A New Discrete Element Sea-Ice Model for Earth System Modeling

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Supplement for Collaborations

Collaborating institutions:

Los Alamos National Laboratory	Adrian K. Turner (Lead and BER PI)
Sandia National Laboratories	Kara Peterson (ASCR PI)
Naval Postgraduate School	Andrew Roberts (Co-PI)

Leadership structure of collaboration:

Individual institutions will be responsible for management of research and budgets assigned to their institutions. Institution PIs will communicate with the lead PI for project coordination and preparation of project reports.

Facilities, equipment, and resources available to the collaborative group:

Shared resources will be obtained from separate computing resource proposals and each institution will use internal computing resources for the initial model development.

Budget by PI/institution ($ in thousands)

Partnership		**Y1**	**Y2**	**Y3**	**Total**
Adrian Turner	LANL	395	400	207	1002
Andrew Roberts	NPS	117	126	68	311
BER Total		512	526	275	1313
Kara Peterson	SNL	503	521	262	1286
ASCR Total		503	521	262	1286
Total		1015	1047	537	2599

Budget by tasks ($ in thousands)

Task	**Task Leader**	**Y1**		**Y2**		**Y3**		**Total**
		BER	**ASCR**	**BER**	**ASCR**	**BER**	**ASCR**	
Task 1	LANL	105	25					130
Task 2	LANL	116	101	140	130			486
Task 3	SNL		151	58	156	8	52	426
Task 4	SNL		126		130		92	348
Task 5	NPS	80		55				135
Task 6	LANL	163	101	162	104			530
Task 7	NPS	48		111		267	118	543

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1 Introduction to High-Resolution Sea-Ice Modeling

1.1 Sea Ice is a Granular Material

Figure 1: Colliding sea-ice floes in the Southern Ocean near the Mertz Glacier in August 1999, scaled against the R.V. Aurora Australis icebreaker (magenta box is approximately 100 m wide).

Sea ice forms a frozen crust of sea water floating in high-latitude oceans. It is a critical component of the Earth system because its formation helps to drive the global thermohaline circulation, and its seasonal waxing and waning in the high north and Southern Ocean significantly affects planetary albedo. Usually 4–6% of Earth's marine surface is covered by sea ice at any one time, which limits the exchange of heat, momentum, and mass between the atmosphere and ocean in the polar realms. Snow accumulates on sea ice and inhibits its vertical growth, increases its albedo, and contributes to pooled water in melt ponds that darken the Arctic ice surface in the spring. Ice extent and volume are subject to strong seasonal, inter-annual and hemispheric variations, and climatic trends, which Earth System Models (ESMs) are challenged to simulate accurately (*Stroeve et al.*, 2012; *Stocker et al.*, 2013). This is because there are strong coupled feedbacks across the atmosphere-ice-ocean boundary layers, including the ice-albedo feedback, whereby a reduced ice cover leads to increased upper ocean heating, further enhancing sea-ice melt and reducing incident solar radiation reflected back into the atmosphere (*Perovich et al.*, 2008). A reduction in perennial Arctic sea-ice during the satellite era has been implicated in mid-latitude weather changes, including over North America (*Overland et al.*, 2015). Meanwhile, most ESMs have been unable to simulate observed inter-annual variability and trends in Antarctic sea-ice extent during the same period (*Gagné et al.*, 2014).

Arguably the most challenging aspect of sea-ice physics to simulate is its drift, deformation, and morphology forced by winds and currents (*Thorndike*, 2000; *Kwok et al.*, 2008). The pack may be approximated as a non-Newtonian fluid on scales exceeding about 10 km (e.g., *Hibler*, 1977; *Hutchings et al.*, 2005; *Tsamados et al.*, 2013), but there is scant justification for such an aggregation in higher resolution models than this (*Coon et al.*, 2007). Sea ice is not a continuous material, but is composed of fractured sheets or floes with scale-invariant size from less than the meter-scale to above 100 km (*Weiss*, 2001), intimated in Fig. 1. Because of its discontinuous nature, it may be modeled as a granular composite (*Hopkins*, 2004a). Up to now, computing power and modeling techniques have been unavailable to simulate sea ice as discontinuous granular elements on decadal to centennial timescales, especially not in coupled models. This proposal addresses that problem.

1.2 Current Sea-Ice Models

Sea-ice models used in current generation ESMs trace their heritage to a class of mechanics models that emerged during the period of the Arctic Ice Dynamics Joint Experiment (AIDJEX) in the 1970s (*Coon*, 1980), the most prominent of which was incorporated into *Hibler* (1979). These models sought a diagnostic solution to the two-dimensional sea-ice stress tensor, σ_{mn} (m,$n=1$,2) used in the momentum equation:

$$M\frac{D\boldsymbol{u}}{Dt} = \boldsymbol{\tau}_a + \boldsymbol{\tau}_w + M\mathrm{f}\mathbf{k}\times\boldsymbol{u} - M\hat{\mathrm{g}}\boldsymbol{\nabla}\eta + \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} \tag{1}$$

Here, $\boldsymbol{u}$ is the sea-ice velocity vector, M is the sea-ice mass per unit area over the ocean surface with normal vector $\mathbf{k}$, $\boldsymbol{\tau}_a$ and $\boldsymbol{\tau}_w$ are the wind and ocean current stress, respectively, f is the Corolis parameter, $\hat{\mathrm{g}}$ is acceleration resulting from gravity, and η is the sea surface height. Several constitutive relations for σ_{mn} were proposed during AIDJEX that assumed that sea ice behaved as a two-dimensional Reiner-Rivlin fluid over length scales of $\sim$100 km (*Rivlin*, 1947), with a bulk and shear viscosity proportional to the compressive strength, P, of sea ice. These models assumed that the pack included a sufficient number of interstices, such as leads and cracks, that their horizontal orientation could be homogenized in an isotropic continuum within each model grid cell at the designated $\sim$100 km scale. The modeled pack was assumed to have no tensile strength, even though it was known that individual floes possessed compressional, flexural, and tensile strength, but the latter two were usually less than the former (*Mellor*, 1986). Reconciling the aggregation of local, floe-scale mechanical properties of sea ice with those measured over 10–100 km, sometimes referred to as the 'geophysical scale' in past literature, was largely the aim of the *Hibler* (1979) viscous-plastic (VP) sea-ice rheology. It assumes that for periods of 1 day or more, and at low strain rates, sea ice behaves as a viscous fluid up to a plastic limit, determined by the relative proportion of smoothly varying shear and compressive stress fields, and the failure compressive threshold, P (*Hibler*, 1977). This criteria forms the basis for the much-used Elastic-Viscous-Plastic (EVP) rheology of *Hunke and Dukowicz* (1997) that adds a non-physical elastic component to the VP rheology to facilitate computational solutions of Eqn. (1) on ocean eddy-permitting grids using many hundreds of computing cores (e.g., *Roberts et al.*, 2015). This EVP rheology, with modifications including those in *Hunke* (2001), was used in more than ten ESMs cited in the last IPCC report (*Stocker et al.*, 2013).

Aligned with AIDJEX efforts to establish a continuum model to solve equation (1), *Rothrock* (1975) and *Thorndike et al.* (1975) derived an approximation for sea-ice compressive strength. Within floes, P is affected by ice thickness, h, temperature, T, salinity, S, and micro-porosity, ϕ_μ, from brine and air pockets (*Kovacs*, 1997; *Timco and Weeks*, 2010). Of these, *Rothrock* (1975) implicitly assumed that, at geophysical scales, P is only dependent upon ice thickness, and described it in terms of the sea-ice thickness distribution, $g(h)$, which has a continuity equation following *Thorndike et al.* (1975), expressed here with a material derivative:

$$\frac{Dg}{Dt} = \Theta + \Psi - g(\nabla\cdot\boldsymbol{u}) \tag{2}$$

$g(h)$ represents sea-ice morphology in terms of the relative proportions of ice with different thicknesses $h \in [0,\infty)$ over a continuous region of the pack, where Θ determines thermodynamic growth and melt, and Ψ describes mechanical redistribution from ridging and rafting where floes collide or thin ice compresses. There are many difficulties associated with solving Eqn. (2), mostly related to the term $\Psi = \Psi(\dot{\epsilon}_{mn}, \omega_R)$, which is a function of both strain rate, $\dot{\epsilon}_{mn}$, and a 'ridging mode', ω_R, that describes how ice thicknesses increases in $g(h)$ during ridging (*Thorndike et al.*, 1975; *Rothrock*, 1986).

Ridge tectonics are constrained by the fact that flexural and tensile strength of undeformed floes ranges over about 0.1–1.5 MPa and 0.2–0.8 MPa, respectively, whereas their compressive strength is typically much more (0.5–5 MPa) (*Moslet*, 2007; *Timco and Weeks*, 2010). It is, thus, most efficient for floes to buckle, subduct, and overthrust at their edges than to compressively fracture within, unless the ice is particularly thin or ductile (*Weeks*, 2010). For this reason floes seldom break under internal compression, but instead cleave under tension, flexure, or shear, dividing into smaller floes. New ridges then form along the edges of these new plates in subsequent convergence. When the ridges form, overriding or subducting ice sheets fracture under flexure into rubble piles (*Tucker et al.*, 1984) with inter-block macro-porosity, ϕ_R, that has been reliably measured up to $\phi_R \approx 0.4$ (*Bowen and Topham*, 1996; *Høyland*, 2007; *Nuber et al.*, 2013). However, Ψ cannot explicitly represent this process because $g(h)$ is an incomplete morphological description of sea ice that does not describe the arrangement, shape, nor macro-porosity of ridges within a region. As a result, Eqn. (2) is a scale-dependent descriptor of sea-ice continuity with a minimum-length threshold of ∼10 km in the Arctic Ocean (*Flato*, 1998).

With the limitations of representing ice morphology solely using $g(h)$, *Hibler* (1980) combined the VP rheology of *Hibler* (1979) with the *Rothrock* (1975) compressive-strength approximation to represent ice strength as:

$$\sigma_{mn} = P\, f_{mn}\left(\frac{\partial u_j}{\partial x_k}\right), \quad P = C_f\, \delta\mathcal{P}(\omega_R), \quad (j,k=1,2) \tag{3}$$

where $\delta\mathcal{P}$ is the change in potential energy per unit area of the pack during ridge formation, and is therefore dependent upon the ridging mode, ω_R. Following *Hunter* (1983), f_{mn} is a tensor function of spatial velocity differentials in parentheses ($u_j = \boldsymbol{u}$) describing the sea ice yield criterion, such as the VP elliptic yield curve of *Hibler* (1979). Most importantly, without being able to fully describe energy dissipation from ridge tectonics by only using ω_R, it is assumed that compressive strength P is proportional to $\delta\mathcal{P}$, where C_f is a proportionality constant ranging between about 10 and 22 in most models (*Lipscomb et al.*, 2007), and based upon simulations of individual ridges by *Hopkins et al.* (1991) and *Hopkins* (1994, 1998). The fundamental problem with this approach, aside from the scale limitation of $g(h)$, is that it assumes the entire pack is isostatic, even though deviations from isostasy are often observed in sea ice (*Melling et al.*, 1993; *Doble et al.*, 2011; *Geiger et al.*, 2015). Moreover, it scales the largest energy sink in ice deformation – frictional loss, which accounts for about 95% of deformational energy consumption – against a comparatively small increase in potential energy, $\delta\mathcal{P}$. This energy sink is another scale limitation of AIDJEX-era models.

1.3 Breakdown of Continuum Model Assumptions at High Resolution

All told, the limitations of Eqns. (1) to (3) render them inappropriate to model sea ice at resolutions of less than 10 km. Using evidence from both remote sensing and in situ observations, *McNutt and Overland* (2003) developed a spatial hierarchy for sea-ice dynamics where ∼10 km represented a transition scale below which emergent properties of regional sea-ice dynamics become dominant to individual floes. Only above this scale, they argue, is the continuum approximation of sea ice valid. Below ∼10 km, individual floe interactions become important and the sea-ice behavior is granular. Yet the continuum Eqns. (1) to (3) are regularly being integrated at higher spatial resolutions than this in regional models (e.g., *Gao et al.*, 2011; *Maslowski et al.*, 2012; *Schweiger and Zhang*, 2015).

Several observational studies, including those during AIDJEX, cast doubt on the basic assumptions underlying the continuum isotropic sea-ice models, even within the 10–100 km scale range. *Thorndike and Colony* (1978) concluded that the assumption of isotropy within even ∼100 km grid cells is unjustified. Sea-ice deformation is demonstrated to be scale-free and highly heterogeneous by *Marsan et al.* (2004) using a multi-fractal analysis of RGPS (RADARSAT Geophysical Processor System; *Kwok*, 1998) strain-rate fields, contradicting the homogeneous assumption made in current models. Similarly, using an in-situ stress gauge, *Weiss and Marsan* (2004) find that stress measurements were highly intermittent and scale-invariant in time. An analysis of satellite-derived strain rates by *Weiss et al.* (2007a) show that sea-ice strain rate is not, in general, proportional to the applied stress, contrary to that expected for a viscously flowing material. Instead of a viscous flow, they find that even moderately loaded ice cover deforms in a brittle manner and does not behave plastically in the way assumed by a VP constitutive law. They also find that tensile stresses are rather frequent, again counter to the assumptions made in AIDJEX-era models, and that, while stress states are shown to be confined within an envelope, this yield surface is scale and rate dependent, rather than fixed. Finally, by looking at the dispersion properties of sea-ice buoys from the International Arctic Buoy Program (IABP; *Rigor*, 2002), *Rampal et al.* (2008) also show that Arctic basin-scale, sea-ice deformation does not mimic viscous flow.

Even though VP-derived sea-ice mechanics were designed for $\sim$100 km grid resolutions, nearly all global coupled models that use VP or EVP rheologies are routinely integrated at spatial resolutions far exceeding this target. Two examples are the Community Earth System Model (CESM; *Hurrell et al.*, 2013) and the Department of Energy's Accelerated Climate Model for Energy (ACME), which use the EVP rheology in the Los Alamos National Laboratory (LANL) sea-ice models, CICE (*Hunke et al.*, 2013) and MPAS-Seaice (*Turner et al.*, In Prep.). These coupled models are routinely run with fidelity far in excess of the aforementioned 100 km and 1 day aggregation scales, both for the Arctic and Southern Ocean. ACME, in particular, is routinely being used to simulate sea ice at about 5 km resolution, yet only a few expansive leads or cracks may be assumed to be present in grid cells with this dimension. In this confined space, sea-ice deformation is both highly anisotropic and discontinuous, contrary to assumptions underlying VP and EVP. Moreover, CICE and MPAS-Seaice approximate sea-ice morphology using only a thickness distribution and, most importantly, model ice morphology and frictional dissipation using Eqns. (2) and (3). Therefore, ACME sea-ice physics remain scale limited in more ways than one.

