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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSOR/MONITOR'S ACRONYM(S) ARO 11. SPONSOR/MONITOR'S REPORT NUMBER(S) 67433-EV-YIP.31

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13. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

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a. REPORT	b. ABSTRACT	c. THIS PAGE			WaiChing Sun
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RPPR Final Report
as of 21-Aug-2019

Agency Code:

Proposal Number: 67433EVYIP
Agreement Number: W911NF-15-1-0581

INVESTIGATOR(S):

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DUNS Number: 049179401
EIN: 135598093
Report Date: 14-Dec-2018
Date Received: 26-Jul-2019
Final Report for Period Beginning 15-Sep-2015 and Ending 14-Sep-2018
Title: Understanding Hydro-mechanical Coupling Mechanism of Wetted Granular Matters Beyond the Pendular Regime
Begin Performance Period: 15-Sep-2015
End Performance Period: 14-Sep-2018
Report Term: 0-Other
Submitted By: WaiChing Sun
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STEM Degrees: 3 **STEM Participants:** 3

Major Goals: Many granular processes involve particles that are not completely dry or fully saturated. In particular, liquids in between particles may form liquid bridges (in the pendular regime), clusters (i.e. in the funicular and capillary regimes) and partially filled with air bubble. The capillary force due to the water in void space is of great importance to both the micro- and macroscopic hydro-mechanical behaviors of granular materials. While significant signs of progress have been made on developing phenomenological models that collectively consider air-water-solid as a macroscopic continuum, how liquid and solid interact at the microscopic origins, upon subjected to external hydraulic and mechanical loadings, remains poorly understood. In retrospect, discrete mechanics may bring insight on granular microstructures that are either completely or nearly dry (via a Young-Laplace model). Nevertheless, deriving a unified micromechanical theory that accurately captures the hydro-mechanical responses of granular matters across different degrees of water saturation remains an incredibly difficult task that has yet been established. A model applicable to predict the granular responses across the full spectrum of degree of water saturation is the key to understand earth surface processes, ranging from sediment transport, vehicle movement and natural disasters to tunnel detection and thus highly relevant to the ARO's mission.

The goal of this YIP research is to develop a micro-marco-coupling model for wetted granular matters that can predict the micromechanical topological changes of the grain-contact and liquid force chains and link these topological changes to macroscopic field-scale problems. The proposed research will combine (1) computational multiscale models that capture the particle-fluid interactions, (2) laboratory suction-controlled experiments that provide both macroscopic and grain-scale data through X-ray CT imaging technique and (3) mathematical tools such as graph theory to analyze the simulated and experimentally captured liquid and solid force chain networks. To overcome the geometrical constraints imposed by the Young-Laplace equation (i.e. particles must be spherical and liquid bridges must be axial symmetrical), the proposed research will explicitly model the pore-scale particle-fluid interaction via a lattice Boltzmann-discrete element coupling scheme and faithful capture the fluid-solid interactions among liquid and particles of varying shapes and sizes. The capillary effect of granular assemblies with different grain size distributions, porosities, loading rates and degree of saturation will be systematically analyzed.

Accomplishments: PDF document uploaded.

Training Opportunities: This project provided crucial support to three Ph.D. students, Eric Bryant, Kun Wang, Nikolas Vlassis, and SeonHong Na. Kun Wang is the student who received the majority of the funding from the YIP program. Through the support, 4 graduate students are developing new technical skills while refining their presentation and social skills in a close-knit research group. The PI met the students and postdoc on a daily basis and provided mentorships to them. Kun Wang has published 9 papers in top journals during the YIP program, while SeonHong has published 6 papers and Eric has published 3 papers.

The Ph.D. students received training through one-on-one work with the PI. The YIP program also provides support for students such that each student at least gets one fully supported opportunity to present at one of the major conference in soil mechanics (ASCE EMI), computational mechanics (USNCCM) or geophysics (AGU Fall Meeting) each year.

The PI also hold special meetings to work with the Ph.D. graduate of the research group to get feedback for their presentation skills and prepare for a job interview. Currently, three of the group members have found tenure-track faculty position from the PI's group -- SeonHong at McMaster university, Jinhyun Choo at University of Hong Kong and Yang Liu at Northeastern University. Ph.D. student Kun Wang will join Los Alamos National Laboratory, a DOE laboratory as a postdoctoral research scientist in the fall of 2019.

Results Dissemination: The YIP program provided the majority of the support for Mr. Kun Wang's PhD study and a portion of the summer salary of the PI. From September 15, 2015 to September 14, 2018, the research group has produced 31 articles, including 27 journal articles. These articles provided the documentation of the research progress of the research group.

In addition, the PI has also been invited to give department seminars, invited lectures, keynotes and a semi-plenary talk at various conferences that are listed below.

W.C. Sun, An adaptive micromorphic-regularized Cam-clay-type model for fluid-infiltrating geological materials, Cold Regions Research and Engineering Laboratory, US Army Corps of Engineers, Hanover, New Hampshire, 2019
W.C. Sun, A cooperative two-player game for automated generations of elasto-plasticity theories and models with AI-guided experimentation, the 3rd Mesoscale Modeling of Explosive Initiation Workshop, Fort Walton Beach, Florida, 2018.
W.C. Sun, Meta-modeling of geological materials: generating mathematical models by hybridizing theory and data, Los Alamos National Laboratory, 2018.
W.C. Sun, Meta-modeling of porous media with strain localization and embedded strong discontinuities, Sandia National Laboratories, 2018 (scheduled, November 7).
W.C. Sun, A multiscale damage-plasticity model for capturing brittle-ductile transition in anisotropic fluid-infiltrating porous rock, Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, 2018 (scheduled, Oct 24).
W.C. Sun, A reinforcement learning approach for modeling the brittle-ductile transition in geological materials, ExxonMobil Research and Engineering Company.
W.C. Sun, Deep-learning enabled multiscale poromechanics: from brittle fracture to ductile flow, Department of Civil and Environmental Engineering, Duke University, 2018.
W.C. Sun, K-fold validation for hybridized theory-based/data-driven anisotropic path-dependent constitutive models for geological materials and beyond, Naval Research Laboratory, 2018.
W.C. Sun, A multiscale damage-plasticity model for anisotropic fluid-infiltrating crystalline rock salt, Department of Civil and Environmental Engineering, the George Washington University, 2018.
W.C. Sun, Computational poromechanics for civil engineering at Columbia University, Research Training Group, Mineral-bonded composites for enhanced structural impact safety (GRK 2050), Technical University of Dresden and German Science Foundation, Germany, 2018.
W.C. Sun, Data-driven computational geomechanics, Department of Civil Engineering, the University of Hong Kong, 2017.
W.C. Sun, Accelerating multiscale discrete-continuum modeling of fluid-infiltrating geomaterials with deep learning, Department of Civil and Environmental Engineering, Hong Kong University of Science and Technology, 2017.
W.C. Sun, Hybrid data-driven multiscale modeling of brittle and ductile responses of fluid-infiltrating geomaterials, 2017 AFOSR Young Investigator Research Program Meeting, Basic Research Innovation and Collaboration Center (BRICC), Arlington, 2017.
W.C. Sun, A multiscale damage-plasticity model for compaction band and fractures in anisotropic fluid-infiltrating porous media, Department of Earth Science and Engineering, Imperial College London, the United Kingdom, 2017.
W.C. Sun, Data-driven multiscale modeling of fractured porous media with cross-validations, Lund University, Lund, Sweden, 2017.
W.C.Sun,Data-driven multiscale geomechanics,Geomechanics Department,Sandia National Laboratories, 2017.
W.C. Sun, A discrete-continuum coupling model for fractured porous media with embedded branched-discontinuities in the finite deformation range, Department of Civil and Environmental Engineering, Princeton University, 2017.
W.C. Sun A critical comparison of variational phase field and eigen-erosion modeling of fractures in fluid- infiltrating porous media: from brittle faulting to cataclastic flow, Department Seminar, Department of Civil and Environmental Engineering, Georgia Institute of Technology, 2017.
W.C. Sun Data-driven computational poromechanics across length scales, Henry L. Pierce Laboratory Seminar Series, Massachusetts Institute of Technology, 2017.
W.C. Sun Multiscale discrete-continuum modeling of porous media in extreme environments, Department Seminar, Department of Civil and Environmental Engineering, New Jersey Institute of Technology, 2017.
W.C. Sun, Data-driven multiscale poromechanics for cold region applications, Cold Regions Research and Engineering Laboratory, US Army Corps of Engineers, Hanover, New Hampshire, 2016.
W.C. Sun, A variational eigen-deformation model for simulating compaction band and fracture propagation in fluid-infiltrating porous media, Jointed Department Seminar, Department of Civil and Environmental Engineering,

