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Multi-Scale, Multi-Physics Advanced Plasma Hybrid Algorithms, Modeling, and Simulations

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Goals of Initiative

Modern plasma physics devices, experiments, and problems of interest involve multiple physical processes occurring over a wide range of spatial, temporal, and plasma density scales, usually with complex boundaries. Often these kinds of problems are treated with a hierarchy of models to approximate the systems and separately treat the range of densities and physical phenomenon found at different times and locations in the systems. Progress has been made with these sorts of approximations. In many cases, however, these multi-scale plasmas and physical phenomena coexist and interact with each other, and thus many traditional approximations miss essential physics in the operation of these systems. Furthermore, many plasma problems of interest involve highly non-equilibrium and non-Maxwellian plasmas, in which plasma distribution functions are essential to the physics of interest and which are simply not treated in the fluid modeling limit. Boundaries are often approximated in simulations as ideal – e.g., as smooth, uniform, homogeneous, passive, non-interacting or immobile layers, without self-consistent plasmas forming at the surfaces. Such boundary plasmas actually have a critical influence on the operation and performance of plasma devices – e.g., in plasma containment systems (MFE), high-energy particle accelerators, and pulsed power facilities. Thus, boundary physics must be included in the modeling of these systems to have any fidelity in design or in comparisons with experimental data.

There is therefore a need for a multi-scale, multi-physics plasma simulation capabilities that can treat the real physics at the boundaries of devices, including self-consistent, time-dependent plasma formation and evolution, and simultaneously treat both high-density and low-density plasma regions away from the boundaries. Numerical methods and algorithms are needed to simultaneously and seamlessly simulate plasma in both the fluid and PIC-kinetic (Particle-in-cell) regimes, depending on the fidelity demanded by the evolving plasma conditions. These methods must handle plasmas that transition between these two limits and plasma that evolves from boundaries.

These methods should be integrated into **predictive plasma engineering design tools with a level of maturity found in other disciplines**, such as electromagnetics, solid mechanics, or thermal transport. Such a capability could significantly advance the rate of progress across our entire field. The absence of a mature plasma engineering design capability has significantly limited the speed of progress in many plasma problems of interest. As is well known, plasma physics can be dominated by empirical (or “artisan”-based) engineering approaches rather than design-driven methods.

Due to the anticipated size and complexity of such multi-scale, multi-physics simulations, the algorithms and codes must be able to run on the next generation DOE high-performance computing (HPC) platforms that are anticipated in the next 5 to 10 years. Due to the uncertainty of the node technology that will be selected for these HPC capabilities, an important consideration is that the code be born using algorithms, solvers, and libraries that are “performance portable”. Best practices from modern computational science and code engineering should be adopted.

Other problems of interest for multi-scale plasma modeling with boundary effects include: low temperature plasmas and plasma processing, laser-driven hohlraums, modeling of Laser plasma interactions, particle acceleration in short-pulse laser target interaction, z-pinch implosion and stagnation, inertial fusion energy systems (including modeling of standoff and the target chamber performance and operation), high-power microwave systems, high-power vacuum diodes, and plasma sheath formation.

At Sandia, multi-scale model development and experimental validation is of such high importance that a “Grand Challenge” LDRD (Laboratory Directed Research & Development) project was initiated to stimulate lab-wide activity on these problems, cutting across traditional organizational divides. However, the initial investment is only funded for 3 years; it is intended to stimulate new, large-scale research activity in this area at Sandia. Future investments to continue these efforts will need to be championed by the DOE Office of Science and HED community at large.

Description of the Initiative

The initiative should include work in a number of general areas:

- Algorithm development to simultaneously simulate multi-fluid to kinetic density ranges.
- Multi-material evolution with appropriate equations of state, with of order 10 materials.
- Extended MHD (XMHD), or asymptotic preserving multi-fluid algorithms and codes to treat expanded density ranges.
- Methods to reduce (or eliminate) the use of numerical density or conductivity floors.
- Fast and scalable field preconditioners, solvers, and particle pushers.
- Memory management techniques, including particle merging methods.

