parameter identification, Functionally graded materials.

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An Alternative Optimization Algorithm to Analysis of Structure by Hybrid Artificial Neural Network-Isogeometric Finite Element Program

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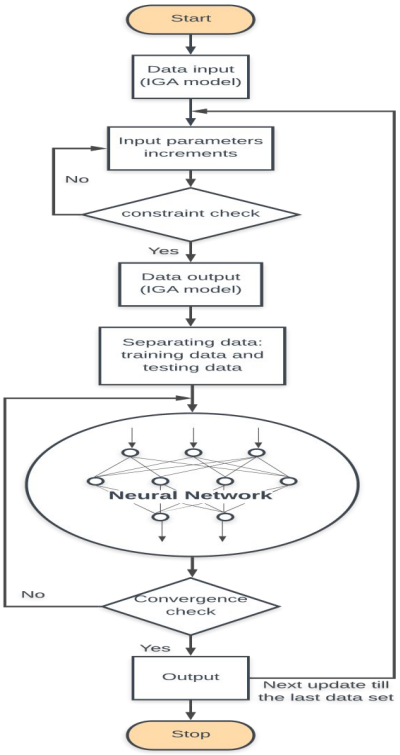
Abstract: The artificial neural network (ANN), which is a system of computing, has its ability to learn the performance task without being programmed and makes attempts to model abstraction in high level in data [1]. And Isogeometric Analysis (IGA) [2] is a computational approach, which offers the possibility of integrating methods for numerical analysis into NURBS-based Computer Aided Design tool, studies the case in which the geometry is more complicated. The hybrid method which is the combination of ANN and IGA (called hybrid IGA/ANN) takes its advantages of these methods to study numerical problems. In the present paper, beside introducing hybrid IGA/ANN (Fig. 1), an optimization algorithm to train data in Neural Network, called *adadeltamax*, is proposed (Algorithm 1). I-shape beam problem with changing in cross-section geometry was applied. The results, gotten from a*dadeltama*x in hybrid method, were compared to those from other optimization algorithms-*sgd*, *nesterov*, *adagrad*, *adadelta*, *rmsprop*, *rmsprop-nesterov*, *adam*, and *nadam*, prove to be an acceptable advantage to use (Fig. 2, Tab. 1). In order to visualize more specifically the result, after training data with more time of iterations, the values of relative error larger than 10 percent are quite small while those of the relative error less than 2.5 percent mostly make up for the huge proportion (Figs. 3,4). The optimization algorithm proves to be a choice to train the data in Neural Network.

Keywords: Neural network, Isogeometric analysis, I-shape beam, Optimization algorithm.



Require: Decay rate ρ, constant ϵ, initial weight parameter θ

Require: Initialize accumulation variables $E[g^2]_o = 0, E[\Delta\theta^2]_o = 0$

1: **While** criteria met **do**

2: Sample a mini-batch of N examples $((x^{(i)}, y^{(i)}),..., (x^{(N)}, y^{(N)}))$ from training set

3: Compute Gradient: $g_t \leftarrow \frac{1}{N}\nabla_{\theta_{t-1}} \sum_i L(f(x^{(i)}; \theta_{t-1}), y^{(i)})$

4: Accumulate Gradient: $E[g^2]_t \leftarrow \max(\rho E[g^2]_{t-1}, |g_t|)$

5: Compute Update: $\Delta\theta_t \leftarrow -\frac{\sqrt{E[\Delta\theta^2]_{t-1}+\epsilon}}{E[g^2]_t+\epsilon} g_t$

6: Accumulate Updates: $E[\Delta\theta^2]_t \leftarrow \rho E[\Delta\theta^2]_{t-1} + (1-\rho)\Delta\theta_t^2$

7: Weight updates: $\theta_{t+1} \leftarrow \theta_t + \Delta\theta_t$

8. **end while**

Algorithm 1: Adadeltamax Optimization Algorithm

Figure 1: Flow chart of Artificial Neural Network-Isogeometric Analysis Hybrid Method

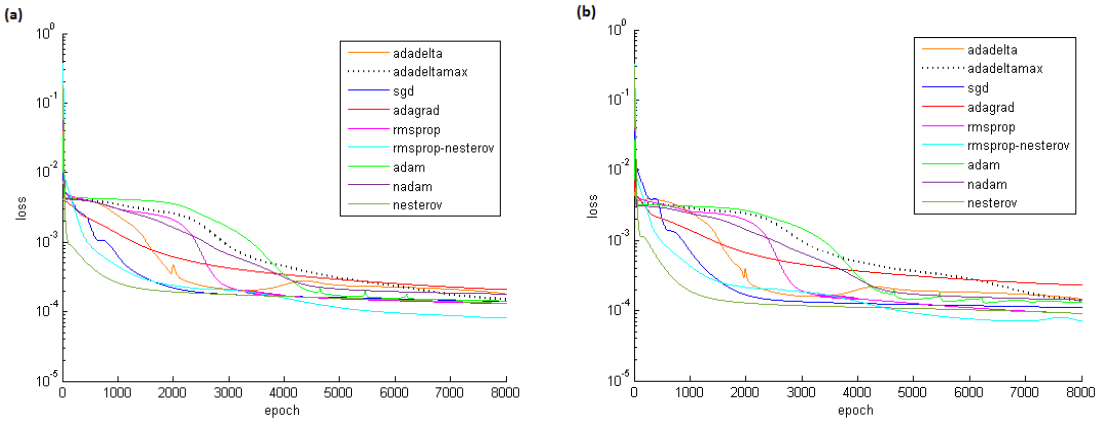


Figure 2: Mean Square Error (MSE) for (a) training data set and (b) testing data set in comparison among number of optimizers. (Y axis in log scale.)

