LESSONS FROM NUCLEAR ENERGY: BUILDING SNOW AND AVALANCHE SIMULATION TOOLS USING A COMMON OPEN-SOURCE FRAMEWORK

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ABSTRACT: The Department of Energy (DOE) is currently investing millions of dollars annually into various modeling and simulation tools for all aspects of nuclear energy. An important part of this effort includes developing applications based on the open-source Multiphysics Object Oriented Simulation Environment (MOOSE; mooseframework.org) from Idaho National Laboratory (INL).

Thanks to the efforts of the DOE and outside collaborators, MOOSE currently contains a large set of physics modules, including phase field, level set, heat conduction, tensor mechanics, Navier-Stokes, fracture (extended finite-element method), and porous media, among others. The phase field module, in particular, is well suited for micro-structure evolution simulations, including solidification. The phase field module was also used, in conjunction with the heat conduction module, to build a multiscale snow modeling application (Pika) which was presented at the 2014 International Snow Science Workshop. The development of MOOSE and its modules is ongoing, and will eventually include ray-tracing and shallow water equation applications, two tools which are of particular interest to the snow research community, in the near future.

The snow science community can learn from the nuclear industry and harness the enormous effort underway to build simulation tools that are open, modular, and share a common framework. In particular, MOOSE-based multiphysics solvers are inherently parallel, dimension agnostic, adaptive in time and space, fully coupled, and capable of interacting with other applications. The snow science community should build on existing tools to enable collaboration between researchers and practitioners throughout the world and advance the state-of-the-art in line with other scientific research efforts.

KEYWORDS: modeling, open-source, simulation

1. MOTIVATION

Significant time and effort has been given to the development of simulation tools for snow. Modeling approaches are broad and include theoretical (Adams and Brown, 1989; Brown et al., 1999), non-equilibrium thermodynamics (Bartelt and Lehning, 2002), microstructural (Kaempfer and Plapp, 2009; Miller and Adams, 2009; Slaughter et al., 2014; Johnson, 2015), avalanche flow (Christen et al., 2010)), and operational Franz et al. (2008). Of course, the most widely used and perhaps most well-developed snow models are SNOWPACK (Bartelt and Lehning, 2002; Lehning et al., 2002b,a) and CROCUS (Brun et al., 1989, 1992).

Due to the success of current modeling efforts, particularly the models used operationally, a need for a modern, unified snow model has been identified. In fact, at the 2016 European Geophysical Union meeting, a splinter group defined the basic criteria for the next generation snow models (Löwe et al., 2016). The findings from the meeting drive the motivation behind this paper, in particular that next generation models "be inspired from what happens in other communities."

Nuclear energy is a critical component of the world's infrastructure, with the United States of America being a major player. The U.S. Department of Energy invests significant capital to support and advance this industry, and a portion of this investment is aimed at modeling and simulation, including the development of the Multiphysics Object Oriented Simulation Environment (MOOSE; www.mooseframework.org). In the current fiscal year, approximately $8.5M has been invested by the Idaho National Laboratory (INL) to develop MOOSE and MOOSE-based applications. The snow research community has an opportunity to capitalize on this investment and utilize this open-source framework for the development of the next generation snow model.

As detailed in the following sections, the desires defined by Löwe et al. (2016) for next generation snow models are well aligned with the design objectives of MOOSE, with many of the requirements inherent to the framework. Section 2 provides a brief overview of

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the framework, in Section 3 the community developed physics modules are described, and in Section 4 the development strategy for MOOSE is discussed.

2. MOOSE OVERVIEW

Löwe et al. (2016) states that next generation models "should be modular," which is central to the design of MOOSE at multiple levels. Foremost, MOOSE is designed around the creation of physics "kernels" for describing a single operator within a set of differential equations (e.g., the diffusion term in heat conduction; $\nabla \cdot k\nabla T$). Many common operators already exist (see Section 3) and new operators are easily added by expanding upon the existing kernels. This modular approach allows kernels representing a set of fully coupled equations to be assembled, while maximizing code reuse. Additionally, over 30 other systems—such as outputs, material properties, and postprocessing—leverage this same modular approach. In the end, developers use the existing components in MOOSE to create the building blocks to meet their own needs, resulting in a custom MOOSE-based application.

