Predictive Community Computational Tools for Virtual Plasma Science Experiments

J.-L. Vay, E. Esarey, A. Koniges

Lawrence Berkeley National Laboratory

J. Barnard, A. Friedman, D. Grote

Lawrence Livermore National Laboratory

Frontiers of Plasma Science Workshops - Town Hall

June 30-July 1, 2015

Advanced simulations play an increasingly important role in plasma science .

Plasmas exhibit **very complex interrelated multi-scale multi-physics** phenomena:

➔ full understanding = **simulations** + **theory** + **experimentation** +/or **observation**.

Advances in algorithms and supercomputing hardware:

➔ predictions with **increasing accuracy and fidelity**: relax and wait?

~~Relax and wait~~: even with recent and projected progress (in software & hardware), **computational frontiers plasma physics** will still be a **very challenging endeavor.**

E.g., **laser–driven high-energy density plasmas** involves **many phenomena**:

- laser-plasma interaction, plasma formation, plasma waves and instabilities, (impact- and photo-) ionization, scattering, radiation, electron-positron pair creation.
- **not possible now** to describe all those phenomena **consistently from first principles**.
  - ➔ various levels of descriptions are used for each of the phenomena
  - ➔ lead eventually to incomplete physics, insufficient resolution, …

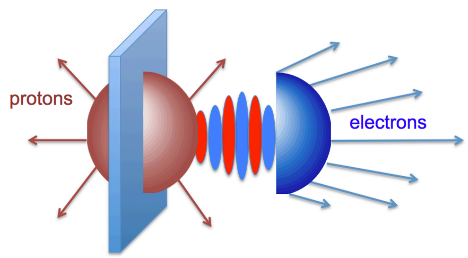
Exascale computing + algorithm advances will **boost the predictive power** of sim.

Ultimate goal: real-time virtual plasma experiments.

High-res. multi-scale multi-physics modeling of plasmas is stressing computational resources

Examples

Ion acceleration



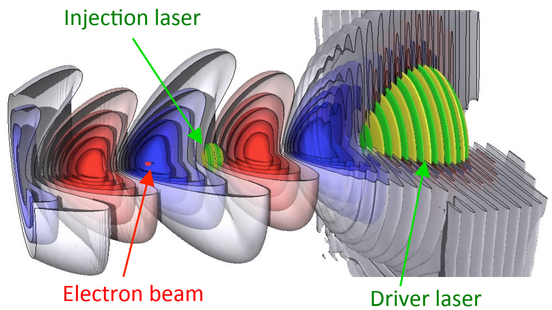
Now: 10^6-10^7 CPU-hours

2025: 10^8-10^{10} CPU-hours

For modeling of plasma-based ion accelerator (laser driven):

Requires $10^4 - 10^7$ steps through :
- O(10^{12}-10^{13}) grid cells
- O(10^{12}-10^{15}) plasma macro-part.
- 10s-100s cases

Electron acceleration



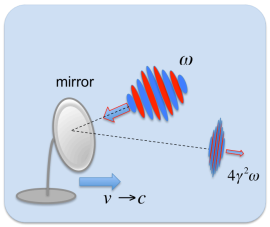
Now: 10^6-10^7 CPU-hours

2025: 10^8-10^{10} CPU-hours

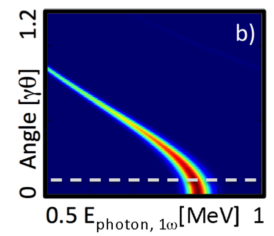
For modeling of plasma-based electron accelerator (beam or laser driven):

Requires $10^4 - 10^7$ steps through :
- O(10^{10}-10^{12}) grid cells
- O(10^{12}) plasma macro-part.
- 10s-100s cases

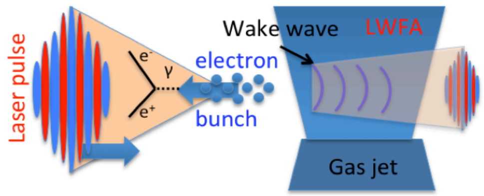
Flying plasma mirrors



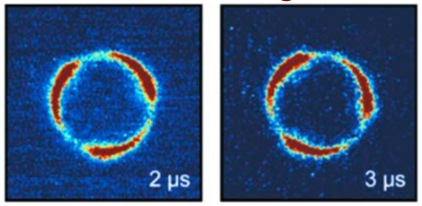
Laser-driven X-ray sources



High-intensity laser-matter interactions



Self-organization in ExB discharges



Exascale will bring tremendous computational power but imposes significant developments

Plasma codes are transitioning to **deeper multi-level parallelism**:

- intra-core: vectorization
- **intra-node: multi-threaded openMP/CUDA (newest)**
- inter-nodes: MPI (can be multi-level: e.g. using MPI groups)
- ensemble: parallel optimization, U.Q.

Scaling to large # of cores will necessitate **efficient dynamic load balancing**

- scaling of EM-PIC with constant uniform plasma is easy
- general case of highly-evolving non-uniform plasma is much harder

A **broad range of solvers need to scale** to large # of cores

- 2^{nd} order FD, high-order FD, FV & FE, spectral (FFT), multi-grid
- regular cartesian and irregular meshes
- adaptive mesh refinement (not mainstream and will need extra development)

High-volume of data increases the need for **efficient parallel IO/in-situ analysis/viz.**

A **community based program** is needed to develop the **next generation** of simulations tools

Computational toolkits that are capable of virtual experimentation **can rival** (and even surpass) the **complexity of individual experiments**

- needs to reproduce the **complexity of experimental setups**,
- discretization -and other numerical artifacts- add **another layer of complexity** that needs to be **fully understood and controlled**.

A **coordinated, community effort** with sustained support would be **most effective**:

- develop & maintain **integrated comprehensive** kit is an **enormous task**:
    - collection of exascale-ready (PIC, MHD, fluid, radiation, QED, MD, EOS, etc.) modules,
- **co-development across institutions** (national labs, universities, …):
    - **optimize resources** through **reuse** and minimization of **redundancy** (enabled by modularity, interoperability with common APIs),
    - **speedup development** and port of **exascale-ready** algorithms,
    - **speedup progress** in understanding and mitigation of **numerical effects**,
- **ecosystem** of modules to enable **selection of best algorithms** while preserving **diversity** of solutions and **creativity**,
- **open source** to be encouraged for easier co-development, verifiability and adoption,
- will enable **standardized interface** that will boost productivity of users.

Summary and Impact

Plasma physics involves tightly coupled non-linear multi-scale/physics phenomena

- **large-scale modeling**, w/ theory/experiment, is **key to understanding of complexity**

Exascale computing will narrow gap toward goal of real-time virtual experiments

- but not silver bullet: **significant investments are needed** to develop exascale-ready toolkit

A **coordinated, community effort** will be **most effective**

- **cross-institutional development** of integrated comprehensive kit **to maximize resources**

New tool to **accelerate discoveries** across plasma science and beyond

- **computational methods are very general** and applicable to a wire range of applications involving plasmas, beams and laser-plasma interactions.
- benefits to society over a wide range of applications
    - **medical technology** (e.g. ion-driven cancer therapy, light sources for bioimaging),
    - **energy** (e.g. fusion sciences),
    - **basic physics** (e.g. HEDLP science, space plasmas science, charged particle traps),
    - **accelerators** (e.g. HEP and rare isotope facilities),
    - **industry** (e.g. plasma processing),
    - **national security** (e.g. science-based stockpile stewardship, gamma sources).

Thank you.