In Situ Visualization of Laser-Plasma Interaction

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Abstract:

Thorough understanding of ultra-intense laser-plasma interaction may enable new routes in fundamental research as well as a wide range of applications [1]. However, such systems involve collective behavior of particles in self-consistent electromagnetic fields which is, in general, complex and strongly non-linear problem that can be investigated only with the help of numerical simulation.

An exponential increase of computational throughput of supercomputers enables researchers to perform simulations with unprecedented accuracy. Using the conventional post-processing approach of data analysis, such simulations would require extremely large amount of data to be stored on a persistent storage. The storage bandwidth performance, however, has not grown up as rapidly as the computational power. In practice, the data coming from the simulations have to be stored only at several time-steps or at much coarser resolution than the original data, the rest is just discarded. Therefore, a significant part of information may be potentially lost.

The technique where the simulation data are concurrently analyzed and visualized while it is being generated is usually referred to as in situ processing. In situ processing could circumvent the bottleneck of data transfer. By coupling the visualization and simulation together, one may process and analyze the simulation data at high spatial and temporal resolutions without the necessity of involving the storage resources.

Recently, we have instrumented the code EPOCH [2] with the ParaView Catalyst [3]. EPOCH is massively parallel, multi-dimensional plasma physics simulation code based on the particle-in-cell (PIC) method. ParaView Catalyst is a library that has been designed for in situ coupling of numerical codes with the state-of-the-art visualization system. Here we present our implementation strategy, performance analyses and demonstrate the in situ capabilities on several large-scale laser-plasma simulations.

References:

[1] G. A. Mourou, T. Tajima and S.V. Bulanov, *Rev. Mod. Phys.* **78**, 309 (2006)
[2] T. D. Arber et al., *Plasma Phys. Control. Fusion* **57**, 11 (2015)
[3] A. C. Bauer, B. Geveci and W. Schroeder, *ParaView Catalyst User's Guide*, Kitware, Inc. (2017)

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INTRODUCTION:

Traditional (post-processing) approach:

1) specify input parameters
2) run simulation
3) analyze generated data

Computational power increases:

- More accurate simulations
- More data to be stored on a disk

Storage and network bandwidth performance has not grown up as rapidly:

- Output takes time
- Data occupy large disk space
- Processing and analysis of data difficult

In practice:

- Data stored only at several time-steps
- Or at much coarser resolution

➢ rest of the data just **discarded**
➢ significant part of information potentially **lost**

In situ processing:

= technique where the simulation data are concurrently analyzed and visualized while it is being generated without the necessity of first storing the data on persistent storage

Solutions: VisIt libsim, ParaView Catalyst, Ascent, Sensei

Benefits:

- Circumvents the bottleneck of data transfer
- Allows to analyze simulation data at high spatial and temporal resolution in memory during the simulation runtime
- Allows to visually explore simulation data and modify the simulation parameters in order to observe immediate impact

Drawbacks:

- Potential increase in executable size caused by linking Catalyst and its dependencies
- Memory overhead caused by copying simulation data structures to VTK data structures

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IMPLEMENTATION STRATEGY:

EPOCH + ParaView Catalyst:

Coupling via **Adaptor** (simulation interface):
- Not to disturb main code
- Simplify the build process

Contains 3 methods:

1) Initialize Catalyst:
- Executed only once (beginning of simulation)
- Configures input channels (one for Cartesian grid, one for each particle species)
- Loads visualization pipelines (what operations to perform, how to output the data, IP address + port of PV server)

2) Run coprocessor:
- Executed at each time-step (operation performed only at pre-defined time-steps or when some condition is fulfilled)
- Builds VTK data-structures:
  - vtkMultiBlockDataSet + vtkRectilinearGrid for Cartesian grid and its decomposition including ghost cells
  - vtkUnstructuredGrid for each particle species
  - Recalculated only when the local domain changes (e.g. particle cross boundary, load-balancing)
- Maps simulation data onto VTK data structures – no deep-copying (structure-of-arrays memory layout - vtkSOADataArrayTemplate):
  - Cartesian grid: electric field (E), magnetic field (B), current density (J)
  - Particles: momentum (p), weight (w)
- Invokes data processing specified in the pipelines