Department of Mechanical Engineering, Northwestern University, 2016.
W.C. Sun, Multiscale discrete-continuum modeling of fluid-infiltrating, partially-frozen and quasi-brittle porous media, Lawrence Livermore National Laboratory, Livermore, California, 2016.
W.C.Sun, Modeling fluid-infiltrating,partially-frozen and quasi-brittle porous media with nonlocal discrete- continuum techniques, Lecture Series on Interaction Modeling in Mechanized Tunneling, Ruhn-University Bochum, Germany, 2016.
W.C. Sun, Computational mechanics for porous media in extreme environments, Department Seminar, Technical University of Dresden, Germany, 2016.
W.C. Sun, Computational geomechanics for fluid-infiltrating, thermal-sensitive and partially frozen granu- lar materials, Machine-ground Interaction Consortium Workshop: Next Generation Mobility Modeling and Simulation, the Suburban Collection Showplace, 46100 Grand River Avenue, Novi, Michigan, 2016.
W.C. Sun, Modeling and validating a micropolar multiscale model for wetted granular matters, keynote Lecture, the International Symposium on Plasticity and Its Current Applications, Keauhou Bay, Hawaii, 2016.
W.C. Sun, Some remarks on modeling fluid-infiltrating, thermal-sensitive, and partially-frozen porous media across length scales, Applied Mechanics Colloquia, John A. Paulson School of Engineering and Applied Sciences, Harvard University, 2016.
W.C. Sun, Computational Thermoporomechanics, University of Perugia, Perugia, Italy, 2015.
W.C. Sun, Validation and Verification of Discrete-continuum coupling modeling of granular materials, 3D Printing and Digital Rock Physics Workshop, Santa Fe, New Mexico, 2015. Albuquerque, New Mexico, 2015.
W.C. Sun, Coupling dissimilar hydromechanical models for fluid-saturated porous media from grain to field scales, Los Alamos National Laboratory, Los Alamos, New Mexico, 2015.
W.C. Sun, Multiscale Modeling for fluid-infiltrating fractured porous media, Claude R. Hocott Lecture, Department of Petroleum and Geosystems Engineering, the University of Texas at Austin, Austin, Texas, 2015.

Honors and Awards: •NSF CAREER Award, National Science Foundation (Mechanics of Materials and Structures Program, Civil, Mechanics and Manufacturing Innovation Division), 2019. The NSF's most prestigious award in support of junior faculty who exemplifies the role of teacher-scholar through outstanding research and excellent education.

• EMI Leonardo Da Vinci Award, the Engineering Mechanics Institute of American Society of Civil Engineers, 2018. The purpose of the award is to recognize outstanding young investigators early in their careers for promising ground-breaking developments in the field of Engineering Mechanics and Mechanical Sciences as relevant to Civil Engineering understood in the broadest sense. The award is given annually to a young investigator, generally under 35 years of age or have worked no more than 7 years since receiving their doctoral degree, and whose contributions have the promise to define new directions in theory and application of Engineering Mechanics, in the vein of Leonardo da Vinci (1452-1519), a man of unquenchable curiosity and feverishly inventive imagination. The EMI of ASCE selected the PI "for his fundamental contributions to computational multiscale poromechanics".

• Zienkiewicz Numerical Methods in Engineering Prize, Institution of Civil Engineers (ICE) and John Wiley & Sons, 2017. Instituted following a donation by John Wiley & Sons Ltd to commemorate the work of Professor Olgierd Cecil Zienkiewicz CBE. DSc FRS FREng of the Institute for Numerical Methods in Engineering, University of Wales , Swansea. The medal is awarded biennially by the Institution of Civil Engineers (ICE) to a researcher under 40 for the paper which contributes most to research in numerical methods in engineering, among 8 prime peer-reviewed journals published by ICE or Wiley, i.e., Géothechnique, Géothechnique Letters, International Journal for Numerical Methods in Engineering, International Journal for Numerical Methods in Biomedical Engineering, International Journal for Numerical Methods in Fluids, International Journal for Numerical and Analytical Methods in Geomechanics, International Journal of Numerical Modelling: Electronic Networks, Devices and Fields, and ICE Proceedings.

• AFOSR Young Investigator Program Award, Air Force Office of Scientific Research, US Air Force, 2017. The Air Force’s Young Investigator Program (YIP) award is one of the most prestigious honors bestowed by the US Air Force to outstanding scientists beginning their independent careers. The program is designed to identify and support talented scientists and engineers who show exceptional promise for doing creative research in order to encourage their teaching and research careers.

• Dresden Fellowship, Technische Universität Dresden, 2016.

• Recognition Award, for original work and authorship of Albany, Sandia National Laboratories, Department of Energy, 2016.

• Mindlin award (Kun Wang), Department of Civil Engineering and Engineering Mechanics, Columbia University, 2019

• Postdoctoral Fellowship (Kun Wang), Los Alamos National Laboratory, Department of Energy, 2019.

• Travel Scholarship (Kun Wang), 20th International Conference on Finite Elements in Flow Problems, Northwestern University, Evanston, 2019.

• Travel Scholarship (Kun Wang and Chuanqi Liu), Workshop on Meshfree and Particle Mechanics: Application and Theory, Santa Fe, 2018.

• Mindlin award (SeonHong Na), Department of Civil Engineering and Engineering Mechanics, Columbia University, 2018.

• Travel Scholarship (Eric Bryant), 3rd Biennial CO2 for EOR as CCUS conference, Petroleum Research School of Norway, 2017.

• Dongju Lee Memorial Award (SeonHong Na), Department of Civil Engineering and Engineering Mechanics, Columbia University, 2017.

• 2nd Place in Best Paper Student Competition (SeonHong Na), Engineering Mechanics Institute, Modeling Inelasticity and Multiscale Behavior Committee, EMI 2016 & PMC 2016, Vanderbilt University, Nashville, TN, 2016.

• Best Poster Presentation Award (Yang Liu, now an assistant professor at Northeastern), USNCCM San Diego, San Diego, CA, 2015.

Protocol Activity Status:

Technology Transfer: The PI has hosted Dr. John Clayton, group leader of the impact physics laboratory from the Army Research Laboratory for a half year visit during the YIP program. In addition, the PI had also visited the Army ERDC Cold Regions Research and Engineering Laboratory in 2016 and in 2019. During the site visit, the PI gave talks on the research conducted via the YIP program and discussed the possibility for future collaborations. The PI is currently working with a research scientist from CRREL, Devin O'Conner on phase-field modeling of ice growth in frozen soil.

PARTICIPANTS:

Participant Type: PD/PI
Participant: WaiChing Sun
Person Months Worked: 5.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Kun Wang
Person Months Worked: 12.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Eric Bryant
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: SeonHong Na
Person Months Worked: 4.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Jinhyun Choo
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
International Collaboration:

International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Nikolas Vlassis
Person Months Worked: 12.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Nikolas Vlassis
Person Months Worked: 12.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Research Experience for Undergraduates (REU) Participant
Participant: Anish Avasthi
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Research Experience for Undergraduates (REU) Participant
Participant: Lauren Brooke
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Undergraduate Student
Participant: Tracy Paltoo
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Other (specify)
Participant: Luca Tassini
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:

International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

ARTICLES:

Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: International Journal for Numerical Methods in Engineering
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Volume: Issue: First Page #:
Date Submitted: 6/28/18 12:00AM Date Published: 5/1/17 12:00AM
Publication Location:
Article Title: A hierarchical sequential ALE poromechanics model for tire-soil-water interaction on fluid-infiltrated roads
Authors: Ines Wollny, WaiChing Sun, Michael Kaliske
Keywords: fluid-solid systems, finite element methods, tire-soil-water interaction; poromechanical ALEformulation; hierarchically staggered iteration scheme
Abstract: This paper introduces a hierarchical sequential arbitrary Lagrangian-Eulerian (ALE) model for predicting thetire-soil-water interaction at ?nite deformations. Using the ALE framework, the interaction between a rollingpneumatic tire and the fl?uid-in?ltrated soil underneath will be captured numerically. The road is assumed tobe a fully saturated two-phase porous medium. The constitutive response of the tire and the solid skeletonof the porous medium is idealized as hyperelastic. Meanwhile, the interaction between tire, soil, and waterwill be simulated via a hierarchical operator-split algorithm. A salient feature of the proposed framework isthe steady state rolling framework. While the finite element mesh of the soil is ?xed to a reference frameand moves with the tire, the solid and fluid constituents of the soil are ?flowing through the mesh in the ALE model according to the rolling speed of the tire.
Distribution Statement: 1-Approved for public release; distribution is unlimited.
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: DOI Publication Identifier: 10.1016/j.cma.2017.10.009
Volume: 330 Issue: First Page #: 1
Date Submitted: 6/28/18 12:00AM Date Published:
Publication Location:
Article Title: Coupled phase-field and plasticity modeling of geological materials: From brittle fracture to ductile flow
Authors: Jinhyun Choo, WaiChing Sun
Keywords: phase fi?eld, plasticity, fracture, strain localization, brittle-ductile transition, geomaterials
Abstract: ?e failure behavior of geological materials depends heavily on con?ning pressure and strain rate. Under a relatively low con?ning pressure, these materials tend to fail by brittle, localized fracture, but as the con?ning pressure increases, they show a growing propensity for ductile, di?use failure accompanying plastic ?ow. Furthermore, the rate of deformation o?en exerts control on the brittleness. Here we develop a theoretical and computational modeling framework that encapsulates this variety of failure modes and their brittle-ductile transition.?e framework couples a pressure-sensitive plasticity model with a phase-fi?eld approach to fracture which can simulate complex fracture propagation without tracking its geometry. We derive a phase-?eld formulation for fracture in elastic-plastic materials as a balance law of microforce, in a new way that honors the dissipative natureof the fracturing processes.
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Publication Identifier Type: DOI Publication Identifier: 10.1007/s11440-018-0703-0
Volume: 14 Issue: 4 First Page #: 923
Date Submitted: 7/19/19 12:00AM Date Published: 7/23/18 7:00AM
Publication Location:
Article Title: Open-source support toward validating and falsifying discrete mechanics models using synthetic granular materials Part I: Experimental tests with particles manufactured by a 3D printer
Authors: Ritesh Gupta, Simon Salager, WaiChing Sun, Kun Wang
Keywords: 3D printing, X-ray CT, particle shape, discrete DIC, oedometer test, compression and recompression index
Abstract: This paper presents a new prototype test designed to analyze the particle shape effects of granular materials on mechanical response, and to establish an experimental database of individual particle movement using Xray CT and DIC techniques to calibrate for verification of micro-mechanical models. The prototype test consisted of a procedure that extracts particle shape features from micro-CT images of a real sand grain and replicates the geometrical features of sand grain using a 3D printer. The quantitative measurement of particle shape descriptors revealed that the synthetic particles inherit some attributes such as aspect ratio and sparseness of the real materials, while exhibiting marked differences for sphericity and convexity. Oedometric compression tests are conducted on specimen of the printed particles of identical size and shape to create benchmark for discrete element model.
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
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Volume: 334 Issue: 1 First Page #: 337
Date Submitted: 6/28/18 12:00AM Date Published: 6/1/18 4:00AM
Publication Location:
Article Title: A multiscale multi-permeability poroplasticity model linked by recursive homogenizations and deep learning
Authors: Kun Wang, WaiChing Sun
Keywords: dual-porosity, data-driven modeling, directed graph, embedded discontinuity, recurrent neural network, multiscale method
Abstract: This article presents a hybrid data-driven method designed to capture the multiscale hydro-mechanical coupling effect of porous media with pores of various different sizes. At each scale, data-driven models generated from supervised machine learning are hybridized with classical constitutive laws in a directed graph that represents the numerical models. By using sub-scale simulations to generate database to train material models, an offline homogenization procedure is used to replace the up-scaling procedure to generate cohesive laws for localized physical discontinuities at both grain and specimen scales. Through a proper homogenization procedure that preserves spatial length scales, the proposed method enables field-scale simulations to gather insights from meso-scale and grain-scale micro-structural attributes.
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Volume: 334 Issue: First Page #: 216
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Article Title: An updated Lagrangian LBM-DEM-FEM coupling model for dual-permeability fissured porous media with embedded discontinuities
Authors: Kun Wang, WaiChing Sun
Keywords: discrete-continuum coupling, strong discontinuity, machine learning, LBM-DEM-FEM, dual-permeability, fractured porous media
Abstract: Many engineering applications and geological processes involve embedded discontinuities in porous media across multiple length scales (e.g. rock joints, grain boundaries, deformation bands and faults). Understanding the multiscale path-dependent hydro-mechanical responses of these interfaces across length scales is of ultimate importance for applications such as CO2 sequestration, hydraulic fracture and earthquake rupture dynamics. While there exist mathematical frameworks such as extended finite element and assumed strain to replicate the kinematics of the interfaces, modeling the cyclic hydro-mechanical constitutive responses of the interfaces remains a difficult task. This paper presents a semi-data-driven multiscale approach that obtains both the traction-separation law and the aperture-porosity-permeability relation from micro-mechanical simulations performed on representative elementary volumes in the finitedeformation range.
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Journal: International Journal for Multiscale Computational Engineering
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Volume: 15 Issue: 6 First Page #: 525
Date Submitted: 6/30/18 12:00AM Date Published:
Publication Location:
Article Title: A SURROGATE MODELING APPROACH FOR ADDITIVE-MANUFACTURED MATERIALS
Authors: Haohui Xin, WaiChing Sun, Jacob Fish
Keywords: additive manufacturing, discrete element method, orthotropic GTN model, computational homogenization of discrete media
Abstract: We introduce a surrogate modeling approach to approximate the mechanical responses of objects manufactured by 3D printers. In particular, we propose a systematic procedure where material parameters of the low-fidelity orthotropic Gurson-Tvergaard-Needleman (GTN) model are inferred from microstructures generated from the high-fidelity discrete element simulations that replicate the additive-manufactured procedure. The calibrated low-fidelity model is validated against experimental data.
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Volume: 318 Issue: First Page #: 667
Date Submitted: 6/30/18 12:00AM Date Published: 5/1/17 12:00AM
Publication Location:
Article Title: Computational thermo-hydro-mechanics for multiphase freezing and thawing porous media in the finite deformation range
Authors: SeonHong Na, WaiChing Sun
Keywords: Finite strain thermo-hydro-mechanicsPoromechanicsGeneralized hardening ruleCritical stateStabilization procedure
Abstract: A stabilized thermo-hydro-mechanical (THM) finite element model is introduced to investigate the freeze–thaw action of frozen porous media in the finite deformation range. By applying the mixture theory, frozen soil is idealized as a composite consisting of three phases, i.e., solid grain, unfrozen water and ice crystal. A generalized hardening rule at finite strain is adopted to replicate how the elasto-plastic responses and critical state evolve under the influence of phase transitions and heat transfer. The enhanced particle interlocking and ice strengthening during the freezing processes and the thawing-induced consolidation at the geometrical nonlinear regimes are both replicated in numerical examples. The numerical issues due to lack of two-fold inf–sup condition and ill-conditioning of the system of equations are addressed.
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Volume: 16 Issue: First Page #: 345
Date Submitted: 7/19/19 12:00AM Date Published: 11/1/18 7:00AM
Publication Location:
Article Title: An adaptive reduced-dimensional discrete element model for dynamic responses of granular materials with high-frequency noises
Authors: Xinran Zhong, WaiChing Sun
Keywords: discrete element method, proper orthogonal decomposition, energy-preserving algorithm
Abstract: We present a dimensional-reduction framework based on proper orthogonal decomposition (POD) for non-dissipative explicit dynamic discrete element method (DEM) simulations. Through Galerkin projection, we introduce a finite dimensional space with less number of degree of freedoms such that the discrete element simulations are not only faster but also free of high-frequency noises. Since this method requires no injection of artificial or numerical damping, there is no need to tune damping parameters. The suppression of high-frequency responses allows larger time step for faster explicit integration. To capture the highly nonlinear behaviors due to particle rearrangement, an automatic mode-update scheme is formulated such that the most efficient basis can be used to predict mechanical responses. Numerical examples including, the wave propagation simulations and uniaxial extension and compression tests are used to demonstrate the capacity of the reduced order model.
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Volume: 346 Issue: First Page #: 216
Date Submitted: 7/19/19 12:00AM Date Published: 4/1/19 7:00AM
Publication Location:
Article Title: Meta-modeling game for deriving theory-consistent, microstructure-based traction–separation laws via deep reinforcement learning
Authors: Kun Wang, WaiChing Sun
Keywords: Meta-modeling,Traction–separation law, Data-driven computational mechanics, Path-dependent responses, Fracture opening and closure
Abstract: This paper presents a new meta-modeling framework that employs deep reinforcement learning (DRL) to generate mechanical constitutive models for interfaces. The constitutive models are conceptualized as information flow in directed graphs. The process of writing constitutive models is simplified as a sequence of forming graph edges with the goal of maximizing the model score (a function of accuracy, robustness and forward prediction quality). Thus meta-modeling can be formulated as a Markov decision process with well-defined states, actions, rules, objective functions and rewards. By using neural networks to estimate policies and state values, the computer agent is able to efficiently self-improve the constitutive model it generated through self-playing, in the same way AlphaGo Zero (the algorithm that outplayed the world champion in the game of Go) improves its gameplay. Our numerical examples show that this automated meta-modeling framework does not only produces models which outperfo
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Article Title: Circumventing mesh bias by r- and h-adaptive techniques for variational eigenfracture
Authors: Aurel Qinami, Eric Cushman Bryant, WaiChing Sun, Michael Kaliske
Keywords: Eigenerosion, Mesh sensitivity, R-adaptivity, H-adaptivity
Abstract: This article introduces and compares mesh r- and h-adaptivity for the eigenfracture model originally proposed in Schmidt et al. (Multiscale Model Simul 7:1237–1266, 2009), Pandolfi and Ortiz (J NumerMethods Eng 92:694–714, 2012), with the goal of suppressing potential mesh bias due to the element deletion. In the r-adaptive approach, we compute the configurational force at each incremental step and move nodes near the crack tip parallel to the normalized configurational forces field such that the crack propagation direction can be captured more accurately within each incremental step. In the h-adaptive approach, we introduce mesh refinement via a quad-tree algorithm to introduce more degrees of freedom within the non- local epsilon-neighborhood such that a more refined crack path can be reproduced with a higher mesh resolution. Our numerical examples indicate that the r-adaptive approach is able to replicate curved cracks.
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Article Title: Shift boundary material point method: an image-to-simulation workflow for solids of complex geometries undergoing large deformation
Authors: Chuanqi Liu, WaiChing Sun
Keywords: Material point method Shift domain, Image-based simulations, Nonlocal damage, Granular materials
Abstract: We introduce a mathematical framework designed to enable a simple image-to-simulation workflow for solids of complex geometries in the geometrically nonlinear regime. While the material point method is used to circumvent the mesh distortion issues commonly exhibited in Lagrangian meshes, a shifted domain technique originated from Main and Scovazzi (J Comput Phys 372:972–995, 2018) is used to represent the boundary conditions implicitly via a level set or signed distance function. Consequently, this method completely bypasses the need to generate high-quality conformal mesh to represent complex geometries and therefore allows modelers to select the space of the interpolation function without the constraints due to the geometric need. This important simplification enables us to simulate the deformation of complex geometries inferred from voxel images.
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Article Title: A micromorphically regularized Cam-clay model for capturing size-dependent anisotropy of geomaterials
Authors: Eric C. Bryant, WaiChing Sun
Keywords: Gradient critical state plasticity, Micromorphic regularization, Size-dependent anisotropy
Abstract: We introduce a regularized anisotropic modified Cam-clay (MCC) model which captures the size-dependent anisotropic elastoplastic responses for clay, mudstone, shales, and sedimentary rock. By homogenizing the multiscale anisotropic effects induced by clay particle aggregate, clusters, peds, micro-fabric, and mineral contact across length scales, we introduce two distinctive anisotropic mechanisms for the MCC model at the material point and mesoscale levels. We first employ a mapping that links the anisotropic stress state to a fictitious isotropic principal stress-space to introduce anisotropy at the material point scale. Then, the mesoscale anisotropy is introduced via an anisotropic regularization mechanism. This anisotropic regularization mechanism is triggered by introducing gradient-dependence of the internal variables through a penalty method such that the gradient-enhanced plastic flow may exhibit anisotropic responses non-coaxial to the stress gradient of yield function.
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Article Title: A cooperative game for automated learning of elasto-plasticity knowledge graphs and models with AI-guided experimentation
Authors: Kun Wang, WaiChing Sun, Qiang Du
Keywords: Directed multigraph, Data-driven constitutive modeling, Multi-agent deep reinforcement learning, Combinatorial optimization, Computational combinatorics
Abstract: We introduce a multi-agent meta-modeling game to generate data, knowledge, and models that make predictions on constitutive responses of elasto-plastic materials. We introduce a new concept from graph theory where a modeler agent is tasked with evaluating all the modeling options recast as a directed multigraph and find the optimal path that links the source of the directed graph (e.g. strain history) to the target (e.g. stress) measured by an objective function. Meanwhile, the data agent, which is tasked with generating data from real or virtual experiments (e.g. molecular dynamics, discrete element simulations), interacts with the modeling agent sequentially and uses reinforcement learning to design new experiments to optimize the prediction capacity. Consequently, this treatment enables us to emulate an idealized scientific collaboration as selections of the optimal choices in a decision tree search done automatically via deep reinforcement learning.
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Authors: SeonHong Na
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Final Report: Understanding hydro-mechanical coupling mechanism of wetted granular matters beyond the pendular regime

