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14. ABSTRACT

15. SUBJECT TERMS
freeze-thaw action, thermohydromechanics, geomechanics, triaxial compression test, suction-control experiment, critical state plasticity

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RPPR Final Report
as of 02-Jul-2018

Agency Code:

Proposal Number: 66791EVRIP **Agreement Number: W911NF-15-1-0442**

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Report Date: 14-Nov-2016 Date Received: 01-Jul-2018
Final Report for Period Beginning 15-Aug-2015 and Ending 14-Aug-2016

Title: Cryo-mechanics of unsaturated frozen soils during freeze-thaw cycle.

Begin Performance Period: 15-Aug-2015 **End Performance Period:** 14-Aug-2016
Report Term: 0-Other

Submitted By: WaiChing Sun Email: wsun@columbia.edu
Phone: (212) 851-4371

STEM Degrees: 4 **STEM Participants:** 1

Major Goals: The objective of this DURIP research is to advance the fundamental understanding of the path dependent behaviors of soils during freeze-thaw cycles. An experimental triaxial cell system equipped with a climate control system and an unsaturated soil triaxial module will be used to vary temperature, axial and radial stresses, as well as air and water pressures of soils monotonically and cyclically. The stress-strain history, water retention behavior and relative permeability will be at various stages of loading cycles will be recorded. By examining the cryo-deformation of specimens subjected to various combinations of drainage conditions, degree of saturations and loading paths, this research will bring the much needed new insights on how crystallization and thawing of ice crystal inside the pore space affects the macroscopic responses of frozen soils. A large strain thermo-poro-plasticity constitutive model will be used in complement with this experimental research to develop validated theory that explains the thermo-hydro-mechanical responses frozen soil during freeze-thaw cycles.

Accomplishments: See PDF Attachment.

Training Opportunities: The PI has short one-on-one meeting with each individual group member every working day. The research group also holds monthly group meeting. In addition, the PI has constantly invited renowned researchers around the world to give seminar on the topics of computational geomechanics, including Claudio Tamagnini from University of Perugia from Itay, Guenther Meschke from Ruhr University Bochum, Germany Yixiang Gan from University of Sydney, among others.

The PI has supported PhD students to attend seminars and conferences, including the EMI-San Diego EMI-MIT conference, World congress of computational mechanics, AGU Fall Meeting, and US Congress of Computational Mechanics.

The PI's group has achieved a level of success in securing tenure-track positions for graduate and postdoc associate. Former PhD student Yang Liu started her tenure-track assistant professor position in the department of Mechanical and Industrial Engineering at Northeastern University in January 2018. Upon completing a very successful postdoc training and published 3 papers with the research group, former postdoctoral research scientist started his tenure-track assistant professor position at the University of Hong Kong. Meanwhile, current PhD student, SeonHong Na has been interviewed for tenure-track position from UIUC, UT Austin, UW Madison, National Taiwan University, McMaster University, Sandia National Laboratory and Lawrence Livermore National Laboratory and has received tenure-track offer from National Taiwan University with a $250,000 US dollar startup package, and another tenure-track offer from McMcaster University in Canada with a $200,000 US dollar startup fund. We expect the research group will continue to maintain a healthy size and consist of highly capable PhD students and postdoctoral scholars.

Results Dissemination: In addition to the journal articles published in top journals, the PI has given following invited seminars:

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.

The PI has also participated in summer internship program to mentor two high school students in addition to undergraduate students from underrepresented groups to enhance the diversity of STEM.

Honors and Awards: 1. 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 in- vestigators 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".

2. 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., Ge?othechnique, Ge?othechnique 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, In- ternational Journal of Numerical Modelling: Electronic Networks, Devices and Fields, and ICE Proceedings.

3. 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.

4. Dresden Junior Fellowship, Technische Universität Dresden, 2016.

Protocol Activity Status:

Technology Transfer: 1. The research group has hosted Dr. John Clayton, the leader of the impact physics group from Army Research Laboratory at Columbia University from October to December 2016.

2. The PI has attend 2-day workshop at AFOSR at Washington DC to present researches supported by this project.

3. The PI has discussed with Dr. John Michopoulos from Computational Multiphysics Systems Lab from Naval Research Laboratory for possible future collaboration on 4/30/2018.

PARTICIPANTS:

