In situ Visualization and Analysis of Particle Accelerator Simulations using WarpVisIt

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1) Science Problem

The available I/O bandwidth and data storage capabilities are decreasing relative to computation, limiting the amount of data that can be saved for post-process analysis. To enable particle-in-cell (PIC) simulations using Warp [1] to: i) more efficiently utilize high-performance computing resources, ii) perform analysis at high temporal resolution, and to iii) enable knowledge discovery from large-scale simulations, we are implementing a three-fold strategy:

1. Couple general-purpose, state-of-the-art *in situ* visualization technology using VisIt [2] with Warp to make new advanced analysis capabilities accessible to Warp and to enable *in situ* processing of the complete data in parallel, which is not possible using the current approach based on OpenDX (see Fig 1.1).
2. Integrate *in situ* query capabilities with Warp and the visualization to enable identification of data features and data subsets of interest, reducing the amount of data that needs to be visualized and stored.
3. Integrate high-performance I/O libraries with Warp to improve parallel I/O performance.

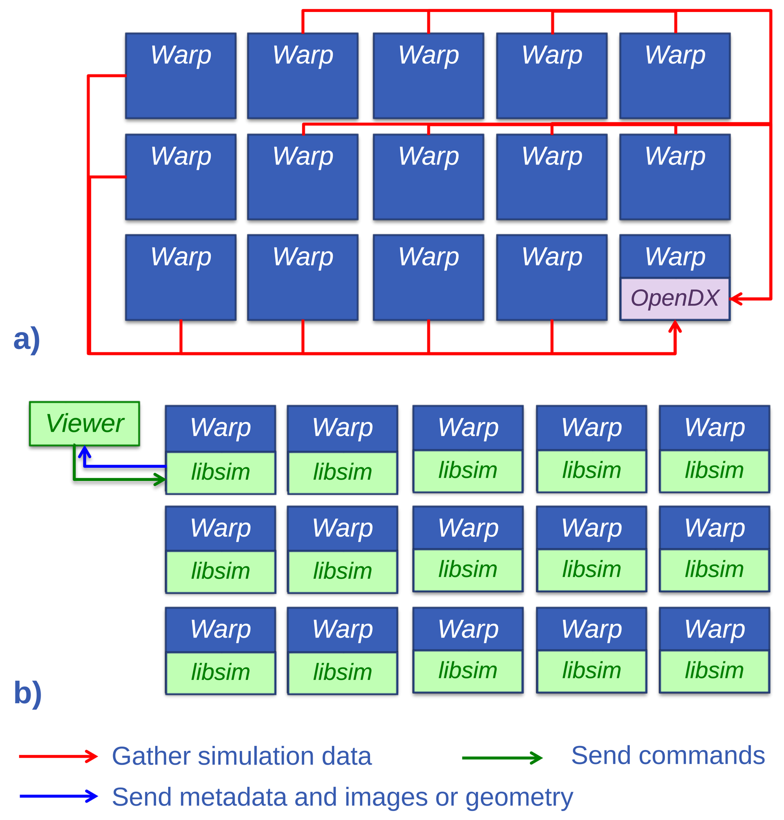


Fig. 1.1 *In situ* visualization using a) Warp+OpenDX and b) Warp+VisIt. VisIt processes the simulation data in parallel and in place, enabling large-scale visualization of the complete data while reducing communication cost.

