

PROJECT ABSTRACT

Ultra-Realistic Simulation and Visualization of Arctic Sea Ice Dynamics

The opening of the Arctic Ocean as sea ice recedes is accompanied by expanding navigational, scientific and economic opportunities. The new Arctic also presents more challenging competitive and national security environments, which put greater demands on the U.S. Navy and U.S. Coast Guard. A central challenge in meeting these demands and in advancing the science and economics of the Arctic Region is to improve our ability to simulate, predict and visualize key sea ice processes and the interaction of sea ice with various structures. A recently developed computational framework offers the potential to transform the simulation and visualization of Arctic sea ice dynamics, with its capability of accurately simulating rheologies ranging from fluid to solid. This mathematical and computational framework, based on the so-called Material Point Method (MPM), has been applied to simulating the beautiful yet varied dynamics of snow, yielding a new level of insight and predictability into the complex mechanics of avalanches and wet sand. What particularly distinguishes this approach, beyond adherence to the basic physics, is the striking, quantum leap in visual realism, as evidenced by the MPM-produced snow scenes in the Academy Award winning animated Disney film *Frozen*.

Here we propose to build an MPM framework for sea ice to bring this new level of realism, resolution and physical accuracy to modeling key dynamical processes in the Arctic ice pack, such as the formation of ridges and leads, and the interaction of ocean waves with sea ice. Such methods will also enable us to create realistic simulations of ships and submarines interacting with sea ice. As phase change and thermo-mechanical processes fall within MPM modeling capabilities as well, we will consider the freezing and melting of sea ice, such as pancake formation in a wave field and the evolution of surface ponding and floe break-up. We will develop an MPM framework designed to efficiently treat the wide range of material parameters, rheological characteristics, collisions, fracture, phase transitions and topological changes arising in complex sea ice scenes; to capture the essential physics and create *ultra-realistic* visual representations of these processes.

Extensive algorithm and software development will be key to building a realistic MPM framework for sea ice. However, there are other critical components of this framework which must be addressed, such as determining the constitutive equations describing the rheological behavior of sea ice over a range of length and time scales, and incorporating the results of field studies into the numerical simulations. As a material, sea ice is a multiscale polycrystalline composite of an ice host with brine and air inclusions. The ice pack itself has a complex multiscale structure of ice floes, typically covered with a snow layer, in an oceanic host. We will bring to bear advanced methods of mathematical homogenization to determining the effective rheological properties of these multiscale composite media, which are key inputs in the proposed sea ice MPM. Moreover, our project features participation in major field campaigns on Arctic sea ice dynamics, with access to extensive data on the scenarios we are simulating. MPM is particularly well suited to the efficient incorporation of these data into the models to achieve a new level of realism and accuracy.

The challenges we must confront in creating this new framework for simulating sea ice dynamics will lead to major advances in mathematical and numerical modeling of complex multiscale media with a broad range of rheological characteristics. This project has the potential to transform the modeling and visualization of sea ice processes, and provide a significant leap forward in addressing future naval, scientific and economic challenges in the Arctic Region.

Approved for Public Release

TECHNICAL PROPOSAL

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FY2019 VANNEVAR BUSH FACULTY FELLOWSHIP

DoD Technical Subject Category #5: **Applied Mathematics and Statistics**

Ultra-Realistic Simulation and Visualization of Arctic Sea Ice Dynamics

Bringing transformative mathematical and computational technology used to create ultra-realistic snow in Disney's movie *Frozen* to modeling and visualizing Arctic sea ice.

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Technical Proposal:
Ultra-Realistic Simulation and Visualization of Arctic Sea Ice Dynamics

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1 Statement of Objectives

The emerging dynamics of the changing Arctic marine environment are complex and highly variable, yet increasingly important to understand and predict as human activities in the region expand. The sea ice cover has bearing on almost any considerations of Arctic operations or studies of the polar marine system. However, much of the previous modeling work has treated sea ice at fine scales as a composite material, or on much larger large scales when incorporating it into climate models. Current large scale numerical models are generally unable to accurately simulate or resolve key processes in the formation, ridging, fracture, deformation, melting, and break-up of sea ice. This inhibits our ability to accurately predict the dynamics of the ice cover on scales of meters and kilometers in space and hours and days in time. These intermediate scale model studies of basic sea ice behavior and interactions can form the building blocks for fundamental advances in larger scale predictive models of sea ice dynamics. Such studies can also be pivotal in the strategic and tactical use of sea ice predictions for military and civilian operations in the Arctic.

Here we propose to directly address this intermediate range of scales by building a new MPM-based computational framework that we believe can revolutionize the mathematical modeling and visualization of sea ice dynamical processes. We will develop this framework with the objective of providing simulations and visual renderings of model dynamic scenarios that reach an unprecedented level of realism, resolution, and adherence to the physics. Reaching this new level of realism and accuracy will be facilitated by the assimilation of field data that we will have access to as well as gather ourselves. Moreover, we will employ advanced techniques of homogenization theory to compute, estimate, and bound the effective rheological behavior of sea ice on the smaller scales needed as input into the MPM framework, and in developing larger scale rheological models of sea ice from our intermediate scale studies.

Our initial focus will be to develop an efficient, user-controllable sea ice constitutive model integrated with a hybrid Eulerian/Lagrangian MPM to simulate ridge formation, fracture and lead development, the influence of waves, currents and winds, and the evolution of ponding and break-up. We will also study the interaction of sea ice with solid structures such as an icebreaker or a surfacing submarine. Toward these objectives, in particular, in the proposed research we will:

- Design novel thermo-mechanical constitutive models for multi-species interactions with sea ice, snow and water mixtures that are accurate at macro- and micro-scales.
- Explore the accuracy of rheological models for different scenarios and scale regimes.
- Develop novel MPM algorithms for discretizing and coupling water, snow and ice phases, as well as their fracture, failure, cohesion and related interactions.
- Employ homogenization methods to obtain constitutive equations for sea ice rheology on scales of centimeters to tens of meters as input into MPM; determine effective rheology of sea ice as a polycrystalline porous composite.
- Create GPU and HPC implementations of MPM discretizations that allow for simulations with 100 million to 10 billion particles, and extremely high visual resolution.
- Incorporate extensive observational data from the major field experiments MOSAiC and ONR SIDEx, and other Arctic sea ice data sets into the MPM computational framework.
- Participate in various field campaigns, obtaining video of dynamic sea ice processes (such as cracking and ridging, ice interaction with vessels, floes interacting in swell) for comparison with simulations.

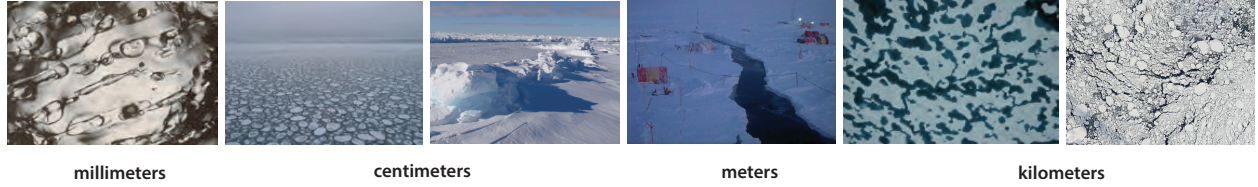


Figure 1: Ice pack building blocks – floes, ridges, leads and ponds. From left to right: millimeter scale brine inclusions [120]; centimeter scale pancake ice forming in a wave field (Golden); pressure ridge in sea ice (Golden); lead in Arctic sea ice (Perovich); Arctic melt ponds (Perovich); large scale view of the Arctic ice pack (NASA).

2 Research Effort

2.1 Introduction

Among the greatest scientific challenges of the 21st century are the observation, understanding, modeling and predicting the pronounced changes in Earth’s polar regions. In the Arctic Ocean, which has seen perhaps the most dramatic changes in recent years, the science, navigation and economics are often dominated by considerations of the sea ice cover. The Arctic ice pack is a key player in Earth’s climate system, it constrains military and commercial navigation, and is typically a critical factor in economic activity in the Arctic marine environment, such as in tourism and resource extraction. The recent losses in sea ice extent and thickness have created new opportunities in the region, which place greater demands on the military, and the U.S. Navy and U.S. Coast Guard in particular. An increasing level of military and civilian activities in the Arctic then requires significant advances in our ability to simulate and predict key sea ice processes and the interaction of sea ice with various structures such as ships and stationary platforms.

Here we propose to build the most advanced, most visually realistic and physically accurate computational framework to simulate and visualize key processes in the dynamics of Arctic sea ice. We believe such a project has the potential to significantly impact (i) our capability to predict the mechanical and rheological behavior of sea ice over a range of length and time scales, (ii) the science of the Arctic Ocean and the climate system, and (iii) the engineering of structures which must interact with sea ice. The idea is to initially focus on creating extremely high resolution, ultra-realistic simulations and visual renderings of the basic building blocks of sea ice dynamics, such as the formation of ridges and leads on the floe scale, the interaction of sea ice with waves, ponding and sea ice break-up, and a ship or submarine breaking through sea ice. We expect this work to provide a penetrating advance in our understanding and capability of predicting the mechanics and rheology of sea ice on *intermediate* length and time scales. Much of the modeling of sea ice conducted previously has concentrated on its fine scale behavior as a material, or on its coarse-grained representation in climate models. Here we focus on sea ice scenes on length and time scales relevant to what a person on a ship may observe. This type of research at these scales has generally not been a part of efforts ranging from canonical modeling of sea ice physical phenomena to how sea ice is represented and incorporated in general circulation models.

To achieve these objectives, the PI initiated a collaboration with Joseph Teran of UCLA, the principal creator and developer of probably the most advanced, realistic computational framework for simulating the dynamics of snow. This fascinating material is a key part of the sea ice system, and like sea ice exhibits a wide range of rheological behaviors from fluid to solid. Teran’s recent development of an extremely flexible, hybrid Eulerian/Lagrangian particle-based Material Point Method (MPM), has been used to revolutionize snow modeling. We believe this approach has the

potential to transform how we model sea ice.