Participant Type: PD/PI
Participant: WaiChing Sun
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: SeonHong Na
Person Months Worked: 6.00 **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: 5.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Luca Tassini
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: Albert Martini
Person Months Worked: 12.00 **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: Journal of Geophysical Research: Solid Earth
Publication Identifier Type: DOI Publication Identifier: 10.1002/2016JB013374
Volume: Issue: First Page #:
Date Submitted: 8/21/17 12:00AM Date Published: 6/30/17 8:00PM
Publication Location:
Article Title: Effects of spatial heterogeneity and material anisotropy on the fracture pattern and macroscopic effective toughness of Mancos Shale in Brazilian tests
Authors: SeonHong Na, WaiChing Sun, Mathew D. Ingraham, Hongkyu Yoon
Keywords: Brazilian Test, phase field fracture, heterogeneous materials
Abstract: For assessing energy-related activities in the subsurface, it is important to investigate the impact of the spatial variability and anisotropy on the geomechanical behavior of shale. The Brazilian test, an indirect tensile-splitting method is performed in this work, and the evolution of strain field is obtained using digital image correlation. Experimental results show the significant impact of local heterogeneity and lamination on the crack pattern characteristics. For numerical simulations, a phase field method is used to simulate the brittle fracture behavior under various Brazilian test conditions. In this study, shale is assumed to consist of two constituents including the stiff and soft layers to which the same toughness but different elastic moduli are assigned. Microstructural heterogeneity is simplified to represent mesoscale (e.g., millimeter scale) features such as layer orientation, thickness, volume fraction, and defects.
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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.2017.01.017
Volume: 318 Issue: First Page #: 1
Date Submitted: 8/9/17 12:00AM Date Published: 4/30/17 10:00PM
Publication Location:
Article Title: A unified variational eigen-erosion framework for interacting brittle fractures and compaction bands in fluid-infiltrating porous media
Authors: Kun Wang, WaiChing Sun
Keywords: Compaction band; Eigen-erosion; Porous media; Hydraulic fracture; Anti-crack; Hydraulic aperture
Abstract: The onset and propagation of the cracks and compaction bands, and the interactions between them in the host matrix, are important for numerous engineering applications, such as hydraulic fracture and CO2 storage. While crack may become flow conduit that leads to leakage, formation of compaction band often accompanies significant porosity reduction that prevents fluid to flow through. The objective of this paper is to present a new unified framework that predicts both the onset, propagation and interactions among cracks and compaction bands via an eigen-deformation approach. By extending the generalized Griffith's theory, we formulate a unified nonlocal scheme that is capable to predict the fluid-driven fracture and compression-driven anti-crack growth while incorporating the cubic law to replicate the induced anisotropic permeability changes triggered by crack and anti-crack growth.
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Publication Type: Journal Article Peer Reviewed: Y **Publication Status:** 1-Published
Journal: Acta Geotechnica
Publication Identifier Type: DOI Publication Identifier: 10.1007/s11440-018-0682-1
Volume: Issue: First Page #:
Date Submitted: 6/28/18 12:00AM Date Published: 6/9/18 8:00AM
Publication Location:
Article Title: Coupled flow network and discrete element modeling of injection-induced crack propagation and coalescence in brittle rock
Authors: Guang Liu, WaiChing Sun, Steven M. Lowinger, ZhenHua Zhang, Ming Huang, Jun Peng
Keywords: Brittle rock, Crack coalescence, Discrete element method, Flow network, Fluid-driven fracture
Abstract: We present a numerical analysis on injection-induced crack propagation and coalescence in brittle rock. The DEM network coupling model in PFC is modified to capture the evolution of fracture geometry. An improved fluid flow model for fractured porous media is proposed and coupled with a bond-based DEM model to simulate the interactions among cracks induced by injecting fluid in two nearby flaws at identical injection rates. The material parameters are calibrated based on the macro-properties of Lac du Bonnet granite and KGD solution. A grain-based model, which generates larger grains from assembles of particles bonded together, is calibrated to identify the microscopic mechanical and hydraulic parameters of Lac du Bonnet granite such that the DEM model yields a ratio between the compressive and tensile strength consistent with experiments. The simulations of fluid injection reveal that the initial flaw direction plays a crucial role in crack interaction and coalescence pattern.
Distribution Statement: 1-Approved for public release; distribution is unlimited.
Acknowledged Federal Support: **Y**