New rheological models have ventured to address the anisotropic and granularity problems, and CICE now includes an option to use the Elastic-Anistropic-Plastic (EAP) rheology of *Wilchinsky and Feltham* (2006), in place of EVP. This option was recently used for a hydrological investigation at eddy-permitting resolutions ($\sim$9 km) in the Regional Arctic System Model (RASM) by *Hamman et al.* (2017). However, EAP still uses a continuum approximation and finite-difference mesh, and is therefore constrained in an analogous way to previous approximations of pack granularity within continuum frameworks by, for example, *Tremblay and Mysak* (1997). EAP requires that the angle between linear kinematic interstices, cracks, or leads is parameterized at a fixed value (*Tsamados et al.*, 2013). It assumes that sea-ice floes are diamond shaped with a constant vertex angle, when in reality floe shapes are emergent properties of the system. One need only look to aerial images of ice fracture, such as Fig. 1, to find contraventions of the diamond-shaped floe rule. Also, EAP only makes changes to the function f_{mn}, not to the compressive stress term P. Several other attempts have been made to improve the sea-ice constitutive relation (*Schreyer et al.*, 2006; *Rampal et al.*, 2016), but these models continue to use a continuum assumption. Other recent work has looked to represent ice morphology as a floe size distribution in continuum models (e.g., *Zhang et al.*, 2016), but this research does not change the yield criteria f_{mn}, nor does it affect the way in which friction is parameterized in P (Eqn. 3). It also does not address the fundamental constraint in current models of $\phi_R = 0$, where sea-ice ridges are assumed to be imporous. To address all of the problems highlighted here, we propose instead to model sea ice as a true collection of discrete elements and incorporate new developments in modeling porous ridges between them to accommodate for isostatic deviation and frictional dissipation.

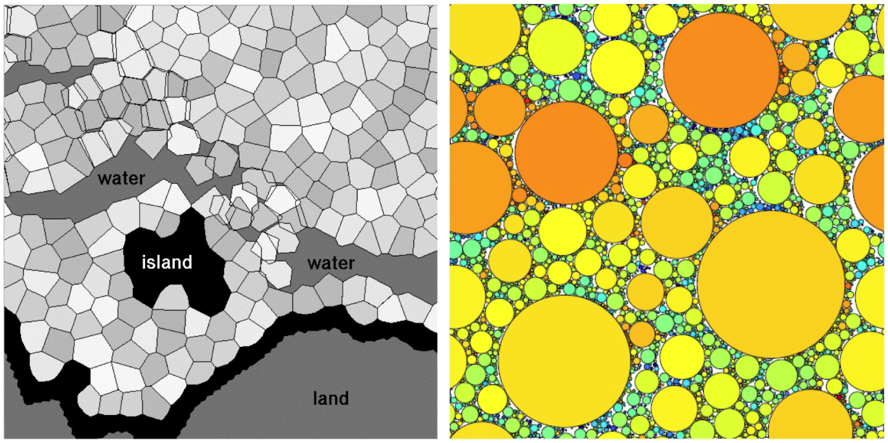

Figure 2: (left): Polygonal discrete elements in the DEM sea-ice model of *Hopkins and Thorndike* (2006). (right): Circular discrete elements in the sea-ice model of *Herman* (2012).

1.4 Discrete Element Method Sea-Ice Models

An alternative modeling paradigm that corrects for the deficiencies of current continuum sea-ice models at high resolution is the Discrete Element Method (DEM). The first DEM model was developed by *Cundall and Strack* (1979) to simulate granular materials. With this method, individual elements of the granular material are explicitly modeled in a Lagrangian framework. Contact forces between elements are determined and the equations of motion for individual elements are integrated in time to determine their motion. Several sea-ice DEM models have been developed. *Hopkins* (2004a); *Hopkins and Thorndike* (2006) developed a DEM sea-ice model that uses polygonal elements, with each element representing a distribution of individual floes. Simulations of the Arctic basin were performed and deformation fields and lead distributions determined. *Herman* (2012), *Li et al.* (2014), and *Xu et al.* (2012) all used circular floe elements in their models rather than polygonal elements, simplifying the calculation of contact forces. Example floe distributions for the polygonal element model of *Hopkins and Thorndike* (2006) and the circular element model of *Herman* (2012) are shown in Fig. 2.

A DEM sea-ice model would solve many of the issues with continuous sea-ice models described in Section 1.3. As floes and their contact forces are explicitly simulated, no averaging to produce a continuum is performed. Consequently, as the resolution of a DEM model increases, the model accuracy increases until the physical floe-size distribution is explicitly reproduced. In contrast, as the resolution of continuum models increases, the assumptions used to derive them become unsupported and accuracy decreases. Also, because DEM models consist of discrete elements with explicit orientated leads between them, the highly heterogeneous and anisotropic nature of the deformation field found in observations can be simulated directly. DEM models can easily simulate complex contact force laws and can simulate the elasto-brittle nature of the pack, as is seen in observations. Continuum models by contrast are restricted in the complexity of force laws that can be simulated using f_{mn}. The need for discrete element sea-ice models at high resolution was highlighted at a recent Department of Energy (DOE) Office of Biological and Environmental Research (BER) Exascale computing requirements review (*Arkin et al.*, 2017).

A DEM sea-ice model would have other advantages over current continuum models when used in Earth system simulations. As the model is fully Lagrangian, there is no need for an advective transport scheme to move tracers between grid cells. Consequently, DEM sea-ice models do not experience any numerical diffusion associated with advection as continuum models do. Thus, they are able to accurately represent discontinuities in the ice cover. Also, transporting tracers represents a significant computational burden for continuum models and considerable effort is spent developing computationally efficient transport schemes (e.g., *Lipscomb and Hunke*, 2004). This computational burden will only increase in the future as biogeochemical and other sea-ice processes add additional tracers to sea-ice models. Because DEM sea-ice models do not need transport schemes, additional tracers may be added with no additional computational burden from transport.

Short-term sea-ice forecasting has recently been made a national research priority (*The White House*, 2014). Within the associated implementation document, the Department of Energy is explicitly listed as a supporting agency for this activity. The United States Navy has a strong interest in improving Arctic forecasts and in developing a capability consistent with the changing nature of the Arctic Ocean (*Chief of Naval Operations*, 2014; *DOD*, 2016). DEM sea-ice models have certain advantages over continuum models for sea-ice forecasting (*Song*, 2014), one of which is the ability to accurately model ocean wave/sea-ice floe interactions and the wave-induced break up of the sea-ice pack (*Xu et al.*, 2012). Consequently, DEM sea-ice models may produce superior simulations of the marginal ice zone at the periphery of the pack.

While several DEM sea-ice models exist, no discrete element sea-ice model has been used in a global climate simulation. The principal reason for this non-use is that DEM models have been traditionally too computationally expensive to be used for the resolutions and simulation lengths needed for global simulations. The model of *Hopkins* (2004a), for instance, requires a time step no more than $\sim$0.5 seconds for a minimum floe size of $\sim$5 km. Such short time steps prohibit the use of discrete element models for simulations other than process studies and short basin-scale simulations. DEM models require short time steps to accurately track the elastic forces that arise when two floes collide with each other. During such a collision, the stiffness of sea ice results in a floe contact ("bounce") time of a fraction of a second, and multiple time steps must occur during the collision to accurately track it. Most DEM models use explicit time stepping because, even with implicit time stepping, multiple time steps must occur during a collision to track it sufficiently. Consequently, implicit methods can only increase the time step by a factor of a few, an insufficient gain to offset the increased complexity of the implicit method (*Samiei*, 2014).

Inelastic contact forces between elements may be stipulated in terms of sea-ice ridging, and we intend to make use of the new multiscale morphology being developed at the Naval Postgraduate School for this purpose. This new physics applies the Principle of Stationary Action for nonconservative systems (*Galley*, 2012; *Galley et al.*, 2014) to a reduced set of ridging equations to emerge from the discrete element modeling of ridges by *Hopkins et al.* (1991). The new method calculates frictional dissipation that is associated with the bending, buckling, and grinding in porous ridge state spaces, instead of scaling the frictional loss with the relatively minor potential energy gain ($\delta\mathcal{P}$). This new method lends itself easily to DEM modeling because frictional work is minimized in Lagrangian coordinates as part of the method, and angles of repose of ridge sails and keels, as well as porosity and ridge width, can easily be transported without the cost of treating them as tracers in a traditional sea ice model. The same multiscale morphology method can be used to calculate thickness changes from sea-ice mechanics in the interior of discrete elements, and to provide a spectrum of ridge shapes for calculating atmospheric and oceanic form drag on each discrete element as an advance on the method put forward by *Tsamados et al.* (2014) for continuum models. Thus ice in each element can have both micro-porosity, ϕ_μ, associated with brine and air pockets, and macro-porosity, ϕ_R, associated with deformed rubble. Although elements as a whole will be assumed to be isostatic, ice at individual points within the element need not be isostatic.

1.5 Accelerated Computing Architectures and Geophysical Fluid Dynamics

As mentioned previously, incorporation of DEM sea-ice models into ESMs has been impeded partly by the large computational requirements of these models. The use of advanced accelerated computing architectures, currently being adopted by leadership computing facilities, offers a method of improving DEM computational performance. Efficient porting of geophysical fluid dynamics codes to use these new computing architectures has, in general, proved difficult. Creating numerical models that are computationally efficient on both GPU and multicore based computing facilities is, in general, a difficult task. These architectures often require different programming styles (ordering of indices, memory management, etc.) for target codes to be efficient. Geophysical fluid dynamics codes also generally lack a compact computational kernel that dominates the compute time, and that can be transferred to efficiently run on GPUs. A recent National Oceanographic Partnership Program project tried to port the Los Alamos sea-ice model, CICE, to use GPUs, but significant performance gains proved elusive. Acceleration of particle methods, such as the Discrete Element Method, on GPUs has enjoyed some success. Several examples of DEM models have been ported to GPUs (*Govender et al.*, 2014) and multicore processors (*Shigeto and Sakai*, 2011), and some have shown impressive increases in speed. The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS, *Plimpton* (1995)), developed by Sandia National Laboratories (SNL) has been successfully ported to accelerated architectures using the Kokkos programming model, and has been used for DEM calculations.

The next set of leadership-class platforms to be installed at Lawrence Livermore National Laboratory (LLNL) and Oak Ridge National Laboratory (ORNL) will have heterogeneous architectures using GPUs for acceleration. The machines will employ the upcoming Volta GPU from Nvidia and POWER9 chip from IBM (*Nvidia*, 2014). When compared with the current GPU-accelerated platform, Titan, the next leadership-class platform at ORNL, Summit, is expected to deliver five times the performance with fewer than one-sixth the number of nodes, yet only require one additional megawatt of power. However, not all future leadership-class computing facilities will use GPUs. Phase-2 of Cori, at Lawrence Berkeley National Laboratory (LBNL), and Aurora, to be installed at Argonne National Laboratory (ANL), will use Intel Xeon Phi processors. These massively parallel, multicore processors incorporate a large number of separate compute cores on a single physical processor. ACME and next-generation sea-ice models will need to use these new machines efficiently.

2 Objectives

The objective of this proposal is to develop a discrete-element sea-ice model suitable for Earth system modeling and suitable for inclusion as the sea-ice component in ACME. We will refer to this proposed model as the Discrete Element Model for Sea Ice (DEMSI). If funded, we expect this proposal to improve the ACME model in two main ways:

- First, we expect DEMSI to significantly improve the fidelity of sea-ice simulations within ACME. As discussed in Section 1.4, a discrete-element sea-ice model would correct many of the deficiencies mentioned in Section 1.3 in the current continuum ACME sea-ice model by allowing complex dynamical processes to be captured by the model of the contact forces between elements.

- Second, DEMSI will use a programming model that will take advantage of the heterogeneous computing architectures being developed for the next generation of the DOE leadership-class computing facilities. By using the accelerators present in these heterogeneous machines, we expect to achieve excellent computational performance in ACME.

Direct Impact on ACME Science Questions: As well as generally improving the sea-ice simulations in ACME, DEMSI will have specific benefits for the main current ACME science questions. The first ACME scientific focus is the global water cycle and aims to investigate how the hydrological cycle and water resources in general interact with the climate. The recent Arctic sea-ice decline has been linked to mid-latitude weather changes, including in North America (*Overland et al.*, 2015). Accurate modeling of sea-ice dynamics will very likely have implications for water resources in non-polar regions. Another ACME focus area is the interaction of biogeochemical cycles and the climate system. The biogeochemical cycles represented in recent sea-ice models have become increasingly sophisticated. Such increased sophistication comes at the expense of needing an increased number of passive tracers and increased computational expense to transport those tracers around an Eulerian grid. A discrete-element sea-ice simulation would not require an explicit transport scheme, and extra passive tracers come at no additional transport computational cost. With a discrete-element model, transport would not limit the number of passive tracers used. The final ACME focus area looks principally at land-ice/ocean interactions in the Southern Ocean. Sea ice is an important player in the climate of the Southern Ocean. Brine rejection from growing sea ice contributes to the formation of oceanic water masses and the sea ice near the coast plays an important role in modifying sub-ice shelf waters. Improved sea-ice dynamics is likely to have a significant impact on Southern Ocean dynamics and ocean/ice-shelf interactions.

Phase-1 Objectives: The phase-1 goal of this project is to demonstrate the feasibility of developing a discrete-element sea-ice model for global Earth system applications. We will develop a fully functional discrete-element sea-ice model, including dynamics, mechanical redistribution, and vertical thermodynamics, applied to the northern hemisphere sea ice domain. We will determine how the physical fidelity of sea-ice simulations is improved by using a discrete-element formulation. We will also demonstrate sufficient computational efficiency to allow the model to be used in ACME, and develop the algorithms needed to allow coupling between the discrete-element model and more traditional Eulerian models.

Phase-2 Objectives: If funded, phase-2 of this project would focus on coupling DEMSI to the ACME model using the coupling algorithms developed in phase-1. We would assess the physical fidelity and computational performance of the model in a coupled configuration, with the aim of validating the model for production ACME simulations. This work will naturally involve expansion of model validation activities to the Southern Ocean sea ice domain.

3 Previous Results

3.1 LAMMPS Development at SNL

DEM calculations in this proposal will be carried out with the LAMMPS software package (*Plimpton*, 1995). LAMMPS was developed at Sandia National Laboratories (SNL) to perform high-performance molecular-dynamics simulations, but has also been modified to perform discrete-element calculations. The basic computations required for DEM are the calculation of pairwise contact forces between elements, and the integration of the equations of motion. Both steps have exact analogues in molecular dynamics, which makes the LAMMPS framework ideal for DEM simulations. Extensive capabilities for DEM simulations are already mature within LAMMPS and include many of the computational features essential to the models of interest in this work: 2D/3D granular dynamics; complex contact interactions, including contact history-dependent friction and cohesion; dynamic load balancing; and capabilities for coupling to other codes. The current DEM implementation in LAMMPS can be tailored to capture various contact physics and has been successfully applied to study a broad range of problems in granular materials (e.g., *Silbert et al.* (2001); *Landry et al.* (2003); *Cheng et al.* (2006)) and suspension flows (e.g., *Schunk et al.* (2012); *Bolintineanu et al.* (2014)).

3.2 DEM Sea Ice Modeling at LANL

The deficiencies of Los Alamos National Laboratory's sea-ice models, CICE and MPAS-Seaice, described in Section 1.3 have been known at LANL for some time, and we have been actively investigating possible ways to correct for these deficiencies. To that end, we have been performing preliminary work in determining what would be needed to implement a fully functional DEM sea-ice model for Earth system applications. To that end, we have implemented a simple prototype DEM sea-ice model that focuses on the contact force model between elements and the integration of the equations of motion of the elements. Results of the prototype for a simple square domain and vortex wind field are shown in Fig. 3.

