MOOSE: A FRAMEWORK TO ENABLE RAPID ADVANCES AND COLLABORATION IN MODELING SNOW AND AVALANCHES

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ABSTRACT: Using the open-source Multiphysics Object Oriented Simulation Environment (MOOSE; `www.mooseframework.org`) from Idaho National Laboratory (INL) the genesis of a modular, collaborative, and multi-scale set of simulation tools for snow was developed with the primary objective of demonstrating the capabilities of the MOOSE framework.

Two independent applications were created: a meso-scale continuum model and a micro-structure model. The continuum model, named Ibex, solves the transient heat equation and accounts for short-wave and long-wave irradiance as well as latent and sensible heat exchange. The micro-structure model, named Pika, was developed following the work of Kaempfer and Plapp (2009) and is a fully-coupled 3D finite element, phase field model capable of tracking the phase transition and capturing the heat and mass transfer at the micro-structure scale in the ice matrix and pore space.

The key feature of the models developed is that each was developed using MOOSE and therefore is inherently parallel and expandable, allowing for model expansion including coupling of additional physics (e.g., solid mechanics) and development of multi-scale simulations. Any application developed with MOOSE supports running, in parallel, any other MOOSE-based application. Each can be developed independently, but still easily communicate with one another (e.g., conductivity in the meso-scale model Ibex could be a constant input just as easily as a complete micro-structure Pika model evaluation) without additional code being written. These two models were then coupled into a single multi-scale simulation, named Yeti.

This method of development has proven effective at INL and the work presented herein aims to be the beginning of a truly collaborative snow modeling effort that greatly increases our current ability to develop sophisticated and sustainable simulation tools.

KEYWORDS: modeling, micro-structure, multi-scale, vapor diffusion, phase-change

1. MOTIVATION

Generally, snow metamorphoses via one of two processes: kinetic or equilibrium metamorphism. Efforts to simulate this behavior use a range of approaches and frameworks and include purely statistical models, continuum bulk property formulations, and complete numerical 3D constructs. Despite the wide spectrum of snow and avalanche models that exist, currently there is no unified modeling effort to allow true collaboration across models as scales. Given the broad range of approaches for snow and avalanche research (see Section 2) a new paradigm is needed for simulations that fosters rapid development and collaboration. This paper aims to demonstrate the capabilities of the open-source Multiphysics Object Oriented Simulation Environment (MOOSE; `www.mooooseframework.org`) as a framework for future snow and avalanche model development.

MOOSE is a finite-element framework that aids in application development by harnessing state-of-the-art fully-coupled, fully-implicit multiphysics solvers while providing automatic parallelization, mesh adaptivity, and an ever-expanding set of physics modules including solid mechanics, phase-field, Navier-Stokes, and heat conduction. MOOSE natively supports multi-scale models allowing linking of MOOSE-based applications, thus fostering collaborations (Gaston et al., in review). Finally, MOOSE follows a rigorous development strategy that ensures software quality at both the framework and application level (Gaston et al., 2014).

This paper briefly demonstrates the capabilities of MOOSE by:

1. developing a meso-scale continuum model for

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heat-condition, named Ibex, following the methods of Slaughter (2010) in Section 3,

2. developing a snow micro-structure model (Pika) based on the work of Kaempfer and Plapp (2009) in Section 4, and
3. coupling the two models together into a single, multi-scale simulation (Yeti) in Section 5.

The purpose of the work is not to provide a validated, fully-operational model for snow, but to take existing modeling approaches and re-implement them using a single framework to demonstrate the capabilities of MOOSE for solving snow and avalanche problems. The tools developed here are the basis for a completely new approach to modeling snow, an approach that aims to bring groups together to build a myriad of different, open-source simulation tools utilizing a common framework to allow for coupling and co-development.

2. BACKGROUND

Modeling the thermal behavior of snow is not a new endeavor; LaChapelle and Forecaster (1960) cites a paper from 1892 that examined temperature profiles of snow. A significant amount of work has examined snow using a continuum mechanics theory of mixtures (e.g., Adams and Brown (1989); Brown et al. (1999). Using a thermal non-equilibrium approach, Bartelt et al. (2004) indicated that temperature differences between the pore air and ice particles and interfacial heat exchange between snow crystals played a significant role in determining the temperature profile. Perhaps the most comprehensive model developed to date is the SNOWPACK model (Bartelt and Lehning, 2002; Lehning et al., 2002a,b), that accounts for heat transfer, water transport, vapor diffusion, and mechanical deformation. Research conducted in an attempt to validate the SNOWPACK model yielded reasonable results, yet Fierz and Lehning (2001) encouraged additional work regarding the initial stage of snow metamorphism, specifically the processes involving particles changing to small faceted or rounded crystals. Miller and Adams (2009) provided a unique approach for modeling this transition. They were able to develop a model capable of faceted growth, but the model is limited in a number of ways, including an assumed spherical geometry.