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as of 02-Jul-2018

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: 3/1/18 12:00AM
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: Geomaterials, Phase field, Plasticity, Fracture, Strain localization, Brittle–ductile transition
Abstract: The failure behavior of geological materials depends heavily on confining pressure and strain rate. Under a relatively low confining pressure, these materials tend to fail by brittle, localized fracture, but as the confining pressure increases, they show a growing propensity for ductile, diffuse failure accompanying plastic flow. Furthermore, the rate of deformation often 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. The framework couples a pressure-sensitive plasticity model with a phase-field approach to fracture which can simulate complex fracture propagation without tracking its geometry. We derive a phase-field formulation for fracture in elastic–plastic materials as a balance law of microforce, in a new way that honors the dissipative nature of the fracturing processes.
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.2018.01.044
Volume: 335 Issue: First Page #: 347
Date Submitted: 6/28/18 12:00AM Date Published: 6/1/18 12:00AM
Publication Location:
Article Title: Cracking and damage from crystallization in pores: Coupled chemo-hydro-mechanics and phase-field modeling
Authors: Jinhyun Choo, WaiChing Sun
Keywords: In-pore crystallization, Chemo-hydro-mechanics, Fracture, Phase field, Effective stress, Reactive flow
Abstract: Cracking and damage from crystallization of minerals in pores center on a wide range of problems, from weathering and deterioration of structures to storage of CO2 via in situ carbonation. Here we develop a theoretical and computational framework for modeling these crystallization-induced deformation and fracture in fluid-infiltrated porous materials. Conservation laws are formulated for coupled chemo-hydro-mechanical processes in a multiphase material composed of the solid matrix, liquid solution, gas, and crystals. We then derive an expression for the effective stress tensor that is energy-conjugate to the strain rate of a porous material containing crystals growing in pores. This form of effective stress incorporates the excess pore pressure exerted by crystal growth – the crystallization pressure – which has been recognized as the direct cause of deformation and fracture during crystallization in pores.
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Journal: Computer Methods in Applied Mechanics and Engineering
Publication Identifier Type: Publication Identifier:
Volume: Issue: First Page #:
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Publication Location:
Article Title: A mixed-mode phase field fracture model in anisotropic rocks with consistent kinematics
Authors: Eric Bryant, WaiChing Sun
Keywords: mixed-mode fracture, secondary crack, phase field fracture
Abstract: Under a pure tensile loading, cracks in brittle, isotropic, and homogeneous materials often propagate such that pure mode I kinematics are maintained at the crack tip. However, experiments performed on geo-materials, such as sedimentary rock, shale, mudstone, concrete and gypsum, often lead to the conclusion that the mode I and mode II critical fracture energies/surface energy release rates are distinctive. This distinction has great influences on the formation and propagation of wing cracks and secondary cracks from pre-existing flaws under a combination of shear and tensile or shear and compressive loadings. To capture the mixed-mode fracture propagation, a mixed-mode I/II fracture model that employs multiple critical critical energy release rates based on Shen and Stephansson, IJRMMS, 1993 is reformulated in a regularized phase field fracture framework. We obtain the mixed-mode driving force of the damage phase field by balancing the microforce.
Distribution Statement: 1-Approved for public release; distribution is unlimited.
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Journal: Journal of Geophysical Research: Solid Earth
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Date Submitted: 7/1/18 12:00AM Date Published: 4/30/18 4:00AM
Publication Location:
Article Title: Prediction of hydraulic and electrical transport properties of sandstone with multiscale lattice Boltzmann/finite element simulation on microtomographic images
Authors: WaiChing Sun, Teng-fong Wong
Keywords: Digital rock physics, Computed tomography, Hydraulic permeability, Formation factor
Abstract: In Fontainebleau sandstone, the evolution of transport properties with porosity is related to changes in both the size and connectivity of the pore space. Microcomputed tomography can be used to characterize the relevant geometric attributes, with the resolution that is sufficiently refined for realistic simulation of transport properties based on the 3D image. In this study, we adopted a hybrid computation scheme that is based on a hierarchical multi-scale approach. The specimen was partitioned into cubic sub-volumes for pore-scale simulation of hydraulic permeability and formation factor using the lattice Boltzmann method. The pore-scale results were then linked with finite element simulation in a homogenized scheme to compute and upscale the transport properties to specimen scale. The simulated permeability and formation factor have magnitude and anisotropy that are in good agreement with experimental rock physics data.
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CONFERENCE PAPERS:

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Conference Name: European Congress on Computational Methods in Applied Science and Engineering
Date Received: 21-Sep-2016 Conference Date: 22-Sep-2016 Date Published: 22-Sep-2016
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Paper Title: A semi-implicit micropolar discrete-to-continuum method for granular materials
Authors: Kun Wang, WaiChing Sun
Acknowledged Federal Support: **Y**

Publication Type: Conference Paper or Presentation **Publication Status:** 1-Published
Conference Name: AGU Fall Meeting
Date Received: 01-Jul-2018 Conference Date: 12-Dec-2015 Date Published: 12-Dec-2016
Conference Location: San Francisco, CA
Paper Title: Crack Propagation considering material heterogeneity and anisotropic surface energy using phase field approach
Authors: SeonHong Na, WaiChing Sun, Jinhyun Choo, Hongkyu Yoon
Acknowledged Federal Support: **Y**

Publication Type: Conference Paper or Presentation **Publication Status:** 1-Published
Conference Name: AGU Fall Meeting
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Paper Title: Computational thermo-hydro-mechanics for freezing and thawing multi scale geological media in the finite deformation range
Authors: SeonHong Na, Luca Tassini, WaiChing Sun
Acknowledged Federal Support: **Y**

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Publication Type: Thesis or Dissertation
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Date Received: 01-Jul-2018 Completion Date: 6/30/18 10:31PM
Title: Multiscale thermo-hydro-mechanical-chemical coupling effects for fluid-infiltrating crystalline solids and geomaterials: theory, implementation, and validation.
Authors: SeonHong Na
Acknowledged Federal Support: **Y**

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Description: Group webpage.

Final Report: Cryo-mechanics of unsaturated frozen soils during freeze-thaw cycles

6/30/2018

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Grantee Proposal Number:
Period of Performance (Reporting Period for this report)
Start: Aug, 15 2015 End: Aug, 14 2016

SUBMITTED BY

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- WaiChing Sun, Assistant Professor, Civil Engineering and Engineering Mechanics, Fu Foundation School of Engineering and Applied Science, Columbia University

Postdoc Research Scientist

- Jinhyun Choo, postdoc research scientist (now assistant professor at the University of Hong Kong).