Table 1: Train and Test MSE ($\times 10^{-3}$) in comparison among different optimizers after 8000 epochs

Optimizers	***adadelta***	***adadelta max***	***sgd***	***adagrad***	***rmsprop***	***rmsprop-nesterov***	***adam***	***nadam***	***nesterov***
Train loss	0.1804	**0.1491**	0.1403	**0.2073**	0.1297	**0.0807**	0.1422	0.1794	0.1311
Test loss	0.1459	**0.1388**	0.1099	**0.2292**	0.0911	**0.0709**	0.1312	0.1423	0.0911

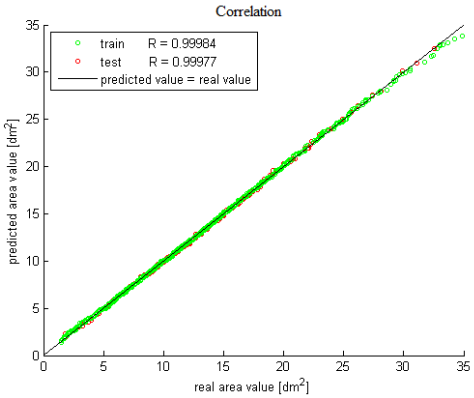


Figure 3: Correlation between the values gotten from real values and predicted values regarding training set and testing set after 21000 epochs in adadeltamax optimizer.

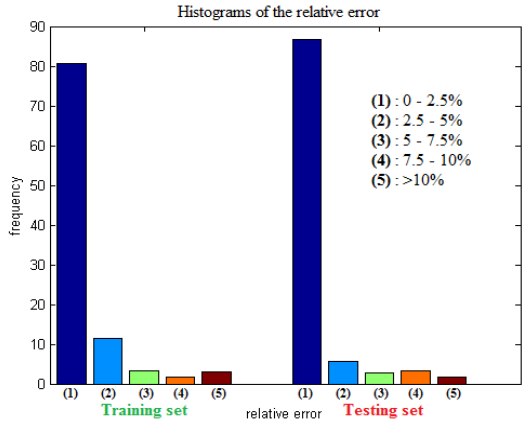


Figure 4: Histograms of relative error regarding trainging set and testing set after 21000 epochs in adadeltamax optimizer.

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Deep learning algorithm for solving PDEs for fluid flow field

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Abstract: How to exactly model fluid flow field in underground engineering has been a longstanding computational challenge and the deep-learning approach provides new perspectives for solving this. We propose to solve the governing PDEs of fluid flow by approximating the solution with a deep neural network. We train the network to satisfactorily obey the differential operator, initial condition, and boundary conditions. The implementation is meshfree compared with the traditional FEM simulations for fluid flow. Without using a mesh, the neural network is trained on batches of randomly sampled time and space points and in this way the deep learning algorithm provides the general solution to the continuity equation of fluid flow. The used method has a similar spirit to Galerkin methods, with the solution approximated by a neural network instead of a linear combination of basis functions. We also compare the results obtained from the deep learning approach and the analytical solution, which shows a satisfactory agreement.

Keywords: Deep learning, PDEs, Fluid flow, Neural network.

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DML based artificial neural network approach to solve transient wave equation using the Collocation method

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Abstract: The working mechanics of a human brain (made-up of neurones) can be mimicked through artificial neural networks (ANN). ANN operates by reducing a given task to a mathematical function, and hence the ability to easily apply several mathematical operations using high-level open source libraries like Tensorflow, Keras, Pytorch, to name a few. Therefore, this technique has been extended to solve several ordinary and partial differential equations (PDEs) [1]. ANN is also applied to solve non-linear PDEs of higher order, thereby addressing the problems associated with finite element and finite difference methods. Furthermore, deep machine learning (DML) consisting of some extra layers (hidden layers), significantly enhances the capacity to resolve complex issues. Therefore, ANN in conjunction with classical methods can result in efficient solution technique for several physical problems involving PDEs. Two popular approaches to solve the governing PDEs are: (i) collocation method and (ii) energy minimisation method [2]. In collocation method, the idea is to choose a finite-dimensional domain with a specified number of points in the selected domain, known as collocation points, and train the network such that the governing equations and the boundary and initial conditions are satisfied with minimum error at the selected points. The energy minimisation approach involves the formulation of governing equations in terms of energy and solve for the response by minimising the energy [3, 4]. Neural networks combined with collocation approach was employed to solve problems satisfying the laws of physics, known as physics informed neural networks (PINNs), for instance: Burger's equation, Schrödinger equation, Allen-Cahn equation, Navier-Stokes equation [5], to name a few.