The particles in Teran’s MPM are small pieces of a continuum model of the material under study. For sea ice – which displays complex composite structure over a wide range of length scales – these small pieces are composites themselves. As a material sea ice is composed of a pure ice host with a porous microstructure of brine and air inclusions on the submillimeter scale, a polycrystalline microstructure on the centimeter scale, and larger brine channels on the meter scale. As the rheological properties of these “particles” are key inputs into the MPM, the PI has involved Elena Cherkaev and Andrej Cherkaev in the Math Department at Utah for their expertise in the effective rheological properties of composites in general and porous media in particular. Pedro Ponte Castañeda of the University of Pennsylvania has expressed strong interest in this project and its close connection to his ONR-funded research on homogenizing the rheological properties of polycrystalline sea ice, and is happy to collaborate and contribute his valuable expertise.

Moreover, to achieve the new levels of realism and physical accuracy that we propose, it is critical for the success of this project to be able to incorporate data from observations of the processes and scenarios under study into the computational framework. Thus the PI initiated a collaboration with Jennifer Hutchings of Oregon State University, an expert in both modeling and measuring sea ice dynamical processes, and co-director of two of the most important Arctic sea ice dynamics field campaigns over the next few years, ONR SIDEx and the dynamics component of MOSAiC. Extensive field measurements of the mechanical and rheological properties of sea ice will be made. The PI’s colleague Donald Perovich of Dartmouth College, who is sea ice team co-coordinator on MOSAiC, has indicated his strong interest in and support of this project, and will act as a data liaison for us. We will have timely access to these critical measurements, and the data will be used to help us calibrate the models, determine the best parameters, and develop MPM-based data assimilation techniques in order to achieve the ultra-realism we seek.

In this project we will exploit the robustness and flexibility of the MPM approach and the range of fluid and solid rheologies that it can handle to bring an unprecedented level of simulation and visualization capabilities to basic sea ice processes. We will develop a modeling and computational framework that efficiently and deftly treats the wide range of material parameters, rheological behaviors, collisions, fracture and phase changes arising in dynamic and thermodynamic sea ice scenarios. We will create realistic simulations of a range of sea ice processes, on scales that have generally not been looked at in any depth.

We believe that this proposed project will indeed open a new chapter in sea ice modeling, with the potential to provide a major leap forward in addressing one of the central challenges that the U.S. Navy and U.S. Coast Guard face in meeting increased demands of the changing Arctic. Finally, this project will offer the postdoctoral, graduate, and undergraduate investigators unique and unusual learning experiences at the exciting interface of cutting edge applied mathematics, transformative computational methods, mechanics of composite materials, and Arctic field science. With the direct connection of the proposed work to the Academy Award winning Disney movie *Frozen*, and our focus here on visual realism, we anticipate that the future success of this project could become a focal point of outreach to students and the general public regarding DoD research and its impact on matters of public, as well as academic and military interest.

2.2 VBFF Senior Personnel

Kenneth Golden (PI) is a Distinguished Professor of Mathematics and Adjunct Professor of Biomedical Engineering at the University of Utah. He contributes expertise on multiscale model-

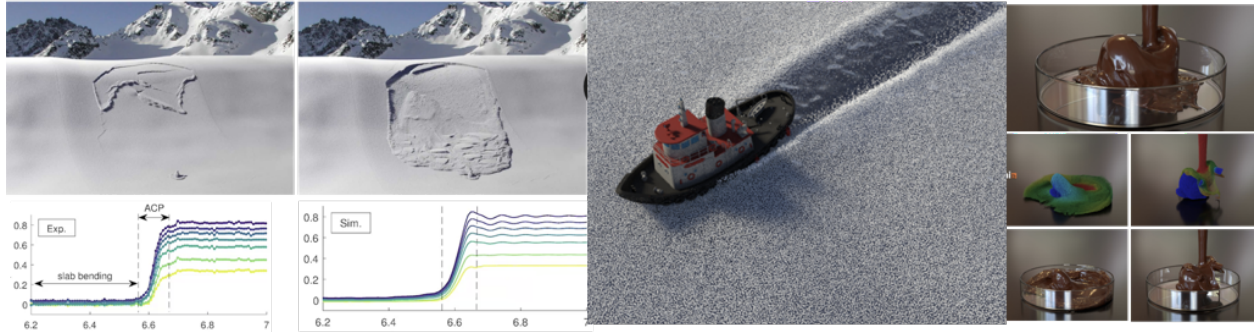


Figure 2: MPM simulation of snow, ice and phase change. Left: Teran *et al.* (2018) developed a novel constitutive model for remotely triggered avalanches. Left top: Slope scale simulation of avalanche with 30 million particles. Left bottom: Plot shows that the model reproduces experimental field data with a comparison of snow slab bending and failure. Middle: Initial MPM simulation with one hundred thousand particles of an ice breaker interacting with ice/snow on top of water. Right: Teran and colleagues (2014) demonstrate successful simulation of phase change with a thermo-mechanical MPM approach and a simulated molten chocolate example.

ing of composite materials, particularly sea ice, using mathematics of homogenization, stochastic processes, inverse problems, statistical mechanics and phase transitions. Golden has substantial field experience since 1980 in measuring dynamic, thermodynamic and transport properties of sea ice in the Arctic and Antarctic, from ice breakers and ice camps. He has led several large, multi-university, multi-disciplinary sea ice-related projects funded by ONR and NSF since the 1990s.

Joseph Teran is a Professor of Mathematics at the University of California, Los Angeles. He contributes expertise in scientific computing, parallel computing, Material Point Method algorithm design, elastoplastic constitutive design, porous mixtures of liquid and granular materials, as well as inverse problems for determining material parameters from observed data. Teran has written over 40 research papers since 2003, with 11 related to simulating snow and similar materials with the Material Point Method. Teran is a former ONR Young Investigator and PECASE awardee.

Jennifer Hutchings is an assistant professor in the College of Earth, Ocean, and Atmospheric Sciences at Oregon State University. She has over 20 years experience in modeling and observation of sea ice dynamics and mechanics. This includes leading field campaigns to inform sea ice dynamics models. Through her leadership roles she will be a direct liaison with upcoming campaigns including ONR SIDE_x and MOSA_iC.

Andrej Cherkaev is a Professor in the Department of Mathematics at the University of Utah. He is an expert in variational methods for composite materials, optimization and optimal structures, damage propagation, and dynamics of multistable solids. He has published two books and more than a hundred papers. He will contribute his expertise toward sea ice homogenization on various scales, modeling of floe fracture, lead formation, and the dynamics of crack propagation.

Elena Cherkaev is a Professor in the Department of Mathematics at the University of Utah. She is a specialist in inverse problems, numerical methods, optimization, and composite materials and is author of more than ninety publications dealing with large scale inverse problems, damage and wave propagation, and mathematical and numerical modeling of heterogeneous materials. She contributes her expertise in analysis and homogenization of sea ice, in particular, in effective viscoelastic behavior and other rheological properties.

2.3 Background

2.3.1 Numerical Modeling of Sea Ice Rheology and Dynamical Processes

Sea ice moves under the influence of ocean currents and winds. On time scales shorter than days the largest terms in the force balance are wind stress τ_a , ocean drag τ_o , inertia and the divergence of the ice stress σ . We can ignore body forces due to gravitational acceleration down the sea surface and the Coriolis force on the intermediate scale. Typically ice is considered to be a thin plate, and the forces and stresses are depth integrated, resulting in an equation for the momentum balance,

$$m \frac{D\mathbf{v}}{Dt} = \tau_o + \tau_a + \nabla \cdot \sigma, \quad (1)$$

where m is ice mass, \mathbf{v} is ice velocity and t is time. The stresses at the upper and lower ice surfaces are estimated with boundary layer parameterizations and weather/ocean model winds and currents. In 2-D models the tensor σ has two principle stresses. These models describe how the mass of sea ice is distributed with a thickness distribution function, and a transport equation tracks changes in area of ice of a given thickness through melt, growth and mechanical redistribution via ridging or opening of leads. Our proposal to produce visually realistic simulations of ice dynamics requires that we simulate these processes with a 3-D representation of ice in the ocean, where τ_o and τ_a are applied to the upper and lower boundaries of the simulation and are zero inside the material. The internal ice stress is given by the second-order Cauchy stress tensor, with 3 normal stress components and 6 shear stress components. The ice mass must obey a continuity equation

$$\frac{Dm}{Dt} - m \nabla \cdot \mathbf{v} = F, \quad (2)$$

where F is a thermodynamically governed rate of ice melt or growth, which tracks the changing density of ice as its structure evolves and changes phase, and \mathbf{v} is ice velocity.

In modeling the kinematics and stress state of sea ice and snow one needs to relate the deformation, or strain rate $\dot{\epsilon} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$, to the stresses in the ice or snow pack. This relationship can be viscous, elastic and/or plastic and is modeled with constitutive relationships expressed as a rheological model, that aggregates behaviour over defined scales, or through expressions describing particle interaction.

Typically, modeling the intermediate scale has been performed to support civil engineering projects. Various approaches have been effective, recently using hybrid finite element and discrete methods [74, 64]. Previous efforts have focused on idealized simulations with the discrete element method (e.g. [57, 56, 123, 85]) and engineering problems tackled with Particle-In-Cell (PIC) methods (e.g. [41, 5, 100]). These methods either assume a continuum that requires a rheological model relating stress to strain that is homogenized to the model resolution or they are discrete methods that assume viscous, elastic and/or plastic behavior when particles of ice interact. Discrete methods are computationally expensive and require reinitialization for simulations longer than several days, however they are effective at modeling granular and plastic behavior and can be used as a research tool to identify appropriate constitutive relations for continuum models (e.g. [102]). Continuum approaches are computationally cheaper and should be employed where homogenization of the stress-strain relation is appropriate. The PIC models took advantage of the homogenized nature of the viscous-plastic rheology [52, 53] (which arguably is not appropriate at the scale of ice-structure interaction) to increase efficiency of numerical solution of sea ice momentum balance while allowing precise representation of discrete features in the ice pack such as the ice edge.