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7. Luca Tassini, Visiting Scholar, University of Perugia, Italy (supported by University of Perugia, Italy)
8. Lauren Brooke, Research Experience for Undergraduates Participant.
9. Anish Avasthi, Research Experience for Undergraduates Participant.

Major Activities:

The support has been used to support research activities of the Sun Research Group at Columbia University. This YIP grant provides the funding proven to be critical for the success of the number of research ideas that eventually lead to articles published in well-respected peer-reviewed journals and the career growth of the PI, the PhD students and postdoc research scientists involved.

The major research activities involve the derivation, testing, verification and validation of the theoretical and computational models and the reporting of the major results in journals. To ensure the impact of the research to the Army's and DoD's missions, the research group had both hosted Army researcher at Columbia (John Clayton, group leader of the impact physics group from Army Research Laboratory at Aberdeen Providing Ground) and also visited the Cold Regions Research and Engineering Laboratory twice during the YIP research program with Dr. Julia Barzyk who helps us established the connections with the scientists at CRREL. The research group also takes effort to support undergraduate and high school students from underrepresented groupsa for summer research visit to stimulate their interest in STEM career and learn the scientific process of research that is of relevant to Army's mission and the scope of the research project.

Specific Objectives:

The goal of this YIP research is to develop a micro-marco-coupling model for wetted granular matters that can predict the micromechanical topological changes of the grain-contact and liquid force chains and link these topological changes to macroscopic field-scale problems. The proposed research will combine (1) computational multiscale models that capture the particle-fluid interactions, (2) laboratory suction-controlled experiments that provide both macroscopic and grain-scale data through X-ray CT imaging technique and (3) mathematical tools such as graph theory to analyze the simulated and experimentally captured liquid and solid force chain networks. To overcome the geometrical constraints imposed by the Young-Laplace equation (i.e. particles must be spherical and liquid bridges must be axial symmetrical), the proposed research will explicitly model the pore-scale particle-fluid interaction via a lattice Boltzmann-discrete element coupling scheme and faithful capture the fluid-solid interactions among liquid and particles of varying shapes and sizes. The capillary effect of granular assemblies with different grain size distributions, porosities, loading rates and degree of saturation will be systematically analyzed

Significant Results:

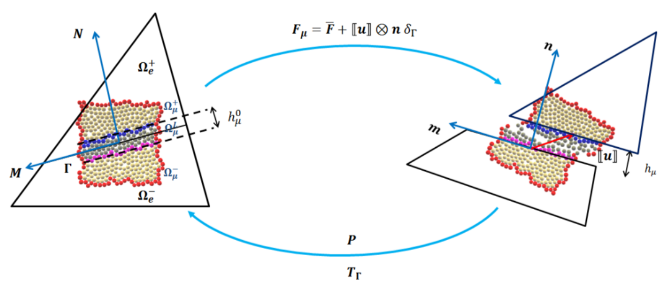

Figure 1: homogenization of DEM/flow network simulations with embedded strong discontinuities.

The support has been used to support research activities of the Sun Research Group at Columbia University. During this reporting period, the YIP support is used to provide the salary and tuition support for graduate student Kun Wang and the part of the time of the PI used to conduct the results. During this reporting period, the research group has submitted 31 papers, including 27 journal articles. A brief summary of the major results is provided below. Note that parts of the descriptions may also include in the progress report.

Discrete-continuum coupling DEM-LBM-FEM solver

The research group has published a series of papers that describe a new proposed model in which grain-scale simulations are used to obtain macroscopic responses at the finite deformation range (cf. Liu et al. 2016, Wang & Sun, 2016, Wang & Sun, 2018, 2019). This work shows that (1) it is possible to formulate theoretical, mathematical and computational framework that links the hydro-mechanical responses of porous media and that (2) also generate evidence to reveal the importance of incorporating characteristic length for hierarchical DEM-FEM multiscale simulations, which was incorrectly thought to be mesh independent in some literature. The research group has therefore invented new methodology to overcome this problem while incorporating the hydro-mechanical responses for the wetted granular matters. In particular, The Army YIP project has led to the creations of two models, one focuses on using micro-polar kinematics and higher-order responses (coupled stress), another one is for embedded strong discontinuities and embedded strong discontinuities (see Figure 1). From a physical perspective, the embedded strong discontinuities are of ultimate importance for numerous geological systems across length scales, such as geomaterials consist of micro-cracks, deformation bands, rock joints, granitic rock, shale formation and oceanic crust. Meanwhile, the micro-polar homogenization can be a significant improvement for the existing hierarchical multiscale DEM-FEM method as it takes account of the micro-rotation mechanisms which is critical to explain the relationship between the mechanics of frictional contact and the macroscopic shear strength.

Deep-learning-based multiscale model

Another important discovery we have found and could be highly important for various engineering and military applications is the incorporation of machine learning for multiscale modeling. While training the feedforward neural network to replicate stress-strain curve has been documented since the 90s, the rapid advancements of deep learning and other new neural network models have breathed new lives to the decades' old problems.