- Rapid meshing and zoning tools, including the ability to efficiently import geometries from engineering CAD models.
- Adaptive meshing to resolve boundary heating and energy deposition near surfaces, with fewer zones in regions that are not as demanding.
- Multi-scale modeling techniques such as Density Functional Theory (DFT), Molecular Dynamics (MD), and/or Grand Canonical Monte Carlo (GCMC) to develop fundamental physics of boundary dynamics, desorption, melting, and vaporization, collision rates, permittivities and ionization and recombination rate models which are required to properly close the physical models.
- Reduced models of multi-scale boundary modeling, to incorporate into numerical codes.
- Sub-scale or sub-zone techniques for modeling ionization of boundary plasmas.
- Zoning methods that can smoothly treat complex shapes.
- Incorporation of radiation transport, particle collisions, relativistic fluids, boundary layers, and plasma ionization kinetics.
- Development of integrated research codes and eventually production codes.
- Close integration of modeling approaches with experimental diagnostics to prioritize and validate physical and numerical models.

Due to highly variable numerical effects arising from multi-scale methods and uncertainties introduced through necessarily imprecise engineering, methods developed by this initiative must be underpinned by rigorous uncertainty quantification approaches. This will be particularly challenging given the highly nonlinear, multi-scale nature of these problems that may introduce strong bifurcations in macroscopic plasma behavior.

There is also the need for an analytical modeling effort that forms the basis for verification and eventually validation of the codes. This effort is especially complex due to the highly coupled nature of the models proposed here.

Multi-institution collaborations are needed to advance this research.

Existing and future DOE-funded HPC would be used to develop these methods and simulations. We envision simulations with scalable performance to encompass large fractions of future computing platforms.

National laboratories have developed mature production codes, into which new algorithms and methods can be introduced. Access to these codes is controlled on a case by case basis with user agreements to ensure appropriate protection of potentially OUO/Export Controlled Information. National laboratories have also developed research codes. Once again, access could be negotiated with particular programs and controlled with user agreements.

Industry has advanced multi-scale and hybrid simulation techniques quite far [1-5] and would be partners in this effort. Industry presently has some engineering capabilities in hybrid simulation, that have been tuned to be valuable in certain limited domains. Additional capabilities would be incorporated into industry codes to improve the domains over which the codes can be used predictively, and to conduct verification and validation on such codes. Such codes would then be available to users for modest licensing fees.

Programmatic Benefit

As is well known, plasma physics can be dominated by empirical (or "artisan"-based) engineering approaches rather than design-driven methods. **Predictive plasma engineering design tools with a level of maturity found in other disciplines**, such as electromagnetics, solid mechanics, or thermal transport would significantly advance the rate of progress across the entire plasma physics field by enabling a design-driven approach to experiments on present systems. Once these multi-scale design tools are validated, they would permit extrapolation of both performance and design-based scaling for present and future facilities. The absence of a mature plasma engineering design capability significant limits the speed of progress in many plasma problems of interest.

In addition, recent studies have highlighted the needs for hybrid modeling techniques for multiple applications, including [6-9]:

• "Plasma Science: Advancing Knowledge in the National Interest", National Academies Press (2007)
• "Advancing HED Laboratory Plasmas", 2009 DOE OFES Advisory Committee Report
• The 2012 Plasma Roadmap" (Review), J. Phys. D: Applied Physics, (2012)
• Foundations of Modelling Non-Equilibrium Plasmas" (Review), Plasma Sources Sci. Tech. (2018)

Specifically, a multi-scale, multi-physics plasma simulation tool could enhance the rate of progress in a variety of fields and problems. Two fields that could be impacted are discussed below. There are many others.