In this paper, the collocation method is used to solve one and two dimensional problems governed by transient wave equation. The collocation points are chosen by dividing the domain uniformly in both space and time. The methodology is implemented using Tensorflow library in Python language. Xavier Initialisation method to used initialise the neural network. The mean square error at the collocation points is calculated and minimised while training the ANN. The relative normalised error is observed to be less than 5% in both of the cases.

Keywords: Artificial neural networks, Deep machine learning, Collocation method, Energy minimisation, Transient wave equation

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Phononic Crystal Band-Gap Detection by Machine Learning Technique

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Abstract: Phononic crystal metamaterial has recently received tremendous development to deliver peculiar features that cannot be found in conventional material, such as cloaking, super-lenses and signal-filtering [2]. Such properties can be revealed from the determination of dispersion relation of the phononic crystal, which associates the eigen-frequencies and wave number of a unit cell due to the Bragg's scattering phenomenon or local resonant. In numerical studies, the dispersion relation, apparently depends on the material properties of the constituents as well as the topology of the unit cell, is normally computed from solving the eigenvalue problem by means of Finite element method (FEM) as [4]

$$\boldsymbol{K}(\mathrm{k})\ \boldsymbol{v} = \omega(k)^2 \boldsymbol{M}\boldsymbol{v}$$

where **K** and **M** are the finite-element-assembled stiffness and mass matrices, respectively, ω is the angular frequency and k is the wave vector defined in the reciprocal space.

In this work, we propose an alternative approach to determine the energy gap in the dispersion relation of 2D phononic crystal using Deep Learning Neuron Network. The proposed approach consists of two procedures described as following.

First of all, in 2D phononic crystal, the unit cell can belong to one of the 5 Bravais lattices grouped into four crystal families [3], that are monoclinic, orthorhombic, hexagonal and tetragonal. Therefore, in the first stage of the method, the type of unit cell will be determined by a classification-trained Neuron Network. By doing this, we can obtain the lattice unit vectors as well as the reciprocal lattice unit vectors so that the Brioullin zone or the Irreducible Brioullin zone can be defined and used for the computation of the dispersion relation. It should be noted that, not only geometry of the unit cell is identified but also the material distribution. In the limitation of linear isotropic material, each constituent is assumed to be defined by two Lame's parameters and mass density.

Once the unit cell setting up is prepared, the training process can start. As described, the material parameters of the constituents defined discretely are taken to be the inputs. Moreover, as we were able to identify the type of unit cell in the first step, specific wave number for different type of unit cell can also be taken as the input parameter. We expect the eigenvalue ω, which will be collected into a vector corresponding to different eigenmode, to be the output [1].

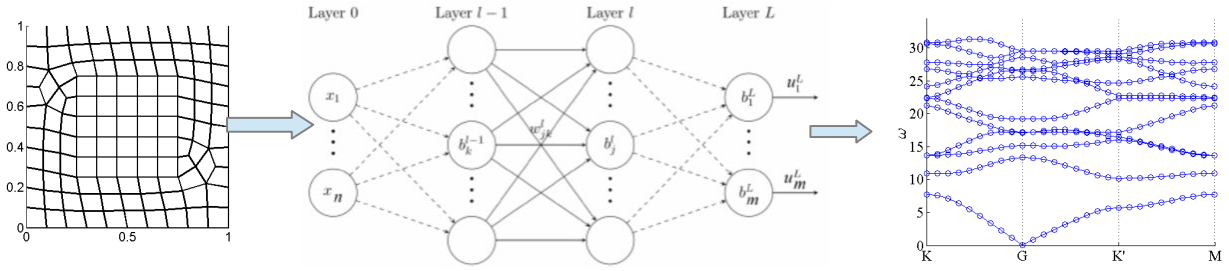

Figure: Schematic of Neural network to predict phononic energy band gap

Keywords: Machine learning, Phononic crystal, Band-gap, Dispersion relation, Energy band diagram.

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Extended isogeometric-meshfree collocation methods without branch enrichment for cracks analysis under contact loading

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Abstract: Collocation methods have been developed as a powerful alternative to Galerkin's method in the context of isogeometric analysis (IGA) characterized by a significantly reduced computational cost, but still guaranteeing higher order convergence rates. In this work, we develop a novel adaptive isogeometric-meshfree collocation method (IGAM-C) for simulating cracks in an elastic half space under contact loading. The concept of IGAM-C method is based upon the correspondence between the isogeometric basis functions and the moving least-squares meshfree shape functions, which provides the flexibility of meshfree adaptive refinement for isogeometric analysis. The proposed method does not require special treatment for essential boundary condition and the time-consuming integration of a weak form. The integrals are evaluated directly in the parametric space following the framework of IGA. Moreover, the elastic crack problems are successfully solved without branch enrichment. The near-tip field is accurately captured by special nodal arrangements around the tip. Furthermore, the resolution of the nonlinear equations governing the contact problem is derived from a strong form to avoid the disadvantages of numerical integration. The implementation of the proposed method is simplified, and the computational effort is reduced. The accuracy and robustness of the presented method are demonstrated through its application to several numerical examples.