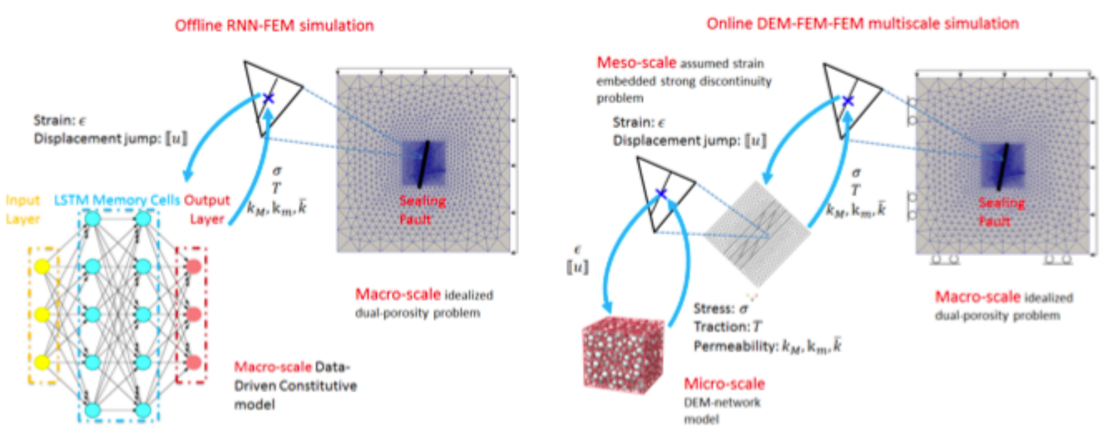

Figure 2: Offline multiscale machine learning based on recurrent neural network (LEFT) and the conventional hierarchical DEM-FEM simulations for earth systems

Figure 2 shows the comparison of the offline DEM-FEM simulation and the conventional hierarchical counterpart. Here the sub-scale simulations are used to generate or supplement the training and validation data. Then, the neural network is trained. Since most of the problems interested by US Army and the geomechanics community are related to materials that exhibit dissipative behaviors due to plastic deformation, damage, and fractures, we designed a specific training and validation procedure for the types of neural networks that are suitable for the task --- the recurrent neural network. Furthermore, while implementing the data-driven model, we also discover that the transformation from Lie group to Lie algebra may yield better results for predictions that requires information from Lie group as input for the neural network. This is particularly useful for tensors in the special orthogonal group (e.g. rotation). In those cases, we employ the spectral decomposition for the second-order tensors, for instance,

$$\boldsymbol{\sigma}' = \sum_{A=1}^{3} \sigma'_A \boldsymbol{n}_\sigma^{(A)} \otimes \boldsymbol{n}_\sigma^{(A)}, \quad \boldsymbol{\epsilon} = \sum_{A=1}^{3} \epsilon_A \boldsymbol{n}_\epsilon^{(A)} \otimes \boldsymbol{n}_\epsilon^{(A)}, \quad \boldsymbol{k} = \sum_{A=1}^{3} k_A \boldsymbol{n}_k^{(A)} \otimes \boldsymbol{n}_k^{(A)}$$

where we take advantage of the fact that the eigenvectors are all orthogonal to each other and that the eigenvalues or other invariants are not changed due to the coordinate system or frame we choose. As a result, we simply represent any second-order tensors in terms of their corresponding eigenvalues and orthonormal eigenvectors. When the input and the output tensors are not co-axial to each other (for instance, strain and stress relation of an anisotropic elastic material), the rotation of the principal directions are computed in the Lie algebra in which the infinitesimal spin is used, i.e.,

$$\boldsymbol{R} = \exp[\tilde{\boldsymbol{\Psi}}] = \sum_{k=0}^{\infty} \frac{\tilde{\boldsymbol{\Psi}}^k}{k!} \; ; \; \boldsymbol{\Psi} = \log \boldsymbol{R} = \sum_{k=0}^{\infty} \frac{(-1)^{n-1}}{n} (\boldsymbol{R} - \boldsymbol{I})^n$$

An interesting application we are currently working on is the simulation of damaged geological material in which localized fractures, micro-cracks, and cavities are idealized as embedded strong discontinuities and the constitutive responses of these localized fractures are captured via the neural network-based data-driven model. As such, there is no need for using traction-separation law. From a physical standpoint, one important technical barrier this new technique overcome is the generation of traction-separation laws for cyclic opening and closure of the cracks. This is particularly important for the cases where the closing of cracks is following by other mixed mode shears, as shown in Figure 3.

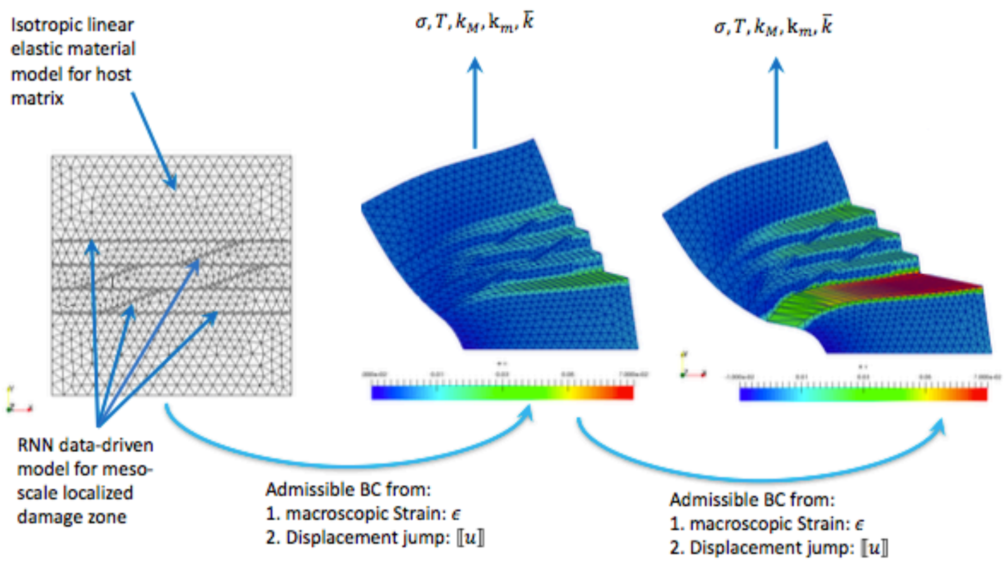

Figure 3: Simulations of RNN-FEM model with embedded strong discontinuities.

<u>Meta-modeling for geomechanics models</u>

In this research, our goal is to leverage the three major machine learning techniques (supervised, unsupervised and reinforcement learning) to discovery new physics of path-dependent materials that cannot be otherwise determined from hand-crafted models. For a given set of data, we seek to find way to gain knowledge not necessarily from excess curve-fitting from training materials, but from finding the right relationships among physical quantities. In a nutshell, the key departure of our work from the other ML applications for constitutive laws and computational mechanics is that we are not attempting to write a surrogate model or constitutive laws from data. Instead, we are attempting to modeling the actions and behaviors of a mechanician who is tasked with writing a constitutive laws for a given set of data. As such, we introduce a game whose objective is to write a predictive constitutive law and then re-cast a modeler as a player in this game with mathematically defined reward, action, state and environment.

Many machine learning models used in mechanical computer simulations employ supervised and unsupervised learning techniques to make predictions with little or no interpretability. This disconnection with human knowledge makes it difficult to assess and manage risk when using such black-box models for engineering applications. In this talk, we present a new framework in which the AI is not simply tasked to make predictions on a mechanical process, but to mimic the actions of a human engineer to create, validate and test hand-crafted models that make predictions. As such, we introduce the concept of meta-modeling in which two AI agents, an experimentalist that generates data and a modeler that interprets data, are tasked with building a directed graph that represents the knowledge of the physical process with the least amount of data required.
In this meta-modeling framework, all data accessible by the agents is modeled as labelled vertices (e.g. porosity, permeability) and all possible ways to connect those vertices are modeled as directed edges (e.g. mathematical expression, neural nets, support vector machine). Therefore, all the possible actions of the agents are mathematically represented by a labeled directed multi-graph. The learning process is therefore re-cast as the procedure to find a directed graph that links the input and output data with the optimal set of edges that maximize the reward (the objective function that measures the prediction qualities). With well-defined agents, reward, action space and environment, the AI modeler will then improve its ability to write the models through self-practicing in a deep reinforcement learning framework. Like humans, it will attempt to take different actions to write a model, then estimate the reward of each action via a deep neural network in a Monte Carlo tree search. By leveraging the ability of the AI modeler to repetitively practice and improve its modeling skills, we demonstrate that the proposed algorithm is able to both discover new hidden hierarchical structures of mechanics knowledge and rediscover well-known mechanics knowledge without any human intervention. In the case where availability of data is limited, the meta-modeling algorithm also explores the weakness of links in the constitutive laws and explores the optimal set of experiments to yield the best forward predictions under a limited budget.

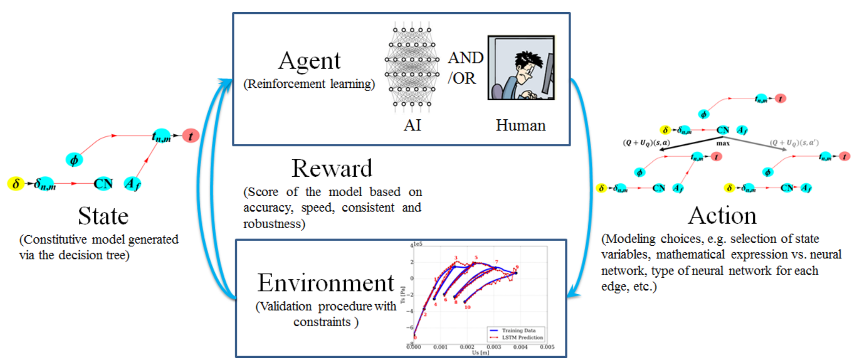

Figure 4: The meta-modeling model: a modeling effort to model the agent that writes constitutive laws.