On a larger level, MOOSE-based applications are themselves modular. Using the extensible "MultiApp" system (Gaston et al., 2015), it is possible to couple multiple applications together. Slaughter et al. (2014) demonstrated this capability by coupling a macro-scale heat-conduction model with a phase field microstructure model of snow. This system may also be used to execute external models, thus would allow for existing tools to be used in union, "ensuring some compatibility with current modeling applications" (Löwe et al., 2016).

Löwe et al. (2016) suggest that a next generation model at "its lowest level of complexity should correspond to the current level of SNOWPACK and Crocus," both of which are one-dimensional and finite-element based (Bartelt and Lehning, 2002; Vionnet et al., 2012). MOOSE is a finite-element framework that harnesses state-of-the-art fully coupled, fully implicit multiphysics solvers while providing automatic parallelization, mesh adaptivity, and dimension agnostic programming. Therefore, with some effort, the desirable components of SNOWPACK and Crocus could be ported to a MOOSE-based application, and immediately gain the ability to run large (15 billion degrees of freedom in Wang et al. (2015)), massively parallel (100,000+ cores) problems in 3D using adaptive and mixed element meshes.

3. PHYSICS MODULES

The next generation model "should be developed including all the 'state-of-the-art' snow physics and be as physically based as possible" (Löwe et al., 2016). MOOSE includes an ever-expanding set of physics modules that could be extended to model snow behavior from the micro- to macro-scale. The following list briefly highlights a portion of the available modules that are of particular interest for modeling snow:

- **Phase Field:** The phase field module provides pre-made kernels to solve the Allen-Cahn and the Cahn-Hilliard equations and is already capable of modeling dendritic solidification (see Fig. 1).
- **Tensor Mechanics:** The tensor mechanics module provides the tools needed to solve solid mechanics problems using a syntax which is natural in the context of tensor mathematics. Objects have been created for all the necessary tensors used in mechanics, including rank-two and rank-four tensors, as well as elasticity tensors and rotations.
- **Heat Conduction:** The heat conduction module in MOOSE is primarily focused on solving the heat equation, and is capable of handling time-, space-, and orientation-dependent material properties.
- **Navier-Stokes:** This module provides the necessary kernels to solve the compressible and incompressible Navier-Stokes equations, including stabilization.
- **Chemical Reactions:** The reactive transport module of MOOSE solves general advection-diffusion-reaction equations, as frequently encountered in other physics, such as porous media flows.
- **Richards:** The Richards module solves the variably saturated single-phase and multi-phase Richards equations that govern slow flow through porous materials.
- **Contact:** The contact module includes algorithms to enforce constraints between moving and deforming bodies, and models the physics of contact, sliding, and friction between them.
- **XFEM:** The extended finite-element method (XFEM) module allows for modeling of discontinuities within a mesh, such as fracture propagation through a material.
- **Level Set:** The level set method is a common technique for tracking the advection of a phase boundary; this module includes standard algorithms for solving the related equations. Currently under development.

- **Ray Tracing:** A module to provide a massively parallel, fully-integrated ray-tracing capability for finite-element applications. Currently under development.
- **Shallow Water:** A module to solve the shallow water equations. Currently under development.

The growing body of scientific research published with MOOSE-based applications suggests it will also be capable of solving the types of complex problems defined by Löwe et al. (2016). These include snow micro-structure, water vapor exchange, transport, chemical processes, and snow optical and mechanical properties, all of which should be a part of the next generation of snow models. For example, Johnson (2015) demonstrated the use of the heat conduction, phase field, and Navier-Stokes modules to model natural convection at the micro-structure level in snow (see Fig. 2).

4. DEVELOPMENT STRATEGY

Within the nuclear energy industry, safety and code reliability is obviously paramount. Therefore, MOOSE employs a rigorous and well-documented development strategy. In fact, MOOSE and many of its derived applications are currently in the arduous process of earning an NQA-1 certification.[1] In order to accomplish this task, a comprehensive set of tools for testing and documenting are being used and rapidly developed. In particular, testing of both MOOSE and MOOSE-based applications is of primary importance (approximately 3M automated regression tests are run each week in the course of day-to-day development). Changes are only merged into the framework once manual code review and the automated tests have ensured the changes are compatible with the applications. Since MOOSE is an open-source project, the testing process is publicly available at www.moosebuild.org.