Keywords: IGA, Meshfree Method, Collocation, Contact Mechanics, Fracture Mechanics.

Introduction

Computational fracture mechanics has been dominated by weak form-based methods for decades. Among these methods, the classical finite element method (FEM) has been applied for crack modeling. The extended FEM (XFEM) [1] was further developed to avoid time-consuming re-meshing in crack problems, whereas it suffers from low computational efficiencies due to the implementation of enrichment functions. On the other hand, the strong-form methods do not require numerical integration and thus perform more efficiently than weak-form methods. Meshfree methods [2] are viewed as next-generation computational techniques for problems involving large deformation, fracture and fragmentation and contact problems. Since the meshfree methods do not rely on a fixed topological connectivity between nodes, they are expected to be more adaptive and robust in resolving the problems where the classic grid-based methods are not suitable. Compared to the finite element method (FEM), meshfree methods are able to save computational time by avoiding re-meshing after each crack extension. Nevertheless, the meshfree method usually has less computational efficiency than the FEM, as higher computational cost is required for meshfree interpolation and numerical integration. The isogeometric analysis (IGA) was first proposed by Hughes *et al.* [3] as a powerful and reliable tool for computation and simulation of engineering problems. By adopting the non-uniform rational B-splines (NURBS) which are widely used in computer-aided designs as basis functions, IGA is not only applicable to engineering analyses but also capable of delivering accuracies superior to the standard FEM in many applications including contact mechanics. However, IGA based on NURBS is difficult to locally refine due to its tensor product nature, which leads to an excessive overhead of control points with increasing refinement. With the goal of overcoming the limitations of NURBS for IGA, adaptive IGA has been studied with T-splines, PHT-splines, hierarchical B-splines, LR-splines, etc. However, constraint equations are required on these methods, increasing the complexity and effort in their implementation. Recently, within the isogeometric collocation (IGA-C) context, several strategies have been studied to reduce the computational cost for Galerkin methods by using higher-order isogeometric basis functions [4].

This paper aims to investigate crack problems via an adaptive isogeometric analysis meshfree collocation (IGAM-C) approach which is a strong form-based approach. In comparison to weak-form approaches, the present approach exhibits advantages inheriting from the IGAM method and the collocation method, such as the flexibility of adaptive

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refinement, elimination of numerical integration, and convenient treatment of essential boundary conditions. The IGAM-C approach utilizes the linear reproducing points which are calculated by a knot vector as the collocation points and achieves the adaptive refinement in a straightforward manner. The adaptive refinement procedure uses a gradient-based error estimator to efficiently determine meshes with large errors. In modeling cracks via the IGAM-C approach, the strong discontinuity along crack surfaces is introduced by the visibility criterion. To achieve a smooth approximation around crack tips, the diffraction method is further employed. Besides, the singularity around crack tips is implemented by the adaptive refinement without requiring the enrichment functions [5]. It is shown that the IGAM-C approach is more efficient and accurate through the adaptive refinement, and successfully captures the near-tip fields for the accurate calculation of stress intensity factors.

Numerical example

Consider a central-cracked plate frictionally contacting with a cylinder as shown in figure 1. This model is loaded with a vertical displacement u = 0.002 and a horizontal displacement v = 0.00075. The geometrical configuration with the following parameters: radius R = 1, width w = 2, high h_1 = 0.3, h_2=0.5, crack length a = 1/4w, b = 1/4w. Young's modulus E = 1, ν = 0.3 and the coefficient of friction μ = 0.2. The penalty parameters are ε_n = 1000 and ε_t = 100.