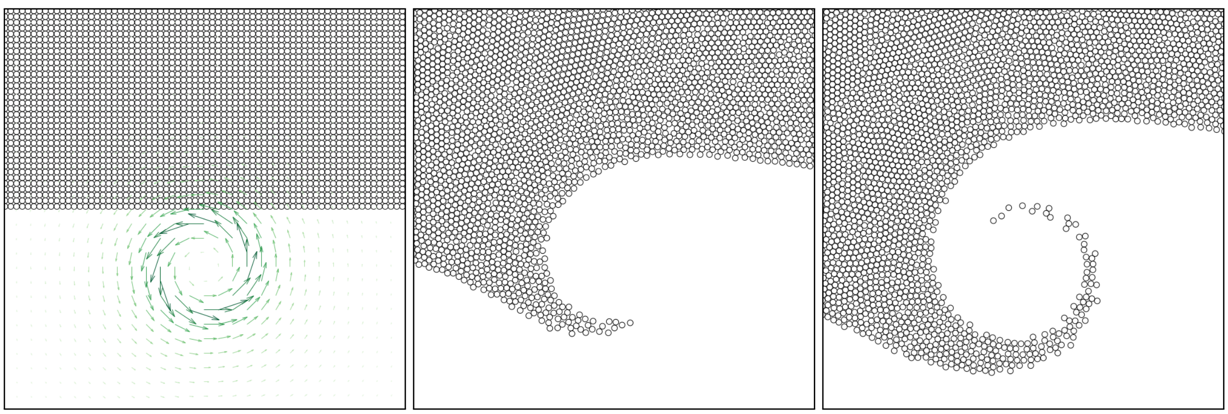

Figure 3: Simulation output from the LANL prototype DEM sea-ice model. Circular elements of equal 5 km are advected by the standard test-case vortex wind field of *Flato* (1993). (*left*): Initial condition with applied wind field shown in green. (*middle*): Simulation after two days. (*right*): Simulation after four days. Different elements experience compression, shear and free-drift.

Development of this prototype has been instrumental in highlighting potential issues with developing a DEM sea-ice model for climate, and guiding the writing of this proposal. Especially useful has been the work performed in determining how to modify the *Hopkins* (2004a) contact force to work with circular elements instead of polygonal elements, and experimental work on the most efficient way to produce a random but tightly packed initial distribution of circular elements.

3.3 Morphological Model Development at NPS

Current limitations in modeling the relationship between horizontal sea ice mechanics and vertical thickness evolution were discussed in section 1.2, and these limitations are equally applicable to discrete element sea ice models. Ridges and floes evolve together, and the contact force model used in a DEM sea ice simulations is dependent upon frictional dissipation incurred during thickness evolution. The minimum horizontal scale of discrete elements is computationally limited, and in this project will be nominally set at 1 km. Therefore the ridge and floe morphology within discrete elements must be modeled separately from inter-element mechanics, leading to a multi-scale sea ice model where ridges and sub-element floe-sizes, when they exist, are represented within discrete elements, the properties of which affects inter-element mechanics. Naval Postgraduate School, in collaboration with Los Alamos National Laboratory, has developed a new way to model sea ice thickness evolution that differs from the AIDJEX-era methods reviewed in section 1.2. It can be used to model multi-scale sea ice physics in discrete element sea ice models (*Roberts et al.*, In Prep.)

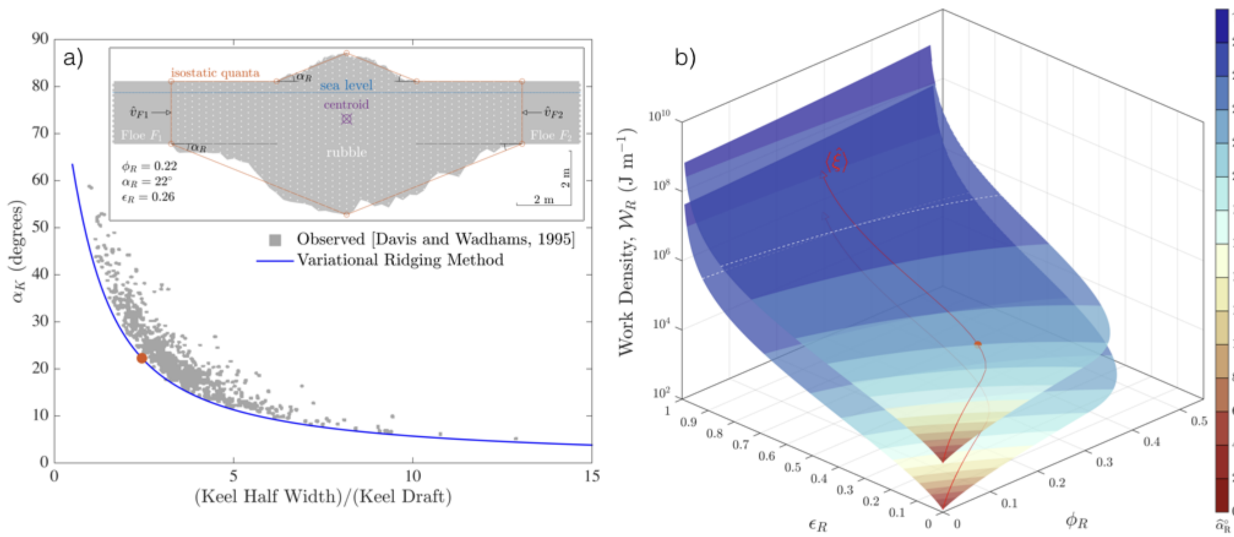

Figure 4: a) Example of a course-grained porous ridge state for a given macro-porosity, ϕ_R, angle of keel and sail repose α_R, and compressional strain, ϵ_R for two converging floes (velocities $\hat{v}_{F1,2}$) and no horizontal shearing (θ_R=0). The ridge as a whole is assumed to be isostatic, but all rubble within it is not. The particular ridge state is compared to submarine data from *Davis and Wadhams* (1995) (orange marker), and sits on the expected ridging path $\langle\hat{\xi}\rangle$ of the ridging work manifold $\mathcal{W}_R$ where $\mathcal{S}$ is minimized in (b). The two leaves in (b) represent ridging ice with thickness 0.5 m (lower leaf) and 2.0 m (upper leaf), and optimal angles of repose, $\hat{\alpha}_R$ (shading color). Every point in the manifold represents a unique ridge state in terms of porosity, angle of repose, ridge width and keel (sail) depth (height). White dashed contours indicate maximum observed sail heights by *Tucker et al.* (1984), which is 7.41 m for the upper leaf.

The new NPS ridging physics represents evolving sea ice thickness with a morphological state space that is expanded from the simple thickness distribution, $g(h)$, to a multivariate construct $\mathfrak{g}(h, h_s, \epsilon_R, \phi_R, \alpha_R, \theta_R)$. This construct describes the shapes and sizes of ridges in a given element as a distribution of ice and snow thickness, h and h_s, ridge strain, ϵ_R, ridge porosity, ϕ_R, angle of ridge repose, α_R, and horizontal shearing angle between discrete elements, θ_R. The theory applies the principle of stationary action for nonconservative systems of *Galley et al.* (2014) to ridge energetics, allowing the determination of an *expected* ridging path $\langle\hat{\xi}\rangle$ from an infinite but bounded possible number of ridge states on a ridging work manifold $\mathcal{W}_R$ demonstrated in Fig. 4. The manifold can be foliated into leaves representing the energy function for a deforming parent ice floe which minimizes the nonconservative ridging action $\mathcal{S} = \int_{t_i}^{t_f} \mathcal{Y} dt$, similar to that described by *Galley* (2012) for discrete non-conservative systems. $\mathcal{Y}$ is the nonconservative Lagrangian energy density per unit ridging area that explicitly accounts for frictional loss and inelastic deformation.

Frictional and inelastic dissipative energy sinks are determined using Rankine's theory to represent Coulombic failure in ridge cross sections following *Hopkins et al.* (1991), which allows the prediction of an optimal angle of repose for keels and sails, $\hat{\alpha}_R$, for each thickness leaf in $\mathcal{W}_R$

(Fig. 4). From this, the redistribution function, $\Psi(\omega_R, \dot{\epsilon}_{mn})$, and compressive strength, P, of discrete elements can be determined. Just as importantly, the method predicts the spatial separation of ridges within elements, and therefore serves as a proxy for sub-element scale floe size distributions. These naturally evolve as scale-invariant size from the mechanics, without any parametric constraints. The method is computationally efficient because the minimization of $\mathcal{S}$ is an eigenvalue problem solved in run-time with a Frobenius companion matrix, or approximated using precomputed look-up tables. Therefore detailed bending and buckling of sea ice associated with ridging can be 'course-grained' in a basin-scale DEM simulation of sea ice, rather than using the simplification of frictional loss reviewed in ection 1.2, which we have found to be highly inaccurate for immature ridges and, hence, for determining inelastic contact forces between elements. This work will form the basis for representing mechanically-induced ice morphology within elements in our proposed research.

4 Proposed Research and Methods

4.1 Overview

Based on the experience gained with the LANL prototype DEM sea-ice model, discussed in Section 3.2, we will develop DEMSI to use circular elements. Previous DEM sea-ice models have either used polygonal or circular elements (see Section 1.4). We choose circular elements for our model because calculations of contact force terms are more computationally efficient with circular disks, as polygonal elements require complex computational geometry algorithms to determine element overlap. Distortions of polygonal elements during simulations also require regular redistributing of those elements back to an original undistorted distribution. Part of this issue is removed by constraining the elements to remain circular, although the reduction in size of elements during ridging must still be accounted for (see Section 4.7). We will use two separate Cartesian polar stereographic planes for a model mesh (one each for the Arctic and Southern Ocean domains), rather than modeling them collectively on an ellipsoid. This process will improve computational efficiency by simplifying the search for element neighbors. The following sections describe in detail the steps needed to develop DEMSI.

4.2 LAMMPS

We will use LAMMPS for the dynamical core of DEMSI. LAMMPS is designed to perform massively parallel computations using the Message Passing Interface (MPI) system and is one of the top applications on DOE leadership-class computing facilities (e.g., Titan: https://www.olcf.ornl.gov/titan/). Using LAMMPS as the dynamical core of DEMSI has a number of advantages. First, we are able to leverage the large amount of computational science effort that has been and continues to be invested in LAMMPS, and rely on a well-tested, mature code base. This effort includes an efficient parallel implementation with dynamic load balancing and support for heterogeneous computing architectures. Second, LAMMPS provides an extensive infrastructure for various particle types and interactions, and has been designed to allow easy customization, including new particle types and force models. This ability is one of the key strengths of the LAMMPS framework and has led to hundreds of contributions from users from all over the world, both in the form of new physical models and new algorithms. The compartmentalized design of LAMMPS makes it possible for users to focus on physical models without needing to modify the core functionality of the code, while custom additions do not adversely impact the performance of existing models or algorithms.

We will take full advantage of these features to add customized models of pairwise discrete-element interactions relevant to sea-ice modeling. From the perspective of algorithm design, the features of discrete-element modeling needed for this work closely mirror the granular materials models that are already well-matured and optimized within LAMMPS. In particular, the contact model described below will require creating, storing, and communicating additional data structures associated with each element-element contact for its entire duration; these capabilities already exist in LAMMPS in the context of cohesive and frictional granular contacts and have been developed and used by members of our team, so we expect minimal difficulties in extending them to the models of interest for this work. Additional features will include element creation/destruction and coupling to other simulation codes, as described below. LAMMPS has proven capabilities in all of these areas, so we likewise do not expect these customizations to present major challenges from the LAMMPS perspective.

Initial tests of the computational throughput we can expect from LAMMPS are promising. For instance, we compare LAMMPS performance against MPAS-Seaice in ACME. The highest-resolution sea-ice mesh used in ACME at the moment has $\sim$6 km resolution in the polar regions. Currently, with this resolution MPAS-Seaice is achieving approximately three simulated years per day (SYPD) of computations using 12,000 cores on the Titan supercomputer at ORNL. For a discrete-element simulation with this resolution, we could expect to use $\sim 10^6$ elements and $\sim$0.5-second time steps (*Hopkins*, 2004a). LAMMPS has been tested on 1000 cores of the Serrano cluster at SNL using 10^6 elements and a contact force law with a history dependent friction. We estimate that computational throughput would be approximately seven SYPD for a 0.5-second time step and that Serrano is approximately three times faster than Titan per core. Thus, LAMMPS should achieve approximately the same throughput as MPAS-Seaice with an order of magnitude fewer cores, even without the proposed improvements in computational performance described in Section 4.4. Such comparisons are only approximate: the MPAS-Seaice computations include thermodynamics ($\sim$0.5 of the runtime), whereas the LAMMPS computations do not and a different LAMMPS contact force law is used than that which will be implemented. However, these estimates give us confidence that we can develop a discrete element sea-ice model with at least as good performance as current models.

4.3 Element Contact Model

One key aspect of developing a DEM sea-ice model is the choice of element contact model. This choice determines the horizontal contact forces produced by element neighbor interactions and the horizontal fracture properties that will distinguish the relative strength of ice under compression, shear, and tension. Our starting point for DEMSI will be the contact force model of *Hopkins et al.* (2004b), adapted to be compatible with our morphological model. Individual elements within this model and our own represent a collection of physical floes rather than a single sheet, as the scale-invariant nature of sea ice means that some real-world floes can have horizontal length scales as low as ten meters or even less. By contrast, we anticipate a minimum element size of about 1 km. To represent the freezing of floes, elements in this contact model can be bonded together with elastic forces. As the stress on these bonds increases beyond either a tensile or compressive limit, fracturing propagates from each end until the bond becomes fully fractured. Once elements are no longer bonded, they interact with a contact force model with plastic, elastic, and viscous terms. If compressive forces between elements exceed some limit, the thinnest of the interacting elements undergoes ridging, shrinking the element while increasing its thickness. We will use the course-grained ridging and the morphological construct $\mathfrak{g}$ described in Section 3.3 to determine the compressive strength, P, of floe collections represented as elements. A number of different contact models will be tested that make use of P, including Coulombic failure criteria akin to that used by, for example, *Schulson and Hibler* (2004) or *Weiss et al.* (2007b), with tensile strength being proportional to and less than P, which is determined from the minimization of ridging action $\mathcal{S}$ within elements. The code for the multiscale morphology will be incorporated into the CICE column physics library, as discussed in section 4.8 below.

The DEM model of *Hopkins et al.* (2004b) uses polygonal elements, so their contact force model will need to be adapted for the circular elements to be used in DEMSI. Implementing this contact force model will be an important first step in developing DEMSI. As we develop the contact model, we will construct a hierarchy of models with increasing complexity, from very simple elastic contact models to a fully complex sea-ice appropriate contact model. This construction will allow us to assess the trade off between model complexity and performance.

A major part of validating any contact force model used will be the standard validation metrics described in Section 4.9. In addition to these metrics, we will investigate the validity of the contact force model by performing very high-resolution, floe-scale simulations in small test domains. These floe-scale elements will be subjected to an external forcing and their dynamic response compared with an equivalent simulation with the standard elements. High-resolution floe-scale simulations are also useful for determining larger scale parameters used in the contact force model of the standard sized elements. For example, *Bathurst and Rothernburg* (1988) determined the Poisson ratio and elastic modulus from a high-resolution simulation that *Hopkins et al.* (2004b) then used in the contact model in their basin-scale simulations.