2) WarpVisIt: Overview

2.1) Controlling the Simulation and Visualization

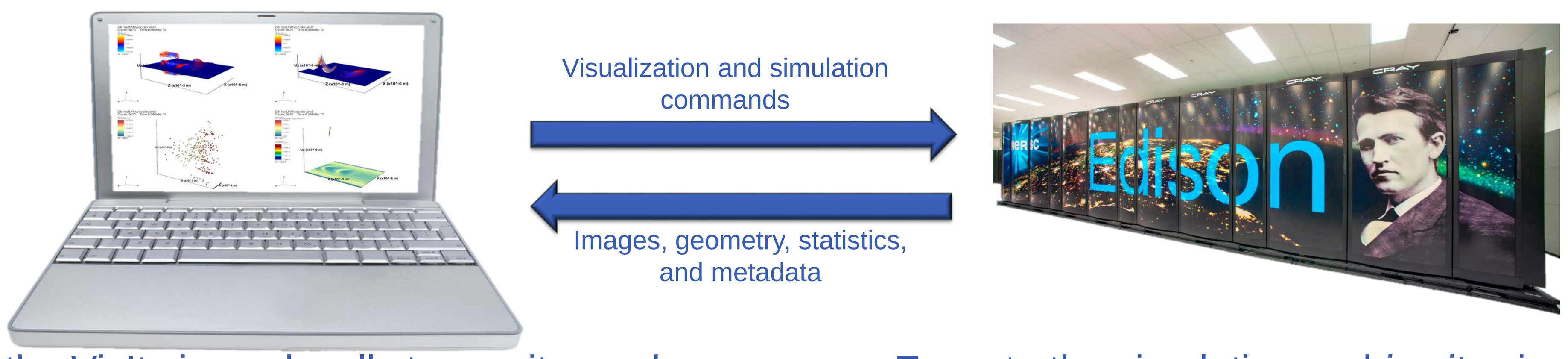
Monitoring Mode
The simulation runs independently while the user connects periodically to the simulation via the visualization to check results and perform *in situ* analysis.

Batch Mode
The simulation and visualization are executed in concert without external user control.

Interactive Mode
The user controls the simulation from the visualization GUI or Python shell while exploring the simulation data as it is being generated.

Shell Mode
The user controls the simulation and the visualization directly from the simulation shell.

2.2) *In Situ* Remote Data Analysis and Visualization



Run the VisIt viewer locally to monitor and interact with the visualization and simulation

Execute the simulation and *in situ* visualization and analysis on remote HPC system

2.3) Other Advanced features

Multiple Field and Species Support: WarpVisIt supports introspection of available particle species and fields to ease interaction with dynamic, solver- and model-depended collections of particle species, fields, and variables.

***In situ* Filtering:** WarpVisIt supports filtered species, enabling users to dynamically expose derived particle species to the visualization, enabling i) flexible *in situ* analysis of particle feature, ii) analysis and collection of data subsets of interest at higher temporal frequency, and iii) reduced cost for subsequent visualization and I/O.

Yee-cell: WarpVisIt supports accurate visualization of Yee-cell meshes used for simulation via dedicated re-interpolation methods.

Custom I/O: WarpVisIt adds support for VTK I/O and eases the integration of new I/O routines

3) Public Release

We released WarpVisIt to the public in June 2015: ***https://bitbucket.org/berkeleylab/warpvisit***

4) *In situ* Visualization and Analysis of Laser-driven Ion Accelerator Simulations

The generation of short pulses of ion beams through the interaction of an intense laser with a plasma sheath offers the possibility of compact and cheaper ion sources for many applications: radiography, deflectometry, cancer therapy, injection into conventional accelerators, fast ignition, isochoric heating of matter, positron emission tomography, nuclear physics among others.

High-resolution 3-D simulations are needed to resolve the short wavelength physics of a solid density plasma at scale. *In situ* visualization and data analysis provide key insight into the dynamics of the electrons and ions acceleration processes.

