White Paper for *Frontiers of Plasma Science Panel*

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Indicate the primary area this white paper addresses by placing "P" in right column.
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	"P", "S"
• Plasma Atomic physics and the interface with chemistry and biology	
• Turbulence and transport	S
• Interactions of plasmas and waves	P
• Plasma self-organization	S
• Statistical mechanics of plasmas	S

Indicate type of presentation desired at Town Hall Meeting.

	"X"
Oral	X
Poster	
Either Oral or Poster	
Will not attend	

Title:	Predictive community computational tools for virtual plasma science experiments.
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Research frontier and importance of the scientific challenge.

Plasmas, especially those under extreme conditions, exhibit very complex interrelated multi-scale multi-physics phenomena that can only be fully understood through advanced particle and fluid simulations coupled to theory, experimentation and/or observation [1][2]. In particular, progress in large-scale simulations, based on advances in algorithms and supercomputing hardware, provide predictions with continuously increasing accuracy and fidelity. However, even in light of all the recent, ongoing and projected progress in both software and hardware, computational studies at the plasma physics frontiers will continue to be a very challenging endeavor. The promise of exascale supercomputing coupled with the computational complexity brought on by emerging architectures and languages poses a challenging yet very promising venue for computational plasma physics that will continue to stress algorithmic development while boosting the predictive power needed for the ultimate goal of real time virtual experimentation (e.g. simulations that reproduce the complexity of experiments at scale and run within seconds to minutes).

The physics of laser–driven high-energy density plasmas involves many phenomena including: laser-plasma interaction, plasma formation, plasma waves and instabilities, (impact- and photo-) ionization, scattering, radiation, electron-positron pair creation. It is not possible, using present technologies, to describe all those phenomena consistently from first principles. Hence various levels of descriptions are used concurrently (or separately) for each of the phenomena. The method of choice for the fully kinetic modeling of laser-plasma interactions is the Particle-In-Cell method [3] where the plasma is described as a collection of charged macro-particles that evolve self-consistently with their

electromagnetic fields, which are resolved on an Eulerian mesh. Collisional effects are usually modeled using Monte-Carlo methods [4]. Radiative processes are described using Monte-Carlo or solving radiative transfer PDEs. Dense regions can be too challenging to model fully kinetically and can in some instances be accurately modeled using Ohm's law [5]. In the exascale context, so-called "Vlasov algorithms", which describe the plasma on a 6-D Eulerian mesh, may become an attractive option for part or all of the simulation particle species/domain and may become increasingly under consideration.

Computational toolkits that are capable of virtual experimentation can rival (and even surpass) the complexity of individual experiments. In addition to having to ultimately reproduce the complexity of experimental setups, discretization -and other numerical artifacts- add another layer of complexity that needs to be fully understood and controlled. The power of the computational tools resides in their versatility for reuse among many applications, and their ability to access phenomena in regimes that are out of reach or cannot be isolated through experimentation or observation. A coordinated effort with sustained support is needed to develop and maintain the suites of computational tools that are required to realize fully the potential that they offer, with tremendous benefits to plasma science activities.

Approach to advancing the frontier and indicate if new research tools or capabilities are required.

The development of the next generation of frontier plasma science modeling tools that will be capable of virtual experiments necessitates an integrated toolkit of a collection of interoperable modules with specialized functionalities. Interoperability will be ensured via well-defined sets of Application Program Interfaces (APIs) and will be essential for efficient co-development across institutions. Thanks to modularity, individual components will be reusable across applications within the framework, as well as by other codes or frameworks. It will also enable easy swapping of components for testing of newly proposed alternate or improved algorithms, and facilitate the adoption of the new modules that prove to perform better. For maximum impact, it is essential for open source to be adopted for most (if not all) of the components. This will also encourage modularity, interoperability and reuse.

High-resolution of the modeling of laser-driven ion acceleration [6][7], flying plasma mirrors [6], high-intensity laser-matter interaction [8], laser-driven X-ray sources [9] or self-organization in ExB discharges [10], for example, necessitate a very large number of cells and macro-particles that stress computational resources. It is thus essential to develop algorithms and implementations that allow multi-level parallelism, and to optimize these on the shared compute node fine-grain level as well as maintain their ability to scale at extreme concurrency. The electromagnetic-PIC approach has been shown to scale to hundreds of thousands of cores or beyond when the distribution of macroparticles is regular. Realistic distributions can be highly irregular spatially, limiting the scaling significantly for production runs. Efficient load balancing algorithms, ultimately coupled to the use of Adaptive-Mesh-Refinement, that scale to very high concurrency will be needed. It is expected that for detailed high-frequency data analysis, the required I/O performances will greatly surpass the expected availability, necessitating efficient data reduction and in-situ analysis/visualization capabilities.