Previous modeling efforts have been limited by uncertainty in rheological relationships for the intermediate scale and a lack of validation data for these models. In this proposal we introduce a

novel approach addressing this. Advances in computer technology now support modeling at scales previously not achieved for sea ice except in limited DEM experiments [118]. We will use the Material Point Method (MPM), with such high resolution and large numbers of small scale particles that for the scenarios we initially investigate we have much more certainty and methods of analysis of the relevant homogenized rheology for polycrystalline sea ice with porous microstructure. MPM been applied on much larger scales for sea ice [110] and is an improvement on the older PIC methods. MPM enables unique strategies for modeling compared to previous Lagrangian or semi-Lagrangian methods, such as mixed phase/media modeling and efficient 3-D simulation. We believe MPM will initially be appropriate for meter to km scales as the homogenization methods we will employ will be valid for ice structure at these scales.

To date models have treated water, ice, snow and air as separated from each other, handling their interaction as fluxes between these constituents controlled by parameterized processes that do not resolve spatio-temporal variability at intermediate scales. Three dimensional MPM simulations will allow us to resolve these interactions directly in mass and momentum transfer between constituents. Developing such models will provide test beds for designing larger scale models, in particular providing avenues for testing candidate constitutive models for meter to sub-km scales.

2.3.2 Material Point Methods

The Material Point Method [109] was designed as a generalization of Particle-In-Cell (PIC) [49] and Fluid Implicit Particle (FLIP) [13] to history dependent materials such as elastoplastic granular solids. Particle-In-Cell techniques of this type are characterized by their hybrid usage of unstructured particles and structured regular grids. The hybrid nature allows for efficient resolution of topology change, e.g. for fracture and failure as well as automatic resolution of self contact and multi-material interactions. These aspects of PIC, combined with the algorithmic insights of the history dependent MPM developers [109] make these techniques ideally suited to computational problems related to a wide range of materials and time scales. Teran *et al.* have proven that MPM is capable of simulating snow and ice for both primarily visual applications like Walt Disney’s “Frozen” [107] as well as engineering applications like avalanche modeling in *Nature Communications* [42]. Given the abundance of multi-material interactions between water, sea ice and snow during ocean wave propagation in marginal ice zones as well as the fracture/failure and multi-material contact incurred during formation of ridges and leads, we believe MPM based techniques can provide a revolutionary improvement in simulation technology for these materials, particularly in visual and spatial resolution accuracy. Furthermore, melt pond evolution and other thermo-mechanical behaviors can be easily incorporated into MPM, as was done by Teran *et al.* [108].

Despite the natural advantages of MPM approaches for simulating snow and related materials, novel algorithmic improvements are needed to model problems in sea ice dynamics. In particular, while the unstructured particle nature of the approach allows for automatic resolution of topology change with fracture/failure, it is difficult to isolate individual cracks and fissure. Ironically, since the method automatically resolves these phenomena, it cannot detect exactly where they are. We will develop algorithmic modifications to MPM that allow for explicit tracking and modeling of cracks and fissures. A natural way to do this is by augmenting MPM with a Lagrangian mesh, as was done in [65]. This removes MPM’s natural treatment of topology change by computing spatial derivatives with the help of the Lagrangian mesh, albeit while enslaved in an updated Lagrangian manner to grid based degrees of freedom during the momentum update stage. However, fracture and failure can be introduced in a controlled manner via damage and plasticity in the

Lagrangian mesh. Another challenge is resolving wide ranges of stiffness in the encountered materials. Implicit time stepping is particularly challenging with elastoplasticity since the linearization of the systems of equations arising in implicit time stepping are not symmetric (by virtue of the plasticity). Resolving these aspects in a manner that is both accurate and that scales well with HPC will be a challenging aspect of the work.

2.3.3 Homogenization for Rheological Properties of Composite Structures

Mechanical behavior and effective properties of heterogeneous materials depend on their constituents as well as on the microstructure. There has been extensive work in the past on estimating and bounding the effective properties of composites. The classical variational Hashin-Shtrikman-Walpole bounds [50, 51] derived in the 1960s were significantly improved by Cherkaev and collaborators who developed a powerful translation method [78, 79, 77] for finding optimal bounds on the elastic energy stored in a composite, which generate optimal bounds for the effective stiffness C^* and compliance S^* of the composite:

$$W_\epsilon(\epsilon_0) = \epsilon_0 : C^* : \epsilon_0 = \min_{\epsilon : \langle \epsilon \rangle = \epsilon_0} \langle \epsilon_0 : C : \epsilon_0 \rangle, \quad \text{and} \quad \epsilon = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2, \quad (3)$$

$$W_\sigma(\sigma_0) = \sigma_0 : S^* : \sigma_0 = \min_{\sigma : \langle \sigma \rangle = \sigma_0} \langle \sigma_0 : S : \sigma_0 \rangle, \quad \text{and} \quad \sigma = \sigma^T, \quad \nabla \cdot \sigma = 0. \quad (4)$$

Here \mathbf{u} is material displacement and ϵ and σ are tensors of strain and stress, respectively, and ϵ^0 (σ^0) is a constant strain (stress) tensor. The fourth order tensors $C(\mathbf{x})$ and $S(\mathbf{x})$ are the spatially varying stiffness and compliance tensors which depend on the properties of the phases. The characteristic function $\chi = \chi(\mathbf{x})$ takes the value 1 if $\mathbf{x} \in \Omega_1$ and zero if $\mathbf{x} \in \Omega_2$, where Ω_2 is region occupied by the second phase.

Various methods for calculating the effective properties from known microstructural information have been developed using the variational approach and asymptotic homogenization theory [98, 67, 84]. An alternative approach to deriving rigorous bounds on the effective complex permittivity ϵ^* of composites is the analytic continuation method, where the effective parameter is treated as an analytic function of the ratio of the component parameters [82, 8, 66, 43]. These bounds assume that the complex permittivities ϵ_1 and ϵ_2 of each component are known and that there is some partial information available about the microstructure. The method is based on a Stieltjes integral representation for the function $F(s) = 1 - \epsilon^*/\epsilon_2$, $s = 1/(1 - \epsilon_1/\epsilon_2)$, which is analytic off $[0, 1]$ in the complex s -plane, involving a positive measure μ which is the spectral measure of a self-adjoint operator $\Gamma\chi$, with $\Gamma = \nabla(-\Delta)^{-1}(\nabla \cdot)$, and Δ the Laplacian operator. The analytic continuation method was extended to viscoelastic shear modulus in [10, 28, 87, 25] with the operator Γ changed to the corresponding operator related to elasticity.

2.4 Formulation

2.4.1 Sea Ice Rheology

In modeling the motion of deforming solid materials, a rheological model is required to relate strain in the material to its internal stress field. This stress is described by a Cauchy stress tensor σ , and this is estimated as a function of strain or strain-rate and material properties such as Young's modulus, viscosity and the yield stress at which plastic failure occurs. These constitutive relationships are often found empirically in laboratory experiments, and such an approach is successful for simulating sub-meter scale processes. On larger scales it is not possible to measure stress and strain over the same scales such that an empirical rheological model can be developed. Hence past efforts have relied on co-opting models from different scales (e.g. [55]) or making *ad-hoc*

assumptions regarding the isotropic or anisotropic nature of sea ice, compressive strength of ice being approximated by its thickness [53], or ice having no tensile strength and obeying an isotropic yield relationship. Some of these assumptions are still open to debate or are suggested to be flawed [33], and it is not well defined what a suitable constitutive relation should be for intermediate or larger scales. The most commonly used rheological model for sea ice is the viscous-plastic (VP) model [53]. However a variety of models have been developed to handle proposed anisotropy in the sea ice yield stress [117, 122, 103] or to simulate brittle fracture (e.g. the elastic-brittle model [92]) which is more realistic compared to the ductile yielding implied [114, 52] by the VP model.

For continuum models we require that the stress field is described by an average stress at the model resolution. For other materials, homogenization approaches have been successful in identifying such relationships, however it is important that the material strain is not discontinuous within elements. This suggests these methods are appropriate when the resolution is orders of magnitude smaller than the size of ice floes, which varies from kilometers in the consolidated winter ice pack to centimeters in the marginal ice zone. In such a rheology the mean stress across an element is related to material properties and the strain ϵ . For plastic materials the yield stress is described as a curve or surface in principle stress space, which for large scale 2-D sea ice simulations might be assigned as either the cone described by Mohr-Coulomb theory [116, 55], a tear-drop shape based on (potentially flawed [93]) energetic considerations in ridging of ice [95], an ellipse for analytic and computational efficiency [53], or sine lens shaped based on homogenization over randomly orientated cracks [119]. This variety, and uncertainty in which models to apply, highlights unknowns in sea ice mechanical properties at large scales that are difficult to resolve with observations and current knowledge. At sub-meter scales we can identify material properties in the laboratory, in the field, or using homogenization, and these properties can be reasonably scaled up to tens of meters (e.g. [36]). We can take advantage of recent advances in computation to resolve the small scales for which we have knowledge to simulate the intermediate scale.

At the smaller intermediate scales the vertical and horizontal dimensions of pack ice become similar and 3-D models are more appropriate than the thin plate approximation for the stress field used to justify 2-D models at larger scales. Observational evidence [104] suggests a Mohr-Coulomb relationship, with a cap representing the ice strength to normal stress, is suitable at sub-meter scales. This behaviour can be scaled to tens of meters [6, 37] and has been used to model ice-structure interaction [99, 64]. Hence we will take this as a starting point for our simulations, recognizing a caveat that under some confining stresses ice failure might occur in other modes not indicative of Coulombic faulting [97] or that brash (non-consolidated small ice pieces) might collectively be better represented by a Von-Mises yield criteria [101].