Recent approaches to modeling the snowpack are based on the 3D images of the snow micro-structure. One notable article by Kaempfer et al. (2005) utilized X-ray micro-tomography (μ-CT) to build a 3D image of a snow sample to which a finite element model was applied for modeling the heat transfer through the sample. Kaempfer and Plapp (2009) demonstrated that phase-field methods may be applied to snow metamorphism and concludes that with the model "snow metamorphism can be studied in details not possible heretofore." This approach is used as the staring point for the work presented in this paper.

3. IBEX: MESO-SCALE MODEL

The meso-scale model presented here is comprised of a single relationship, the heat-equation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot k_{eff} \nabla T + s, \tag{1}$$

where t is time, T is temperature, s is a heat source term, and the material properties ρ, c_p, and k_{eff} are the bulk density, specific heat, and thermal conductivity for snow, respectively. The model developed includes incoming short-wave irradiance that is absorbed within the snow (i.e., the s source term in Eq. (1)), including absorption that differs with wavelength as detailed by Slaughter (2010, Ch.4). On the surface the effects of incoming and outgoing long-wave irradiance as well as sensible and latent heat are included as detailed in Slaughter (2010).

To demonstrate the accuracy of the model, Exp. #2 of Morstad et al. (2007) was reproduced using a 1D Ibex simulation. The simulation was set up using the parameters detailed in Slaughter (2010, Ch.4) including incoming short- and long-wave radiation set to 650 W/m^2 and 235 W/m^2, respectively and the albedo in the visible, near-infrared, and short-wave infrared defined as 0.94, 0.80, and 0.59, respectively.

Fig. 1 includes the simulation results and a comparison with the experimental data of Morstad et al. (2007) after 8 hours; qualitatively the 1D Ibex model is capable of capturing the general trend of experimental data. Providing the complete details, fine tuning, and validated parameters for Ibex is beyond the scope of this demonstration paper.

Since, Ibex was built using MOOSE, it is dimension agnostic, thus the same code that produced the 1D results above is also capable of running in 3D with adaptive meshing, as shown in Fig. 2, without altering anything except the input file. This simulation uses the same input parameters as mentioned above, except applies the incoming short-wave irradiance as a function of space and time. This demonstrates the flexibility of MOOSE-based applications to build flexible and extensible tools, which will be further demonstrated in the next section.

4. PIKA: MICRO-STRUCTURE MODEL

A phase-field micro-structure model based on the work of Kaempfer and Plapp (2009) was developed

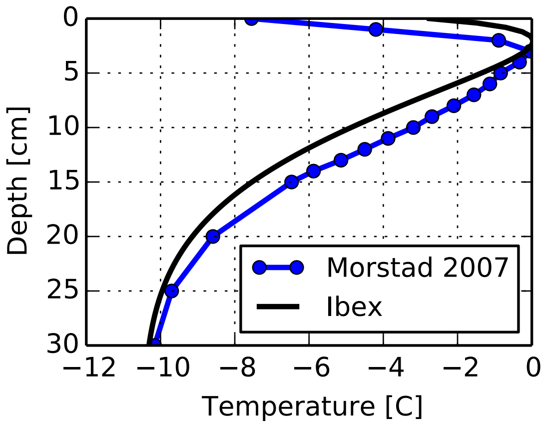


Fig. 1: Comparison of experimental data and 1D Ibex simulation.