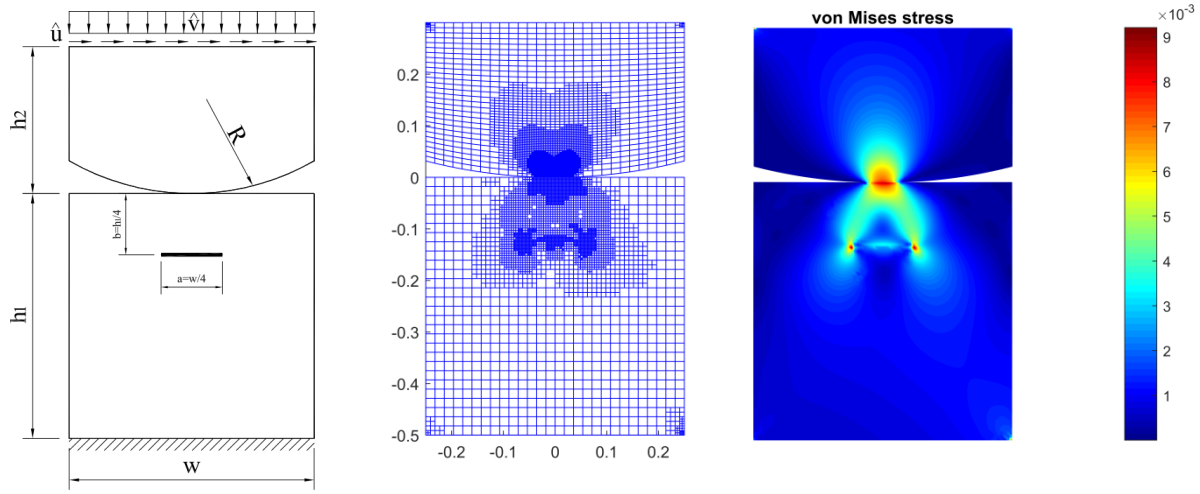

Figure 1: Schematic of the cylinder on plane Hertzian with crack under contact loading: (a) Geometrical modeling, (b) adaptive mesh after 4 refinement steps, (c) contour plots of von Mises stress.

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Numerical simulation of Von-Karman plate problem by nonlocal operator method

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Abstract: Nonlocal operator method as a recently proposed numerical approach shows great potential in solving various physical problems. Some features of this method include nodal integration or numerical integration, variational formulation or weighted residual formulation, free of shape function in conventional method, C^n continuity of the operators, meshless, non-uniform discretization. The method is ready for explicit/implicit analysis of solid mechanics involved geometrical nonlinearity. Owning to its high continuity, the method can solve higher order problems directly without resorting to the mixed formulation, which introduces the intermediate fields and requires a large number of degree of freedoms. In this paper, we apply the nonlocal operator method to solve the Von-Karman plate problem. The numerical results in terms of in-plane and out-of-plane displacement are verified by that of Abaqus with S4R element formulation.

Keywords: Nonlocal operator method, plate theory, Von-Karman plate.

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Data Driven solution for 1D Cahn-Hilliard Equation

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Abstract: The artificial neural network (ANN) is a class of machine learning tools, which is inspired by the structure and behavior of biological neural systems. ANN recognizes the patterns in a series of input and output values and using the acquired 'knowledge' it then predicts the unknown output values for a given set of input values. However, despite its excellent performance in the domain of image processing and computer science, it cannot ensure that the essential physical laws associated with an engineering problem are satisfied. Recent development in the field of machine learning, propose the use of physics informed/constrained neural networks (PINN) for solving partial differential equations (PDE) [1]. In PINN methods, the neural networks are trained to solve supervised learning problems while respecting any given law of physics described by general non-linear partial differential equations.

The Cahn-Hilliard equation is a time dependent fourth-order PDE that describes the phase separation process. The high order operators that appear in the Cahn-Hilliard equation are the main obstacle to obtain an accurate solution. Numerical methods like finite element analysis are often not capable enough to solve the PDEs directly; instead, the fourth-order equation is decomposed into two second-order equations using various assumptions. Moreover, the curse of dimensionality, present in the traditional numerical methods is a hindrance for solving higher order PDE's in higher dimensions [2]. In this context, we propose a PINN based approach to solve the Cahn-Hilliard equation. In this work, we consider the one-dimensional Cahn-Hilliard equation with periodic boundary conditions. The governing equation with periodic boundary conditions could be stated as:

$$
\begin{aligned}
&\frac{\partial u}{\partial t}+\frac{\partial^4 u}{\partial x^4}-\frac{\partial^2\left(F'(u)\right)}{\partial x^2}=0, x\in[0,2\pi], t\in[0,8500],\\
&F=\frac{1}{4}\left(u^2-1\right)^2,\\
&u(0,t)=\cos(2x)+\frac{1}{100}e^{\cos(x+1/10)},\\
&u(t,0)=u(t,2\pi),\\
&\frac{\partial u(t,0)}{\partial x}=\frac{\partial u(t,2\pi)}{\partial x},
\end{aligned}
\tag{1}
$$

where, u ∈ [-1, 1] denotes the phase, F is the free energy function and x represents the spatial co-ordinates. In this problem, we consider $\epsilon = 0.18$. The training data set is generated by solving the Cahn-Hilliard equation with a spectral Fourier discretization, using the toolbox chebfun [3], with N = 512 points to discretize the domain and a time step, $\Delta t = 0.1$. Fig. 1 shows the training points at time t = 8300s. The neural network is set up with four hidden layers of 500 neurons each. For optimization, we use the Adam (adaptive momentum) optimizer. For the time integration, we use the fourth-order implicit Runge-Kutta method with q stages, where q = 100. Using this setup, the mean squared error of the governing equation at n collocation points is minimized, where n = 512. The loss function is defined as:

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$$
\begin{aligned}
&L = LSE_{int} + LSE_{bound},\\
&LSE_{int} = \sum_{i=1}^{q+1}\sum_{j=1}^{n}\left(u_i^n\left(x_j^{n,i} - u^{n,i}\right)\right)^2,\\
&LSE_{bound} = \sum_{i=1}^{q}\left(u^{n+c_i}(0) - u^{n+c_i}(2\pi)\right)^2 + \left(u^{n+1}(0) - u^{n+1}(2\pi)\right)^2\\
&+\sum_{i=1}^{q}\left(\frac{\partial u^{n+c_i}(0)}{\partial x} - \frac{\partial u^{n+c_i}(2\pi)}{\partial x}\right)^2 + \left(\frac{\partial u^{n+1}(0)}{\partial x} - \frac{\partial u^{n+1}(2\pi)}{\partial x}\right)^2,
\end{aligned}
\tag{2}
$$

where LSE_{int} denote the loss in the interior points and LSE_{int} denote the loss in the boundary points. For training the data set, we use $\Delta t = 0.2$. The convergence of the minimization of the loss function is shown in Fig. 1, along with the comparison of the predicted and expected solution. The time step and number of stages were determined such that the theoretical error is below the machine precision ($\Delta t^{2q} \leq 10^{-16}$). To measure the accuracy of the proposed approach, the relative L_2 norm is computed using:

$$
L_2 = \frac{\sqrt{\int (c_{pred} - c_{exact})^2 dx}}{\sqrt{c_{exact}^2 dx}} \tag{3}
$$

For the proposed approach, $L_2 = 0.006\%$. This proves the ability of the method to efficiently predicted the solution for one-dimensional Cahn-Hilliard equation.

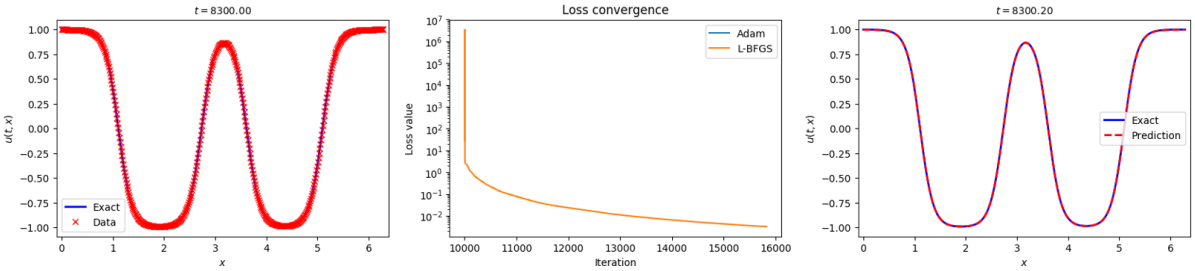

Figure 1: From left to right: Training points over the exact solution of the Cahn-Hilliard equation. Convergence of the training Loss function. The training is done at time t = 8300 s, and comparison between prediction and expected solution of the Cahn-Hilliard equation at t = 8300.2 s

Keywords: Machine learning, Differential equations, Cahn-Hilliard equation.

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Probabilistic characterization of rock mass deformation modulus from P-wave velocity based on information criteria

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Abstract: Determination of rock mass deformation modulus (E_{rm}) is a very important but very challenging task in rock mechanics and rock engineering. Since direct measurements of E_{rm} by in situ tests are expensive, time-consuming and sometimes even impossible, many empirical methods for estimating E_{rm} have been developed by using geotechnical classification indices. However, in many cases, accurate determination of classification indices is not an easy task. Since the nondestructive and easy geophysical method is commonly used to measure the P-wave velocity (V_p) in the field, this paper has developed an empirical correlation between E_{rm} and V_p based on 834 collected datasets by considering both inherent and transformation uncertainties. To do that, first information criteria are employed to select the best model for deriving a general empirical correlation; maximum likelihood estimation (MLE) methods are used to specify the incorporated parameters of each candidate model; and computational intelligence techniques like particle swarm optimization (PSO), artificial bee colony (ABC) and differential evolution (DE) algorithms are adopted to derive the optimal solutions for MLE. Then, based on the derived general empirical equation, a Bayesian equivalent sample approach using Markov Chain Monte Carlo (MCMC) simulation is applied to conduct probabilistic characterization of E_{rm} by combining prior knowledge and project-specific observed V_p data. Comparative studies of the results from the Bayesian equivalent sample approach and in situ measured E_{rm} values suggest that the proposed method is effective and validate the applicability of the derived general empirical correlation.

Keywords: Rock mass deformation modulus, P-wave velocity, Empirical correlation, Maximum likelihood estimation, Computational intelligence techniques, Markov Chain Monte Carlo simulation.