We assume sea ice can be treated as a continuum at scales an order of magnitude smaller than floe dimensions and that it is a quasi-brittle material, following [7], with elastic behaviour prior to yield. Cracking can be represented through weakening of the ice on yielding, and freezing accounted for by temperature and time dependent strengthening. Slip-stick behavior is observed in fractured ice that indicates frictional processes are rate and temperature dependent on times scales of seconds, suggesting healing at low strain rates and weakening at higher strain rates [75]. Values for Young's modulus and the compressive, tensile and flexural strength of sea ice are found to be temperature and ice structure dependent [113]. The temperature and time dependence have not been considered directly in simulations of ice interaction before, we will use this observed information (reviewed in [113], friction angle informed by [63]) to inform parameter choice to realistically simulate deformation with synoptic to seasonal variability in material properties. Along

any plane in stress space the shear stress τ can be related to normal stress σ_N as $\tau = \sigma_N \tan(\phi) + c$, where ϕ and c are the material properties friction angle and cohesion, respectively. At yield the material can deform, and the rate of deformation is described by a flow rule that relates yield stress to strain rate. Typically this flow law is taken to be an associative law where strain is normal to the yield curve, though we will consider a non-associative flow law that allows for dilation in shear by setting strain normal to a cone defined by a dilation angle $\delta \neq \phi$. Within the yield curve we expect the behaviour is linear elastic $\boldsymbol{\sigma} = C\boldsymbol{\epsilon}$, where C is a stiffness tensor. This assumption will be tested by the SIDEx team who we expect will provide insight into the nature of C .

2.4.2 Material Point Method

Continuum model: The thermo-mechanical governing equations arise from conservation of mass, momentum, as well as heat transfer,

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v} \quad (5)$$

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}^b + \mathbf{f}^s \quad (6)$$

$$\rho \frac{Du}{Dt} = -\nabla \cdot \mathbf{q}, \quad \mathbf{q} = \kappa \nabla T, \quad c = \frac{\partial u}{\partial T}. \quad (7)$$

Here \mathbf{f}^b is the material body force (e.g. gravity), \mathbf{f}^s is stress applied along the material boundaries (e.g. wind and ocean drag), ρ is the mass density, \mathbf{v} is the velocity, $\boldsymbol{\sigma}$ is the Cauchy stress, u is the stored heat energy per unit mass, T is the temperature, \mathbf{q} is the heat flux, κ is the heat conductivity and c is the heat capacity per unit mass. The stress can often be expressed in the form $\boldsymbol{\sigma} = \frac{1}{J} \frac{\partial \Psi}{\partial \mathbf{F}^E}(\mathbf{F}^E, T) \mathbf{F}^{E^T}$, where $\Psi(\mathbf{F}^E, T)$ is the potential energy density, $J = \det(\mathbf{F})$ is the determinant of the flow map Jacobian \mathbf{F} and where \mathbf{F}^E (\mathbf{F}^P) is the elastic (permanent) part of the material deformation $\mathbf{F} = \mathbf{F}^E \mathbf{F}^P$. This decomposition is consistent with plastic deformation, mathematically we use the decomposition to satisfy a yield condition on the stress, $f(\boldsymbol{\sigma}) \geq 0$. We will design novel thermo-elastoplastic models capable of reproducing experimental observations of the formation of ridges and leads, ocean wave propagation in marginal ice zones, melt pond evolution and more. As noted by Hibler [54] and Feltham [40], sea ice constitutive modeling is an open and challenging area of research involving various aspects of engineering and physical and mathematical rigor. For example, sea ice is isotropic at large time and length scales, and such an assumption can greatly simplify the definition of the elastic potential and yield criteria. Feltham has shown that some evidence suggests sea ice cannot withstand tensile stress and that the yield surface can be accurately approximated by an isotropic model defined in terms of an ellipsoidal region in compressive/shearing stress space. However, other evidence suggests anisotropic models are necessary at more general scales, which can complicate the model considerably. Furthermore, although we primarily discuss elastic aspects, viscous stress must also be incorporated into the model (Hunke et al. [61]). Notably, Teran *et al.* [42] have designed an elastoplastic formulation for snow and anticrack propagation in weak layers exhibited by remotely triggered avalanches (see Figure 2). This appeared in *Nature Communications* and was recently highlighted in *Wired Magazine*. We will build on these efforts to complete the proposed model.

To resolve the composite behavior of sea ice as mixture of air, water, snow and ice, we will also incorporate aspects of multispecies porous media. This requires some modifications to the governing equations where mixture theory is used to incorporate volume and mass fractions of the different species and to resolve the momentum, mass and energy exchanges. MPM is well suited

for these types of problems, as Teran *et al.* have shown [112]. To model the distinct phases as well as the collective behavior of the mixture, one first introduces individual kinematics and dynamics of each phase, where each material is responsible for its own flow map, mass density and stress states [2]. The species dependent generalization is indicated with a superscript α where the $\alpha = 0$ indicates liquid water, $\alpha = 1$ indicates ice, $\alpha = 2$ indicates air and $\alpha = 3$ indicates snow. For example, the velocity of phase α is \mathbf{v}^α . The mass and momentum of phase α is given by ρ^α and $\rho^\alpha \mathbf{v}^\alpha$ respectively. The total mass density of the mixture is the sum $\rho = \sum_\alpha \rho^\alpha$ and total momentum is the sum $\rho \mathbf{v} = \sum_\alpha \rho^\alpha \mathbf{v}^\alpha$. Each species obeys conservation of mass with respect to its own motion $\frac{D^\alpha \rho^\alpha}{Dt} + \rho^\alpha \nabla \cdot \mathbf{v}^\alpha = 0$, which by summing over α implies conservation of mass of the mixture. Each species also obeys conservation of linear momentum as $\rho^\alpha \frac{D^\alpha \mathbf{v}^\alpha}{Dt} = \nabla \cdot \boldsymbol{\sigma}^\alpha + \mathbf{p}^\alpha + \rho^\alpha \mathbf{g}$ where \mathbf{p}^α represents the transfer of momentum due to the relative motion of the constituents, $\boldsymbol{\sigma}^\alpha$ is the partial stress tensor associated with species α , and \mathbf{g} is the gravitational acceleration. Summing over α yields conservation of linear momentum for the mixture $\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}$, where $\boldsymbol{\sigma} = \sum_\alpha \boldsymbol{\sigma}^\alpha$ is Cauchy stress.

MPM discretization: In MPM, the discrete state consists of a collection of particles that partition the domain based on initial volumes V_p^0 , with time t^n , positions \mathbf{x}_p^n and with masses m_p computed from the initial mass density as $\rho(\mathbf{x}_p^0, t^0) V_p^0$, and linear and affine velocities $\mathbf{v}_p^n, \mathbf{C}_p^n$ used for APIC particle/grid transfers [65]. Each particle additionally stores the elastic portion of the deformation gradient $\mathbf{F}_p^{E,n}$ and yield surface size τ_{Cp} . An MPM time step from time t^n to t^{n+1} typically consists of three steps: (1) mass (m_p) and momentum ($m_p \mathbf{v}_p^n$) are transferred from particles to grid using weights ($w_{ip}^n = N(\mathbf{x}_p^n - \mathbf{x}_i)$) defined by Eulerian grid interpolating functions $N(\mathbf{x})$ that describe the degree of interaction between particle p and grid node i , (2) the grid momentum ($m_i^n \mathbf{v}_i^n$) is then updated in a variational way from the potential energy in the system, and finally (3) the motion of the grid under the updated momentum is interpolated to the particles. In step (2), the deformation gradient is stored per particle and is updated using an updated Lagrangian view. With this assumption the deformation gradient is computed as the product of the time t^n deformation gradient \mathbf{F}_p^n and the deformation of the grid (evaluated at the particle) over the time step $\hat{\mathbf{F}}_p^{n+1} = (\mathbf{I} + \sum_i \mathbf{v}_i^{n+1} \nabla w_{ip}^n)$ where $\nabla w_{ip}^n = N \mathbf{x}(\mathbf{x}_p^n - \mathbf{x}_i)$ is the derivative of the grid interpolating functions.

2.4.3 Homogenization of Multiscale Composites

Sea ice is a multiscale multiphase highly anisotropic composite material with complex structure on many length scales. Its rheological response depends on a variety of different factors [62, 37, 39], it varies depending on the scale, on the state of the microstructure as well as on previous deformations and damage events. It also depends on the time of the season. For instance, the winter ice pack could be modeled as a solid plate with a random distribution of cracks, but in summer, the network of leads results in viscoplastic behavior.

Homogenization theory provides results that can be applied to sea ice at small scales. Sea ice is a polycrystalline composite material of pure ice with brine and air inclusions. The effective properties of such polycrystalline composites (or bounds for them) can be calculated using variational methods [50, 51, 98, 46, 21, 17, 83, 18] or Stieltjes integral representations [82, 66, 43, 44, 28]. Nonlinear homogenization methods have been developed [89, 91, 72] that use linear comparison media or estimate the effective behavior using low-order statistics of the microstructure [34]. These results should be incorporated into the mesoscale models that account for the relevant physics, geometries and thermodynamics as well as the modes of damage [54, 55, 16, 76]. For instance, in columnar ice, with highly anisotropic elongated grains which easily glide along basal planes

[1, 38], this microstructure strongly influences the macroscopic response and the rheological properties of sea ice, as well as the direction and propagation of cracks.

2.5 Proposed Research

Sea ice and snow exhibit a broad range of rheological behaviors depending on length and time scale, temperature, forcing structure, and other factors. These complex media can maintain their shape elastically, but can also fracture, fail or even flow like a granular or fluid medium with sufficient loading. We will create a flexible, particle-based computational framework that can accurately simulate key sea ice processes and interactions, that is highly faithful to the physics, and can provide extremely realistic visual renderings. This framework will be able to encompass a range of relevant rheological behaviors, from fluid to solid, with temperature determining phase changes. We will develop a new thermo-mechanical model capable of producing simulations that accurately recreate – physically and visually – observed phenomena. We will develop novel Material Point Methods to discretize our model. The MPM is a Particle-In-Cell technique designed for history dependent materials. It is very efficient for simulating elastoplastic and related rheologies, and it naturally resolves large deformation, plastic straining, fracture, failure, cracking and coupling with varied materials. Despite its history with these types of materials, we will develop novel MPM’s with unprecedented spatial and visual resolution.

2.5.1 Dynamical Scenarios

We propose to investigate, in detail, several typical processes and scenarios in the dynamics and thermodynamics of Arctic sea ice. As we develop our MPM framework, these are the examples that we keep in mind to simulate and visualize with extreme accuracy and realism. The structures and scenarios we consider will serve as building blocks for larger scale models and simulations.