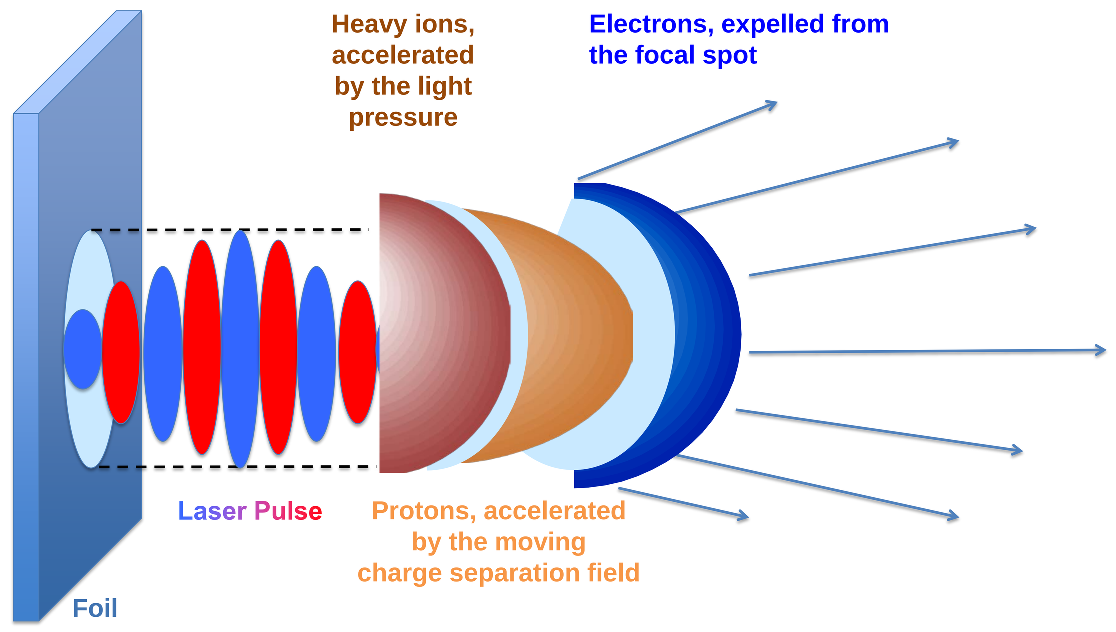
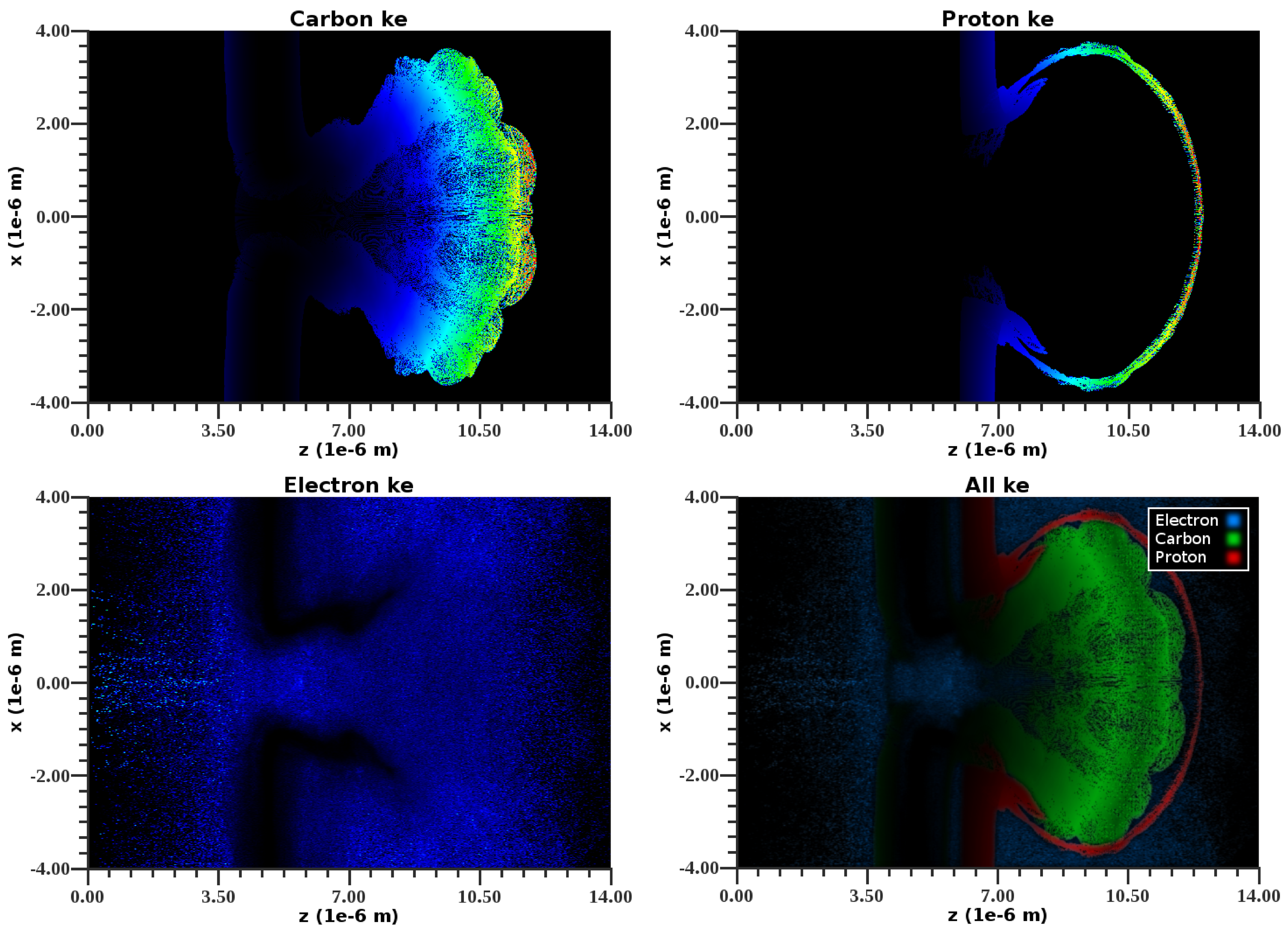