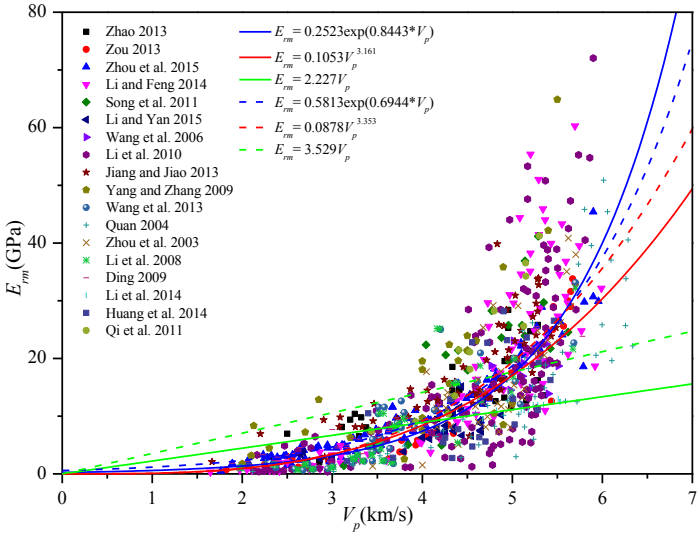

Fig. 1 Database employed and derived empirical correlations between rock mass deformation modulus E_{rm} and P-wave velocity V_p

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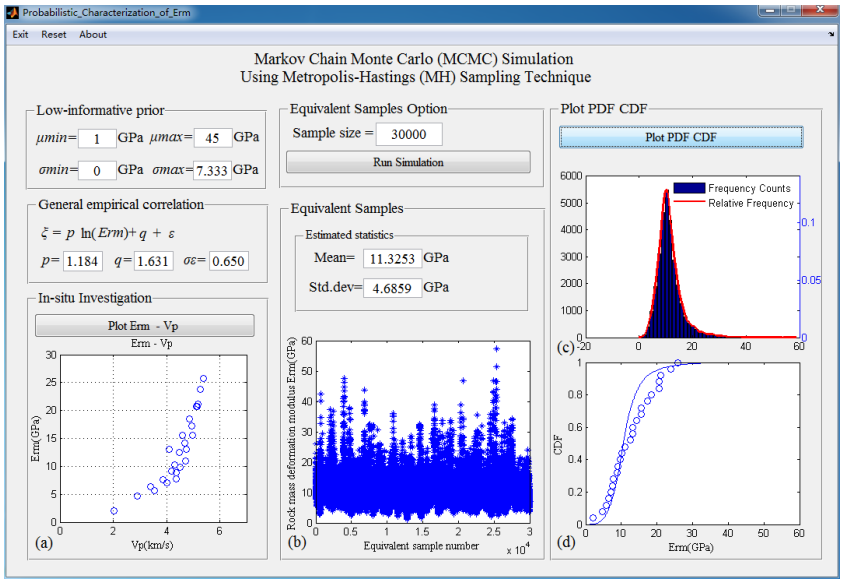

Fig. 2 (a) 25 sets of E_{rm} and V_p data at Longkaikou hydropower station (Zhou et al. 2015); (b) Scatter plot of the 30,000 equivalent samples of E_{rm} from MCMC simulation; (c) Histogram and relative frequency (PDF) of the equivalent samples for E_{rm}, and (d) Validation of the probability distribution for E_{rm} estimated from the equivalent samples

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Stochastic multiscale modeling of thermal properties of Polymeric clay nanocomposites and global sensitive analysis

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Abstract: We propose a stochastic multiscale modeling based on sensitivity analysis(SA) methods to quantify the most significant input parameters influencing the heat conductivity of polymeric clay nanocomposites(PCNs). The effect of the conductivity of cylinder, the conductivity of epoxy, interficial resistance, volume fraction and aspect ratio on the conductivity of composites is systematically studied by using Finite Element Method(FEM). We use global sensitive analysis to rank how much influence the different input parameters can achieve. We also use surrogate model to describe the true model in this paper. According to our results, all surrogate models in stochastic methods predict the same conclusion that the biggest sensitive index from key input parameters is aspect ratio. However,interficial Resistance has no significant effect on thermal properties of the PCNs since sensitive index is nearly 0. We also compare with different surrogate models, all of them are suit for sensitivity analysis, and they all have high precision to the thermal model.

Keywords: Uncertainty quantification, Polymeric nanocomposites(PCNs), thermal properties, Stochastic modeling , Multiscale modeling.

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Uncertainty Analysis of Engineering Structures by Time Domain Spectral Element Based Modeling

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Abstract: This work investigates the use of time domain spectral element method (TSEM) for the uncertainty analysis and modeling of beam structures. We have considered both Timoshenko beam (TB) and sandwich beam to perform the analysis. Beam is one of the key building blocks of different engineering structures and depending upon the choice of applications the material properties differ. With the advent of new materials, over the years the material systems for engineering structures changed from isotropic to composite depending upon the field of applications. Aerospace industry prefers lightweight structures with desired stiffness and strength. In this age, composites and Sandwich structures have replaced isotropic materials in many aerospace applications. The analysis and design of composite structures are complex and the prediction of responses become more difficult in the presence of uncertainty. Uncertainty is unavoidable in engineering structures. So, to obtain a reliable design, it should be considered into modeling. The uncertainty can be in material as well as in geometric properties and it occurs due to the manufacturing process. This kind of uncertainty is termed as aleatory uncertainty which is inherent and cannot be reduced. The other kind of uncertainty is epistemic uncertainty which is basically due to the assumptions in the mathematical model we are using. So, to predict the response we have to consider probabilistic modeling to obtain reliable design. In this work, we explain the effect of aleatory uncertainty on the response behaviour of beam structures through Monte Carlo simulation [1]. Also, a stochastic time domain spectral element method (STSEM) is proposed for the uncertainty analysis and modeling of beam structures [2].