4.4 Improved Performance

Poor numerical performance has prevented DEM sea-ice models from performing global climate simulations. We will pursue two research tracks to improve the computational performance of DEMSI. First, we will investigate the acceleration on GPUs using Kokkos. LAMMPS has already made significant progress in porting both basic and advanced algorithms to use the Kokkos framework for shared-memory parallelism, and our project team includes a current LAMMPS developer who has experience of porting parts of LAMMPS to GPUs. LAMMPS testing is regularly performed on GPU platforms using the Kokkos CUDA configuration. Projects that build on the foundation of LAMMPS, including DEMSI, can leverage the existing work on LAMMPS GPU performance, which also serves as a clear guide and reference for further use of Kokkos in newly developed features. Single GPU cards are beginning to outperform their multi-core and many-core CPU competitors for increasingly complex problems. For example, the NVIDIA P100 GPU has stacked memory with bandwidth over twice that of typical CPU RAM, which has been the main bottleneck in certain single-GPU scientific applications (*Nvidia*, 2014). In the case of GPUs, the second important bottleneck is bandwidth between the CPU and GPU, and software development should be carried out with a focus on preventing such transfer and moving as much computation as possible onto the GPU.

Second, we will investigate whether techniques developed in the granular materials field for increasing DEM time step duration can be applied to a sea-ice model without physically degrading the results to an unacceptable degree. As mentioned in Section 1.4, the elastic stiffness of sea ice and the necessity of tracking elastic collisions between floes requires very short time steps. A similar problem is encountered in the granular materials field. Researchers in this field have successfully increased the time step of their simulations by decreasing the elastic stiffness of their particles (e.g., *Kuo et al.* (2002), *Limtrakul et al.* (2003), and *Malone and Xu* (2008)). *Lommen et al.* (2014) decreased the particle stiffness by a factor of 10^7 (and increased the time step by a factor of 100) without affecting the pertinent bulk properties of the material studied. We propose studying the effect of decreasing the elastic stiffness of the sea ice in DEMSI with the intention of demonstrating that the stiffness may be decreased sufficiently to significantly increase the allowable time step. Essentially, we intend to demonstrate that the floe elastic collision time can be increased from a fraction of a second to around a minute without significantly affecting the simulated climate.

4.5 Coupling Discrete Element Models

To use DEMSI in ACME, we will address the challenge of effectively coupling a Lagrangian particle model to other gridded model components. Under this project, we will develop algorithms to accurately and conservatively map fluxes from DEMSI to gridded atmosphere and ocean models. Standard methods for conservatively remapping between fixed grids involve computing conservative interpolation weights based on overlap areas between the two grids. In contrast, interpolating from a Lagrangian-particle sea-ice model requires a method that effectively approximates scattered data distributions. Accurate interpolation can be achieved for scattered data using a least squares approach and we will investigate using generalized moving least squares (GMLS) (*Wendlund*, 2005; *Mirzaei et al.*, 2012). Although this method of interpolation ensures a given order of accuracy it is not property preserving, in general. Members of our team have shown in previous research that property preservation can be efficiently ensured through enforced constraints using an optimization approach (*Bochev et al.*, 2014). We will build on these results to design constraints to be applied in conjunction with the least squares minimization to enforce conservation of fluxes and preservation of bounds.

The ACME coupler currently relies on off-line regridding using precomputed mapping files to pass data between two fixed grids from one model component to another. This strategy is not possible for a sea-ice model with Lagrangian particles that are changing location at each time step. To couple DEMSI, we will develop an efficient in-line regridding method that will incorporate the constrained GMLS algorithms and dynamically remap sea-ice fluxes to the ocean and atmosphere grids. This algorithm will utilize efficient LAMMPS capabilities for finding neighboring elements and dynamic load balancing. LAMMPS also has the capability to define the model domain using a structured grid, and efficiently assign particles (elements) to each grid cell as they move throughout the domain. Using this capability, when running in a coupled setting, we will define the domain boundary of our model as the set of ocean mesh cell edges that form the ocean/land boundary in the ocean component of ACME. This constraint prevents nonconformity of the sea-ice and ocean domains, which is prevented in ACME and other ESMs by requiring that the sea-ice and ocean models be discretized on the same mesh.

4.6 Creation of Elements

Sufficiently cooling atmospheric conditions create new sea ice in regions of open water. Within our new model, this process will be represented as the creation of new elements. While LAMMPS has infrastructure that allows the creation of new elements, a new module will be needed that determines where new elements should be created and what properties those elements should have. During coupled simulations, the ocean model, through the coupler, will provide a mass flux of frazil ice formed in the ocean. If this frazil is formed under existing elements, this mass flux will be added to those elements. If the frazil is formed in open water, then new elements will be created. During stand-alone simulations, DEMSI will need a simple slab-ocean model to calculate the amount of frazil ice formed. This process will require a simple Eulerian model to run in parallel with the discrete model. This simple slab-ocean model will closely follow the implementation in CICE and MPAS-Seaice.

Determining when and where to add new elements is a challenging problem and forms a significant research topic of this project. Placing a new element at random in the existing pack would create extreme contact forces and perturb the pack dynamics, because it is likely the new element would overlap significantly with existing elements. When placing new elements, the existing element distribution will be interrogated to enforce the constraint that new elements do not overlap with the existing distribution of elements. One possible method to achieve this placement is for DEMSI to store a fixed distribution of potential new elements and test those elements to determine if they can be created without negatively affecting the pack. Other possibilities include actively searching for areas of open water and placing new elements dynamically.

4.7 Destruction of Elements

Elements undergoing convergence and ridging will result in ice being transferred from thin to thick thickness categories and a decrease in the element horizontal size, but with increased macro-porosity (Section 3.3). More complex deformations of elements are prevented by requiring the elements to remain circular. Because the maximum allowable time step scales with the size of the elements, for computational efficiency some minimum element size will need to be defined and elements will need to be prevented from shrinking smaller than this limit. Ultimately this limit will be set depending on the computational efficiency of the LAMMPS implementation of the DEM model, with smaller limits being preferred. It will also depend on the resolution of the morphological construct $\mathfrak{g}$, and on whether look-up tables or a run-time solution to $\mathcal{W}_R$ is desired. The advantage of using look-up tables is that they are efficient, while the advantage of a run-time solution is that it can accurately account for the impact of snow cover on ridging and isostasy. Some alteration to the element size distribution must be made once an element undergoes sufficient ridging that its size drops below the lower element size limit. This alteration must conserve ice volume and other conserved quantities and produce the minimum of perturbations to the dynamics of the pack. One possibility is to conservatively remap the entire floe-size distribution back to a starting distribution (as was done by *Hopkins* (2004a)). Less intrusive possibilities include merging neighboring elements or destroying elements by redistributing element quantities to surrounding elements. Determining the best method to limit element size represents a significant research topic for this project.

4.8 Implementation of CICE Column Physics

Several other tasks must be completed in order to develop a fully functional sea-ice model suitable for global Earth system modeling. The largest is to implement the complex vertical physics present in the current generation of sea-ice models. This implementation includes sea-ice thermodynamics and radiation physics, and melt pond and snow morphology. For DEMSI, we will use the same "column physics package" as is currently used by the CICE model and the MPAS-Seaice model in ACME, except with the addition of the new NPS morphology as discussed in Section 4.3. The column package was created in the LANL CICE model by extracting the vertical physics into a separate library. Consequently, CICE and MPAS-Seaice use identical code for their vertical physics. A CICE consortium is currently being created that will facilitate the public distribution of this package. We will integrate the column package provided by the CICE consortium into our sea-ice model, giving us the same vertical physics fidelity as MPAS-Seaice. This task is facilitated by the fact that one of our team members completed the same task for MPAS-Seaice. As part of the implementation of the multiscale morphology, the existing infrastructure in the column physics package will be updated to use the predicted ridge shapes for sea ice form drag.

4.9 Verification, Validation, and Performance Assessment

Verification: To verify the correct implementation of DEMSI, we will implement a series of idealized test cases, each of which tests a specific new development within this proposal. Individual developments within this proposal will define a test case that will test whether that development is performing as expected. Only once the test is passed will the development be considered complete. Once the development is complete, the test case will be added to the repository to allow idealized testing of the new development at later times. As part of this project, we will develop a comprehensive test suite made up of the implemented test cases. Before new developments are merged into the master branch of the repository, this comprehensive test suite will be run to ensure that the new development has not broken previous developments through a series of regression tests. The correct behavior of the model during these test cases will also represent project milestones. Test cases range from the simple (such as single stationary elements to test forcing and thermodynamics, two element test cases to test contact model implementations, and cantilever test cases to test element bonding) to the complex (such as the vortex test case shown in Fig. 3 and the Arctic basin with realistic forcing).

Validation: During Phase-1 of this project, we will test the fidelity of DEMSI Arctic simulations using three methods, initially with the observational datasets listed in Table 1. First, we will use gridded satellite products and submarine draft measurements to evaluate modeled ice concentration, extent, drift, draft, and age mapped to an Eulerian reference frame. Table 1 summarizes the core observations to be applied to this evaluation method, where '*E*' indicates mapping of discrete elements to an Eulerian mesh before quantifying model bias and skill using methods commonly employed for coupled sea ice simulations (e.g. *Jahn et al.*, 2012).

DEMSI diagnostic	Evaluation method and dataset	Duration
Concentration/extent	*E* NOAA Climate Data Record (*Meier et al.*, 2014)	1979-
Drift & deformation	*E* Polar Pathfinder Drift (*Tschudi et al.*, 2016a)	1978-2015
	L International Arctic Buoy Program†	1980-
	L RADARSAT-1 Arctic Ocean deformation§	1997-2008
	L Envisat Arctic Ocean deformation§	2008-2012
Freeboard	*S* ICESat (*Yi and Zwally*, 2010)	2003-2008
	S IceBridge freeboard & snow depth (*Kurtz et al.*, 2015)	2009-
	S CryoSat-2 (*Tilling et al.*, 2015)	2010-
	S ICESat-2 (*Markus et al.*, 2017)	2018-
Draft	*E* U.S. Navy and Royal Navy (*NSIDC*, 2006)	1960-2005
	E SCICEX Submarine Data (pending availability)	2011-2016
Ice age	*E* Arctic sea ice age (*Tschudi et al.*, 2016b)	1978-2015
Mass balance	*L* IMB buoys (*Perovich and Richter-Menge*, 2015)	1993-2017
Ice-ocean flux	*L* Ocean Flux Buoys (*Shaw et al.*, 2008)	2002-2017
Ice-atmosphere flux	*L* SHEBA flux tower data (*Persson*, 2002)	1997-1998

Table 1: Baseline Arctic observational datasets for evaluating DEMSI state space (upper tier) and coupling (lower tier) using: *E* - Eulerian mapping; *L* - Lagrangian observation emulator; and *S* - Satellite altimetric emulator. References: NOAA - National Oceanic and Atmospheric Administration; SCICEX - Submarine Arctic Science Program data; SHEBA - Surface Heat Balance of the Arctic *in situ* data; † - *http://iabp.apl.washington.edu*; § - *https://rkwok.jpl.nasa.gov*.

A second evaluation method will exploit modeling sea ice in a Lagrangian reference frame, and will be critical for evaluating the Element Contact Model (section 4.3). Sea ice drift, deformation and atmospheric and oceanic fluxes will be evaluated along element paths $\boldsymbol{x}_a(t)$ using a Lagrangian observation emulator. Measurements ideally suited to this method are marked 'L' in Table 1. The Lagrangian emulator will make virtual buoy deployments in DEMSI at the same place and time as actual instrument deployments. Velocity, strain rate, internal stress and interfacial flux terms will be recorded along tracer paths, and new model tracer deployments will occur at regular intervals as the model solution diverges from measured tracks, while the existing model tracers continue. This facilitates efficient validation of ice mechanics and fluxes on timescales of hours to decades using wavelet analysis along Lagrangian paths as described by *Roberts et al.* (2015). NPS has since enhanced this analysis method to quantify cyclonic and anticyclonic model velocity performance with *Taylor* (2001) skill scores, and this will be applied to DEMSI. We will also quantify dispersion within DEMSI's dynamics, and compare them against Arctic observations (e.g. *Rigor*, 2002; *Rampal et al.*, 2008). Finally, we will investigate the extent to which spatial and temporal scaling properties of DEMSI deformation mimics measured scaling signals (*Marsan et al.*, 2004; *Hutchings et al.*, 2011), making use of improved deformational datasets where possible (e.g. *Bouillon and Rampal*, 2014).

The third validation method will adapt an altimetric satellite emulator to DEMSI that is in an advanced stage of development in the Regional Arctic System Model (RASM). Using this emulator, we will evaluate sea ice freeboard in DEMSI using satellite (ICESat, CryoSat-2, ICESat-2) and aircraft (IceBridge) measurements denoted 'S' in Table 1. ICESat-2 will be launched in 2018, and we anticipate quickly capitalizing on this new data stream through our ongoing involvement with the ICESat-2 Early Adopter Program (see *http://icesat.gsfc.nasa.gov/icesat2/apps-ea.php*). Part of the design of the satellite emulator is described by *Bench* (2016), and her thesis is available online at *http://hdl.handle.net/10945/49374*. The emulator circumvents inherent uncertainty introduced when converting satellite- and aircraft-measured freeboard to sea ice thickness, which requires knowledge of snow thickness, ice density and ridge porosity that are seldom known with confidence (*Kwok and Cunningham*, 2008). Instead, it evaluates model freeboard, not thickness, which is perfectly known from $\mathfrak{g}(h, h_s, \epsilon_R, \phi_R, \alpha_R, \theta_R)$, and is the actual quantity measured by altimeters, and therefore has a quantified measurement error (e.g. ± 0.14 m along ICESat ground tracks as specified by *Yi and Zwally*, 2010). It is therefore a reliable validation metric of modeled sea ice volume. Using the satellite emulator, model freeboard is sampled within ± 1 hour at the location of each satellite or aircraft measurement. The difference between each altimetric freeboard measurement and modeled freeboard sample takes into account the altimeter footprint on the ice through a spatial ridge distribution determined from $\mathfrak{g}$, and the difference between satellite and modeled freeboard over that footprint is used to construct basin-wide skill scores and bias estimates, and can be summarized on *Taylor* (2001) diagrams. This method is particular relevant to DEMSI, because the ground footprint of LASER altimeters, as used in ICESat, IceBridge and ICESat-2 when it is launched in 2018, is less than 100 m, and by evaluating a model along narrow LASER tracks, we will be capitalizing on the high fidelity of both the observations and the discrete elements.

In addition to these validation methods, we will also intercompare the results for the new discrete-element sea-ice model against ACME's own sea-ice component and MPAS-Seaice (an ACME collaboration agreement will be obtained for this purpose). We will also make use of observations that emerge during this project, including those expected to come from the Multidisciplinary Drifting Observatory for the Study of Arctic Climate (MOSAiC; *http://www.mosaicobservatory.org*). During the course of this project, we will work to build collaborations with MOSAiC scientists.