As a material, sea ice is a polycrystalline composite of pure ice with brine and air inclusions, with effective rheological properties depending on spatiotemporal scales. As winds or currents force sea ice convergence, pressure ridges form, and with divergence and shearing, leads open up. Here we propose to initially focus in on smaller intermediate spatiotemporal scales and consider the interaction of two or three floes on the scale of 10 m – 100 m each. With forces driving the floes together we will study in depth the process of floe collision, material failure, and pressure ridge formation. Likewise, with floes subjected to divergent or shearing forces, we will study in depth the process of floe cracking, material failure, and lead formation.

A wave field can break up sea ice floes, or create large fields of “pancakes” that can accrete into large floes, as shown in Fig. 3. The interaction of ocean waves with sea ice in various forms is of great interest, and the mix of species (water, sea ice, snow, frazil, pancakes) and types of dynamics in these scenes is particularly well suited to the MPM framework we will develop. Subjecting a large unbroken floe to an incident ocean wave, where the floe may have uniform internal structure from quiescent congelation growth or may be formed from “gluing” together smaller floes, will yield fascinating pattern and size distributions of broken pieces. By considering suspensions of frazil ice crystals in a wave field we will be able to simulate the process of pancake formation, which is increasingly prevalent in the Arctic with increasing waves and areas of open ocean.

Typically, sea ice has a layer of snow on top which is important mechanically, thermally, and electromagnetically. The snow may be saturated with brine or sea water, like wet sand, and melting snow forms the iconic blue ponds on top of summer Arctic sea ice as in Figure 1. While numerical simulations of melt pond evolution used in large scale climate models keep track of melt water volume, they do not typically produce digital versions of melt ponds on Arctic sea ice that are

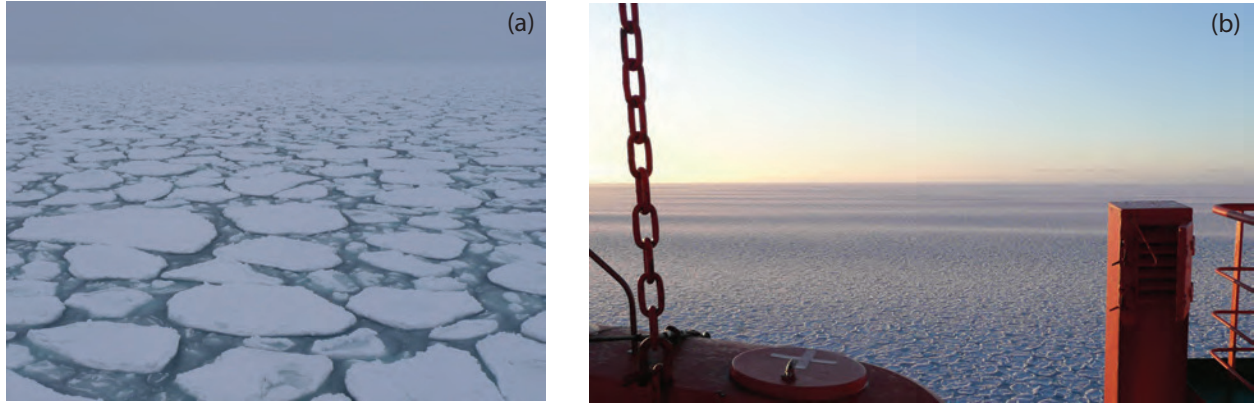


Figure 3: (a) Sea ice broken into floes in the marginal ice zone (Golden). The larger floes are 2 to 3 meters across, and are separated by frazil ice. (b) A field of pancake ice interacting with ocean swells in the marginal ice zone (Golden). The larger floes in the foreground are approximately 1 meter across.

physically and visually accurate representations of real ponds. With the thermo-mechanical MPM framework we propose, we will be able to simulate processes such as the evolution of melt ponds, the formation of snow-ice – the freezing of snow on the ice surface saturated with brine or sea water, and the break-up of rotted, highly porous sea ice saturated with melt water and sea water. We remark that by changing the range of scales and zeroing in on the brine microstructure over a sample of few centimeters, we should be able to simulate – and visualize – the detailed thermal evolution of the brine microstructure and its geometrical and fluid transport characteristics [45].

Not so dissimilar from two ice floes colliding is another class of scenarios that we will focus on, namely, the interaction of ships, submarines and stationary structures with sea ice. As we develop the MPM framework for sea ice interactions, these types of simulations will be within the capabilities of our computational advances. Given the data assimilation techniques that we will develop along with the MPM framework, we expect our simulation, optimization, and visualization capabilities to impact the engineering of structures that are designed to interact with sea ice.

2.5.2 Material Point Method for Sea Ice

While MPM has been used with great effect to simulate snow and other granular materials and mixtures, much work remains to develop a technique capable of achieving the realism desired for the proposed effort. The primary obstacles are (1) development of techniques capable of scaling up to hundreds of millions and even billions of particles, (2) development of novel rheological models, including homogenization considerations that are capable of simulating mixtures of air, water, ice and snow over a wide range of scales, include thermo-mechanical effects, (3) fitting parameters of these models to Arctic sea ice data generated from MOSAiC, ONR SIDEx, and other sources.

Teran has developed many parallel computing techniques for MPM simulations. Indeed every paper written in the Teran Lab related to MPM uses either manycore or GPU level parallelism. Parallelism where kernels scale in tens of cores is necessary for running simulations at high resolution, with many hundreds of thousands up to a few tens of millions of particles. However, manycore and GPU approaches do not have sufficient cores or memory to run simulations at the scale desired in the proposed effort. For example, consider the simple one meter cubed block of snow simulated in Figure 4. 610,000 particles are used to represent the block, this is less than one particle per cubic centimeter. The bulk behavior on the scale of meters is resolved, however we would like to achieve

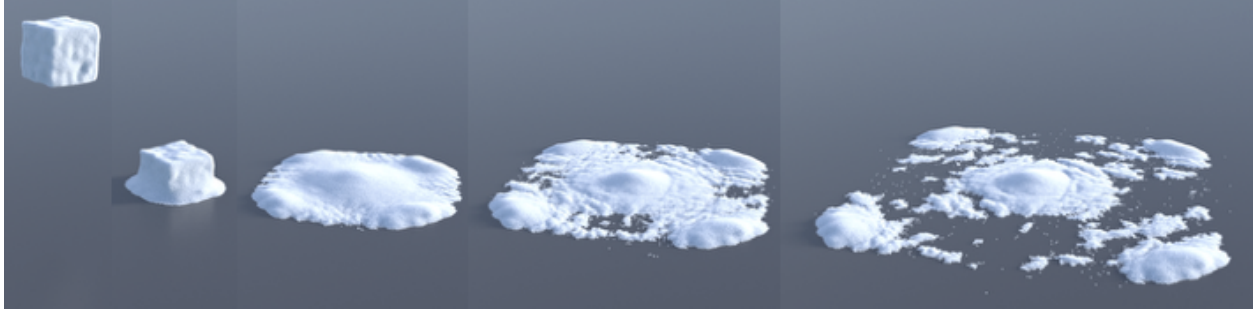


Figure 4: MPM simulation: manycore. We simulate a cubic meter block of snow falling onto the ground with MPM. The simulation was run on an Intel Xeon E5-2690 V2 system with 20 threads and 128GB of RAM. Our techniques scale well up to 20 threads which allows us to simulate the block with a total of 610,000 particles. Our simulation was done with less than one particle per cubic centimeter.

resolution down to the sub-millimeter scale for simple scenarios such as this. Furthermore, at the centimeter scale, we would like to simulate many tens or hundreds of cubic meters of material. In order to provide this performance capability, we will need to use HPC involving multiple machines. We will generalize prior approaches developed in the Teran Lab to this hardware setting and leverage resources at the UCLA IDRE and U. of Utah SCI computing centers.

While Teran and collaborators have developed techniques that include thermo-mechanical and multispecies effects, they have not done so with the level of complexity required in the proposed effort. Furthermore, inclusion of homogenization effects and non-continuum related aspects will require novel treatment. The Teran lab will use much of their existing computing infrastructure to provide this functionality, however many novel algorithmic and modeling advances will be required. The Teran Lab’s existing computing experience and computing infrastructure will provide a strong starting point for these developments.

In order to develop models and simulation techniques capable of reproducing ice floes, ridging, cracking and related phenomena, our models will have to have many tens or even hundreds of rheological parameters. While the flexibility engendered by a wide range of parameters is necessary, it comes at the cost of complicating the process of fitting the model to data. We will have access to a wide range of kinematic and physical data from the MOSAiC and ONR SIDEx projects and it will be critically important that we can choose our parameters so that we can reproduce the observed data. We will develop novel techniques that allow us to do this. We will use traditional approaches such as casting the parameter estimation as an optimization problem as well as using more modern promising ideas such as machine learning enhanced fitting.

2.5.3 Visualization of Dynamical Processes

We will develop ultra-realistic visualizations of sea ice, snow and water simulations. Teran has many years of experience producing visualization of MPM simulation data that are nearly photo-real. Indeed Teran’s MPM simulations have been used in a number of Walt Disney motion pictures, including *Frozen*, *Moana*, and *Zootopia*. We will use the same techniques in the proposed effort that were used to render scenes for the motion picture industry. To achieve maximal realism in rendering, we will use the latest advances from the computer graphics literature related to ray tracing, including global illumination, photon maps, depth of field, ambient occlusion, glossy reflections, soft shadows and bloom. We will use the Mental Ray ray tracer to achieve this. Teran’s students

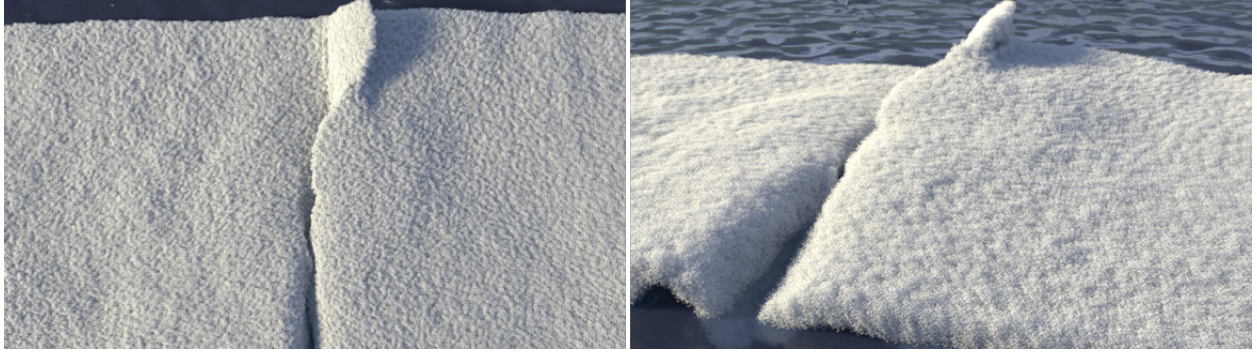


Figure 5: MPM simulation: water and snow. We simulate two slabs of snow using the model from [42] on top of a pool of water. The slabs are driven towards one another by Dirichlet boundary conditions. The impact causes a small ridge, however we do not see the debris and breakage that would be expected. Our failure to capture this effect is likely due to an inaccurate assumption about compressive failure. Currently, we use an ellipsoidal yield surface associative flow and softening. Clearly this is not enough to capture the real phenomena and the proposed effort will address this.

are experts at using these techniques and software. The images in Figures 2 and 4 were rendered by Teran’s group using these approaches.