For instance, in our published work, we have used the deep learning to help us identifying the importance of multiple micro-structural attributes on the macroscopic responses and identify the relative importance of (1) fabric tensor, (2) coordination number of particles and (3) other measurement. Based on the results of the deep learning studies, we then propose models that, for the first time, incorporates the fabric tensors as input for the non-co-axial traction-separation law and yields a model that is suitable to capture the complex damage-plasticity mechanisms of interfaces undergoing a combination of tensile, compressive and shear kinematics (see Figures in the RHS). Our discovery does not only show that the fabric tensor is critical for anisotropic responses of granular materials, but we also find a way to automatically incorporate those influences without hand-crafting a new model every times we want to test a new hypothesis (see Figure 5).

Another related development is the usage of unsupervised learning to generate reduced-basis models (see Figure 6, also Zhang & Sun 2018). The idea behind this is to use previous simulations of similar natures (e.g. periodic responses, repeated procedures in manufacture, mixing) to determine a Galerkin projection that enables simulations carried with very limited degree of freedoms associated with the orthogonal basis rather than the nodal responses of a standard finite element or discrete element models.

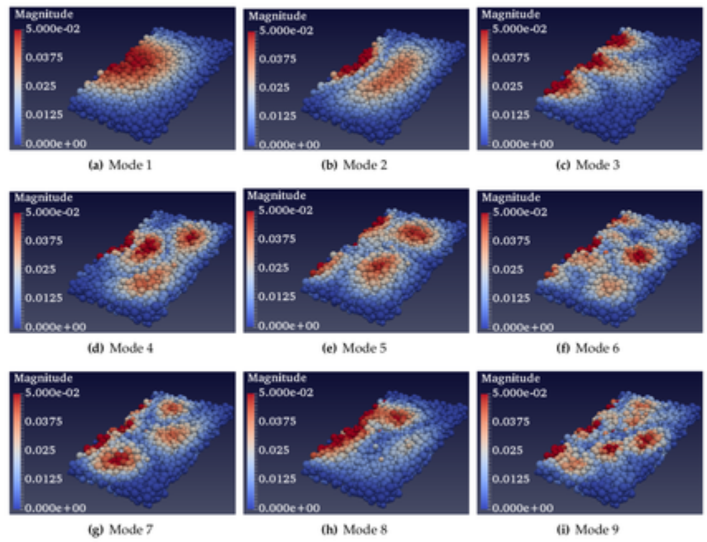

Figure 6: Orthogonal basis obtained from proper orthogonal decomposition for fast DEM simulations.

We also introduce a number of new ideas in the training procedure. For instance, we introduce the usage of long-short-term memory neuron to predict history-dependent responses and employ spectral decomposition to represent evolutions of tensorial input and output information such that the frame-dependent issues exhibited in RNN constitutive laws are corrected. We use a dual-permeability problem as a test bed to demonstrate how this new modeling approach works. More information can be found in the published articles. Meanwhile, the micro-polar homogenization can be a significant improvement for the existing hierarchical multiscale DEM-FEM method as it takes account of the micro-rotation mechanisms which is critical to explain the relationship between the mechanics of frictional contact and the macroscopic shear strength.

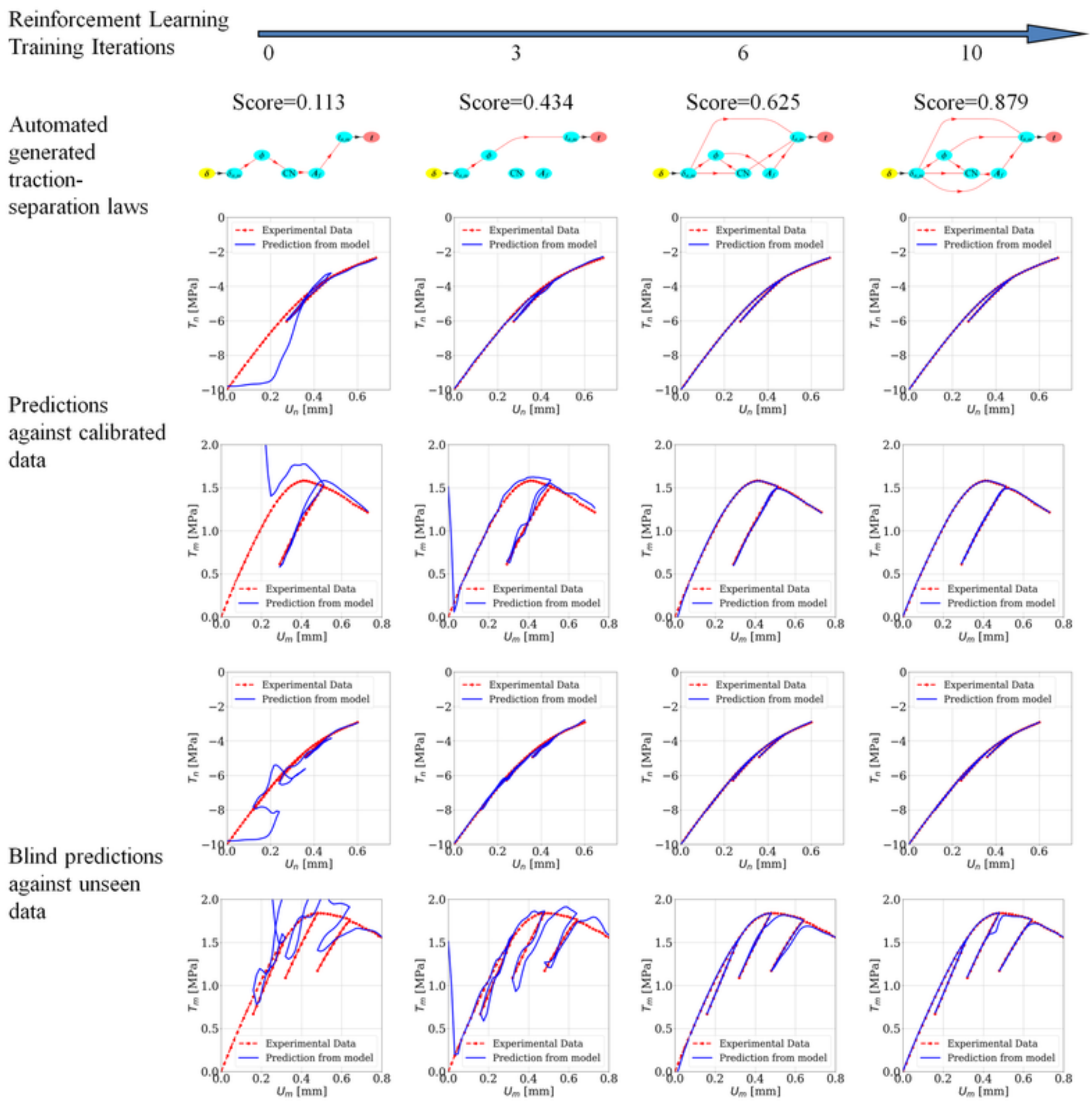

Figure 5: Self-improvement of the computer agent over each constitutive model writing session. Over time, the computer agent learns the directed graph that represents the relationships among physical quantities and employ this knowledge to write constitutive laws.

<u>Validations and inverse problems for earth materials</u>

We also introduce a multi-agent meta-modeling game to generate data, knowledge, and models that make predictions on constitutive responses of elasto-plastic materials. We introduce a new concept from graph theory where a modeler agent is tasked with evaluating all the modeling options recast as a directed multigraph and find the optimal path that links the source of the directed graph (e.g. strain history) to the target (e.g. stress) measured by an objective function. Meanwhile, the data agent, which is tasked with generating data from real or virtual experiments (e.g. molecular dynamics, discrete element simulations), interacts with the modeling agent sequentially and uses reinforcement learning to design new experiments to optimize the prediction capacity. Consequently, this treatment enables us to emulate an idealized scientific collaboration as selections of the optimal choices in a decision tree search done automatically via deep reinforcement learning.

Another important implication of the meta-modeling game is its ability to quantitatively analyze the performance of families of models currently (or historically, if possible, to be inferred from reverse engineering) available in the literature for an intended prediction task. Table 1 shows the post-game analysis of the performance of the 112 models automatically generated from the two-player game. The resultant models are grouped into five different classes based on the types of the edges used in the game. The interesting aspect of the data in Table 1 is that it provides users a quantitative measure that configurations based on generalized plasticity and critical state outperform all the other 90 configurations. This result is consistent with the convention understanding from soil mechanics in which the classical critical state plasticity theory and the resultant plastic dilatancy/contraction predictions is regarded as the key ingredient for predictive constitutive laws. Examinations on models in Class 1 also reveals that three-invariant generalized plasticity with critical state perform the best in the blind predictions, especially when the material states of the granular materials in the calibration tests (e.g. confining pressure, initial void ratio, stress path) are significantly different than the ones in blind predictions.

