Ristra: Multi-physics Simulation for National Security Problems

The property and behavior of various materials under a wide variety of extreme conditions is central to many applications within the realm of national security. Such modeling requires multiple length and time scales and drives requirements for exascale computing. Los Alamos National Laboratory is developing a next-generation multi-physics code for national security applications that focuses on 3D multi-physics, insight at the mesoscale for extreme condition materials, and high-energy density physics simulations.

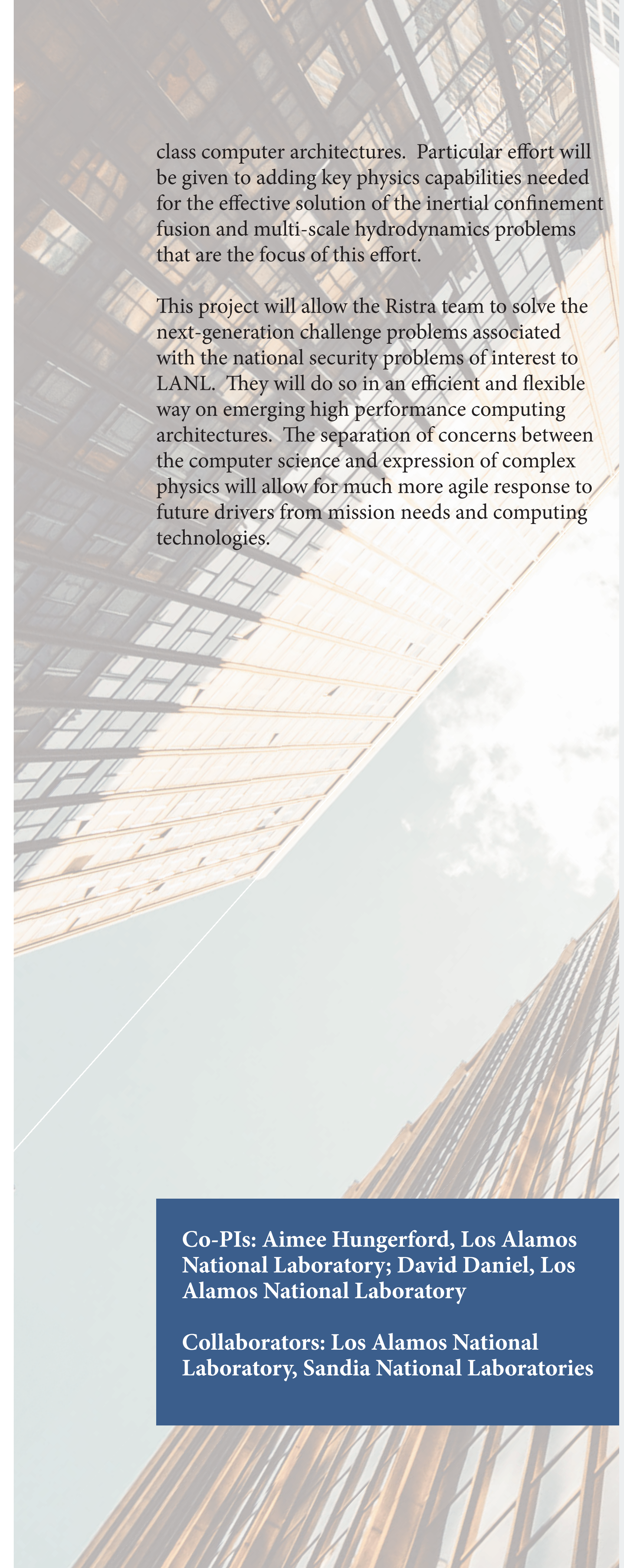
Computer science technologies that allow efficient use of emerging HPC architectures suggest a need for physics algorithms that permit increased concurrency at many scales. This motivates a fresh look at the numerical decisions made throughout the simulation process, from setup through analysis. With this in mind, Ristra is casting a wide net across available physics algorithms for multi-physics simulation and, at the same time, exploring novel programming models for emerging architectures.

Ristra's focus is on two application domains, both of which feature multi-scale methods that will be an important component of extreme-scale multi-physics simulations of the future:

High Energy Density Physics for Inertial Confinement Fusion. Ristra's Symphony code is an unstructured multi-material radiation hydrodynamics application that features a multi-scale algorithm for the radiation solve: a fully-coupled low-order radiation hydrodynamics system is updated by a high-order radiation solver which has the potential to be executed asynchronously (work in progress).

Multi-Scale Hydrodynamics of Materials in Extreme Conditions. Ristra's FUEL code is an unstructured multi-material arbitrary Lagrangian-Eulerian (ALE) hydrodynamics code that can be coupled to complex material models to take account of mesoscale physics, such as grain structure, in the dynamic response of materials. Mesoscale modeling is computationally intensive, and the multi-scale approach has potential for effective use of exascale-class systems, as well as providing a promising target for data-driven machine-learning (ML) techniques.
Key to the architecture of Ristra's applications is FleCSI (Flexible Computer Science Infrastructure), an abstraction layer that provides the desired separation of concerns between computational physics and computer science. FleCSI is a compile-time configurable framework designed to support multi-physics application development. As such, FleCSI provides a very general set of infrastructure design patterns that can be specialized and extended to suit the needs of a broad variety of solver and data requirements. FleCSI provides an abstract data model supporting compile- and run-time configurability for implementing a variety of discretizations (mesh and mesh-free) and physics fields and operators over them. FleCSI also provides an abstract execution model that can target a variety of underlying parallel programming runtimes from well-established options such as MPI, to ambitious new programming systems such as Legion, a data-centric model with out-of-order task execution The intent is to provide developers with a concrete set of user-friendly programming tools that can be used now, while allowing flexibility in choosing runtime implementations and optimizations that can be applied to future architectures and runtimes. This effort also provides a realistic infrastructure for the evaluation of programming models and data management technologies.

Over the course of the ECP project, the Ristra team will continue to push the boundaries on the development of multi-scale, multi-physics applications as well on the programming models needed to demonstrate performance on exascale-class computer architectures. Particular effort will be given to adding key physics capabilities needed for the effective solution of the inertial confinement fusion and multi-scale hydrodynamics problems that are the focus of this effort.



This project will allow the Ristra team to solve the next-generation challenge problems associated with the national security problems of interest to LANL. They will do so in an efficient and flexible way on emerging high performance computing architectures. The separation of concerns between the computer science and expression of complex physics will allow for much more agile response to future drivers from mission needs and computing technologies.

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Progress to date

The initial features of the FleCSI infrastructure are complete, and the Symphony and FUEL codes are maturing to support the required physics modules for a target challenge problem. Recent accomplishments of the project include:

- Demonstrated first results from Ristra's Symphony code, an unstructured mesh, multi-material radiation hydrodynamics code using a novel high-order/low-order (HO LO) multi-scale method for the radiation solver. Symphony was demonstrated using a variety of test problems including 2D and 3D Inertial Confinement Fusion (ICF) calculations.
- Enhanced fidelity in ICF simulations through adoption of new Discontinuous Galerkin low-order radiation solver.
- FleCSI's parallel capability was showcased using Ristra's simpler single material gas hydrodynamics code FleCSALE, demonstrating the ability of a code to connect through FleCSI to distinct parallel backends (MPI and Legion) with no required changes to the physics implementation.
- Enhancements to improve support for multi-material capability were added to FleCSI and demonstrated in Symphony and FleCSALE-mm.
- Demonstrated first results from a new FleCSI-based, serial, unstructured Eulerian and Lagrangian low energy density code FUEL.