MPM is a particle method, and this can pose some challenges for rendering. Typically, there are three options for rendering this type of data: (1) render the raw simulation particles as tiny spheres, (2) splat the particles to a regular grid to define a density function and render based on a light ray’s occlusion with this field, (3) wrap a surface (implicit or explicit) around the particles and render the surface. Option (1) is appropriate for dry snow and sand, but looks too particulate for cohesive, wetter snow. (2) was used in Figures 2 and 4. (3) is more appropriate for water. Part of our efforts will be in developing new variations on these options that increase the achievable visual realism. Teran’s group has recently made great progress in this regard for ductile materials, which may lead to techniques that generalize to rendering brittle ice, snow and water in close proximity.

2.5.4 Homogenization for Multiscale Building Blocks in the Material Point Method

As a multiphase anisotropic composite with complex structure on many length scales, sea ice has different effective properties on different scales and different discretization levels. We propose to develop a multiscale iterative homogenization approach for calculating the properties of the ice “blocks” needed in MPM simulations, over a range of resolutions, or block sizes.

The effective properties on smaller scales will be obtained by analytical and computational homogenization methods [111, 21, 14, 88, 73, 19, 87]. These methods yield homogenized parameters depending on the microgeometry: volume fraction, shape and orientation of brine inclusions, distribution of the c-axes as a polycrystalline composite, and take into account viscoelastic properties [24, 28] and a nonlinear dilatational response [90, 106, 34].

To help simulate floe collisions, fractures, ridge and lead formation, and to inform our MPM development, we propose to develop a numerical multiscale approach based on upscaling the behavior of the inhomogeneous sea ice composite accumulating microdamage [22] on different scales. This damage accumulation can be incorporated into the MPM calculations through the internal variables evolving in time; such evolution can be modeled using a system of differential equations that is solved at each time iteration step [35, 15, 94, 125, 80]. The coefficients of the ODE system are determined by the parameters of the spectral measure in the Stieltjes representation of the effective properties [25]. This spectral measure μ contains all information about the structure of the

composite [43, 28]. We propose to investigate the evolution of μ due to the evolution of the structure of the ice, due to fracture, creep and viscoplasticity, as well as healing of ice (e.g. refreezing leads). This will provide a link between the evolutionary processes that release or dissipate energy and the internal variables used in the upscaled simulation with the MPM method.

The model for damage accumulation and criteria for the propagation of damage and cracks will be developed based on the previous work of Cherkaev for damage accumulation and propagation in nonlinear lattice structures [20, 105, 22]. To facilitate the numerical modeling of the dynamics of ice floes, we will build a model of large scale crack propagation using a stochastic description of inhomogeneous ice structure that might be influenced by the thickness, cracks, leads, and ridges. If we view large floes as inhomogeneous structures “glued” together from smaller floes whose size distribution statistics we have [96, 115, 58, 59] then the locations of potential cracks in the large floe can be modeled as a weakened random ‘pre-crack’ network. Under compressive loadings [121], the ice floes experience frictional sliding and ridging which results in viscoelastic or viscoplastic deformation. We will develop criteria for the opening of leads and the dynamics of ice breakage due to various impacts based on partial damage accumulation developed in [3, 4, 23, 22]. Using accurate forcing MPM simulation data and incorporating a fracture model, we will determine the conditions for ridge initiation, formation, and evolution. This will also lead to a model of ridges and rafting resulting from a fracture due to buckling of a thin compressed plate.

2.5.5 Field Data on Dynamic Sea Ice Processes

High quality data is critical to the success of this project. MOSAiC, Multidisciplinary drifting Observatory for the Study of Arctic Climate, will be a major real-time source of this data (<https://www.mosaic-expedition.org/>). MOSAiC is a large, international, interdisciplinary program with a central scientific question of “What are the causes and consequences of an evolving and diminished Arctic sea ice cover.” The centerpiece of MOSAiC is a yearlong drift experiment in the Central Arctic from September 2019 to September 2020.

MOSAiC will provide an extraordinary data set covering a range of spatial scales over an entire annual cycle. The sea ice observations will encompass spatial scales from computer tomography of sea ice microstructure to satellite observations. MOSAiC will focus on three spatial scales; the Central Observatory (mm to km), the Distributed Network (km to tens of km), and the large scale (tens of km to thousands of km). Measurements will be made over an entire annual cycle. Sea ice measurements of particular value to our project (on various scales) include:

- 3-D maps of ice microstructure (sub-mm)
- Snow stratigraphy (millimeter)
- Surface topography maps (kilometers)
- Ridges: number, shape, spacing (tens of km)
- Floes: size and shape (tens of km)
- High resolution ice deformation (tens of km)
- Electromagnetic signatures (kilometers)
- Sea ice porosity (millimeter)
- Snow depth surveys (kilometers)
- Ice thickness surveys (thousands of km)
- Leads: number, shape, spacing (tens of km)
- Ponds: number, size, geometry (10s of km)
- Internal ice stress (kilometers)
- Partitioning of solar radiation (kilometers)

The Sea Ice Dynamics Experiment (SIDEx) field campaign will track ice pack stress and strain fields on scales from sub-meter to the interaction of floes in the consolidated ice pack. As in MOSAiC, the ice drift, thickness, snow cover, snow stratigraphy and topography will be monitored. We will also be obtaining high resolution video and images of various sea ice scenes of interest.

2.5.6 Assimilation of Data from Field Experiments

The physical model for sea ice will vary with many rheological parameters related to various modes of stress generation. In order to develop a model with sufficient ability to reproduce the many desired modes of deformation, failure and cohesion, it will be necessary to have many tens of parameters. While this will make the models flexible in terms of the phenomena they can recreate, it also makes fitting the parameters to observed data much more difficult.

We will have many types of data available to us, and it is vitally important that we can determine the appropriate rheological parameters to reproduce them. This can be done in many ways, but in most cases it is very useful to differentiate the simulated configurations of the material with respect to rheological parameters. Teran and collaborators [32] recently generated a technique for estimating elasticity related parameters for Kirchhoff-Love thin shell models utilizing an orthotropic hyperelastic assumption. The orthotropic model was designed to be flexible enough to capture modes of stress and strain exhibited by woven fabrics like denim, and silk. From a set of simple laboratory measurements, Teran and colleagues developed a method for determining tens of parameters needed to match observed stress-strain curves from data. This was done by penalizing the least squares deviation in the simulated result from the observed data.

Different smoothing (quadratic) and non-smoothing (total variation) penalization functionals were studied in [9] in applications to an inverse geophysical problem of fitting the parameters of the subsurface to the data measured on the surface of the earth. Reconstruction of spatially varying rheological parameters which requires fitting many hundreds of parameters to observed data can use model order reduction techniques [68, 69] originally developed by Cherkaev and collaborators [70, 71] for magnetotelluric imaging problem.

To provide a more accurate estimate for the rheological parameters, we will use the inverse bounds approach [29] developed by Cherkaev and Golden for evaluation of microstructural parameters of composites. This method takes measurements of the effective properties of composite materials and produces rigorous bounds for the geometric parameters and other properties of the composite [26, 27, 31]. This inverse homogenization approach is based on the reconstruction of the spectral measure in the Stieltjes integral representation for the effective properties of the composite material [26, 30, 124]. The method has been used with complex permittivity data to recover brine porosity in sea ice [29, 86] and connectivity in human bone [11, 47]. Moreover, this approach was extended to polycrystalline materials and tested on sea ice data [48, 81]. An extension of this approach to elasticity was developed and applied to viscoelastic shear modulus measurements for the reconstruction of bone properties and geometric parameters [10, 12, 28].

Hu *et al.* [60] have recently shown that MPM is very useful for optimization and control related problems because the updated Lagrangian nature of the method allows for simple expressions of the derivatives of the simulated states with respect to the rheological parameters.

2.6 High Performance Computing

Figure 2 shows an avalanche simulation with 30 million particles run with manycore-level parallelism on a single desktop PC. While this resolution is sufficient at the slope scale of tens of meters, we are interested in resolving phenomena from larger to much finer scales, which will require resolution only available with high performance computing on large clusters of workstations. We will make use of computing resources at the UCLA IDRE facilities as well as the University of Utah SCI Institute and potentially with the Oak Ridge DOE Summit supercomputing infrastructure.

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4 Management Approach

This project will be directed by the PI Golden, who will play a significant role in all of the major research thrusts, interact with program managers, prepare reports, link with DoD personnel, and be an active participant in DoD activities. The PI's goal here is to build the most advanced, most realistic and physically accurate computational framework to simulate and visualize key processes in the dynamics of Arctic sea ice. The idea is to make a major advance in our understanding and capability of predicting the mechanics and rheology of sea ice at intermediate length and time scales. Such research has been woefully missing from efforts ranging from canonical modeling of sea ice to how it is represented and incorporated in general circulation models.