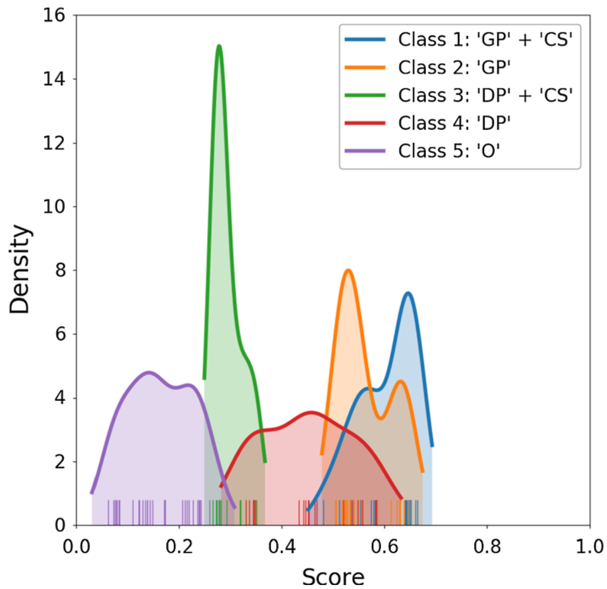

Figure 6: Distribution of the scores of the models generated during the deep reinforcement learning. The models are grouped into five families (see Table 1). The curves present the Gaussian kernel density estimation of the model score distributions.

However, comparisons of the results in Classes 1, 2,3 and 4 shown in above Figure reveal a somewhat surprising conclusion in which the generalized plasticity seems to be consistently the more important ingredient than the critical state theory for yielding predictive models. Although it is important to stress that this conclusion must be interpreted with respect to the types and amount of data available and the intended prediction task, this result does provide further evidence to support the speculations that the generalized plasticity, if calibrated properly, does likely to improve the accuracy of blind predictions of the responses of granular materials in the monotonic triaxial compression tests (see Figure 6, also Wang, Sun & Du, 2019).

<u>Vehicle-soil interaction and off-road mobility</u>

We introduced an Arbitrary-Eulerian-Lagrangian (ALE) model to capture the interaction between elastic porous media and tires. This is the first time an ALE model has been formulated, implemented and verification correctly in the finite deformation range. In particular, the correct capture of the material and geometrical nonlinearities are important to simulate the interactions of the soil and foreign objects that cause severe deformation of the soil and therefore limits the mobility of vehicles. The numerical model employs an operator-split approach which allows commercial code, which is used to model tire and contact, and the research code, which is used to model the soil as a two-phase porous medium, as shown in Figure 4. In the soil model, we employ another operator-split strategy such that the flow simulator and the solid solver updates sequentially and iteratively until the residuals of the system of equations are all reduced to be below the tolerance.

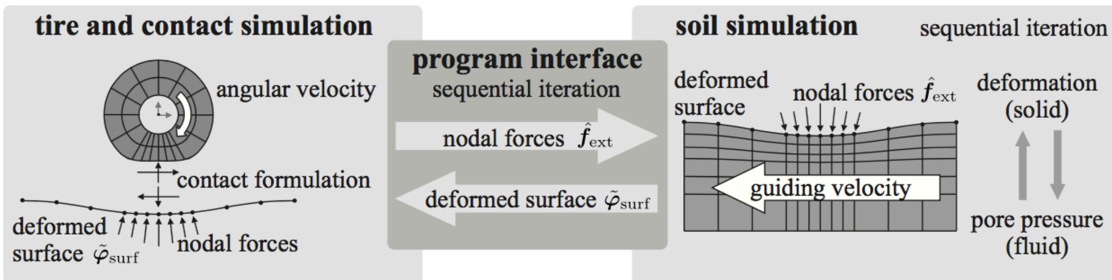

Figure 7: Operator-split model for soil-tire interaction. (cf. Wollny et al., 2017).

Figure 5 shows a snapshot of simulation results obtained from the operator-split model. In this particular case, the diffusion of the fluid depends on the rolling speed of the tire and increasing the moving speed of the vehicle may lead to a surface response that are more dominated by deviatoric deformation mode. One particular promising next step is to simulate the responses of soil under more extreme conditions. For instance, at the cold region where thawing or frozen of ice may lead to softening soil and thawing induced settlement. Furthermore, the unsaturated soil model can also be incorporated to study the effects of raining and other more extreme weather on the durability of the pavement system or the mobility of vehicle in a wet off-road environment.

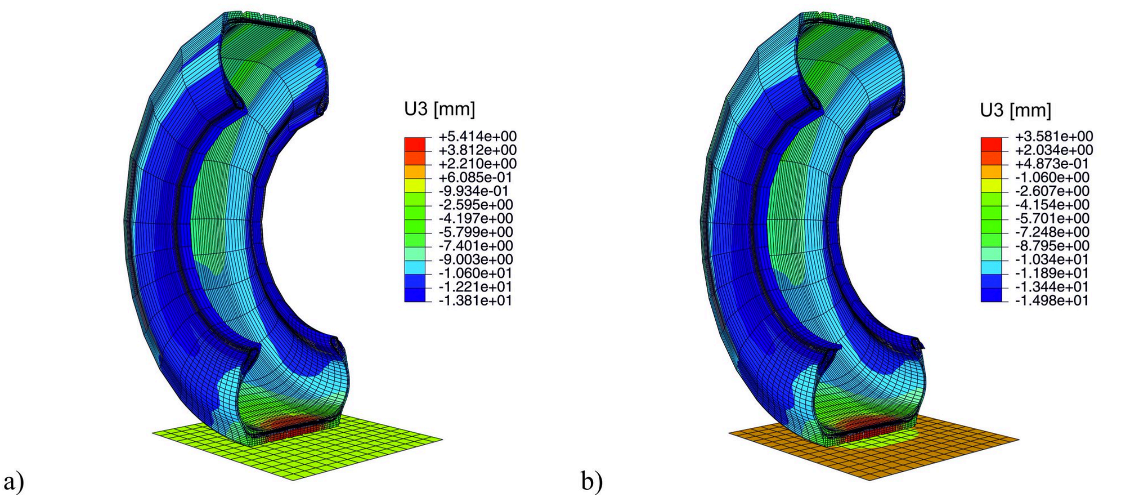

Figure 8: Contact stress of tire at different time step. Figure reproduced from Wollny et al. 2017.

<u>Modified material point method for complex geometries undergoing finite deformation</u>

One key drawback of classical discrete element methods for particulate mechanics is that they cannot generate any kinetic and kinematics information at the sub-grain scales. Nevertheless, many dissipative mechanisms of granular materials are actually originated from path-dependent behaviors at the sub-grain scales where wear, damage, fracture and fragmentation occur. Nevertheless, recovery of these sub-scale information while capturing the geometry and form of each individual grains is inherently a difficult task (Liu & Sun, 2019).

To overcome this issue, we establish an efficient image-to-simulation workflow to overcome this technical barrier. We introduce a mathematical framework designed to enable a simple image-to-simulation workflow for solids of complex geometries undergoing large deformation in the geometrically nonlinear regime. In particular, we adopt the integration scheme of the material point method to resolve the convergent issues for Lagrangian meshes due to mesh distortion, while using a shifted domain technique originated from Scovazzi and coworker to represent the boundary condition implicitly via a level set or signed distance function (see Figure 9).

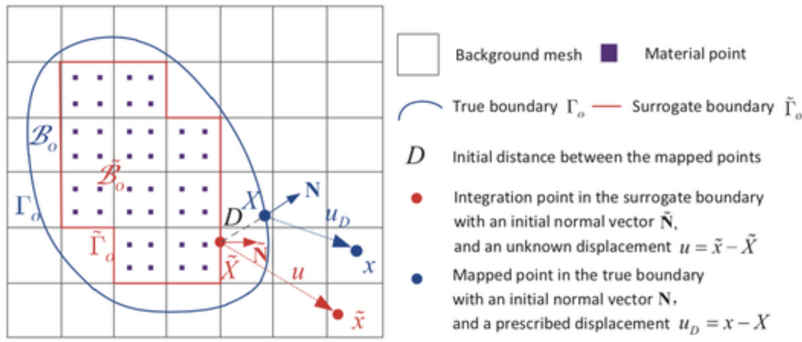

Figure 9: shift domain technique applied to material point method

Consequently, this method completely bypasses the need to generate high-quality conformal mesh to represent complex geometries and therefore allows modelers to select the space of the interpolation function without the constraints due to the geometrical need. This important simplification enables us to simulate deformation of complex geometries inferred from voxel images. Verification examples on deformable body subjected to finite rotation have shown that the new shifted domain material point method is able to generate frame-indifference results. Meanwhile, simulations using microCT images of a Hostun sand have demonstrated that this method is able to reproduce the quasi-brittle damage mechanisms of single grain without the excessively concentrated nodes commonly displayed in conformal meshes that represent 3D objects with local fine details (see Figure 10)

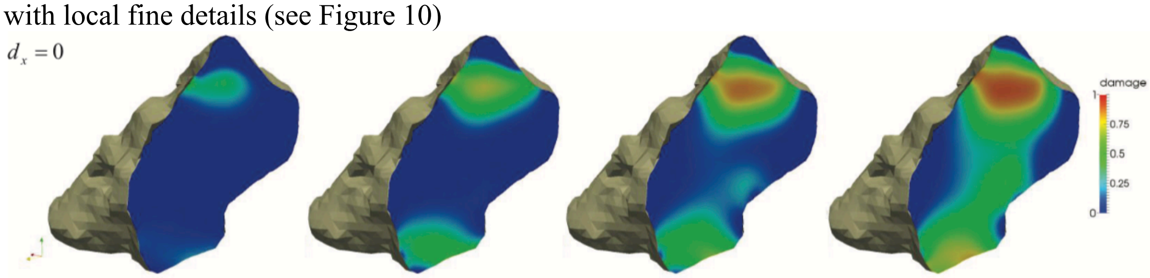

Figure 10: Particle damage occurs during indentation simulated by a nonlocal damage model. Note that classical DEM cannot recover any stress field or energy flux information near the singular tip and hence cannot accurately predict the propagation of crack.