Research Assistant

1. Kun Wang, PhD Candidate Civil Engineering and Engineering Mechanics, Fu Foundation School of Engineering and Applied Science, Columbia University (supported by ARO and Columbia cost share)
2. SeonHong Na, PhD Candidate Civil Engineering and Engineering Mechanics, Fu Foundation School of Engineering and Applied Science, Columbia University (supported by Columbia cost share). Will join McMaster University as assistant professor in Spring 2019.
3. Albert Martini, MS Candidate, Civil Engineering and Engineering Mechanics, Fu Foundation School of Engineering and Applied Science, Columbia University (supported by Columbia cost share)
4. Luca Tassini, Visiting Scholar, University of Perugia, Italy (supported by University of Perugia, Italy)

Major Activities:

The support has been used to support research activities of the Sun Research Group at Columbia University. This DURIP grant provides the funding to purchase an equipment that is critical for the success of the number of research ideas that eventually lead to research works published in peer-reviewed journals and the career growth of the PI and the PhD students. Due to the nature of the research grant is for equipment purchase, the impact of the support goes beyond the original performance period and will last as long as the equipment is continuously being used, as in the case of this project.

The purchase request was sent by the PI as soon as the award letter was issued on August 15, 2015. After finishing various types of paperwork and fulfilling a variety of requirements by Columbia University required to make the purchase, the PI was able to make the purchase order with the support of the Carleton laboratory, on 4/29/2016. The triaxial apparatus was arrived on 5/23/2016. Following this, an engineering from the manufacturer GDS instruments, Mr. Diogo Teles was sent to Columbia to help setting up the apparatus and complete the training. The training sessions are attended by the PI, graduate students SeonHong Na, Kun Wang and Zhijun Cai and visiting scholar Luca Tassini on 6/2/ to 6/3/2016.

Following the training session, the research group has conducted triaxial compression tests under different combination of temperature, strain rate and confining pressure under the undrained condition ever since. We are particularly interested at the behaviors of the frozen soil near the phase transition temperature and hence we designed a series of tests, each with the same undrained loading path, but are conducted under fixed temperature. The majority of the tests are taken place during the visit of Luca Tassini, while graduate student Alberto Martini has undertaken the rest of the test before his MS graduation. The major discoveries and findings are outlined in the next two sections.

In the meantime, we have developed a new poromechanics theory that takes account of the pre-melting theory, the phenomenological effect of thawing and freezing on the shear strength of the materials but also, equally important, the hydraulic and thermal conductivities that vary with the unfrozen water thin film exists between the solid grains and ice crystals. This eventually leads to the first finite strain theory for thermo-hydro-mechanical responses of frozen soil and was published in Computer Methods in Applied Mechanics and Engineering, one of the most prestigious journals, not only in the field of computational geomechanics, but also in computational mechanics. This work mainly done by PhD student SeonHong Na, who has worked with the PI to derive the theory, implement the computer code, and invent new computer algorithms, including a new operator-split algorithm and a new pre-conditioner to make the solver feasible for the highly complex multi-physical problems.

Specific Objectives:

In this DURIP project, our goal is to find answers for the following important scientific questions for frozen soil that could have significant impacts on cold region geotechnical engineering and geomechanics.

1. How does macroscopic thermal effect vary under different degrees of saturation? One key important objective we would like to achieve is to distinguish how yield surface, plastic potential, hardening laws and thermo-elasticity of the soil differ when subjected to (i) small temperature change but no phase transition occurs and (ii) large temperature change that induces the water-ice phase transition?

2. How does stress anisotropy induced by liquid bridge evolve during freeze-thaw cycle? While liquid bridge is well known to induce stress anisotropy in the pendular regime, this anisotropy is often considered insignificant and neglected in the classical Bishop's effect stress theory as liquid bridge is prone to rupture. However, if a volume fraction of water is frozen, this frozen part of the liquid bridge will be solidified and thus potentially intensify the anisotropic effect. On the other hand, the experimental study can also shed light on how anisotropy of stress evolves during thaw-weakening process.

3. How does spatial heterogeneity of material properties driven by temperature and unfrozen water diffusion affect the validity of four-phase mixture theory and strength homogenization scheme between ice- and solid-phase? This is a critical issue that has yet been successfully addressed. Since the heat transfer and flow of the unfrozen water are not in the same temporal and spatial scales, a macroscopic constitutive law without internal length scale might not be valid or sufficient. The data set generated from this research

program can provide evidence to test the validity of the four-phase (ice- solid-water-air) mixture theory originally proposed in Zhou and Meschke [2013] and determine whether classical homogenization scheme based on equivalent inclusion method is sufficient for modeling frozen soil undergoing phase transitions.

4. How do temperature change, phase transition and flow of unfrozen water in pore space affect the onset and propagation of micro-cracks and affect macroscopic behaviors at high confining pressure?