To do this, the PI has initiated a collaboration with Joseph Teran of UCLA, the principal creator and developer of probably the most advanced, realistic computational framework for simulating the dynamics of snow, a material that is a key part of the sea ice system, and which exhibits a wide range of rheological behaviors from fluid to solid, like sea ice. The “points” in Teran’s Material Point Method (MPM) are small pieces of a continuum version of the material under study. In the case of sea ice these small pieces themselves have complex composite structure – with brine inclusions on the submillimeter scale, polycrystalline structure on the centimeter scale, and larger brine channels on the meter scale. The PI has involved close colleagues Elena Cherkaev and Andrej Cherkaev in the Math Department at Utah for their expertise in the effective rheological properties of composite materials. Moreover, in order for this project to have a firm grounding not only in mathematics and computation, but in actual observations and experiments of the key dynamical scenarios we are interested in studying, the PI initiated a collaboration with Jennifer Hutchings of Oregon State University, a sea ice dynamics expert and co-director of two of the most important Arctic field campaigns in this area over the next few years. These data will be incorporated into the models and simulations to achieve new levels of realism and physical accuracy. (Hutchings and Golden have worked together in the past: they were both participants in the Australian Sea Ice Physics and Ecosystem Experiment II off the coast of East Antarctica aboard the icebreaker *Aurora Australis* for 2 months in 2012. They experienced being effectively stuck for 3 weeks as the ice pack was being pushed up against the continent, and witnessed incredible dynamical forces and sea ice mechanical behavior. As we look back, the conversations we had on the ship that were spurred by that experience can be viewed as seeds which are finally germinating here!)

We plan to have one major in-person meeting each year for all project personnel, with monthly skype meetings including the PI and all senior personnel. There will also be several opportunities each year for Golden, Hutchings and Teran to meet together through visits to each other’s universities, as well as at conferences. We also plan for postdocs and students to help facilitate interaction and cross-pollination of ideas and methods among the researchers at Utah, OSU and UCLA by spending time with other groups at other institutions. Within each university, weekly research meetings involving faculty and students will be held.

In addition to the above described collaborations, the University of Utah is home to the well known Scientific Computing and Imaging (SCI) Institute. In the attached letter of support, the Interim Director of SCI Mike Kirby has expressed great support for this project - in ensuring access to their extensive computing and visualization networks, as well as active collaboration in MPM development and other natural areas of common interest, such as scientific visualization. Also, as homogenization for polycrystalline media is a key input into MPM in our project, we have been in touch with Pedro Ponte Castañeda of the University of Pennsylvania. He has conducted significant

ONR-funded research on this problem, and in an attached letter of support has enthusiastically expressed his interest in collaborating with us. With our close connection to the ONR SIDEx field campaign, we are delighted to have in an attached letter the strong support and interest in collaboration from the senior leaders of SIDEx, Chris Polashenski of USA CRREL and Dartmouth, Andy Mahoney of University of Alaska Fairbanks, as well as Dr. Hutchings. Finally, Donald Perovich of Dartmouth, who is sea ice team co-coordinator on MOSAiC, will act as a data liason for this project, providing us with extensive, highly relevant data from MOSAiC. He has expressed his support in this regard in his recommendation letter for the PI Golden.

Project Schedule:

Year 1. Initial MPM development; rheological homogenization on small scales for input into MPM; identification of dynamical scenarios and planning for interactions with field campaigns.

Years 2-3. Development and refinement of MPM for complex sea ice scenes; investigate homogenized constitutive laws for extending MPM to larger scales; extensive data gathering in ONR SIDEx and MOSAiC, and assessment of the data for MPM.

Years 4-5. Incorporation of field data and video recordings of dynamical scenarios into MPM for creation of ultra-realistic simulations and visual renderings; investigation of accuracy of sea ice rheological models; further development of homogenization of sea ice rheology at larger scales and incorporation into MPM framework; analysis and scenario investigation from data and video from field campaigns.

5 Principal Investigator and Senior Personnel Time

PI Kenneth Golden

1. **Current.** NSF Grant DMS-1715680, “Random Matrix Theory for Homogenization of Composites,” Role: PI. Total Award: \$353,794. Period Covered: 08/15/17 – 07/31/20, Summer months per year: 1. ABSTRACT: We explore the spectral properties of random matrices that govern classical transport in random and quasiperiodic media, using analytical and computational tools. We focus on understanding connections between the geometry of the medium and the statistical properties of the spectra, and the appearance of universal distributions.
2. **Current.** ONR Grant N00014-18-1-2552, “Multiscale Homogenization for Sea Ice,” Role: PI. Total Award: \$583,573. Period Covered: 07/01/18 – 06/30/21, Summer months per year: 1. ABSTRACT: We address fundamental questions in sea ice homogenization, where behavior and structure on small scales is incorporated into representations of effective behavior on larger scales, and estimating parameters controlling small scale processes from large scale observations. We consider transport properties of sea ice as a composite, the complex viscoelasticity of the ice pack for waves in the Marginal Ice Zone, and advection diffusion processes in sea ice.
3. **Pending.** ONR MURI “Statistical Dynamics of the Arctic Sea Ice Pack,” Role: PI. Total Award: \$7,500,000. Period Covered: 06/01/19 – 05/31/24, Summer months per year: 1.5. ABSTRACT: We propose to develop a robust, multiscale, multiphysics theory of the probability distributions that characterize the components of the ice pack mesostructure (configurations of ice floes with distributions of sizes, shapes, thicknesses, leads and ridges), its effective rheology and response to forcing. Viewing the evolution of the sea ice pack based on stochastic processes opens new and natural avenues for the assimilation of observational data and the quantification of uncertainty.

The PI is currently serving as research advisor and is responsible for 1 postdoctoral fellow, 4 Ph.D. students, 5 undergraduates, and 1 high school student.

The PI’s time will be allotted roughly as follows:

1. ONR Sea Ice Project (until summer 2021): 15%
2. NSF Random Matrix Theory Project (until summer 2020): 10%
3. This Project if Awarded: 30%
4. Mentoring / Supervising Research Students: 10%

Senior Personnel Joseph Teran

1. **Current.** Department of Defense (W81XWH-15-1-0147), “Virtual Tissue Modeling for Real-Time Surgical and Interventional Procedure Simulation.” Role: CO-PI. Total Award: \$3,501,032.00. Period Covered: 07/1/15 – 06/30/18 (no cost extension), Summer months per year: 0. ABSTRACT: The major goal of this project is to develop and evaluate a new virtual tissue modeling methodology for use in military medical training simulators for forward surgical and interventional care of combat injuries.

2. **Current.** NIH “Improving Diagnostic and Therapeutic Imaging Tools for Better Management of Chronic Obstructive Pulmonary Disease.” Role: CO-PI. Total Award: \$2,338,959.00. Period Covered: 04/01/18-03/31/23, Summer months per year: 1. ABSTRACT: The goal of this proposal is to develop a patient-specific non-invasive COPD imaging biomarker by measuring hyperelastic properties of lung tissues and airflow dynamics studies inside the lung, using data acquired during free breathing.
3. **Pending.** DOE/Oak Ridge National Laboratory (20192697) “A high performance computing model of powder-scale melting and solidification simulations in additive manufacturing of metals via the Material Point Method (MPM).” Role: CO-PI. Total Proposed Amount: \$200k. Period Covered: 2/1/19-1/31/21, Summer months per year: 1. ABSTRACT: The purpose of this work is to aid in the development and implementation of a high performance computing model of powder-scale melting and solidification simulations in additive manufacturing of metals via the Material Point Method (MPM). There are 2 core objectives to this work: (1) develop and apply an accurate MPM formulation of surface tension including Marangoni flow for the modeling of melt pool formation in additive manufacturing, (2) develop and apply accurate MPM constitutive models for heat transfer, melting, solidification, and residual stress formulation in additively manufactured metal components. This includes an exploration of multiscale linkage to phase field, cellular automata, and mesoscale property simulations.
4. **Pending.** ONR MURI “Octopus Connectome-Inspired Design of Decentralized Controllers for High-Dimensional Embodied Systems.” Role: CO-PI. Proposed Amount: \$1,141,463. Period Covered: 6/1/19 - 5/31/24, Summer Months per Year: 1. ABSTRACT: We will develop a rigorous octopus-inspired model for closed-loop sensory-motor control of adaptive, high-dimensional systems with distributed autonomy. Three-fifths of the octopus central neurons form neural networks that control the arms (axial nerve cords) and connect them to one another for complex functions. We will refer to the combination of the axial nerve cords and their interconnections through the inter-brachial plexus as the brachial nervous system (BNS). Little is known about how the interactions between the cerebral ganglion (brain) and the BNS produce behavior such as locomotion and object manipulation. The focus of our project is on the characterization and parametric modeling of the neuromuscular dynamics of octopus arm function in terms of the joint information processing that occurs within and between the cerebral ganglion and the BNS as the octopus solves complex sensorimotor problems. Toward this end, we will develop new techniques for combined behavioral and multi-site electrophysiological studies of the sensorimotor system that controls the octopus arms. We will map the complex circuitry of the BNS in the arm to fully establish a graph representation of the octopus connectome for that appendage by imaging and visualizing isolated brachial chain ganglion (nerve cords) at an unprecedented resolution. By employing principled and data-driven modeling, we will use the collected functional and structural data to devise dynamical models of sensorimotor processing in the cerebral ganglion and BNS. We will integrate these models with structural models of soft arms with distributed sensing and actuation to create the first decentralized feedback controllers that can replicate octopus arms physical responses to sensory information. We will validate these control-oriented models with a 3D biomechanical model that replicates the observed arm spatiotemporal dy-

namics in the marine environment, including interactions with solid surfaces and objects.

Teran currently supervises 6 Ph.D. students. His time will be allotted roughly as follows: (1) 15% NIH Improving Diagnostic and Therapeutic Imaging Tools for Better Management of Chronic Obstructive Pulmonary Disease project, (2) 30% Oak Ridge MPM for 3D printing project (3) ONR MURI: 15% (4) This project if awarded 40%.