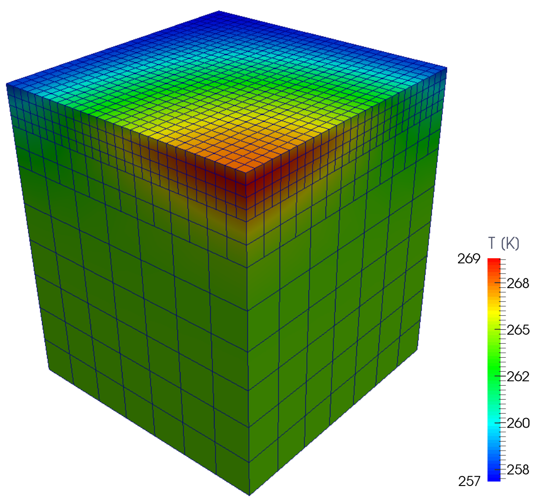


Fig. 2: Demonstration of 3D Ibex simulation with spatial and temporal varying incoming short-wave irradiance.

that tracks heat and mass transfer and includes sublimation and deposition of water-vapor. The MOOSE framework includes a phase-field module (Tonks et al., 2012), thus making this approach a natural choice.

The model is comprised of three relationships: the phase-field, the heat, and the mass transport equations. The phase-field equation, as defined in Eq. (2), allows the phase transition from ice to pore space to be modeled as a continuous, smooth variable allowing for complex geometries to be captured with an arbitrary finite element grid. The phase-field equation is defined as:

$$\tau \frac{\partial \phi}{\partial t} = W^2 \nabla^2 \phi + (\phi - \phi^3) + \lambda [u - u_{eq}](1 - \phi^2)^2, \quad (2)$$

where ϕ is the phase-field variable (1 for ice; -1 for pore), t is time, τ is the phase-field relaxation time, W is the interface thickness, λ is the phase-field coupling constant, u is the dimensionless vapor concentration, and u_{eq} is the dimensionless vapor concentration at equilibrium. The τ and λ terms dictate kinetics of the micro-structure evolution and are detailed by Kaempfer and Plapp (2009).

The heat equation is given in Eq. (3), which includes a forcing term that accounts for the gain or loss of heat due to phase change:

$$C(\phi) \frac{\partial T}{\partial t} = \nabla \cdot [K(\phi) \nabla T] + \frac{L_{sg}}{2} \frac{\partial \phi}{\partial t}, \quad (3)$$

where T is temperature, C and K are the phase-field adjusted heat capacity and thermal conductivity, respectively, and L_{sg} is the latent heat of sublimation.

Eq. 4 is the mass-transport equation that models the diffusion of vapor in the pore space:

$$\frac{\partial u}{\partial t} = \nabla \cdot [D(\phi) \nabla u] - \frac{1}{2} \frac{\partial \phi}{\partial t}, \quad (4)$$

where D is the phase-field adjusted vapor diffusion coefficient.

The model developed here—Pika—generally follows the formulation presented by Kaempfer and Plapp (2009) with two notable exceptions: (1) Pika utilizes a finite element solution as opposed to a finite difference and (2) Pika allows the interface kinetic coefficient (β) and capillary length (d_0), which dictate the τ and λ terms of Eq. (2), to vary with temperature whereas Kaempfer and Plapp (2009) held these terms constant.

Fig. 3 shows the results of a benchmark problem modeled by Kaempfer and Plapp (2009), which is reproduced here for comparison. The problem is based on experiments of a bubble inside a block of ice having a 5 mm square cross section that is subjected to to various temperature gradients (Nakaya, 1956; Stehle, 1965). The results shown here are for a gradient of 543 K/m and match well with those reported by Kaempfer and Plapp (2009). The Pika model exhibited an average interface velocity of 3.73e-9 m/s at 7200 s, which is similar to those reported by Kaempfer and Plapp (2009).

Utilizing simulation settings similar to the benchmark problem a simulation was performed on a μ-CT scanned cross-section of snow measuring 5 mm square. This sample was obtained at the Subzero Science and Engineering Research Facility at Montana State University. Snow samples were extracted and contained within an x-ray translucent container allowing for μ-CT imaging of the undisturbed snow microstructure. Once extracted, a series of x-ray images are