Fig. 4.1 Illustration of the basic ion-acceleration process at the **Directed Coulomb Explosion Regime**:
- The laser pulse accelerates the target by radiation pressure and
- Removes most electrons from the target and in turn the
- Moving charge separation field boosts the protons.

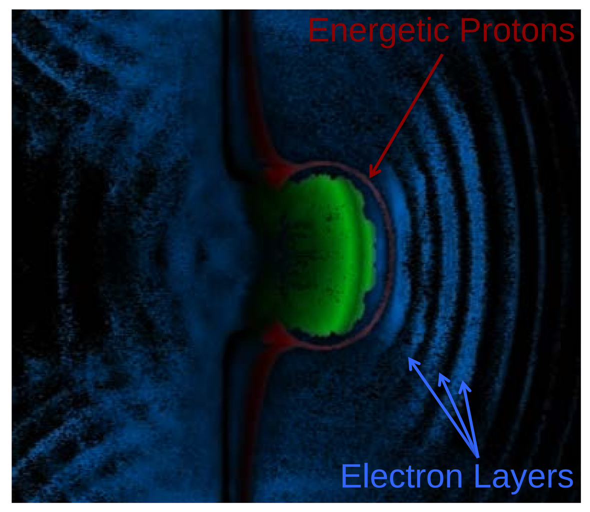
Best designs use high-Z/low-Z layer foils of solid density.