An example of a modular computational toolkit that can integrate a wide collection of plasma models is the Warp open-source Particle-In-Cell framework [11], developed originally within the U.S. Heavy Ion Inertial Fusion research program for the modeling of intense ion beams, and extended to a broader range of applications [12], including laser-plasma interactions. Warp can model all the stages of a laser-driven ion accelerator, including the laser-plasma interaction (see sample result in Fig. 1), ion extraction and transport into an accelerator lattice [13], up-to its final focusing onto a target. Its modern user interface based on the Python scripting language allows for a near-agnostic programming language

paradigm, since modules can be developed using Python, FORTRAN, C, C++, etc., and easily combined through the Python interface. The Python interface itself gives access to a very wide and rapidly growing library of community developed open-source modules for number crunching, parallel computing, data analysis and visualization. It also enables customization through user-programmability, interactivity and rapid prototyping.

Many of the high energy density plasmas are relativistic and it is thus essential to capture relativistic effects accurately. Recent advances in the modeling of relativistic plasmas, including the analyses and mitigation of the so-called 'numerical Cherenkov' instability [14], enable a much more accurate account of relativistic effects. Given the trend of computer hardware, the ratio of the cost of data communication over the cost of computing is increasing. Novel algorithms for parallelization of pseudo-spectral Maxwell solvers that enable spectral (or near-spectral) accuracy while minimizing communications promise to enable scaling of high-fidelity models to very high concurrency [15]. Those recent advances (that have been pioneered in the Warp framework) will provide the basis for tools with unprecedented accuracy, stability and scalability. Augmented with subgrid physics such as collisions and radiation, the new tools will enable the modeling of a very wide range of plasma physics and lead the way toward the ultimate goal of real time virtual experimentation.

Kinetic plasma codes need to be coupled to magnetohydrodynamic (MHD) codes for the modeling of the formation of plasma ahead of the laser main pulse arrival, and to radiation/hydrodynamic codes for the modeling of energy deposition and its effects in targets [16], such as HYDRA, DISH, or ALE-AMR [17][18] (see sample result in Fig. 2), as well as molecular dynamics codes and other specialized codes depending on the experiment. It will be very important to develop MHD tools with AMR that scale to very high concurrency, more accurate ion stopping algorithms, and improved Equations-of-State (EOS) in the warm dense matter regime (also benchmarked with experiment). Surface tension effects need to be incorporated or improved, especially in regimes such as warm dense matter where the state is a mix of plasma, conventional fluid, and solid.

Impact of this research on plasma science and related disciplines and any potential for societal benefit.

Large-scale modeling is key to understanding the multi-scale tightly coupled non-linear multi-physics phenomena in support of theory and experiments at the plasma science frontier. Developing the next generation tools that will enable ultimately real time virtual experiments, at higher accuracy, computational speed and integrating together more phenomena than is possible now. This will speedup the design, operation and analysis of experiments, making them more affordable and able to deliver more science. It will also enable virtual experiments in regimes that are not accessible to experiments or observations over a much wider parameter range than would be possible with existing tools.

Overall, the proposed tools will reduce time to solution, increasing and accelerating scientific discoveries across plasma science and beyond. The computational methods and tools are very general and applicable to a wire range of applications involving plasmas, beams and laser-plasma interactions. Benefits to society range from medical technology (e.g. ion-driven cancer therapy, light sources for bio-imaging) to energy (e.g. fusion sciences), from basic physics (e.g. HEDLP science, space plasmas science, charged particle traps) to broader accelerator applications (e.g. HEP and rare isotope facilities), and from industry (e.g. plasma processing) to national security (e.g. science-based stockpile stewardship, gamma sources) [1][2].