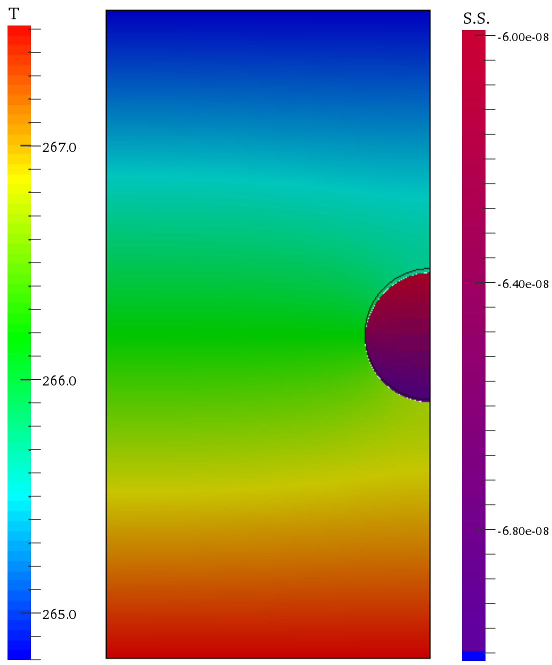


Fig. 3: Benchmark problem of bubble within 5 mm cross section of ice; temperature (T) reported in K and supersaturation (S.S.) in kg/m^3.

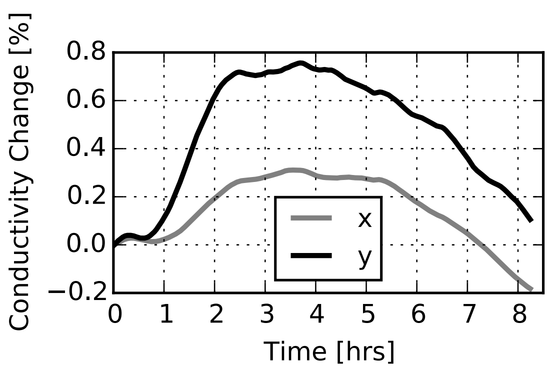


Fig. 4: Percent change in effective thermal conductivity in the vertical (y) and horizontal directions (x) during the simulations.

taken at several positions around the sample utilizing a SkyScan 1173 Micro-CT Scanner. The simulation was subjected to a temperature gradient of 250 K/m for approximately eight hours.

As shown in Fig. 4, during the simulation the effective thermal conductivity (k_{eff}) was computed in the vertical (y) and horizontal directions (x), which were on the order of 1.2 W/mK, the upper limit of what is expected for snow (Sturm et al., 1997). The k_{eff} value accounts for heat transfer by diffusion only, thus in essence is an indicator of the conduction through the ice matrix.

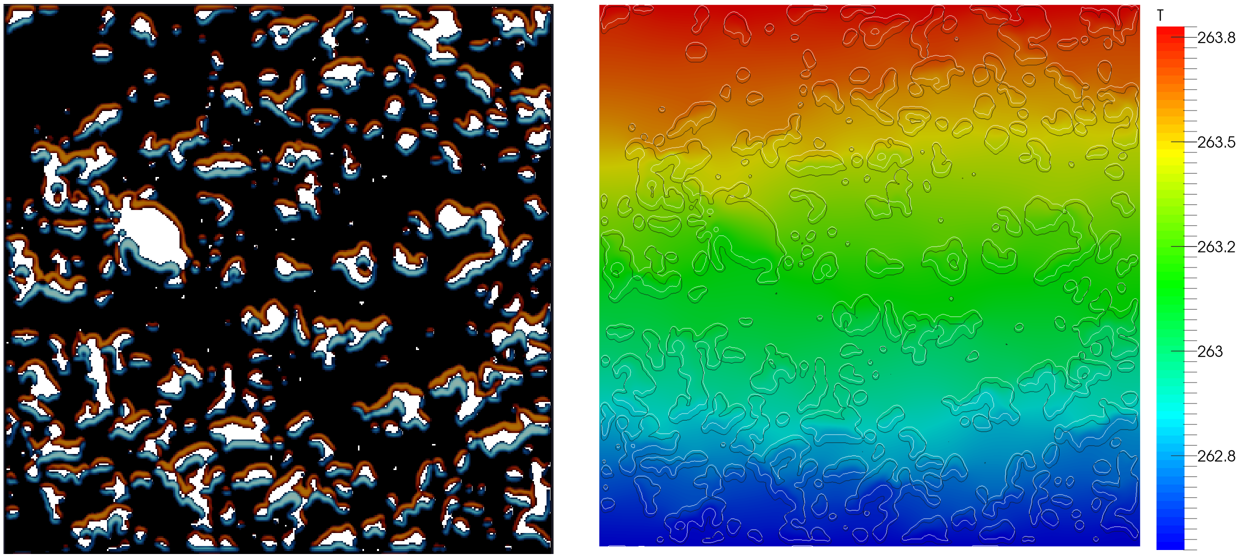
Fig. 5a includes the raw snow image overlaid with the areas that observed sublimation (hot colors) and deposition (cold colors) and Fig. 5b shows the snow the temperature field at the end of the simulation as well as the ice grain locations at the beginning and end of the simulations.