Significant Results:

Experimental Studies on Frozen Soil

During the report period, the Columbia research team has leveraged the cost share to conduct tests on frozen soils. To validate the correct functioning of the machine and the procedure used, the results of one of the tests performed in the laboratory, at room temperature, have been compared with the results provided by VELACS (Verification of Liquefaction Analysis by Centrifuge Studies), also obtained on Nevada Sand samples, with failure point at room temperature. The comparison showed a perfect qualitative correspondence between the results.

Once the machine has been tested, a VELACS test (carried out on a sample of Nevada Sand with a relative density of 40%) has been used for the comparison with the tests carried out at Columbia University. During these experiments, to highlight the basic characteristics of frozen soils (all the tests have been conducted at the same confining pressure), the parameters that were changed are the temperature and axial strain rate.

In addition to the expected changes in the constitutive responses due to the formation and thawing of ice crystals in the pore space, we also found that the crystallization of ice in the pores has a profound influence on the failure mode. Our experiments indicate that while shear band may still form at a temperature low enough to trigger ice crystallization, a slight reduction in temperature may significantly strengthen the ice in the pore space, leads to highly undrained shear strength but also replace the highly localization failure mode with a diffuse one as shown in Figure 1. The research group is currently working on a manuscript to summarize the experimental findings and also to obtain more evidences from experiments conducted by PhD student Nicholas Vlassis.

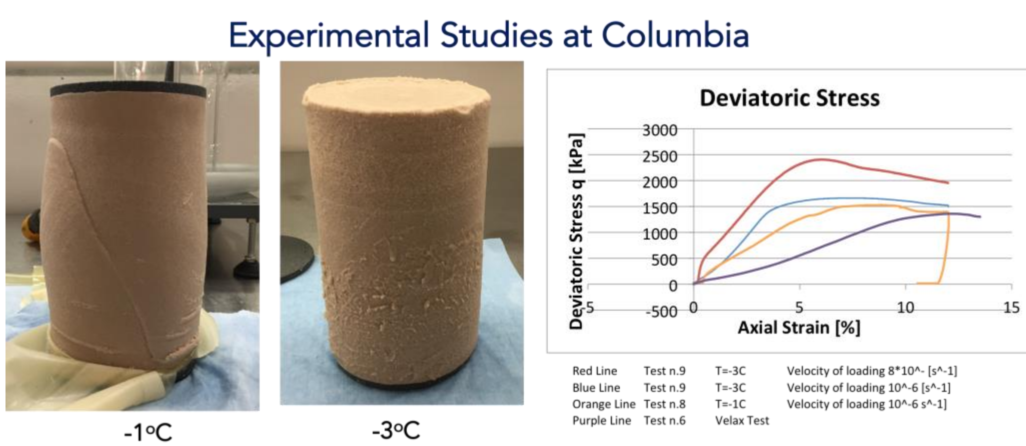

Figure 1: specimen at the end of the undrained triaxial compression test under different temperature (LEFT), the

deviatoric stress vs. axial strain of tests at different temperature and loading rates.

Computational Thermo-hydro-mechanics of Frozen Soil at the Finite Deformation Range

In this paper we present for the first time a finite strain poromechanics theory that fully considers the thermo-hydro-mechanical coupling effect of the mass-exchanging, phase-transiting porous media. Previously, significant contributions have been made to derive thermal-sensitive or degree-of-saturation-sensitive constitutive laws for the frozen soil. An implicit total Lagrangian finite element framework is formulated, while thermal and cryo-suction effects are explicitly captured by a generalized hardening rules that allow the yield surface to evolve based on the volume fraction of ices in the pore space and the temperature. In addition, we also highlight a number of numerical issues that are crucial for developing a practical and robust numerical implementation. Numerical examples are provided for elucidating the mechanical behavior of frozen soil under thawing and freezing conditions. The results indicate that a comprehensive model that explicitly captures the multiple thermo-hydro-mechanical coupling mechanisms of frozen porous media (instead of lumping them together through phenomenological laws) may yield far more accurate and reliable results. This elegant approach also eliminates the needs to introducing excessive amount of ad hoc parameters solely for curve-fitting, and is therefore easier to calibrate and more practical.