Given the requirements for rigor defined by the nuclear energy industry and the significant investment being made by INL, the MOOSE project certainly meets the “careful validation process (e.g., code review, strong code management policy)” requirements of the next generation snow models (Löwe et al., 2016). As with nearly all aspects of MOOSE, the systems for testing, documentation, and the graphical user interface (GUI; Gaston et al., 2014), are modular and extensible as well. Discussing these tools in further detail is beyond the scope of this paper, but a detailed description of development strategies is provided by Slaughter et al. (2015), and future publica-

[1] http://tinyurl.com/hr7ymna

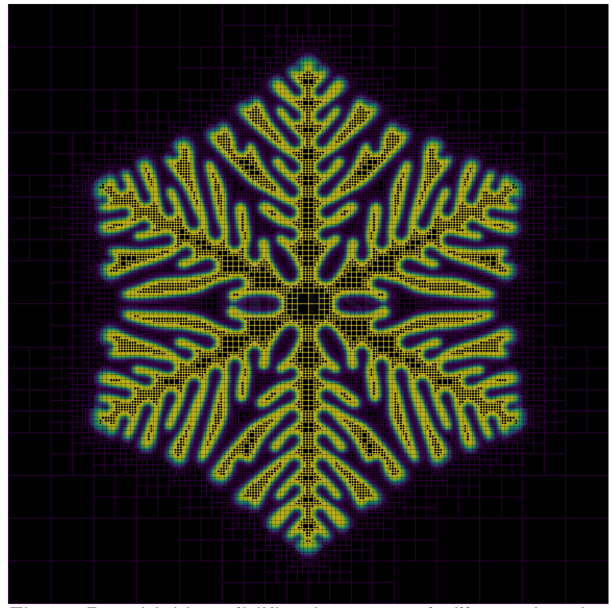

Fig. 1: Dendricitic solidification example illustrating the capabilities of the MOOSE phase field module.

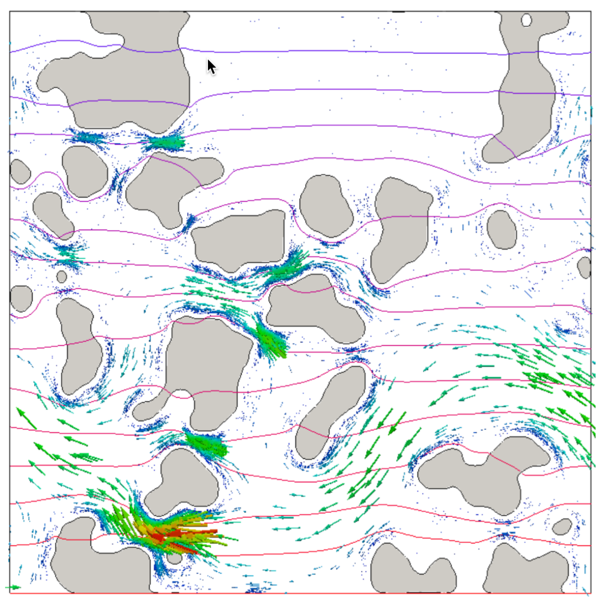

Fig. 2: Simulation of natural convection developed by a 500 K/m temperature gradient in real snow micro-structure on a 30° slope. The vectors indicate flow direction and are colored by velocity magnitude. The horizontal contours are isotherms (red (bottom) is warmer). Reproduced with permission from Johnson (2015).

tions will be dedicated to the documentation strategies and GUI.

5. CLOSING REMARKS

The next generation snow model has been defined based on the criteria of modularity, community development and engagement, software development practices, and simulation capability. Driven by a commitment to quality by INL, MOOSE is one possible framework that meets many of the requirements defined by the snow and avalanche community. The next generation snow models should establish a new paradigm, by leveraging existing work to construct a spectrum of applications using a common, open-source framework to allow access and ease of cross-development for researchers and practitioners.

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