The modeling of sandwich beam considers higher-order sandwich panel theory which can address the core flexibility. The material parameters are modeled as 1-D non-Gaussian random field [3]. Monte Carlo simulation considering computationally efficient time-domain spectral element method is explored to perform the numerical experiments for different boundary conditions as well as for different materials in the sandwich face sheet and core. The effects of material and geometric uncertainty in the response behaviour of a sandwich beam are quantified. Both individual as well as combined effect of uncertain material and geometric parameters are studied for the static, free vibration and dynamic response [1]. For the discretization of non-Gaussian random field expansion optimal linear estimation (EOLE) [3] is used.

In the next phase, the stochastic time domain spectral element method (STSEM) based modeling is proposed. Discretization of the random field is obtained by optimal linear estimation (OLE) [3]. Both lognormal and Weibull type distribution is considered for input random field. The OLE-based discretization of a random field simulates the random fields digitally and the realizations of stiffness, mass matrix, and dynamic stiffness matrix are also obtained. Computationally efficient time domain spectral element method (TSEM) [4] is used to develop the STSEM formulation. For TSEM the degrees of freedom (DOF) are very less and it provides a diagonal mass matrix which requires less computational cost followed by reduction in the CPU time. In this work, STSEM [2] is proposed for beam structures and the effect of correlation length on the response statistics is also studied. The computational efficiency of the proposed method and the deflection statistics of the Timoshenko beam and sandwich beam are obtained. This STSEM formulation can further used for complex structural and computationally demanding wave propagation problems.

Keywords: Time domain spectral element method, Monte Carlo simulation, Random field, Uncertainty, Sandwich beam.

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Probabilistic stability analysis of earth dam slope using extreme gradient boosting method

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Abstract: Probabilistic risk assessment of geotechnical structures has gained increasing popularity in geotechnical engineering, which provides valuable information for the prevention and control of geological hazards[1-3]. It is well recognized that earth dam is the most common type of dam in the world, however, few studies have performed to investigate the effects of uncertainties underlying soil-water characteristic curve (SWCC) on the earth dam slope failure risk. This paper develops a probabilistic risk assessment approach for earth dam slope under the Bayesian framework. The proposed approach shields light on the propagation of SWCC model selection uncertainty and parameter uncertainty on the earth dam slope failure assessment, and allows providing a model-independent estimate of failure risk with the aid of Bayesian model averaging. For illustration, the proposed approach is applied to the risk assessment of Ashigong earth dam located in Qinghai province of China. Results show that the SWCC parameter uncertainty and model selection uncertainty can be rationally quantified under the Bayesian framework making use of the limited test data and prior knowledge. Although the SWCC parameter uncertainty plays a dominant role in the risk assessment compared with the SWCC model selection uncertainty, the earth dam slope failure risk is significantly affected by the SWCC model selection. In geotechnical risk assessment, it is prudently to adopt the model independent estimate obtained from the proposed approach for rational decision making, instead of betting on a single model.

Keywords: Uncertainty quantification, Risk assessment, Soil-water characteristic curve, Earth dam, Bayesian approach.

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Probabilistic Assessment of Serviceability Limit State of Diaphragm Walls for Braced Excavation in Clays using Point Estimate Method

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Abstract:. Bracing systems for deep excavations are commonly required to ensure stability and prevent against excessive deformations in the construction of basements for shopping malls and underground transportation facilities. For excavations in deposits of soft clays, stiff retaining wall systems such as diaphragm walls help to restrain ground movements and wall deflections in order to prevent damage to nearby buildings and utilities. It is quite common for designers to limit the maximum wall deflection to 0.5% times the maximum excavation depth. However, a review of measured diaphragm wall displacements from various published case histories of successful deep excavations show that wall deflections can be up to more than 2% times the excavation depth. Since the allowable threshold wall displacement depends on various influencing parameters, wall deflections should not be limited to an arbitrary value. For the previous reliability studies that on reliability of braced excavation systems, usually a probabilistic framework combining a simplified wall deflection estimation model with reliability methods to determine the probability of serviceability limit state failure. This paper adopts the point estimate method (PEM), which is free from development of a response surface or surrogate models. It then compares the PEM results with the combination of polynomial regression and Monte Carlo simulation, which proves that PEM is more efficient and reliable. This study presents an reasonbale methodology that allows engineers to determine the required threshold limiting normalized wall deflection to meet the different target serviceability reliability indices.

Keywords:. probabilistic assessment, wall deflection; braced excavation; point estimate method

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