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 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.

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.
- Interactive Mode: The user controls the simulation from the visualization GUI or Python shell while exploring the simulation data as it is being generated.
- Batch Mode: The simulation and visualization are executed in concert without external user control.
- Shell Mode: The user controls the simulation and 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-dependent 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 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.

In situ Visualization and Analysis of Particle Accelerator Simulations

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.

Fig. 1.2 Visualization of the kinetic energy for the three main particle species: a) carbon (top left), b) proton (top right), and c) electrons (bottom left) using a heat-map color scale (blue-low, green-medium, red-high).

The bottom right figure shows the joint evolution of the different particle species illustrating the feature highlighting characteristics acceleration features.

Fig. 1.3 Joint visualization of the carbon (green), proton (red), and electron (blue) particles highlighting characteristic acceleration features.

Fig. 1.4 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 the comparative visualization of the density of all three particle species.

The visualizations shown in Fig. 2.2 to 4.4 where generated in situ by WarpVisIt on the 2.39PF/s Cray XC30 supercomputer system Edison at NERSC using 2400 cores.

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