The k_{eff} results are of particular interest; during the first few hours of the simulation both values increase, with the vertical direction increasing at a greater rate. Then both begin to decrease at a similar rate after about four hours. There may be many explanations for this behavior. This decrease may be indicative of the pore space beginning to align in the direction of the gradient, which is expected, thus reducing the ice connectivity. However, considering the simplicity of the phase-change kinetics as well as the method used to compute k_{eff}, which is known to be inaccurate when pores are near the boundaries, such analysis is not appropriate. This plot serves to demonstrate the capabilities and potential to model micro-structure evolution of snow using MOOSE. Pika is intended as a starting point for further research that includes convection in the pore space, more realistic vapor flux boundary conditions, enhanced phase-change kinetics including accounting for ice grain orientation, as well as more robust effective property algorithms.

5. YETI: MULTI-SCALE MODEL

The ability to develop a multi-scale model from existing MOOSE-based applications is a key feature for the framework as it allows for collaboration across scales and developers (Gaston et al., in review). Consider the two applications presented above—Pika and Ibex—that could easily be two modeling efforts underway at different institutions. This section demonstrates how the two models may be coupled together in a single application.

For this demonstration, a 2D Ibex simulation serves as the master application. This simulation is a 2D version of the solution—executed for 24 hours of simulation time—presented in Section 3 with increased short-wave irradiance and reduced albedos to drive large temperature gradients for demonstration purposes. In this case rather than assuming a value of thermal conductivity it is computed using Pika. As illustrated in Fig. 6, Ibex computes the temperature and temperature gradient across the entire domain, then feeds these values to the Pika applications embedded at six locations, as shown in Fig. 7a. Pika then evaluates and computes the effective thermal conductivity



(a) (b)

Fig. 5: (a) The difference between the phase-field variable between initial and final simulations steps demonstrating where mass was gained (blue) and lost (orange) and (b) Tte difference in the ice grains initially (black) and after (white) 8 hours subjected to a 250 K/m temperature gradient.

and returns that value back to Ibex for use in the next timestep.

Each Pika simulation started from the same μ-CT snow image and was fed temperature and temperature gradient information from Ibex and returned the effective thermal conductivity in the vertical direction, which was then linearly interpolated across the entire domain in the master Ibex application. Fig. 7a displays the temperature gradients that were passed to the Pika simulations and Fig. 7b displays the change in thermal conductivity that is passed back to Ibex. Initially the k_{eff} values were approximately 0.58 W/mK. Note, this value differs from the values in Section 4 due to using a larger interface thickness (W) to allow for a coarser finite element mesh to ease the computational requirements for the simulations.

Referring to Fig. 7b, the small initial drop in conductivity is a result of the micro-structure simulation initializing to the supplied temperature gradient, whereas

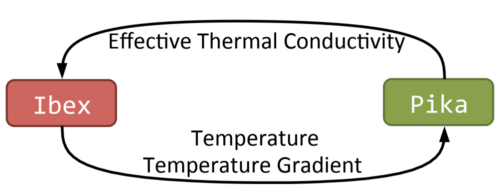
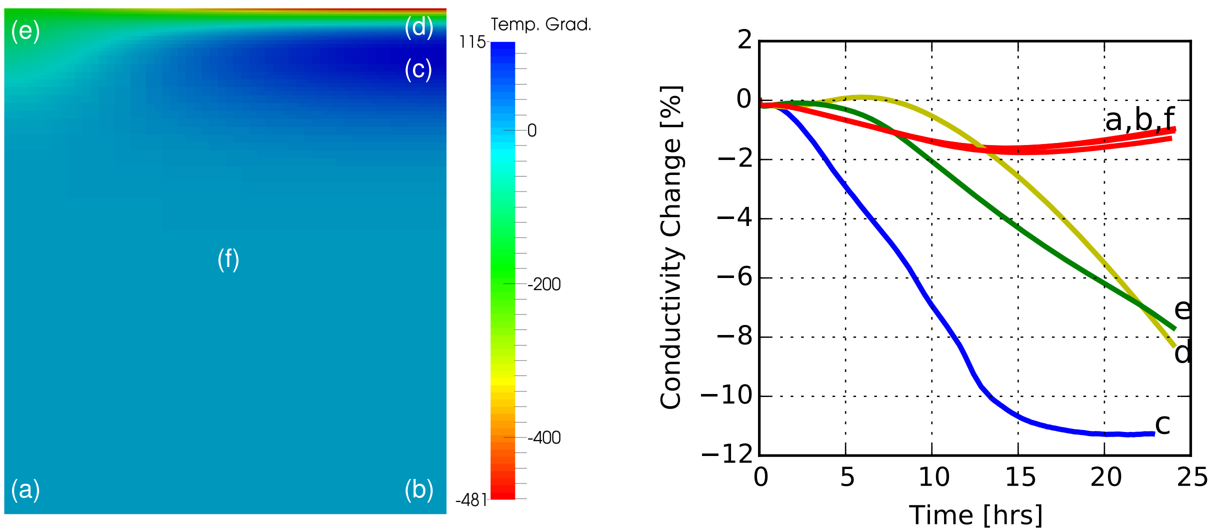