Senior Personnel Jennifer Hutchings

1. **Current.** NSF Grant OPP 1722729, “CR: Thermodynamic and dynamic drivers of the Arctic sea-ice mass budget at MOSAiC” Role: PI. Total Award: \$407,452. Period Covered: 10/01/17 – 09/30/21, Calendar months per year: 1/1/4/3. Abstract: MOSAiC is an international year long drifting station that will be deployed in October 2019 to investigate physical, biological and chemical processes in the new Arctic with increasing seasonal ice. This project supports the framework for monitoring ocean to atmosphere fluxes and a distributed network of autonomous observations that will be used, in conjunction with remotely sensed data, to upscale localized times series to a spatio-temporal understanding of the ice pack and the fluxes. Hutchings is ice dynamics lead for the project, producing the time evolving spatial information needed. MOSAiC also supports ice mechanics experiments from 5 countries, including collaboration with the ONR SIDEx, providing data of use to the current project.
2. **Current.** NSF Grant OPP 1740768, “Scale invariance of sea ice deformation: identifying how boundary conditions define the spatial ranges of these relationships” Role: PI. Total Award: \$469,735. Period Covered: 6/01/18 – 5/31/21, Calendar months per year: 1. Abstract: A combination of discrete element modeling and observational analysis will be used to investigate mechanical behaviour of pack ice. The discrete model will inform suitable constitutive relationships for continuum modelling approaches. Hypothesis driven research includes identifying bounds on scaling behaviour for sea ice deformation and floe size, in collaboration with Takenobu Toyota.
3. **Current.** NASA Grant 80NSSC18K1026, “Observational study to constrain rheological models for sea ice” Role: PI. Total Award: \$319,311. Period Covered: 10/01/18 – 9/30/21, Calendar months per year: 2. Abstract: Structural analysis performed on fracture patterns apparent in remote sensed imagery will be used to inform rheological parameters for pack ice on scales of tens to thousands of kilometers.
4. **Current.** ONR Grant , “A Plan for an Integrated Sea Ice Dynamics Experiment (SIDEx)” Role: PI. Total Award: \$515,312. Period Covered: 01/11/18 – 10/30/2023, Calendar months per year: 2/1/4/2/2. Abstract: A field campaign to identify suitable stress-strain rate relationships for sub-floe to multi-floe scales. Novel measurements will characterize the strain field at previously unachieved precision and spatial resolution. Stress fields will be estimated through inverse modeling constrained with localized measurements of stress. Outcomes will be validation data for models of sea ice interaction and new theory to support these.

5. **Pending.** ONR MURI “Accurate Quantification, Understanding, Assessment and Learning of Sea Ice Dynamics (AQUALID)” Role: PI. Total Award: \$7,520,575. Period Covered: 06/01/19 – 05/31/24, Calendar months per year: 3. Abstract: A framework is proposed to design new sea ice dynamics models with assimilative capabilities for forecasting on scales from the size of ice floes up to the Arctic Basin. We will employ machine learning to identify scales and dynamic zones for which dimension reduction can be achieved through adapting constitutive models and resolution. A Discrete Element Method modeling approach will be taken to design new constitutive models for sea ice, informed with new observational metrics and a detailed investigation of transitions in scaling behaviour of sea ice deformation and floe size informing transitions in the essential physics controlling the sea ice momentum balance.

The investigator’s time will be allotted roughly as follows:

1. Current NSF and NASA projects: 30%
2. ONR SIDEx Project (current): 20%
3. Mentoring / Supervising: 5% 1 undergraduate, 1 graduate, 1 post-doc and 1 research associate
4. This Project if Awarded: 20%

Senior Personnel Andrej Cherkaev

1. **Current.** NSF Grant DMS, “Optimal Multimaterial Composites and Exotic Structures,” Role: PI. Total Award: \$240,000. Period Covered: 07/31/15 – 07/31/19, Summer months per year: 1. ABSTRACT: This project deals with optimization of microstructures of multicomponent composites. The theory requires development of techniques of quasiconvex envelopes. The second part of the project deals with exotically structured materials with unusual properties.

The investigator’s time will be allotted roughly as follows:

1. Current NSF project: 10%
2. This Project if Awarded: 10%

Senior Personnel Elena Cherkaev

1. **Current.** NSF Grant DMS-1715680, “Random Matrix Theory for Homogenization of Composites,” Role: PI. Total Award: \$353,794. Period Covered: 08/15/17 – 07/31/20, Summer months per year: 1. ABSTRACT: We explore the spectral properties of random matrices that govern classical transport in random and quasiperiodic media, using analytical and computational tools. We focus on understanding connections between the geometry of the medium and the statistical properties of the spectra, and the appearance of universal distributions.
2. **Current.** ONR Grant N00014-18-1-2552, “Multiscale Homogenization for Sea Ice,” Role: Co-PI. Total Award: \$583,573. Period Covered: 07/01/18 – 06/30/21, Summer months per year: 1. ABSTRACT: We address fundamental questions in sea ice homogenization,

where behavior and structure on small scales is incorporated into representations of effective behavior on larger scales, and estimating parameters controlling small scale processes from large scale observations. We consider transport properties of sea ice as a composite, the complex viscoelasticity of the ice pack for waves in the Marginal Ice Zone, and advection diffusion processes in sea ice.

3. **Pending.** ONR MURI “Statistical Dynamics of the Arctic Sea Ice Pack,” Role: Co-PI. Total Award: \$7,500,000. Period Covered: 06/01/19 – 05/31/24, Summer months per year: 0.5. ABSTRACT: We propose to develop a robust, multiscale, multiphysics theory of the probability distributions that characterize the components of the ice pack mesostructure (configurations of ice floes with distributions of sizes, shapes, thicknesses, leads and ridges), its effective rheology and response to forcing. Viewing the evolution of the sea ice pack based on stochastic processes opens new and natural avenues for the assimilation of observational data and the quantification of uncertainty.

Elena Cherkaev is currently serving as research mentor and is responsible for 1 postdoctoral fellow, 1 Ph.D. student and 1 undergraduate student.

1. Current NSF projects: 20%
2. ONR Sea Ice Project (until summer 2021): 15%
3. Mentoring / Supervising: 10%
4. This Project if Awarded: 10%

6 Facilities

Utah: The Math Department provides outstanding computing facilities for use by faculty, students, and staff. The fully inter-networked workstation and microcomputer configuration includes almost 300 systems in a range of models from these architectures: Apple, GNU/Linux (Dell & IBM), Solaris (Oracle/SUN), and Sun Ray thin client stations. These include at least one file server from each UNIX architecture. The Center for High Performance Computing (CHPC) offers powerful computing tools for the University of Utah research community, boasting a total of 7 super computer clusters with over 21,000 nodes/cores running with anywhere from 2.1-2.8 GHz of speed.

University of Utah Scientific Computing and Imaging (SCI) Institute

Some of our data analysis, computational modeling and simulations will be performed at the SCI Institute. The SCI research group was founded in 1994 by Drs. Chris Johnson and Rob MacLeod along with five graduate students. In 1996, they became the Center for Scientific Computing and Imaging and in 2000, the SCI Institute. The SCI Institute is now one of eight permanent research institutes at the University of Utah and home to 200 faculty, students, and staff. The 17 tenure-track faculty are drawn from the School of Computing and the Departments of Biomedical Engineering, Mathematics, and Electrical and Computer Engineering.

The SCI Institute has established itself as an internationally recognized leader in visualization, scientific computing, and image analysis applied to a broad range of application domains, including biomedicine, defense, and energy. The overarching research objective is to conduct application-driven research by creating new scientific computing techniques, tools, and systems. SCI Institute researchers also apply many of these computational techniques within their own particular scientific and engineering subspecialties.

The SCI Institute either directs or has been associated with several national research centers: the NIH Center for Integrative Biomedical Computing (CIBC), the DoE Scalable Data Management, Analysis, and Visualization (SDAV), the Center for Extreme Data Management, Analysis, and Visualization, the NIH National Alliance for Medical Image Computing (NA-MIC), the DOD Alliance for Computationally-guided Design of Energy Efficient Electronic Materials, and an NVIDIA Center of Excellence.

SCI Institute Resources

The SCI institute has over 25,000 square feet of functional space within the John and Marva Warnock Engineering Building. The data analysis, computational modeling, and simulation studies that will be performed at the SCI Institute will rely on the expansive computational resources available. The SCI Institute computing facility includes shared memory multi-processor computers, clusters, and dedicated graphics systems. Among the extensive resources are the following:

1. Nvidia DGX-1 with 8X Tesla V100, Dual 20-Core Intel Xeon E5-2698 v4 2.2 GHz Processors, and 128 GB RAM.
2. 264 core, 2.8TB shared memory SGI UV 1000 system, Intel X7542 2.67GHz Processors.
3. 64 node CPU cluster. Each node has 8 cores, 24GB of RAM, with a 4x DDR Infiniband backbone with dual 10G network connections to SCI core switches.
4. 32 node GP-GPU cluster. Each node has 16 cores, 64GB of RAM with Intel E5-2660 2.20GHz processors. Each node has 2x Nvidia k20 GPUs with 2 full speed FDR Infiniband connections. System has a total of 128 56Gb/s Infiniband connections.

5. 10 blade HPE Apollo 6000 cluster system with 10 Xeon-7210 CPUs with 480GB RAM.
6. 64 core, 512GB shared memory HP DL980 G7 with Intel Xeon X7560 2.27GHz processors.
7. 12 core Intel Xeon E5-2640 2.50GHz with 32GB of RAM and 3x K20c GPUs.

UCLA: The University of California, Los Angeles provides the Teran group with lab space dedicated to algorithm development. This includes ample space for whiteboard and impromptu discussions as well as six high-powered desktops with manycore and GPU level parallelism. This space serves as the core meeting and work area for Teran's PhD students and postdocs.

OSU: Oregon State University provides Hutchings with office, lab space, storage and shipping to support her fieldwork and analysis. A Dell Poweredge R430 server is owned by Hutchings, in which disc space can be expanded to support this project.

7 Commitment of Support

Utah: If the proposal is funded, the University of Utah will provide the tuition for the two graduate student lines requested in the proposal. For each student this is \$20,000 per year. Over the 5 year duration of the grant, this totals up to \$200,000. This commitment reflects the very strong, sustained support the administration of the University of Utah (Dean, Chair, Vice President for Research) has provided for the PI's research program.