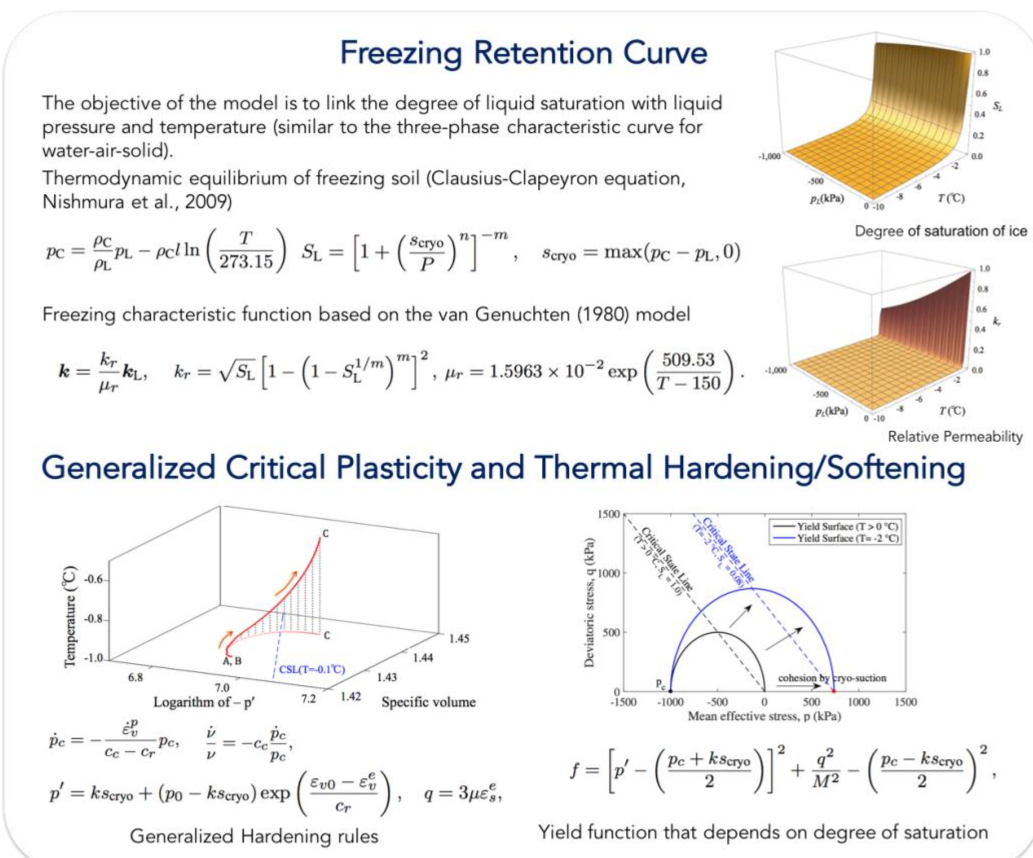

Figure 2: Constitutive laws for the thermo-hydro-mechanical coupling responses of frozen soil. Figure reproduced from Na and Sun, CMAME 2017.

The details of the constitutive law is summarized in Figure 2 in which the degree of saturation of ice is obtained from pre-melting theory such that the ice crystal pressure is a function of temperature, pore water pressure of the unfrozen water and the cryo-suction pressure. Using the idea of generalized critical state plasticity, the Cam-clay model is extended such that the hardening rules of the yield surface depends on the degree of saturation of ice. The upshot of this approach is that the model may seamlessly reduce into the classical soil model in room temperature but also incorporate the effects of freezing and thawing.

Microstructural Analysis of Geomaterials via micro-CT images

In this study, we have adopted a hierarchical multi-scale approach [White et al., 2006; Sun et al., 2011a; 2011b] to simulate hydraulic and electrical transport in three samples of Fontainebleau sandstone that had been imaged using X-ray CT by Lindquist et al. [2000]. Each specimen was partitioned into 8 unit cubes with linear dimensions of 1.08 mm for pore-scale LB calculation of permeability and formation factor. Our analysis of the geometry and percolative structure indicate that dimensions of the unit cubes are sufficiently large for treating them as REV for numerical simulation of the transport properties. The image resolution also seems adequate, and there is not a need to acquire CT images at a more refined resolution for such digital rock physics applications, in agreement with the analysis of Thovert et al. [2001] that focused on the percolation and electrical conductivity.

Unlike previous studies that used different numerical techniques for the hydraulic and electrical transport, we here employed LB simulations for both, which provide a more consistent basis for synthesizing permeability, formation factor and geometric attributes. The LB method has seldom been used to simulate formation factor of porous rock. The methodology we adopted here proved to be effective, but we should also note that by no means is it the only feasible approach for simulating electrical transport. For example, Chai and Shi [2008] have proposed an alternative formulation by adding an additional term on the right-hand side of the evolution equation such that the Chapman-Enskog expansion in time and space would recover the exact Poisson equation when diffusivity is non-zero.