Performance Assessment: Scalability and good performance are crucial properties for a sea-ice model used in long-integration coupled simulations. We will assess the performance of DEMSI for selected benchmark problems on standard CPU systems as well as a variety of testbeds with heterogeneous architectures. Initial testing will focus on measuring the scalability of all components of DEMSI (DEM, column physics, morphology) to numbers of processors comparable with what is used in ACME runs. Once Kokkos support has been implemented in DEMSI, we will test benchmark performance on CPUs with GPU acceleration and on self-hosted Xeon Phis. We will translate the CPU only and heterogeneous platform performance results into a metric of simulated years per day for an equivalent ACME resolution in order to compare with MPAS-Seaice, which will be used as a performance baseline. We will additionally investigate model design impacts on DEMSI performance. These include the impact of data movement and communication implementation on GPU and multicore performance, trade-offs between accuracy and decreasing elastic stiffness in determining an effective time step size, and the impact of element size variation or polydispersity on performance.

4.10 Risks and Rewards

Balancing the risks and rewards of this project can be achieved with two questions: 1) Is it a question of *if* coupled sea ice models transition to discrete element dynamical cores, or *when* will they transition? 2) Are the theoretical developments, numerical methods and computing facilities ready for such a transition? For the first question, we believe the transition to discrete element sea ice models is inevitable, simply because the accuracy of continuum sea ice dynamics can only decrease below $\sim$10 km resolution, but the reverse is true of discrete element sea ice dynamical cores. DEMSI is therefore an investment in the future that will maintain DOE's position as a world leader in sea ice modeling. To answer the second question, we believe that we can build on the theoretical and computational foundations of tools like LAMMPS and Kokkos, as well as theoretical developments in non-conservative classical mechanics applied to sea ice morphology to assemble a new dynamical core ready for the computing facilities of the future. While such a venture inevitably involves risks, perhaps the best protection against these is in the team we have constructed. It includes scientists who are leading sea ice model development in two advanced coupled frameworks (ACME, RASM) and computational scientists at the forefront of code development for next generation processors with expertise in advanced numerical discretizations including DEM. The project will also provide an opportunity for a postdoctoral fellow to be part of DEMSI from its onset, and will provide graduate students at Naval Postgraduate School with a window on methods that may become the backbone of U.S. numerical sea ice prediction in years to come.

5 Project Management Plan

Adrian Turner (LANL, BER) will serve as lead Principal Investigator (PI) and will be the primary contact for communications with DOE program managers. He will organize project workshops, teleconferences, and management tools and serve as the lead for the BER side of the project. He will manage work undertaken at LANL including creating the main DEMSI code into which other modules (e.g. LAMMPS) are integrated, developing a contact force model (4.3), methods to create (4.6) and destroy (4.7) elements consistently, and developing metrics to assess the physical fidelity of the model (4.9). ***Kara Peterson*** (SNL, ASCR) will lead the ASCR side of the project and manage work undertaken at SNL. This work includes development of a new sea-ice type in the LAMMPS model, implementation of the contact model into LAMMPS, implementation of Kokkos acceleration for the discrete element contact force types in LAMMPS, and development of a consistent method for transforming element data into meshes (4.5). ***Andrew Salinger*** (SNL) and ***Steve Plimpton*** (SNL; the creator of LAMMPS) will act as unfunded consultants for this project. ***Andrew Roberts*** (NPS, BER) will manage the BER tasks of developing a new morphological model suitable for a discrete element sea-ice model (3.3) and DEMSI validation tools (4.9), working closely with LANL and SNL on the development of the contact model and other components as described in in section 6. He will host postdoctoral fellow visits to NPS from LANL as part of the project, and involve NPS graduate students in the design of observational emulators at no cost to DOE.

To facilitate management of this project, we will organize tasks and monitor achievement of milestones using a cloud-based project management tool, such as *Asana*. We will hold monthly and impromptu project teleconferences using *WebEx*. We will use the *Slack* instant messaging tool, email, and telephone for day-to-day communications. To meet in person, we have budgeted for yearly workshops where all team members can meet at one of the project institutions and discuss progress on the project face-to-face, with more regular working visits between groups as the need arises. The code developed in this project will be documented through a series of scientific papers published in the peer-reviewed literature. These papers will document each major research development and, also, analyze the overall model performance as defined in Section 4.9.

As our ultimate aim is to integrate our new model into the ACME model, we will follow ACME best practices for code development from the outset. We will host our new code on the same cloud-based repository hosting service as ACME (*GitHub*; DEMSI will, however, be its own standalone github project. LAMMPS and CICE already have their own repositories) using an ACME compatible work-flow. Coding standards will be enforced that ensure the code is readable, well-commented and documented, and modular in design. Before integration into ACME, validation of the model (see Section. 4.9) will be well-documented in an ACME integration design document.

Budget by PI/institution ($ in thousands)

Institution	**PI**	**Role**	**Y1**	**Y2**	**Y3**	**Total**
LANL	Adrian Turner	Lead and BER PI	395	400	207	1002
NPS	Andrew Roberts	NPS PI	117	126	68	311
BER Total			512	526	275	1313
SNL	Kara Peterson	ASCR PI	503	521	262	1286
ASCR Total			503	521	262	1286
Total			1015	1047	537	2599

Budget by tasks ($ in thousands, see section 6 for task definitions)

Task	**Task Leader**	**Y1**		**Y2**		**Y3**		**Total**
		BER	**ASCR**	**BER**	**ASCR**	**BER**	**ASCR**	
Task 1	LANL	105	25					130
Task 2	LANL	116	101	140	130			486
Task 3	SNL		151	58	156	8	52	426
Task 4	SNL		126		130		92	348
Task 5	NPS	80		55				135
Task 6	LANL	163	101	162	104			530
Task 7	NPS	48		111		267	118	543

6 Timetable of Activities

The following tables present a proposed timetable of DEMSI major tasks, sub-tasks and milestones. Institutions assigned to sub-tasks are denoted by letters: L=LANL, S=SNL, N=NPS. The final column signifies the year and quarter the sub-task will be completed in.

***Task 1:* Model integration** (Lead: LANL)		
Set up project management tools/github repository and create main DEMSI code	L	Y1Q1
Create DEMSI sea-ice element type in LAMMPS	S	Y1Q2
Integrate LAMMPS into DEMSI	L	Y1Q2
Create the atmospheric and oceanic forcing routines	L	Y1Q2
Integrate column physics into DEMSI	L	Y1Q4
Add ridging/morphology/form drag improvements to DEMSI column physics	LN	Y1Q4
***Task 2:* Contact force model** (Lead: LANL)		
Investigate possible contact models	LS	Y1Q2
Determine how to implement a realistic contact model with circle elements	LS	Y1Q4
Integrate ice strength from the NPS morphology into the contact model	LN	Y2Q1
Implement and test contact model, validating with observational emulators	LSN	Y2Q3
***Task 3:* Performance** (Lead: SNL)		
Add Kokkos support for DEM LAMMPS	S	Y1Q4
Test ability to decrease element stiffness, increase time step	LN	Y2Q3
Optimize performance on multiple platforms including with Kokkos acceleration	S	Y2Q4
Benchmark DEMSI on Department of Defense computers	N	Y3Q2
***Task 4:* Coupling** (Lead: SNL)		
Determine requirements for coupling DEM sea ice model to a fixed grid atm/ocn	S	Y1Q1
Implement prototype remap method for DEM flux exchange	S	Y1Q4
Implement constrained optimization approach to ensure conservation of fluxes	S	Y2Q3
Test accuracy and conservation in prototype remap code	S	Y2Q4
Implement coupling algorithm in DEMSI and test accuracy and efficiency	S	Y3Q2
***Task 5:* Ridging/Morphology** (Lead: NPS)		
Implement multiscale morphology into the CICE Column Package for DEMSI	N	Y1Q1
Conduct tests to benchmark look-up and run-time morphology solutions	N	Y1Q2
Integrate sea ice redistribution into element size reduction and destruction	LN	Y2Q2
***Task 6:* Element creation and destruction** (Lead: LANL)		
Scope solutions to element destruction	LS	Y1Q2
Implement and investigate disappearing element solutions	LS	Y1Q3
Validate disappearing element methodology	LS	Y2Q1
Scope solutions to element creation	LS	Y2Q1
Implement and investigate element creation solution	LS	Y2Q2
Validate element creation methodology	LS	Y2Q4
***Task 7:* Validation** (Lead: NPS)		
Implement the model I/O framework	LN	Y1Q3
Adapt standard Eulerian sea-ice validation methods from ACME and RASM	LN	Y1Q4
Implement the Lagrangian observational emulator (LOE) in DEMSI	LN	Y2Q1
Create supporting LOE code for wavelet, dispersion and scaling metrics	LN	Y2Q2
Implement ICESat/IceBridge/CryoSat-2/ICESat-2 satellite emulator	N	Y2Q3
Adapt supporting RASM satellite emulator code for DEMSI freeboard metrics	N	Y2Q4
Comprehensive evaluation of Phase-1 Arctic Ocean simulations	LSN	Y3Q1

7 Progress from DOE-Funded Research

7.1 CICE

LANL has received significant support over an extended period from DOE ESM to develop and maintain the CICE sea-ice model (*Hunke et al.*, 2013). Thanks partly to the contributions of community members, including the Naval Postgraduate School (NPS), CICE has become one of the most sophisticated and widely used sea-ice models in the world and it is the sea-ice component for the National Center for Atmospheric Research's (NCAR) Community Earth System Model (CESM; *Hurrell et al.*, 2013). Through the ESM Cloud-Cryosphere project, **Adrian Turner** was funded to develop a new vertical thermodynamics method for the CICE model, based on a "mushy layer" formulation (*Turner et al.*, 2013; *Turner and Hunke*, 2015). This method determines both the temperature and bulk salinity of the sea ice prognostically and parameterizes various processes that modify the sea-ice salinity, such as gravity drainage, flushing, and snow-ice formation. This thermodynamics is the default one used by CICE and MPAS-Seaice. Contributions by **Andrew Roberts** to CICE are listed in section 7.5.

7.2 LANL: MPAS-Seaice and ACME

Over the past several years, **Adrian Turner** has received considerable DOE ESM funding through the Accelerated Climate Model for Energy (ACME) project as lead developer of MPAS-Seaice, a new variable-resolution sea-ice model (*Turner et al.*, In Prep.). This model uses the Modeling for Prediction Across Scales (MPAS) modeling framework, which allows models to use variable resolution Voronoi tessellation meshes. These meshes permit a smooth transition in grid resolution allowing computational resources to be focused in regions of interest. Within its dynamics, MPAS-Seaice uses the same EVP constitutive relation and variational differential operator methods as CICE, but adapted to operate on the polygonal cells of MPAS meshes rather than the quadrilateral cells of CICE. A working version of MPAS-Seaice was required for version 1 of the ACME model, as this version of ACME was scheduled to incorporate the MPAS-Ocean model and ACME requires the ocean and sea-ice components to share a common mesh, making CICE incompatible with this version of ACME. This constraint necessitated a rapid development schedule for MPAS-Seaice, which was partly achieved by the development of the CICE column physics package, wherein the CICE code-base was refactored by placing all vertical physics into a separate library. This library could then be used by both CICE and MPAS-Seaice, and recoding of the extensive vertical physics avoided in MPAS-Seaice. Within the ACME project **Adrian Turner** oversaw the successful coupling of MPAS-Seaice into the coupled system and currently leads the sea ice effort, including overseeing and performing new sea-ice model development and investigating anomalies in the model coupling.

7.3 SNL: Compatible Discretizations and Optimization-based Methods

Over the last several years **Kara Peterson** has actively contributed to an ongoing ASCR-funded project led by Pavel Bochev (SNL) focusing on the development of new classes of compatible and property-preserving numerical methods for mission-relevant applications. Under this project we have developed novel stabilization schemes for drift-diffusion equations and collaborated to implement them in the Sandia Charon semiconductor code (*Bochev et al.*, 2013, 2015). We have additionally developed methods for conservative and monotone optimization-based remap and transport(*Bochev et al.*, 2014). Recently, we have developed new optimization-based partitioned coupling schemes for elliptic equations (*Kuberry et al.*, 2017).

Kara Peterson has also been funded under the BER project Parallel Analysis Tools and New Visualization Techniques for Ultra-Large Climate Data Sets (ParVis) led by Robert Jacob (ANL), which provided high-performance data-parallel versions of several common analysis algorithms for data from Earth science applications. Under this project we developed a Parallel Gridded Analysis Library (ParGAL) that was built from ASCR tools including Trilinos and MOAB and was designed as the core of a parallel implementation of the NCAR Command Language (NCL) (*Jacob et al.*, 2013). Under the BER and ASCR funded project Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC) led by Forrest Hoffman (ORNL) **Kara Peterson** and Iulian Grindeanu (ANL) implemented a finite volume tracer advection scheme that coupled MOAB for mesh intersections with the High-Order Method Modeling Environment (HOMME) spectral element dynamical core.

7.4 SNL: LAMMPS

Advancements in LAMMPS with regard to DEM applications for granular and colloidal systems have historically been partially funded by a variety of Cooperative Research and Development Agreements (CRADAs) between SNL and several industry partners. Further CRADAs with a heavy focus on LAMMPS DEM development are currently being pursued, with potential for funding starting in FY18. More recently, additional development of more sophisticated contact models (e.g. cohesion, history-dependent twisting/rolling friction) as well as the ability to represent complex, moving boundaries in DEM (e.g. geometric primitives, triangulated surfaces) have been funded by an Advanced Scientific Computing - Physics and Engineering Modeling (ASC P&EM) project (PI **Dan Bolintineanu**). This project will continue to be funded in the context of modeling granular flows for additive manufacturing applications. Although the length scales and application spaces are substantially different from the work proposed herein, the development of general DEM capabilities and algorithms within LAMMPS is expected to be highly synergistic.

7.5 NPS: Regional Arctic System Model

Andrew Roberts' previous work on DOE-funded projects has focused on the development, coupling and analysis of the sea-ice component of the Regional Arctic System Model (RASM). He has received funds from one previous DOE BER project and two current projects lead by Wieslaw Maslowski at Naval Postgraduate School: 1) *Collaborative Proposal: Improving Decadal Prediction of Arctic Climate Variability and Change Using a Regional Arctic System Model (RASM)* (DE-SC0005783, complete); 2) *Collaborative Project: Understanding the effects of tides and eddies on ocean dynamics, sea ice cover and decadal/centennial climate prediction using the Regional Arctic Climate Model (RACM)* (DE-SC0005522, current); 3) *Collaborative Research: Advancing Arctic Climate Projection Capability At Seasonal To Decadal Scales* (DE-SC0014117, current). RASM is a fully coupled model of the high north incorporating the Weather Research and Forecasting Model (WRF), Variable Infiltration Capacity (VIC) terrestrial model, the Parallel Ocean Program (POP) and the Los Alamos Sea Ice Model (CICE). It uses the coupling and infrastructure framework of the Community Earth System Model (CESM) and in many respects is a regional analogue of CESM. **Andrew Roberts'** RASM accomplishments so far under DOE BER funding include:

1. First application of the new CICE column package and dynamical core in a fully coupled framework outside of ACME, in collaboration with Elizabeth Hunke at LANL, becoming an example of the use of this new CICE configuration ahead of its initial release by the CICE Consortium in late 2017.