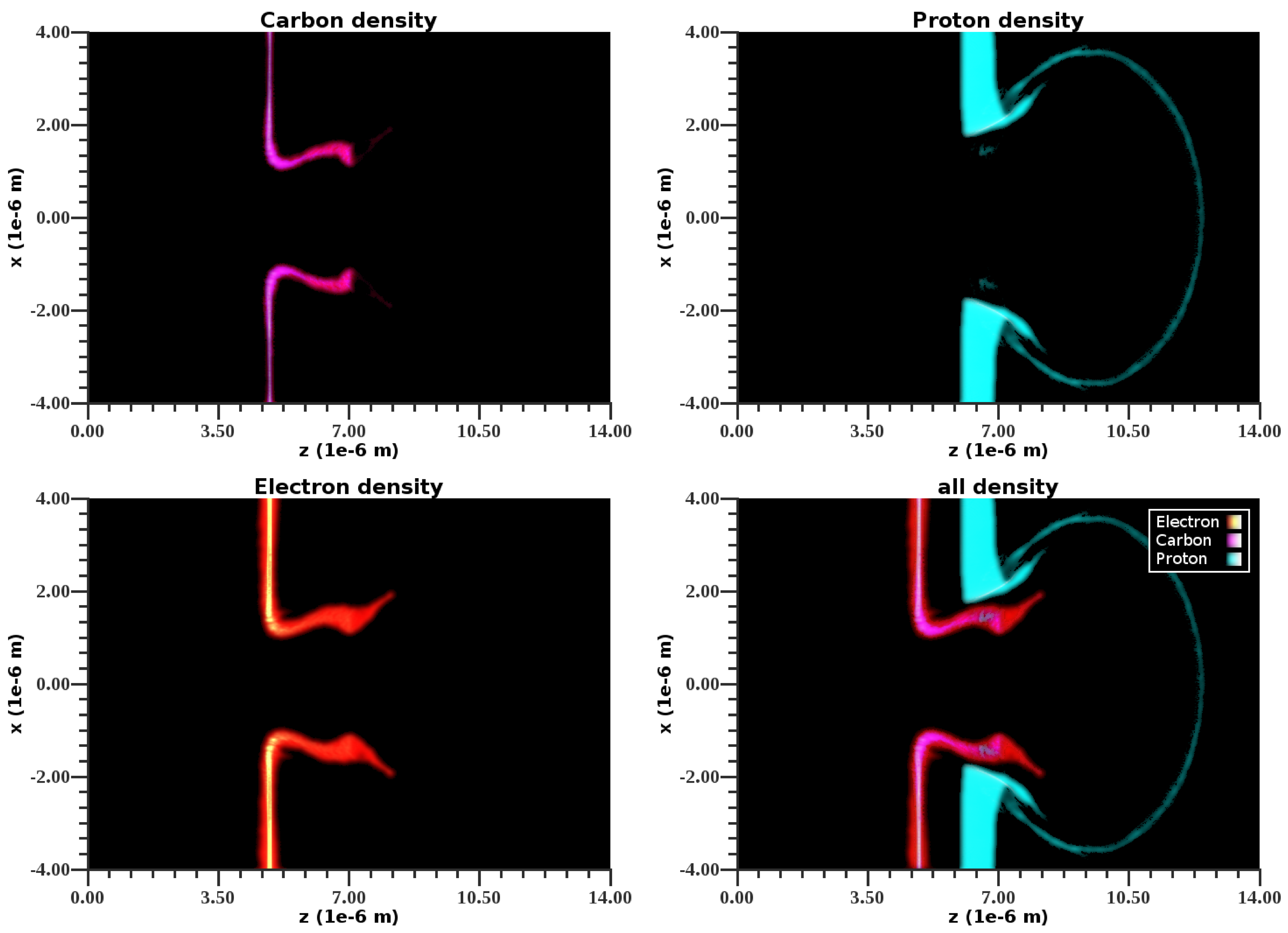


← **Fig. 4.2** Visualization of the kinetic energy for the three main particle species: a) carbon (top left), b) proton (top right), and electrons (bottom left) using a heat-map color scale (blue=low, green=medium, red=high).

The bottom right figure shows a comparative visualization of the kinetic energy of all three particle species illustrating the joint evolution of the different particle species.

↓**Fig. 4.3** Joint visualization of the carbon (green), proton (red), and electron (blue) particles highlighting characteristic acceleration features.





← **Fig. 4.4** Visualization of the particle density for the three main particle species: a) carbon (purple, top left), b) proton (cyan, top right), and c) electrons (red, bottom left) using an intensity color scale.

The bottom right figure shows a comparative visualization of the density of all three particle particle species.

The visualizations shown in Fig. 4.2 to 4.4 where generated *in situ* by WarpVisIt on the 2.39PF/s Cray XC30 supercomputer system Edison at NERSC using 2400 cores.

[1] B. Whitlock, J. M. Favre, and J. S. Meredith. "Parallel in situ coupling of simulation with a fully featured visualization system." Proceedings of the 11th Eurographics conference on Parallel Graphics and Visualization,(2011)
[2] J.-L. Vay, D. P. Grote, R. H. Cohen, and A. Friedman, "Novel methods in the Particle-In-Cell accelerator Code-Framework Warp," IOP Computational Science & Discovery, 5 014019 (2012)
[3] S. S. Bulanov, D. W. Litzenberg, K. Krushelnick, A. Maksimchuk, "Directed Coulomb Explosion regime of ion acceleration from mass limited targets by linearly and circularly polarized laser pulses," arXiv:1007.3963, (2010)