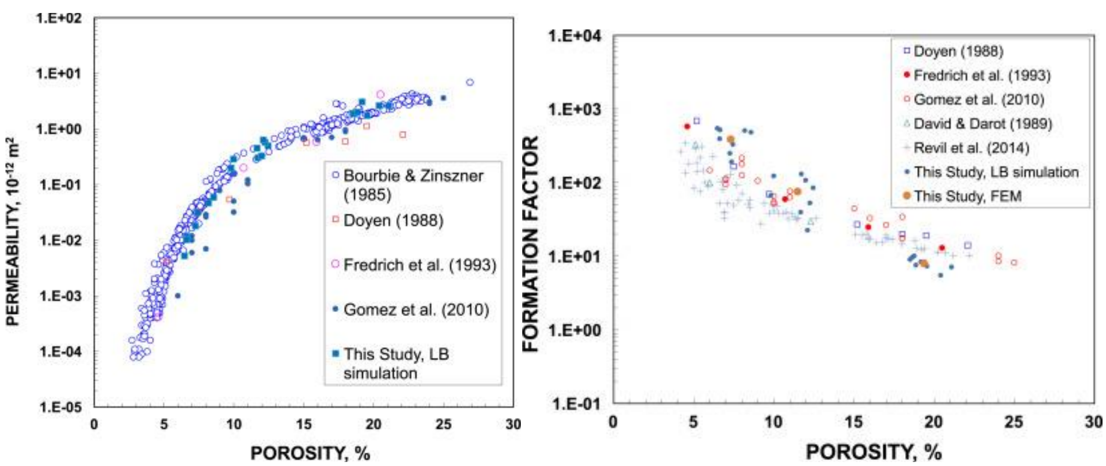

Figure 3: Permeability of Fontainebleau sandstone as a function of porosity. Simulated values from this study (with pressure gradient along the axial direction) are shown as solid squares. For comparison, laboratory data from the following studies are also plotted: Bourbie and Zinszner, Doyen, Fredrich et al. and Gomez et al..(LEFT) and Formation factor of Fontainebleau sandstone as a function of porosity. Values from this study from LB and FE simulations are shown as blue and brown circles, respectively. For comparison, laboratory data from the following studies are also plotted: Doyen, David and Darot, Fredrich et al., and Gomez et al..(RIGHT). Figure reproduced from Sun & Wang,

IJRMMS, 2018.

Our permeability calculation, shown in Fig. 2 is closer to the experimental measurements than previous numerical studies (most of which also used the LB method), especially when the porosity is below 10%. The improvement here may be attributed to several factors. First, advance in computation capability has allowed us to consider a unit cube of larger dimension, that more closely approximates a REV of the porous sandstone. Whereas we considered a sub-volume of 1903 voxels, Arns et al.35 started off with a sub-volume of only 1203 voxels, and to circumvent numerical issues related to percolation in the low-porosity regime, they had to "fine grain" the CT image by replacing each voxel by $2 \times 2 \times 2$ voxels with half the linear dimension. Second, difference in the LB methodology may have contributed to the discrepancy, but in the absence of more detailed description of their numerical procedure, it is difficult to assess this issue. Lastly, difference in segmentation algorithms can also result in subtle differences in pore geometry of segmented images, which would impact permeability values derived from LB simulations.

In our hybrid scheme, the pore-scale LB results were linked with FE simulation in a homogenized approach to compute and upscale formation factor and permeability tensor at specimen scale. White et al.15 have demonstrated the feasibility and effectiveness of such an approach for calculating the permeability of Castlegate sandstone (with porosity of 20–24%). Our study has shown that this hybrid scheme can be extended to calculating both effective permeability and formation factor of a porous sandstone, with porosities over a relatively broad range that is associated with an appreciable change in connectivity.

These results indicate that flow simulations at pore-scale could be used as a tool for predicting both formation factor and permeability of geological materials. This is significant also for the frozen soil problems where important material parameters such as relative permeability for the unfrozen water and the thermal conductivities might not be so easy to extract from experiments. In those cases, microCT images are not only useful to capture the growth of the ice lens and the freezing of the water in the pore space, but also for predicting the evolution of the effective material parameters as a function of porosity, temperature, confining pressure and microstructural attributes.

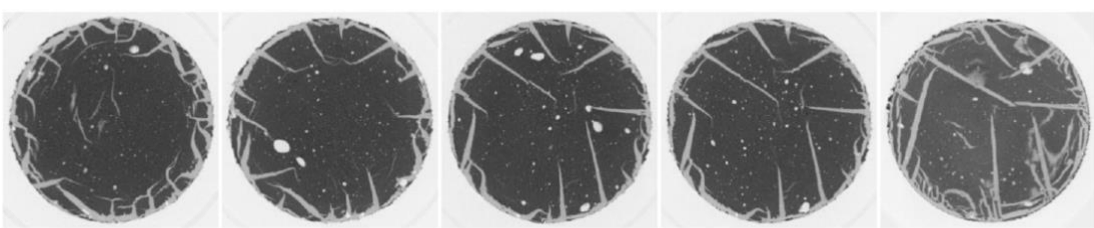

Figure 4: MicroCT images of ice crystral growth in chalk specimen. Figure obtained from collaborator Cino Viggiani

Currently, the PI is preparing a new set of theoretical work that incorporate an important set of experimental work where the growth mechanism of the ice crystal is captured in great details in a series of microCT images done by the Grenoble research group. The PI has obtained agreement between the researchers there to share their microCT images for future analysis, should the opportunity comes for future study on frozen soil.