2. Implementation and validation of CICE Version 5 in RASM and CESM, jointly completed by Naval Postgraduate School and the National Center for Atmospheric Research. This work identified and corrected problems associated with the simulation of melt ponds, form drag and inertial oscillations, and the coupling of mushy-layer thermodynamics that contributed to a new public release of CICE (5.1.2). Associated research includes an inter-comparison of EVP and EAP ice mechanics, using an ICESat emulator to analyze total simulated sea ice mass. A publication is nearing submission on this topic, which has also resulted in completion of two student theses supervised by **Andrew Roberts** (*DiMaggio*, 2014; *Bench*, 2016).
3. Collaborative research with the University of Washington using CICE 5.1 innovations and improvements in RASM for hydrologic studies (*Hamman et al.*, 2016, 2017).
4. Identification of physical constraints in modeling ice-ocean inertia in high-resolution models to accurately simulate the drift of sea ice on timescales of hours to decades (*Roberts et al.*, 2015). A significant problem was discovered in the way some Earth System Models couple ocean, sea ice and atmospheric components that leads to an instability in the ice-ocean boundary layer. Results from this work are now used in ACME and CESM and one thesis was supervised by **Andrew Roberts** on the high-frequency coupling topic (*Mills*, 2012). A spin-off publication from this work is in progress on the positive impact that improved ice-ocean coupling has on CESM's Antarctic sea ice edge.
5. Collaborative work with the University of Colorado to identify a leading cause of poor Arctic sea-ice thickness simulations in the crude representation of cloud liquid droplet size in some atmospheric models (*Cassano et al.*, In Review), and the use of RASM to understand the impact of strong wind events south of Greenland on high resolution atmosphere-ice-ocean boundary layer interactions (*DuVivier et al.*, 2016).
6. Theoretical development of improved representation of form drag through the simulation of ridges in Earth System Models, including expansion to porous ridging, as discussed in this proposal. The first publication for this work is close to submission (*Roberts et al.*, In Prep.).

Research progress has been communicated with the scientific community at international conferences and workshops, including invited presentations. Several substantial software products have been created, including RASM itself, as well as MATLAB packages for off-line ICESat/ICESat-2 model emulators and Lagrangian sea ice drift and deformation analysis.

Appendix 1: Biographical Sketches

The following pages provide biographical sketches for the following personnel:

Adrian Turner	Los Alamos National Laboratory
Kara Peterson	Sandia National Laboratories
Andrew Roberts	Naval Postgraduate School
Dan Bolintineanu	Sandia National Laboratories
Dan Ibanez	Sandia National Laboratories

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Education and Training:

2005	PhD	University of Cambridge, UK	High energy astrophysics
2001	MSci	University of Cambridge, UK	Physics & astrophysics
2001	MA	University of Cambridge, UK	Natural Sciences

Research and Professional Experience:

2013-Present Staff Scientist Los Alamos National Laboratory
Lead developer of the MPAS-Seaice model and sea-ice modeling lead in ACME

2010-2013 Postdoctoral research associate Los Alamos National Laboratory
Developed a new "mushy layer" thermodynamics in the Los Alamos CICE model

2005-2009 Postdoctoral research associate University College London, UK
Developed a regional coupled sea ice/ocean model with CICE and NEMO

Publications:

Urrego-Blanco, J., Urban, N., Hunke, E. C., **Turner, A. K.**, and Jeffery, N., (2016) "Uncertainty Quantification and Global Sensitivity Analysis of the Los Alamos Sea Ice Model", *Journal of Geophysical Research-Oceans*, ***121***, 2709–2732

Turner, A. K. and Hunke, E. C., (2015) "Impacts of a mushy-layer thermodynamic approach in global sea-ice simulations using the CICE sea-ice model", *Journal of Geophysical Research-Oceans*, ***120***, 1253–1275

Turner, A. K., Hunke, E. C., and Bitz, C. M., (2013) "Two modes of sea-ice gravity drainage: A parameterization for large-scale modeling", *Journal of Geophysical Research-Oceans*, ***118***, 2279–2294

Hunke, E. C., Lipscomb, W. H., **Turner, A. K.**, Jeffery, N., and Elliott, S., (2013) "CICE: The Los Alamos Sea Ice Model Documentation and Software Users Manual Version 5.0", Los Alamos National Laboratory, Los Alamos, N. M. LA-CC-06-012.

Hunke, E. C., Notz, D., **Turner, A. K.**, and Vancoppenolle, M., (2011) "The multiphase physics of sea ice: a review for model developers", *Cryosphere*, ***5***, 989–1009

Hunke, E. C., Lipscomb, W. H., and **Turner, A. K.**, (2010) "Sea-ice models for climate study: retrospective and new directions", *Journal of Glaciology*, ***56***, 1162–1172

Elliott, S., Hunke, E., Jeffery, N., **Turner, A. K.**, Maltrud, M., Deal, C., and Jin, M., (2010) "Systems level simulation of sea ice-atmosphere biogeochemistry connections", *SOLAS*, ***11***

Flocco, D., Feltham, D. L., and **Turner, A. K.**, (2010) "Incorporation of a physically based melt pond scheme into the sea ice component of a climate model", *Journal of Geophysical Research-Oceans*, ***115***

Synergistic Activities:

2016	Represented LANL sea-ice models at the NGGPS Community Sea Ice Model Recommendation Workshop
2015-pres.	Sea-ice representative on the ACME coupled sea-ice team
2014	Participant of a SciDAC proposal review panel

Graduate and Postdoctoral Advisors and Advisees:

Graduate advisor	A. C. Fabian (U. Cambridge)
Postdoc advisors	D. Feltham (U. Reading), E. Hunke (LANL)
Student advisees	F. Therrien (U. Montreal)

Collaborators and Co-editors:

R. Aulwes	Los Alamos National Laboratory
D. Bailey	National Center for Atmospheric Research
C. Bitz	Univ. Washington
J. Dukowicz	Los Alamos National Laboratory
S. Farrell	NOAA/NASA
D. Feltham	Univ. Reading, UK
D. Flocco	Univ. Reading, UK
J. Fyke	Los Alamos National Laboratory
M. Holland	National Center for Atmospheric Research
E. Hunke	Los Alamos National Laboratory
D. Jacobsen	Los Alamos National Laboratory
N. Jeffery	Los Alamos National Laboratory
P. Jones	Los Alamos National Laboratory
W. Lipscomb	Los Alamos National Laboratory
S. Price	Los Alamos National Laboratory
T. Ringler	Los Alamos National Laboratory
A. Roberts	Naval Postgraduate School
D. Schroeder	Univ. Reading, UK
N. Urban	Los Alamos National Laboratory
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J. Wolfe	Los Alamos National Laboratory

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Education and Training:

2008	PhD	University of New Mexico, Albuquerque, NM	Applied Mathematics
1994	MS	University of Colorado, Boulder, CO	Astrophysics
1991	BS	New Mexico State University, Las Cruces, NM	Physics

Research and Professional Experience:

2010-Present Senior Member of the Technical Staff Sandia National Laboratories
Optimization-based remap and transport, stabilization for drift-diffusion equations

2008-2010 Postdoctoral research associate Sandia National Laboratories
Elastic-decohesive constitutive model for sea ice, compatible discretizations

1995-2003 Staff/Senior Scientist Applied Research Associates, Albuquerque, NM
Hydrodynamic calculations of airblast effects, conventional weapon effectiveness

Publications:

M. D'Elia, D. Ridzal, **K. Peterson**, P. Bochev, M. Shashkov, (2016) "Optimization-based mesh correction with volume and convexity constraints." *JCP* ***313***, 455–477.

P. Bochev, M. Perego, **K. Peterson**, (2015) "Formulation and analysis of a parameter-free stabilized finite element method." *SINUM* ***53***, 5, 2363–2388.

P. Bochev, **K. Peterson**, M. Perego, (2015) "A multi-scale control volume finite element method for advection-diffusion equations." *IJNMF* ***77***, 11, 641–667.

K. Peterson, P. Bochev and D. Ridzal, (2014) "Optimization-based conservative transport on the cubed-sphere grid." in *Large-Scale Scientific Computing*, Springer Lecture Notes in Computer Science, I. Lirkov, S. Margenov, and J. Wansiewski.(Eds.) ***8353***, 205–212.

P. Bochev and D. Ridzal and **K. Peterson**, (2014) "Optimization-based remap and transport: a divide and conquer strategy for feature-preserving discretizations." *JCP*, ***257*** Part B, 1113–1139.

K. Peterson, H. Schreyer and D. Sulsky, (2012) "Decohesion with Refreezing", *Cold Reg. Sci. Technol.*, ***76-77*** 44–51.

D. Sulsky and **K. Peterson**, (2011) "Towards a New Elastic-Decohesive Model of Arctic Sea Ice", *Physica D*, doi:10.1016/j.physletb.2003.10.071.

K. Peterson and D. Sulsky, (2011) "Evaluating Deformation in the Beaufort Sea Using a Kinematic Crack Algorithm with RGPS Data", In *Remote sensing of the Changing Oceans*, D. Tang, J. Gower, G. Levy, et al., (Eds.) Science Press/Springer ISBN 978-3-642-16540-5.

D. Sulsky, H. Schreyer, **K. Peterson**, M. Coon, and R. Kwok, (2007) "Using the Material-Point Method to Model Sea Ice Dynamics", *J. Geophysical Res* ***112*** C11S903.

Graduate and Postdoctoral Advisors and Advisees:

Graduate advisor	D. Sulsky (University of New Mexico)
Postdoc advisors	P. Bochev (SNL)

Collaborators and Co-editors:

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Peter Bosler	Sandia National Laboratories
Marta D'Elia	Sandia National Laboratories
Forrest Hoffman	Oakridge National Laboratory
Xujiao Gao	Sandia National Laboratories
Iulian Grindeanu	Argonne National Laboratory
Robert Jacob	Argonne National Laboratory
Jayesh Krishna	Argonne National Laboratory
Paul Kuberry	Sandia National Laboratories
Scott Moe	Univ. Washington
Mauro Perego	Sandia National Laboratories
Denis Ridzal	Sandia National Laboratories
Mikhail Shashkov	Los Alamos National Laboratory
Timothy Tautges	CD-adapco
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Nathaniel Trask	Sandia National Laboratories

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Education and Training:

2005	Ph.D.	University of Tasmania, Australia	ASOS
1993	B.Sc.(Hons)	University of Melbourne, Australia	Earth Science

Research and Professional Experience:

2010-present Research Assistant Professor Naval Postgraduate School
Developer of the sea ice component of the Regional Arctic System Model (RASM)

2005-2010 Postdoctoral Fellow University of Alaska Fairbanks
Arctic system and ice-tide modeling

2003-2004 Sea Ice Scientist Australian Antarctic Division
Constructed a sea ice forecast model for the Southern Ocean

2001-2002 Meteorologist Australian Antarctic Division
Created the Australian Antarctic Automatic Weather Station Dataset (http://aws.acecrc.org.au)

Relevant Publications:

Hamman, J., B. Nijssen, **A. Roberts**, A. Craig, W. Maslowski, and R. Osinski (2017): The Coastal Streamflow Flux in the Regional Arctic System Model, *J. Geophys. Res. Oceans*, Accepted, doi:10.1002/2016JC012323.

Hamman, J., B. Nijssen, M. Brunke, J. Cassano, A. Craig, A. DuVivier, M. Hughes, D. Lettenmaier, W. Maslowski, R. Osinski, **A. Roberts**, X. Zeng (2016): Land surface climate in the regional Arctic system model, *J. Climate*, 29(18), doi:10.1175/JCLI-D-15-0415.1.

DuVivier, A., J. Cassano, A. Craig, H. Hamman, W. Maslowski, B. Nijssen, R. Osinski, **A. Roberts** (2016): Winter atmospheric buoyancy forcing and oceanic response during strong wind events around southeastern Greenland in the Regional Arctic System Model (RASM) for 1990-2010 *J. Climate*, 29(3), doi:10.1175/JCLI-D-15-0592.1.

Roberts, A., A. P. Craig, W. Maslowski, R. Osinski, A. DuVivier, M. Hughes, B. Nijssen, J. Cassano and M. Brunke (2015): Simulating transient ice-ocean Ekman transport in the Regional Arctic System Model and Community Earth System Model, *Ann. Glaciol.*, 56, 211-228, doi:10.3189/2015AoG69A760.

Maslowski, W., J. Clement-Kinney, M. Higgins, **A. Roberts** (2012): The Future of Arctic Sea Ice, *Annu. Rev. Earth Planet. Sci.*, 40, 625-654, doi:10.13140/2.1.1828.9441.

Roberts, A., J. Cherry, R. Döscher, S. Elliott, L. Sushama (2011): Exploring the Potential for Arctic System Modeling, *Bull. Amer. Meteor. Soc.*, 92, 203-206, doi:10.1175/2010bams2959.1.

Hutchings, J., **A. Roberts**, and C. Geiger (2011): Spatial and temporal characterization of sea-ice deformation, *Ann. Glaciol.*, 52(57), 360-368, doi:10.3189/172756411795931769.

Roberts, A. F., J. Cassano, R. Döscher, L. Hinzman, M. Holland, H. Mitsudera, A. Sumi, and J. E. Walsh (2010): A Science Plan for Regional Arctic System Modeling, A report to the National Science Foundation from the International Arctic Science Community, *International Arctic Research Center Technical Papers 10-0001*. University of Alaska Fairbanks, 47pp., doi:10.13140/2.1.1828.9441.

Hibler, W. D., III, **A. Roberts**, P. Heil, A. Proshutinsky, H. Simmons, and J. Lovick (2006): Modeling M2 tidal variability in Arctic sea-ice drift and deformation, *Ann. Glaciol.*, 44, 418-428, doi:10.3189/172756406781811178.

Synergistic Activities:

Chair, 2014-2015, Polar Meteorology and Oceanography Committee, American Meteorological Society (AMS), including co-chair, Joint 49th Canadian Meteorological and Oceanographic Society Congress & 13th AMS Conference on Polar Meteorology and Oceanography, 31 May-4 June, 2015.

Co-lead, 2017, dynamical core code maintenance and development for the CICE Consortium sea ice model (*http://oceans11.lanl.gov/trac/CICE/wiki/CiceConsortium*).

PI, 2015-2017, ICESat-2 Early Adopter Program (*http://icesat.gsfc.nasa.gov/icesat2/apps-ea.php*), implementing a satellite emulator in CICE to evaluate simulated sea ice thickness against measured freeboard. Work is funded through existing grants, but involvement provides access to ICESat-2 tools, synthetic data and the mission science team ahead of the satellite launch in 2018.

Scientist, 2016-2017, Global Learning and Observation to Benefit the Environment (GLOBE) International STEM Network (*https://www.globe.gov*), leading an ICESat-2 education and outreach pilot project in a PK-8 school in Monterey, California.

Invited speaker, including at a Gordon Research Conference (2011), American Geophysical Union Fall Meeting (2014), and the Forum for Arctic Modeling and Observational Synthesis (2015).