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Figures

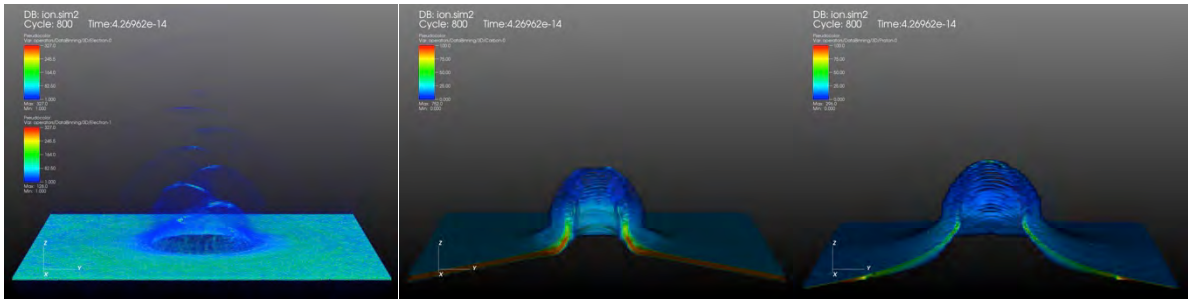

Fig. 1: Warp 3-D simulation of ion acceleration experiment with a short laser pulse impacting a thin foil of carbon and hydrogen. The laser (not shown) is propagating from bottom to top: (left) ejection of electrons from the pre-formed plasma (color according to local density); (middle) carbon ions (color according to local density); (right) protons (color according to local density). Visualization was performed in-situ (i.e., at runtime) using VisIt.

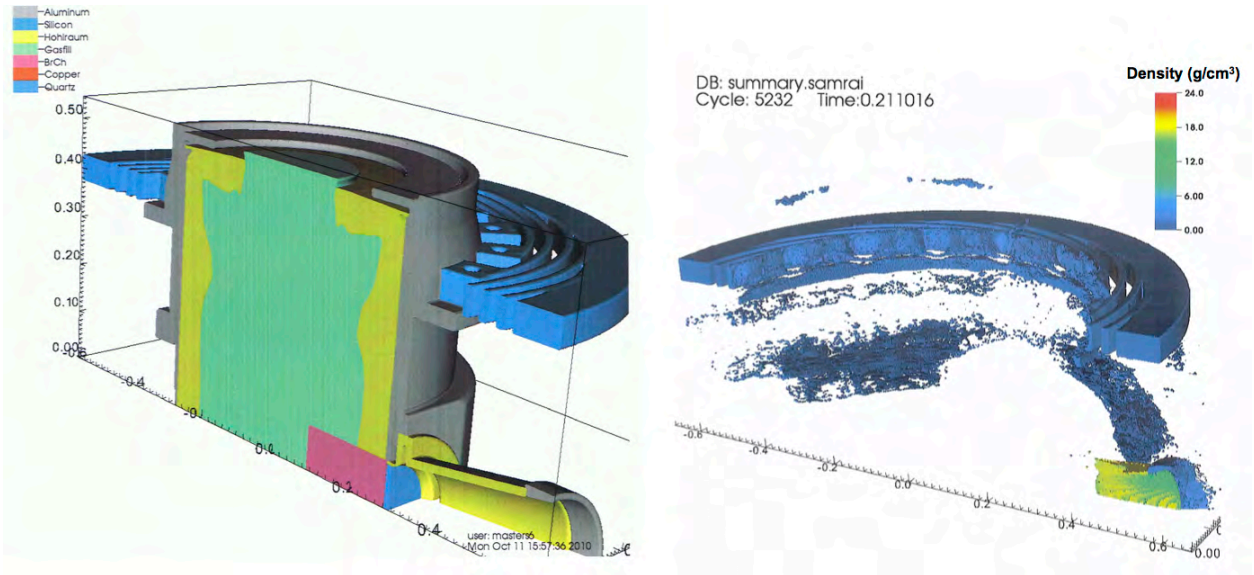

Fig. 2: Left image is initial condition (different colors represent different materials) of a laser heated, gas-filled cryogenic Al hohlraum with an Au liner and Si cooling ring. Symmetry allows us to model only ¼ of hohlraum in the ALE-AMR simulation. A Cu sample inside an attached cone has blown into the gas fill and some of the Au liner. The right image shows the unvaporized material ($T < 3000K$ and $\rho > 0.5$ gm/cm^3) after ALE-AMR simulates blow-off the vaporized material (time = 211 ns).