Fig. 6: Flow chart showing information passing that occurs across scales.

the results in Section 4 started with an initialized temperature field. The areas subjected to negative gradients (e and d) undergo changes resulting in constant or slightly increasing k_{eff} and the location with a postive gradient, c, showed a nearly continous decrease in conductivity. The points subjected to zero gradient—a, b, and f—all behaved almost identically and demonstrated a slight decrease in the conductivity, which may be a function of the phase-field method itself which tends to form circular geometries if not influenced by additional driving forces.

Fig. 8 shows a small subset of the change in microstructure between the various Pika simulations. The changes are in agreement with the results from the effective conductivity calculations and the temperature gradients to which the simulations were subjected. The initial condition, which was the same for all six simulations, is shown in white. The simulations without a gradient (a, b, and f) colored red all behaved similarly but still showed movement that led to changes in k_{eff}. The regions exposed to strong gradients experience larger changes in the micro-structure and the areas exposed to a strong negative gradient, (e) and (d), migrate in the opposite direction to the region with a strong postive gradient (c). Again, due to the simplistic kinetics and method for computation of thermal conductivity, exploring the reasons for the trends briefly described here is not appropriate. Additionally, Pika includes temporal scaling parameters for various terms to make the numerical solution feasible. This was not



(a)

(b)

Fig. 7: (a) Temperature gradient (K/m) after 24 hours of simulation time and approximate locations of micro-structure Pika simulations and (b) the change in thermal conductivity as computed by the six Pika simulations.

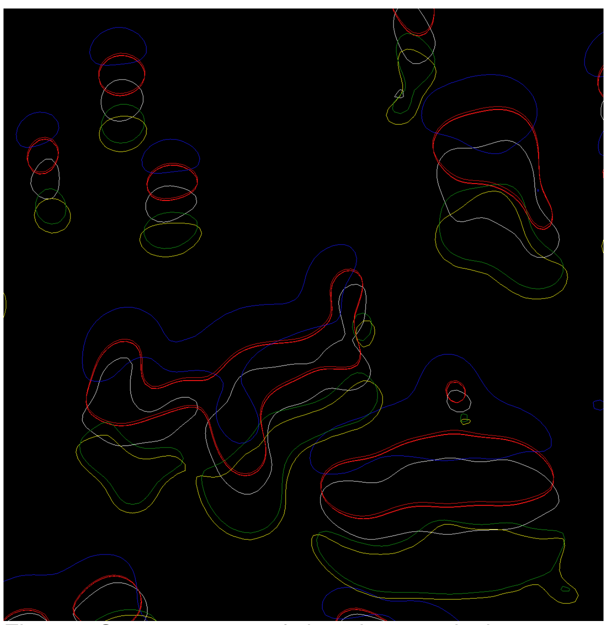


Fig. 8: Small sample of the changes in ice crystal shape from the initial condition (white) for the six Pika simulations: the colors match Fig. 7b where simulations (a), (b), and (f) are red; (c) is blue; (d) is yellow; and (e) is green.

considered in the meso-scale model and likely influenced the feedback between the models. However, as a pure demonstration of the capabilities offered by the MOOSE-framework, this result presents an example of how two separate applications, developed independently, can be easily coupled together to build a multi-scale simulation.