Graduate student and postdoctoral advisees:

Thomas Mills	M.Sc. 2012	Naval Postgraduate School
Dominic DiMaggio	M.Sc. 2014; Ph.D. 2016	Naval Postgraduate School
Kristine Bench	M.Sc. 2016	Naval Postgraduate School
Joseph Hamman	Ph.D. 2016	University of Washington
Shawn Gallaher	Ph.D. 2016	Naval Postgraduate School

Graduate and postdoctoral advisors:

Ph.D. Advisors	William Budd	University of Tasmania, Australia
	Petra Heil	Australian Antarctic Division
	Roger Hughes	University of Melbourne, Australia
Postdoctoral Advisors	William Hibler III	University of Alaska Fairbanks
	Larry Hinzman	University of Alaska Fairbanks
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Co-authors and collaborative co-investigators (past 48 months; no co-editors):

David Bailey	National Center for Atmospheric Research
Mary Batteen	Naval Postgraduate School (Deceased)
Michael Brunke	University of Arizona
John Cassano	University of Colorado Boulder
Jaclyn Clement-Kinney	Naval Postgraduate School
Anthony Craig	Independent contractor
Clara Deal	University of Alaska Fairbanks
Larry Di Girolamo	University of Illinois
Alice DuVivier	National Center for Atmospheric Research
Scott Elliott	Los Alamos National Laboratory
Sinéad Farrell	University of Maryland
William Gutowski	Iowa State University
Matthew Higgins	Central Intelligence Agency
Marika Holland	National Center for Atmospheric Research
Mimi Hughes	National Oceanic and Atmospheric Administration
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Jennifer Hutchings	Oregon State University
Alexandra Jahn	University of Colorado Boulder
Nicole Jeffrey	Los Alamos National Laboratory
Meibing Jin	University of Alaska, Fairbanks
Bonnie Light	University of Washington
Dennis Lettenmaier	University of California Los Angeles
William Lipscomb	Los Alamos National Laboratory
Paty Matrai	Bigelow Laboratory for Ocean Sciences
Matthew Maltrud	Los Alamos National Laboratory
Wieslaw Maslowski	Naval Postgraduate School
Bart Nijssen	University of Washington
Robert Osinski	Polish Institute of Oceanology
Mark Seefeldt	University of Colorado, Boulder
Mark Serreze	National Snow and Ice Data Center
Amy Solomon	National Oceanic and Atmospheric Administration
Slawek Tulaczyk	University of California Santa Cruz
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Education and Training:

2010	Ph. D.	University of Minnesota, US	Chemical Engineering
2005	B. A. Sc.	University of Toronto, Canada	Chemical Engineering

Research and Professional Experience:

2014-Present Technical Staff Sandia National Laboratories
DEM simulations, LAMMPS development, statistical characterization of heterogeneous materials

2011-2014 Postdoctoral Fellow Sandia National Laboratories
Molecular dynamics, colloid suspension modeling, transport in hetergeneous materials

2005-2010 Ph. D. student University of Minnesota
Computational biophysics: molecular dynamics, electrodiffusion modeling

Publications:

Bolintineanu, D. S., Grest, G. S., Lechman, J. B., Silbert L. E., (2015) "Diffusion in jammed particle packs". *Physical Review Letters*, ***115***, 088002.

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Education and Training:

2016	PhD	Rensselaer Polytechnic Institute, US	Computer Science
2012	BS	Rensselaer Polytechnic Institute, US	Compute Science & Systems

Research and Professional Experience:

2016-Present Technical Staff Sandia National Laboratories
Integrating Kokkos with LAMMPS, Albany, etc.

2012-2016 PhD Student Rensselear Polytechnic Institute
Developed mesh adaptation library using Kokkos

Publications:

Ibanez, D. A., Seol, E. S., Smith, C. W., and Shephard, M. S., (2016) “PUMI: Parallel unstructured mesh infrastructure,” *ACM Transactions on Mathematical Software*, ***42***, 17:1—17:28

Ibanez, D., Dunn, I., and Shephard, M. S., (2016) “Hybrid MPI-thread parallelization of adaptive mesh operations,” *Parallel Computing* ***52***, 133–143

Ovcharenko, A., **Ibanez, D.**, Delalondre, F., Sahni, O., Jansen, K. E., Carothers, C. D., and Shephard, M. S., (2012) “Neighborhood communication paradigm to increase scalability in large-scale dynamic scientific applications,” *Parallel Computing*, ***38***, 140–156

Appendix 2: Current and Pending Support

Adrian Turner

Effort will be adjusted if the pending proposal is funded.

Current support

Title: Accelerated Climate Model for Energy (ACME)
Award number: -
PI: Dave Bader (Project PI, LLNL), Todd Ringler (LANL PI)
Program: DOE BER
Period: 7/2014–6/2018
Commitment (person-months): 12.0/year
Total Award: $5.869M/year
Description: Developing an Earth System Model for DOE mission needs.

Pending support

Title : A new discrete element sea-ice model for Earth system modeling (this proposal)
PI: Adrian Turner
Program: DOE BER
Period: 01/01/18 – 06/30/20
Commitment (person-months): 6.0/6.0/3.0
Total Award: $1,001,632

Kara Peterson

Effort will be adjusted if the pending proposal is funded.

Current support

Title: Mathematics and Algorithms for Heterogeneous Numerical Models: An Optimization-Based Approach
PI: Pavel Bochev (SNL)
Program: DOE ASCR
Period: 10/2014–9/2017
Commitment (person-months): 3.0/year
Total Award: $450K/year
Description: Development of compatible, property-preserving discretizations for a variety of application areas using optimization-based methods.

Title: Compatible Particles: a New Paradigm for Structure-Preserving Discretization without a Mesh
PI: Pavel Bochev (SNL)
Program: SNL LDRD
Period: 10/2016–9/2019
Commitment (person-months): 3.0/year
Total Award: $580K/year
Description: Development and theoretical derivation of compatible particle-based discretizations.

Title: Advanced Scientific Computing, Integrated Codes, Charon Support
PI: Joe Castro (SNL)
Program: DOE ASC
Period: 10/2016–9/2017
Commitment (person-months): 4.0/year
Total Award: $1.5M/year
Description: Code and algorithm development for the Trilinos-based Charon semiconductor model.

Title: ATDM Intrepid2 Support
PI: (Intrepid 2 task) Mauro Perego (SNL)
Program: DOE ATDM
Period: 10/2016–9/2017
Commitment (person-months): 2.0/year
Total Award: $1.5M/year
Description: Code development for the Intrepid2 Kokkos-dependent compatible discretization package in Trilinos.

Pending support

Title : A new discrete element sea-ice model for Earth system modeling (this proposal)
PI: Adrian Turner (LANL)
Program: DOE BER/ASCR
Period: 10/01/17 – 06/30/20
Commitment (person-months): 6.0/6.0/3.0
Total Award: pending

Title : Coupling Approaches for Next-Generation Architectures (CANGA)
PI: Phil Jones (LANL)
Program: DOE BER/ASCR
Period: 08/01/17 – 07/30/22
Commitment (person-months): 4.0/year
Total Award: pending

Title : Formulation, Analysis and Computation of Heterogeneous Numerical Methods
PI: Pavel Bochev (SNL)
Program: DOE ASCR
Period: 10/01/17 – 09/30/20
Commitment (person-months): 2.0/year
Total Award: pending

Andrew Roberts

Effort will be adjusted if the pending proposal is funded.

Current support

Title: Collaborative Research: Understanding Arctic Marine Biogeochemical Response to Climate Change for Seasonal to Decadal Prediction Using Regional and Global Climate Models
Award number: IAA1417888
PI: Wieslaw Maslowski
Program: NSF ARCSS
Period: 10/01/14 – 09/30/17
Commitment (person-months): 1.0/1.5/1.5
Total Award: $901,021
Description: Investigating coupled marine ecosystem and physical feedbacks in the Regional Arctic System Model.

Title: Advancing Arctic Climate Projection Capability at Synoptic to Seasonal and Decadal Scales using the Regional Arctic System Model (RASM)
Award number: N0001417WX00563
PI: Wieslaw Maslowski
Program: ONR AGP
Period: 05/01/15 – 04/30/18
Commitment (person-months): 2.46/2.5/2.5
Total Award: $900,551
Description: Developing the Regional Arctic System Model to be used as a forecast tool for seasonal to decadal timescales using the most recent innovations in sea ice physics, and the highest possible resolution on many thousands of compute cores.

Title: Collaborative Research: Advancing Arctic Climate Projection Capability at Seasonal to Decadal Scales
Award number: DE-SC0014117
PI: Wieslaw Maslowski
Program: DOE BER/RGCM
Period: 08/01/15 – 07/31/18
Commitment (person-months): 2.0/4.0/3.5
Total Award: $500,024
Description: Phase 3 of the Regional Arctic System Model project, focused on model analysis and outcomes from developments in RASM phase 2 as funded by DOE.

Title: Collaborative Research: Understanding the role of Arctic cyclones – A system approach
Award number: IAA1603602
PI: John Cassano
Program: NSF ARCSS
Period: 07/01/16 – 06/30/19
Commitment (person-months): 3.0/3.0/3.0
Total Award: $509,454
Description: Investigating changes in atmosphere-ice-ocean coupling in the presence of cyclones in the Arctic on a variety of timescales.

Title: Collaborative Research: Towards Advanced Understanding and Improved Decadal/Centennial Prediction of Arctic Sea Ice State and Climate Change
Award number: IAA1108542
PI: Wieslaw Maslowski
Program: NSF ARCSS
Period: 10/01/12 – 09/30/17
Commitment (person-months): 3.0/2.0/1.0/1.0/1.0
Total Award: $617,323
Description: Investigating the role of high-frequency ice dynamics on the state of sea ice in the Arctic using the Regional Arctic System model

Title: Collaborative Project: Understanding the Effects of Tides and Eddies on the Ocean Dynamics, Sea Ice Cover and Decadal/Centennial Climate Prediction
Award number: DE-SC0005522
PI: Wieslaw Maslowski
Program: DOE BER/SciDAC
Period: 09/15/12 – 09/14/17
Commitment (person-months): 3.0/3.0/2.0/1.0/1.0
Total Award: $733,648
Description: Investigating the role of ocean eddies and tides on the state of the pack and ocean in the Regional Arctic System Model.

Pending support

Title : A new discrete element sea-ice model for Earth system modeling (this proposal)
PI: Adrian Turner
Program: DOE BER/SciDAC
Period: 01/01/18 – 06/30/20
Commitment (person-months): 6.0/6.0/3.0
Total Award: $311,462

Title: A Scalable High-Order Ice-Sheet/Ocean Interaction Model for the Polar Regions
PIs: Francis Giraldo and Wieslaw Maslowski
Program: DOE BER/SciDAC
Period: 01/01/18 – 06/30/20
Commitment (person-months): 3.0/3.0/1.5
Total Award: $1,205,000

Dan Bolintineanu

Effort will be adjusted if the pending proposal is funded.

Current support

Title: Additive manufacturing particle bed deposition and thermal transport modeling
Award number: -
PI: Dan S. Bolintineanu (SNL)
Program: DOE ASC P&EM
Period: 10/2014–
Commitment (person-months): 3.0/year
Total Award: $180k/year
Description: Developing and applying DEM capabilities in LAMMPS to study granular flows for additive manufacturing applications

Title: Corning CRADA: Property prediction and control in heterogeneous materials
Award number: -
PI: Jeremy Lechman (SNL)
Program: CRADA
Period: 10/2014–
Commitment (person-months): 3.0/year
Total Award: $1,488,500
Description: Develop and apply statistical analysis tools to materials with complex microstructures; develop particle simulation methods to model process/structure relationships in particulate materials

Title: Born Qualified Grand Challenge
Award number: -
PI: Allen Roach
Program: DOE LDRD
Period: 10/2015–10/2018
Commitment (person-months): 1.0/year
Total Award: -
Description: Develop tools and knowledge to advance additive manufacturing for SNL mission needs

Pending support

Title : A new discrete element sea-ice model for Earth system modeling (this proposal)
PI: Adrian Turner
Program: DOE BER
Period: 01/01/18 – 06/30/20
Commitment (person-months): 3.0
Total Award: $1,001,632

Title : Connecting polymer physics and microstructure with large-deformation polymer foam mechanics
PI: Sharlotte Kramer (SNL)
Program: DOE LDRD
Period: 10/2017-10/2020
Commitment (person-months): 4.0
Total Award: $1,635,000

Title : Microscale characterization of powder feedstocks for metal additive manufacturing
PI: Dan Bolintineanu
Program: DOE LDRD
Period: 10/2017-10/2020
Commitment (person-months): 4.0
Total Award: $1,290,000

Title : Mesoscale modeling of particulate media and manufacturing processes
PI: Jeremy Lechman
Program: DOE LDRD
Period: 10/2017-10/2020
Commitment (person-months): 3.0
Total Award: $1,425,000

Title : Characterization of powder feedstocks for qualification of metal additively manufactured components
PI: Jeremy Lechman
Program: DOE LDRD
Period: 10/2017-10/2020
Commitment (person-months): 4.0
Total Award: $1,335,000

Daniel Ibanez

Current support

Title: Adaptive & Modular Particle Dynamic Methods
PI: Steven Plimpton (SNL)
Program: WFO
Period: 10/2016–9/2017
Commitment (person-months): 3.0/year
Total Award: $200K (FY17)
Description: Kokkos implementation in LAMMPS

Title: Laboratory for Computational Mechanics (LCM)
PI: Alejandro Mota (SNL)
Program: DOE ASC PE & M
Period: 10/2010–9/2019
Commitment (person-months): 1.6/year
Total Award: $350K (FY17)

Title: FASTMath
PI: Karen Devine (SNL)
Program: DOE ASCR
Period: 8/2011–3/2017
Commitment (person-months): 1/year
Total Award: $4.65M

Pending support

Title : A new discrete element sea-ice model for Earth system modeling (this proposal)
PI: Adrian Turner
Program: DOE BER
Period: 01/01/18 – 06/30/20
Commitment (person-months): 4.0/4.0/2.0
Total Award: pending

Appendix 3: Bibliography and References Cited

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Appendix 4: Facilities and Other Resources

The following pages describe facilities and resources available at the collaborating institutions.

- Los Alamos National Laboratory
- Sandia National Laboratories
- Naval Postgraduate School

Los Alamos National Laboratory

Researchers at LANL and their collaborators have access to substantial state-of-the-art Institutional Computing capabilities as part of institutional support and ongoing funding by DOE Climate Modeling programs. These resources come in the form of production systems that are part of LANL's Institutional Computing resources and additional set of testbed systems devoted entirely to supporting research and development activities. Current funding permits an allocation between 5-10% of the resources below with additional resources available through an annual proposal-driven allocation.

The current available institutional computing systems include:

System	Processor Type	Memory (GB)	Cores / node	Node Count	Network	TFLOPS
Grizzly	Intel Xeon Broadwell	128	36	1,490	OmniPath	1,806
Wolf	Intel Xeon E5-2670	64	16	616	Infiniband Fat-Tree	205
Pinto	Intel Xeon E5-2670	32	16	154	Infiniband Fat-Tree	51.3
Moonlight	Intel Xeon E5-2670 + NVIDIA M2090	32	16	308	Infiniband Fat-Tree	488

All of these clusters are attached to a 10PB Lustre high performance storage system and expandable archival storage that currently has a capacity of several hundred PB. A small high-memory visualization cluster is available for analysis.