<u>Computational Thermo-hydro-mechanics of Frozen Soil at the Finite Deformation Range.</u>

A stabilized thermo-hydro-mechanical (THM) finite element model is introduced to investigate the freeze-thaw action of frozen porous media in the finite deformation range. By applying the mixture theory, the frozen soil is idealized as a composite consisting of three phases, i.e., solid grain, unfrozen water and ice crystal. A generalized hardening rule at finite strain is adopted to replicate how the elasto-plastic responses and critical state evolve under the influence of phase transitions and heat transfer. The enhanced particle interlocking and ice strengthening during the freezing processes and the thawing-induced consolidation at the geometrical nonlinear regimes are both replicated in numerical examples. The numerical issues due to lack of two-fold inf-sup condition and ill-conditioning of the system of equations are addressed. Numerical examples for engineering applications at cold region are analyzed via the proposed model to predict the impacts of a changing climate on infrastructure in cold regions.

In a nutshell, the constitutive model follows the treatment of the Barcelona basic model in which the degree of saturation is hypothesized as an extended internal variable that influences the size and shape of the yield surface. In this particular work, we consider the case where the soil with unfrozen fluid follows the behaviors of a Cam-Clay model. As such, the critical state line is also moved along with the degree of saturation of ice crystal. Due to the pre-melting theory, one may assume that the surface energy difference may lead to the unfrozen water thin film formed in between the ice crystal and the solid skeleton. Therefore, the freezing process can be characterized using a freezing retention curve and that the degree of saturation of ice crystal can be determined from the temperature and the suction pressure, the difference between the mean pressure of ice and unfrozen water,

$$S_{\mathrm{L}} = \left[1 + \left[\frac{-(1-\rho_{\mathrm{C}}/\rho_{\mathrm{L}})p_{\mathrm{L}} - \rho_{\mathrm{C}} l \ln(T/273.15)}{P}\right]^{n}\right]^{-m},$$

where ρ_c and ρ_l are the intrinsic densities of the ice crystal and unfrozen water, P is the reference pressure, T is the temperature, n and m are the material parameters that manipulate the shape of the retention curve. The yield surface therefore reads,

$$f = \left[p' - \left(\frac{p_c + k s_{\mathrm{cryo}}}{2}\right)\right]^2 + \frac{q^2}{M^2} - \left(\frac{p_c - k s_{\mathrm{cryo}}}{2}\right)^2,$$

Figure 6 shows the results of one shear band simulation at undrained state in which the formation of a shear band may heat up slightly (about half Celsius degree) and cause a shrinkage of shear band if the loading rate is sufficiently fast.

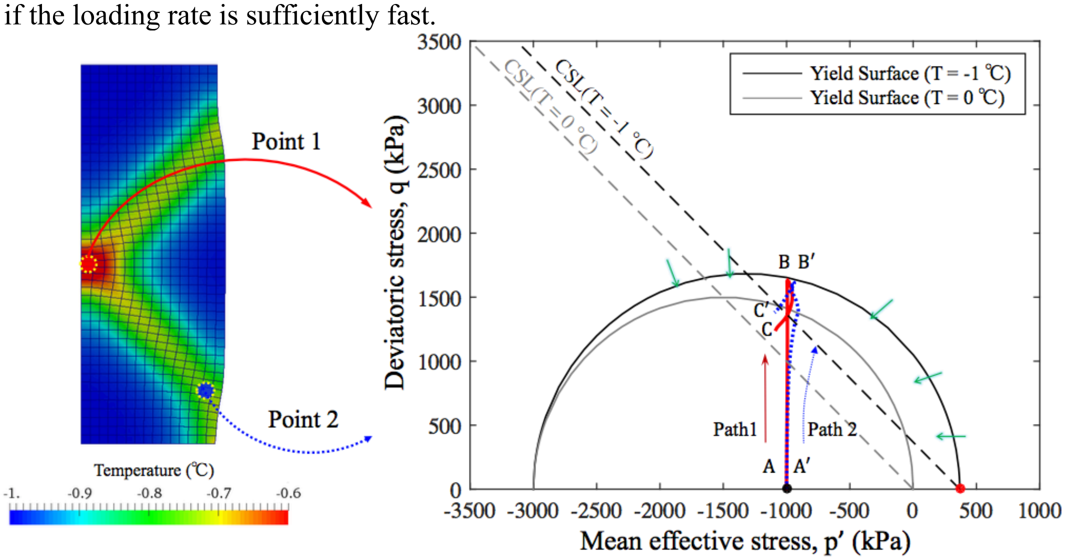

Figure 12: Shrinking of yield surface due to increasing temperature predicted by the frozen soil model. Figure reproduced from Na & Sun, 2017.

This work is also used to simulate one-dimensional freezing and thawing. Shown in Figure 7 is the temperature, suction, porosity and ice saturation profile at 1 hours, 5 hours and 20 hours after a prescribed cold temperature applied on the top of a soil deposit. The initial temperature of the soil is 2 Celsius while the bottom of the soil layer is assumed to be in touch of a thermal reservoir or heat bath such that the temperature at the bottom remains effectively constant. The results shown below indicates that the model is able to predict the major thermo-hydro-mechanical mechanism that leads to freezing and the effect of expansion due to the growth of ice crystals inside the pores. On the other hand, we have also conducted additional study to simulate the thawing and thawing settlement and compared the results against experiments available in the literature. The detailed work has been showcased in *Na & Sun, 2017*. The RA of this work has won multiple awards and poster competitions.

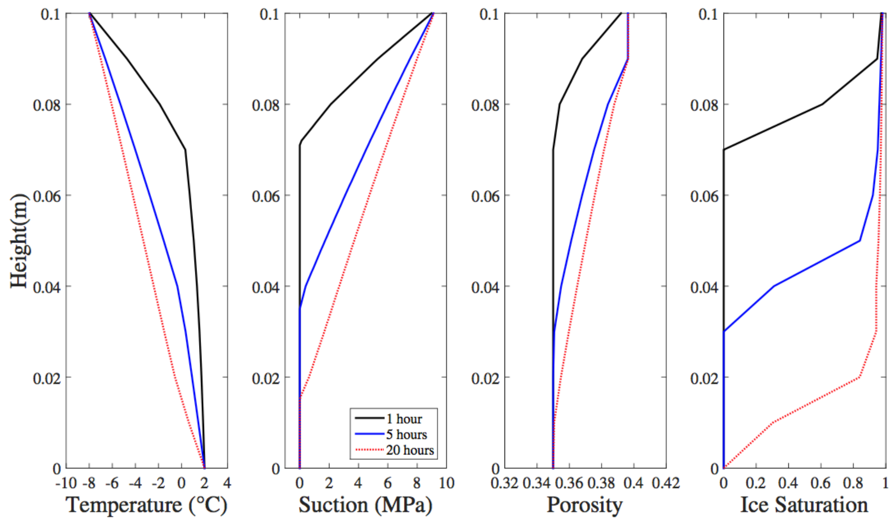

Figure 4: One-dimensional temperature, suction, porosity and ice saturation profile simulated by the THM model. Figure reproduced from Na & Sun, 2017)

<u>Key outcomes or other achievements:</u>

During the YIP program, the PI's research group has graduated three PhD students, SeonHong Na, who is now assistant professor at McMaster University, Yang Liu, who is now assistant professor at Northeastern University and Kun Wang who will join Los Alamos National Laboratory as a postdoctoral research scientist in the Theoretical Division. The success of the research group, in particular, Kun Wang's work, is impossible without the support for the YIP program.

The following peer-reviewed journal articles and conference papers are completed either fully or partially supported by this grant:

1. <u>K. Wang</u>, **W.C. Sun**, Anisotropy of a tensorial Bishop's coefficient for wetted granular materials, *Journal of Engineering Mechanics,* doi:10.1061/(ASCE)EM.1943-7889.0001005, 2015. [PDF] [Bibtex]
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