6. CLOSING REMARKS

The MOOSE framework is a powerful, finite element simulation framework capable of solving complex systems in a fully coupled manner as evidenced by the growing number of MOOSE-based applications under development. The work presented here demonstrates that using MOOSE to model snow at differing scales is possible. Two applications were created as a starting point for future research: a meso-scale model for simulating snow as a continuum and a micro-structure model capable of tracking phase-change and ice grain boundaries. Using these two models, a multi-scale simulation was performed to demonstrate the ability to couple different applications together across scales.

The work performed aims to establish a new paradigm in snow and avalanche modeling: building a spectrum of applications using a common, open-source framework to allow access and ease of cross-development for researchers and practioners.

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8. REFERENCES

Adams, E. and R. Brown, 1989: A constitutive theory for snow as a continuous multiphase mixture. *International Journal of Multiphase Flow*, **15 (4)**, 553–572.

Bartelt, P., O. Buser, and S. A. Sokratov, 2004: A nonequilibrium treatment of heat and mass transfer in alpine snowcovers. *Cold Regions Science and Technology*, **39 (2)**, 219–242.

Bartelt, P. and M. Lehning, 2002: A physical SNOWPACK model for the Swiss avalanche warning: Part I: Numerical model. *Cold Regions Science and Technology*, **35 (3)**, 123–145.

Brown, R. L., M. Q. Edens, and M. Barber, 1999: Mixture theory of mass transfer based upon microstructure. *Defence Science Journal*, **49 (5)**, 393–409.

Fierz, C. and M. Lehning, 2001: Assessment of the microstructure-based snow-cover model SNOWPACK: Thermal and mechanical properties. *Cold Regions Science and Technology*, **33 (2)**, 123–131.

Gaston, D., J. Peterson, C. Permann, D. Andrš, A. Slaughter, and J. Miller, 2014: Continuous integration for concurrent computational framework and application development. *Journal of Open Research Software*, **2 (1)**, URL http://openresearchsoftware.metajnl.com/article/view/jors.as.

Gaston, D., et al., in review: Physcis-based multiscale coupling for full core nuclear reactor simulation. *Annals of Nuclear Energy*.

Kaempfer, T. U. and M. Plapp, 2009: Phase-field modeling of dry snow metamorphism. *Physical Review E*, **79 (3)**, 031 502.

Kaempfer, T. U., M. Schneebeli, and S. Sokratov, 2005: A microstructural approach to model heat transfer in snow. *Geophysical Research Letters*, **32 (21)**.

LaChapelle, E. R. and A. H. Forecaster, 1960: *Critique on Heat and Vapor Transfer in Snow*. Alta Avalanche Study Center.

Lehning, M., P. Bartelt, B. Brown, and C. Fierz, 2002a: A physical snowpack model for the swiss avalanche warning: Part III: Meteorological forcing, thin layer formation and evaluation. *Cold Regions Science and Technology*, **35 (3)**, 169–184.

Lehning, M., P. Bartelt, B. Brown, C. Fierz, and P. Satyawali, 2002b: A physical snowpack model for the swiss avalanche warning: Part II: Snow microstructure. *Cold Regions Science and Technology*, **35 (3)**, 147–167.

Miller, D. and E. Adams, 2009: A microstructural dry-snow metamorphism model for kinetic crystal growth. *Journal of Glaciology*, **55 (194)**, 1003–1011.

Morstad, B., E. Adams, and L. McKittrick, 2007: Experimental and analytical study of radiation-recrystallized near-surface facets in snow. *Cold Regions Science and Technology*, **47 (1)**, 90–101.

Nakaya, U., 1956: *Technical Report Research Paper 13*. Tech. rep., Snow Ice and Permafrost Research Establishment, Corps of Engineers, US Army.

Slaughter, A. E., 2010: *Numerical Analysis of Conditions Necessary for Near-surface Snow Metamorphism*. Ph.D. thesis, Montana State University.

Stehle, N., 1965: *Technical Report Vol. R 421*. Tech. rep., US Naval Civil Engineering Laboratory.

Sturm, M., J. Holmgren, M. König, and K. Morris, 1997: The thermal conductivity of seasonal snow. *Journal of Glaciology*, **43 (143)**, 26–41.

Tonks, M. R., D. Gaston, P. C. Millett, D. Andrš, and P. Talbot, 2012: An object-oriented finite element framework for multiphysics phase field simulations. *Computational Materials Science*, **51 (1)**, 20–29.