• MCF or MFE - It is well known that boundaries play a critical role in MFE systems, and that understanding and modifying the plasma edge properties at the boundary of the plasma at the confinement chamber wall are critical in achieving high confinement modes. Future progress could be made with advanced simulation capabilities self-consistently addressing boundary plasma layer evolution from solid density vessels (10^{23} cm^{-3}), and its interaction with, and the dynamics of the lower density magnetically-confined plasmas (10^{12-14} cm^{-3}).

• ICF or IFE – although target implosion physics is often treated through radiation hydrodynamics or magneto-hydrodynamics simulations, there are lower density plasmas in these systems that need to be treated in a more systematic and integrated fashion. In laser-driven systems, these lower density plasmas lead to laser light reflection from hohlraums, impact both the laser-driven hohlraum energetics and the laser light absorption and x-ray re-emission, and affect the spatial redistribution of the laser drive in both indirect and direct drive approaches. In pulsed-power-driven z-pinch systems, such plasmas perturb the surface of imploding liners and affect the geometrical distribution of current, thus impacting the implosion, stagnation, and compression of the pinch. Such plasmas also impact the current that can be coupled from a pulsed power driver to a target. The modeling of mix layers in ICF implosions might require such a plasma modeling technique, spanning more orders of magnitude in density than traditional fluid treatments. Future progress in developing methods of driver standoff for IFE target chambers (laser, heavy ion, pulsed power) could also benefit from multi-scale, multi-physics modeling tools.

US Leadership and Global Context

The U.S. leads the world in large-scale plasma simulation capabilities, in particular in the DOE and NNSA laboratories. The proposed initiative would expand and extend the U.S. capability to simulate plasmas over a wider range of application space, giving the U.S. a lead for at least 10-years in this new frontier.

Timeline of the Initiative

Investment in this initiative can start today. These new plasma simulation capabilities are needed in 5 to 10 years, if not sooner. This timescale is commensurate with the timescale for development of new HPC capabilities. This timescale is also commensurate with the timescale for several potential future capabilities such as a next generation pulsed power capability (NGPPC), future magnetic confinement devices, or a ramp up in research into Inertial Fusion Energy.

Equipment/Facility Design Details
N/A

Cost Range

We envision development of algorithms, methods, solvers, multi-scale science, modeling of boundary effects, and integrated plasma modeling techniques, including verification and validation, focused on several different exemplars.

We propose a range of funding of $5-10 M/year. One might adopt a MURI model for up to 7-10 years, to fund a multi-institution collaboration to ensure integrated development of understanding and capabilities and to foster a community of practice. Some of the funding could be based on proposals from institutions and multi-institution collaborations. In addition, we propose that a center of excellence in multi-scale plasma modeling should be funded at a level of $3-5 M/year, for a five-year period, with one renewal. Total funding per year, to multiple sites, is estimated at a level of $10-15 M/year. A sustained effort of funding for 10 years at this level would result in a suite of multi-scale, multi-physics production codes, tailored for multiple applications, that would exist on HPC platforms available to users and multiple institutions, to address multiple problems of practical importance at unprecedented scales. Some codes that would be developed would be available via licensing from various entities, either from national laboratories, or industry.

Cross-Cutting Connections

Related activities that are not included in the cost range include:

• Acquisition of data to validate the methods, algorithms, and codes. Programs that intend to utilize these capabilities must develop and fund experimental programs to validate the methods. We don't intend to exclude experiments entirely from the funding of the proposed program, simply to limit the scale of experimental activities. Limited experimental validation activities are envisioned in this program, particularly at university scale. A vigorous and complete validation for large scale applications must be carried out by the main programs.

• The algorithm, solver, method, and code development initiatives must be carried out with close coupling to and collaboration with the DOE ASC program, which is funding the design and construction of large scale HPC systems. Modern HPC platforms are an enabling technology to simulate multi-scale, multi-physics phenomenon. Research must be developed compatible with the future computing platforms.

Possible Advocates of This Initiative

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Dr. Luis Chacon – Los Alamos National Laboratory
Prof. John Verboncouer – Michigan State University
Prof. Charles Seyler – Cornell University
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