<u>Brittle-ductile transition</u>

The test results from experiments also lead us to we to derive a framework that couples a phase-field description of fracture with pressure-sensitive plasticity, for encapsulating a wide range of failure modes of geomaterials from brittle fracture to ductile flow. Particular attention is paid to a realistic capture of the transition of these failure modes with changes in confining pressure and strain rate conditions. In the process of our development, several new contributions are presented to make the two-way coupling between phase-field and plasticity theoretically consistent and numerically robust. They include a microforce-based derivation of a phase-field model that honors the dissipative nature of the fracturing process, the dilative/compactive split and rate-sensitive storage of plastic work, and the use of phase-field effective stress for plasticity. The results are published in Choo and Sun, CMAME 2018 and summarized in Figure 5.

By coupling the phase field fracture model with a cap plasticity, we introduce a new approach where the brittle fracture, quasi-brittle damage, ductile fracture, shear banding and the diffusive failures in high confining pressure can all be simulated and predicted by ***one single model with the same material parameter.*** This consistency is critical for extending the frozen soil model for real-world application, as the formation of the ice will profoundly strength the materials such that the soil may exhibit rock-like behaviors. This is a very interesting problem. As the ice and solid grains may in that case behaves like a two-phase composite, the constitutive responses will become inherently anisotropic and heterogeneous.

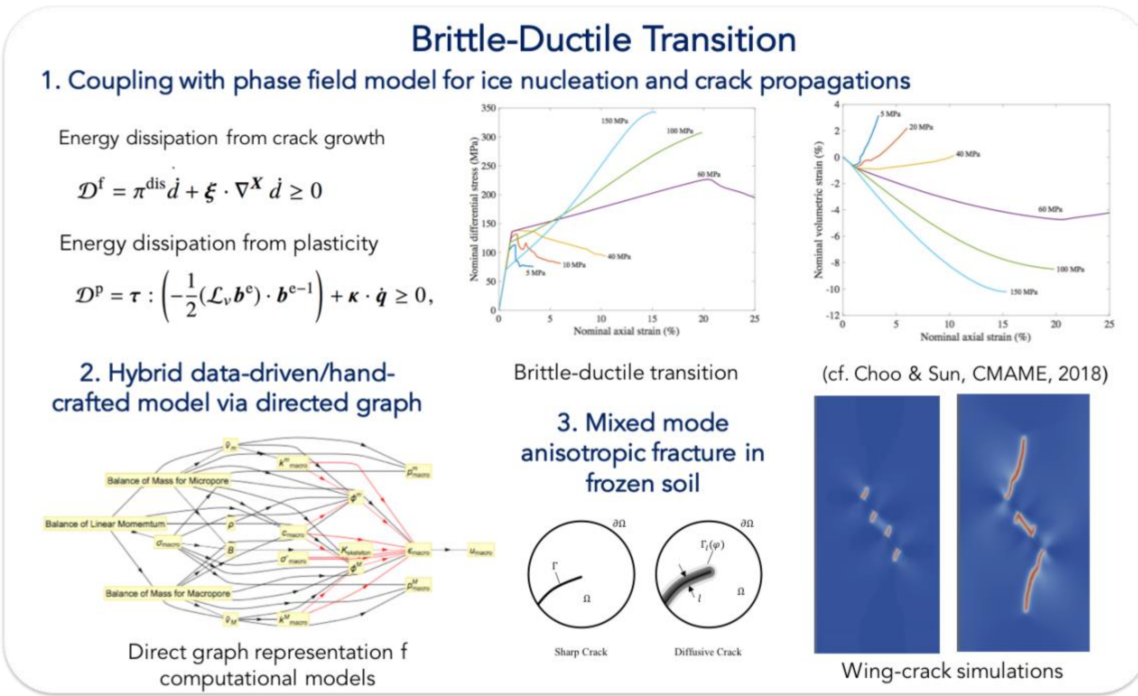

Figure 5: Modeling of brittle-ductile transition of geological materials. Figure reproduced from Choo & Sun, CMAME, 2018.

Key outcomes or other achievements:

From the scientific viewpoint, this work has led to 7 journal articles publication, 1 PhD thesis and 3 conference papers. This project is instrumental to the success of the PI and his students as exemplified by the following major honors the PI received since the beginning of the project. In particular, the PI is the only person who has ever won both the EMI Leonardo da Vinci Award from American Scoeity of Civil Engineers and the Zienkiewicz Numerical Methods in Engineering Prize from the United Kingdom Institution of Civil Engineers, both are the most prestigious honors for the respectively society that has age limits.

1. 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".

2. 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., Geothechnique, Geothechnique 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.

3. 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.

More importantly, the research group has successfully secured three tenure-track positon for three former members, PhD student SeonHong Na (McMaster University, Canada), Jinhyun Choo (the University of Hong Kong, Hong Kong) and Yang Liu (Northeastern University, USA). These results are the testimonial of the quality of the work of this research group.

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

1. K. Wang, 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]
2. Y. Liu, W.C. Sun, J. Fish, Determining material parameters for critical state plasticity models based on multilevel extended digital database, *Journal of Applied Mechanics*, 88(1), doi: 10.1115/1.4031619, 2015. [PDF][Bibtex]
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[PDF] [Bibtex] (PhD Student Yang Liu won 2015 best poster competition at USNCCM San Diego).

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