In addition to these production systems, Laboratory researchers host a number of small clusters and single-node systems that are used to explore Nvidia GPUs and Intel many-core architectures. For example, one collection of testbed systems can be accessed through a common front-end dubbed Darwin. This 128 node cluster is used to explore higher core count designs and accelerator-based computing. The majority of Darwin's nodes contain 48 AMD Opteron cores and either one or two GPUs. Half of the nodes contain dual NVIDIA Fermi-class GPUs and the other half a single AMD GPU. The nodes are interconnected with dual Infiniband QDR interfaces. In addition, each node contains both a solid state and a mechanical disk drive. The system contains additional nodes that explore new processors and systems from Intel, AMD, NVIDIA, and ARM.

Recently, a D-Wave quantum computer was acquired for exploring novel computing techniques.

Sandia National Laboratories

Computer Facilities. Sandia National Laboratories sponsors and uses several high performance computing systems, including large capability and capacity systems for running computational science and engineering applications, and testbed systems to support early access to emerging computing architectures for code development and testing.

Cielo is a Cray XE6 system consisting of 8,944 compute nodes, each comprising two AMD eight-core Opteron processors. The system provides more than 1.374 petaops (PF) of peak performance, and 268 terabytes (TB) of memory. A total of 272 service input/output (I/O) nodes provide access to the 7.6 PB Lustre parallel file system approximately at 160 gigabytes (GB/s) of bandwidth. Cielo is used by scientists at three national laboratories: Los Alamos (LANL), Sandia (SNL), and Lawrence Livermore (LLNL), to solve our nation's most demanding stockpile stewardship problems; that is, the large-scale application problems at the edge of our understanding of weapon physics. Cielo is one of the large capability systems funded by the National Nuclear Security Administration (NNSA) for the Advanced Simulation and Computing (ASC) Program. It is operated by the Advanced Computing at Extreme Scale (ACES) program, a Los Alamos National Laboratory (LANL) and Sandia National Laboratories Partnership. In the 2015-2016 timeframe, ACES will install Trinity, a next generation computing system, for the replacement of Cielo.

In order to support a variety of computational workloads, Sandia has a number of capacity systems for solving large, complex science and engineering problems, and visualizing and interpreting results. Sandia's High Performance Computing (HPC) Linux clusters (systems linked together to provide increased processing capability) are configured with home, projects, and scratch areas and a common user environment. In particular, Chama, Red Sky and SkyBridge and Serrano are the major commodity- based systems that accommodate 19,712, 22,584 and 29,568 x86 (Intel) cores, respectively. For these systems, technical support is available, including cluster integration, system software, management of HPC systems, storage systems, application, networking and hardware. Sandia also leverages expertise from other Sandia corporate resources such as the Advanced Networking, Scalable System Software, Customer Support, Computing Facilities, and Capability Computing.

As part of NNSA's Advanced Simulation and Computing (ASC) project, Sandia has acquired a set of advanced architecture testbeds to help prepare applications and system software for the disruptive computer architecture changes that have, and will continue, to appear, as HPC systems approach Exascale. In contrast to ASC Advanced Technology or Commodity Technology supercomputer platforms, these testbed systems are not for production computing cycles. Instead, they are intended to be pre-production or first-of-a-kind prototypes to support exploration of a diverse set of architectural alternatives that are possible candidates for future pre-Exascale systems. While these testbeds can be used for node-level exploration, they also provide the ability to study inter-node characteristics to understand future scalability challenges. To date, the test bed systems populate 1-6 racks and have on the order of 50-200 multi-core nodes, many with an attached co-processor or GPU.

The testbeds allow for path finding explorations of 1) alternative programming models, 2) architecture-aware algorithms, 3) energy efficient runtime and system software, 4) advanced memory sub-system development and 5) application performance. But that is not all. Validation of computer architectural simulation studies can also be performed on these early examples of future Exascale platform architectures. As proxy applications are developed and re-implemented in architecture-centric versions, the developers need these advanced architecture systems to explore how to adapt to an MPI + X paradigm, where X may be more than one disparate alternative. This in turn, demands that tools be developed to inform performance analyses. ASC has embraced a co-design approach for its future advanced technology systems. By purchasing from and working closely with the vendors on pre-production testbeds, both ASC and the vendors are afforded early guidance and feedback on their paths forward. This applies not only to hardware, but other enabling technologies such as system software, compilers, and tools.

There are currently several testbeds available for use, with more in planning and integration phases. They represent distinct architectural directions and unique features important for future study. Examples of the latter are custom power monitors and on-node solid state disks (SSD).

Computer Science Research Institute. The mission of the Computer Science Research Institute (CSRI), New Mexico, is to conduct collaborative research and development with external researchers (particularly university faculty) in the areas of computer science and mathematics to build Sandia's and DOE's modeling and simulation capabilities. The CSRI has established research in the areas of computer and computational science critical to the laboratories' and DOE's mission. They work to identify external research collaboration that will impact DOE objectives and provide funds for work through university researchers (faculty and students) working at Sandia.

The CSRI provides a mechanism by which university researchers learn about problems in computer and computational science at DOE laboratories, conduct leading-edge research, interact with scientists and engineers at the laboratories, and help transfer the results of their research to programs at the laboratories. The CSRI also enables the laboratories to maintain and expand the computer science and mathematics expertise required for DOE projects and initiatives to be successful. The CSRI is a focal point, both physically and in terms of research collaborations, for university researchers, students, and laboratory staff engaged in computer and computational science, modeling, and simulation. This project will leverage ongoing CSRI activities to foster additional collaborations and interactions with academic and lab researchers. The Sandia staff and visiting collaborators will be housed in the 34,500 sq. ft. CSRI facility, housing 190 researchers comprising 140 full-time staff and 50 visitors including conference rooms and collaborative work areas. The CSRI facility has significant local computing power and with high-bandwidth network connection to large-scale Sandia computing platforms.

Naval Postgraduate School

Work for this project at Naval Postgraduate School (NPS) will be undertaken in the Polar and Global Climate Laboratory in the Department of Oceanography in Monterey, California. This laboratory has a history of sea ice and Arctic oceanographic modeling using Department of Defense supercomputing facilities, and involving NPS postgraduate students in the research.

Computing facilities: Computing resources are available from the Navy Department of Defense Supercomputing Resource Center (NAVY), U.S. Army Engineering and Research Development Center (ERDC), and Air Force Research Laboratory (AFRL) through the Department of Defense High Performance Computer Modernization Program (DOD/HPCMP) at no-cost to this project (*https://www.hpc.mil*). These machines include:

System *Center*	Processor Type	Memory (GB)	Cores / node	Node Count	Network	PFLOPS
Lightning *AFRL*	Intel Xeon E5-2697v2	64	24	2,370	Cray Aries	1.28
Gordon *NAVY*	Intel Xeon E5-2698v3	128	32	1,523	Cray Aries / Dragonfly	1.50
Conrad *NAVY*	Intel Xeon E5-2698v3	128	32	1,523	Cray Aries / Dragonfly	2.00
Topaz *ERDC*	Intel Xeon E5-2699v3 Haswell	128	36	3,456	FDR 14x InfiniBand Hypercube	4.62
Thunder *AFRL*	Intel E5-2699v3	128	36	3,216	FDR 14x InfiniBand Enhanced LX Hypercube	5.62

Of these, Lightning, Topaz and Thunder also include a limited number of GPU nodes. All of NAVY, AFRL and ERDC have secure and substantial tape archive systems, and may be used for long-term storage for data and code retention consistent with Federal Government policies. The NPS PI (Roberts) and his students have dedicated workstations and other computers available locally for data processing, archiving and visualization. All workstations have fast internet connections to remote HPCMP sites. NPS also operates a High Performance Computer (HPC) Center, which supports campus-wide investigators in the areas of visualization and Linux/Macintosh operating systems.

Laboratory Resources: Sufficient office space is available at NPS to accommodate all involved staff, students and visiting scientists associated with this project.

Appendix 5: Equipment

No additional equipment is required for this proposal.

Appendix 6: Data Management Plan

The plan below describes how any data generated from this project will be managed.

A6.1 Data types and sources

This project will be generating sea-ice model simulation output data from verification and validation simulations. This data will be generated from a variety of model domains, from simple idealized test cases to full Arctic and Antarctic basin domains. The model output will represent a variety of simulation durations and realism of atmospheric and oceanic forcing.

A6.2 Content and format

Output data will be generated in netCDF format. The output data will contain sea-ice model prognostic and diagnostic fields, as well as metadata, including the model version and configuration, using Climate and Forecast (CF) metadata conventions. Data will be output by element as well as from fields regridded onto a regular mesh. Data used to validate the model in the published literature will be published using the Earth System Grid Federation (ESGF) system.

A6.3 Sharing and preservation

Simulated data used for model validation and published in the open literature will be made available for public use using the Earth System Grid Federation (ESGF, esgf.org), or other similar cloud-based data storage system. Data will only be publicly released after the data has appeared in a peer-reviewed publication. The model code will be made publicly available through a public release on the project github repository site after the model has been described in the peer-reviewed literature and initial science simulations have been performed and published. Data will be archived at ESGF for a minimum of three years. Determination of whether data will be removed after this minimum period will depend on whether the data is still relevant, has not been superseded by later data, and is no longer cost effective to store.

A6.4 Protection

No PII will be included in simulation data and this research does not involve human subjects. This research is unclassified and simulation results from it will be published in the open literature. Restriction of data access before peer-reviewed publications is intended to protect intellectual property before publication.

A6.5 Rationale

This project is focused on developing and validating a new sea-ice model, and deliverables are in the form of a new code-base and validation simulation output. We expect that broader members of the scientific community may want to reproduce the validation analysis of our new model or use the new model. Release of data and code to the wider community allows this and encourages external testing and development of the code base. Restrictions of release until project team members have published results in the peer-reviewed literature protects the intellectual property of those members, and ensures only properly vetted and validated results are used.

A6.6 Software and Codes

The model code will be made publicly available through a public release on the project github repository site after the model has been described in the peer-reviewed literature and initial science simulations have been performed and published.

Appendix 7: Other Attachments

Letters of support from unfunded collaborators

Sandia National Laboratories

Operated for the U.S. Department of Energy's
National Nuclear Security Administration
by **Sandia Corporation**

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Andrew G. Salinger
Principal Member of Technical Staff
Center for Computing Research

Re: Consultation on DEMSI

March 7, 2017

Dear Adrian,

I am writing to affirm my commitment to consulting on your DEMSI project for a granular flow based model for sea ice.

I have deep familiarity with both the ACME climate project and DOEs computational science capabilities. I have leadership roles on the BER side on as a Software Engineering Group lead on ACME and as PI of the CMDV Software project, and on the ASCR side as an executive council member of FASTMath under SciDAC-3 and Trilinos leader. I was a part of the (in my opinion, highly successful) SciDAC-3 PISCEES project for developing an ice sheet component for ACME, which, like your DEMSI project, included a partnership between BER staff from COSIM at LANL and ASCR staff from CCR at SNL.

Armed with that exposure, I am very intrigued by your project, finding a way to leverage one of DOEs flagship application codes, LAMMPS, to impact a highly visible aspect of Earth system modeling, sea ice dynamics. As a consultant, I will look for ways to further leverage staff and expertise in FASTMath and ACME to accelerate your project's productivity.

In addition, as PI of the CMDV Software project, I can also tell you that are working to upgrade the ACME build system to facilitate the incorporation of external frameworks into ACME for production runs on the LCFs. So, when the time arises, the task of integrating DEMSI/LAMMPS into the ACME download/configure/build/run/test infrastructure should be a minor obstacle.

Regards,

Andrew G. Salinger

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9 March 2017

Re: ***DEMSI***

Hi Adrian,

The purpose of this letter is to confirm my interest in collaborating with you in your proposed work to develop a Discrete Element Method Sea Ice (DEMSI) model that extends in novel ways the DEM implementation we have within our LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code at Sandia.

As an open source code, LAMMPS has a long history of collaborative development with contributions from many users around the world to extend its capabilities. As its originator and lead developer, I can provide expert advice on how to implement new models and features relevant to your sea ice application, as well as on how to optimize code performance for existing and new heterogeneous architectures. In turn, I'm excited that new capabilities developed under your project, including new contact models and use of the Kokkos library to exploit fine-grain parallelism in the discrete element method, will be contributed to the LAMMPS code base. I think this will be exciting for the large LAMMPS user community and impact other research areas such as granular (particulate) modeling generally.

I look forward to our collaboration and the your successful development of a DEMSI model that provides an efficient, scalable sea ice simulation capability for running coupled climate simulations.

Sincerely,

Steve J Plimpton

Steve Plimpton
Distinguished Member of Technical Staff

Acronyms

ACES4BGC	Applying Computationally Efficient Schemes for BioGeochemical Cycles
ACME	Accelerated Climate Model for Energy
AIDJEX	Arctic Ice Dynamics Joint Experiment
ANL	Argonne National Laboratory
ASC P&EM	Advanced Scientific Computing - Physics and Engineering Modeling
ASCR	Office of Advanced Scientific Computing Research
BER	Office of Biological and Environmental Research
CCR	Center for Computing Research
CESM	Community Earth System Model
CF	Climate and Forecast
CICE	The Los Alamos Sea-ice model
CMDV	Climate Model Development and Validation
COSIM	Climate, Ocean and Sea Ice Modeling group
CPU	Central Processing Unit
CRADA	Cooperative Research and Development Agreement
DEM	Discrete Element Method
DEMSI	Discrete Element Model for Sea Ice
DOD	Department of Defense
DOE	Department of Energy
EAP	Elastic-Anisotropic-Plastic
ESGF	Earth System Grid Federation
ESM	Earth System Model
EVP	Elastic-Viscous-Plastic
GMLS	Generalized Moving Least Squares
GPU	Graphics Processing Unit
HOMME	High-Order Method Modeling Environment
IABP	International Arctic Buoy Program
IBM	International Business Machines
ICESat	Ice, Cloud, and land Elevation Satellite
I/O	Input/Output
IPCC	Intergovernmental Panel on Climate Change
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LLNL	Lawrence Livermore National Laboratory
MPAS	Model for Prediction Across Scales
MPI	Message Passing Interface
NCAR	National Center for Atmospheric Research
NCL	NCAR Command Language
NOAA	National Oceanic and Atmospheric Administration
NPS	Naval Postgraduate School
ORNL	Oakridge National Laboratory
ParGAL	Parallel Gridded Analysis Library
ParVis	Parallel Analysis Tools and New Visualization Techniques for Ultra-Large Climate Data Sets
PI	Principal Investigator
PII	Personally Identifiable Information

PISCEES	Predicting Ice Sheet and Climate Evolution at Extreme Scales
POP	Parallel Ocean Program
RAM	Random Access Memory
RASM	Regional Arctic System Model
RGPS	RADARSAT Geophysical Processor System
SCICEX	Submarine Arctic Science Program
SciDAC	Scientific Discovery through Advanced Computing
SHEBA	Surface Heat Balance of the Arctic
SNL	Sandia National Laboratories
SSMI	Special Sensor Microwave Imager
SYPD	Simulated years per day
VIC	Variable Infiltration Capacity model
VP	Viscous-Plastic
WRF	Weather Research and Forecasting Model