3) Finalize Catalyst:
- Executed only once (end of simulation)
- Releases all Catalyst resources

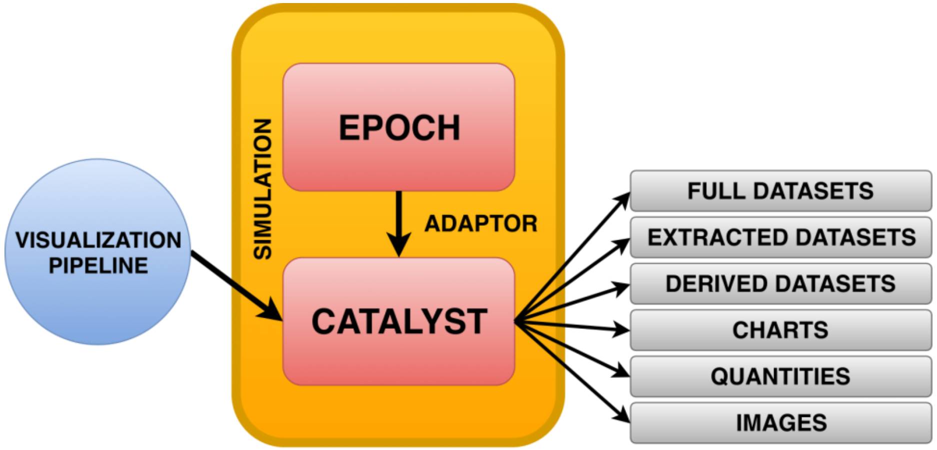

Figure 1: EPOCH workflow for in situ visualization using ParaView Catalyst.

PERFORMANCE ANALYSIS:

2 modes of operation (may run simultaneously):

1) Batch mode:
- Code executes the visualization pipelines automatically
- No need of user intervention

2) Interactive mode:
- User can connect to simulation with ParaView GUI and explore the data as it is being generated
- Allows to steer the simulation (pause, specify breakpoints conditionally)
- invaluable tool for scientific insight, debugging

Performance testing:

- compute time and I/O cost for certain analysis operations on a test 3D simulation
- executed on 16 nodes of the ELI Beamlines cluster (16 x 16 Haswell-EP cores, 128 GB DDR4 RAM, fully non-blocking fat-tree Infiniband QDR network, 40 Gbps bandwidth, storage bandwidth performance approx. 1.8 GB/s)
- The simulation dumped three field quantities (E, B, J) at high frequency (each 10th iteration out of 2100) in double precision
- I/O operations take 95 % of the total time, 8.2 TB of disk space required in the case of dumping whole datasets for post-processing
- ratio between computation and I/O operations much more reasonable regarding the individual Catalyst filters
- using the right visualization pipelines to extract the features of interest drastically reduces the I/O and speed-up the simulation

Type of output	Runtime (hh:mm:ss)	Total size
No I/O	01:46:07	0.0
Full Dataset (SDF)	36:42:52	8.2 TB
Slice (VTM)	02:14:07	19.5 GB
Iso-surface (VTM)	02:27:47	115.1 GB
Plot over line (PVTP)	01:53:12	17.5 MB
Image (PNG) *	01:54:27	13.8 MB

Table 1: Comparison of compute time and I/O cost for several data processing operations. *Images rendered at 1080p using software renderer.

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IN SITU USE CASES:

Laser-plasma interaction:

- High-energy photon generation using the concept of relativistic flying mirrors (RFM)
- Applications: molecular imaging, attosecond spectroscopy, diagnostics of thermonuclear plasmas, experiments on laboratory astrophysics

RFM:

- reflection of counter-propagating laser beam from thin dense electron layers traveling with velocities close to the speed of light
- reflected wave is compressed, amplified and its frequency is up-shifted (due to double Doppler effect)
- Plasma mirror is realized by wake-wave generated by intense laser pulse

- To model this scenario, PIC simulations require very **high spatial and temporal resolution** to accurately describe a large band of frequencies
- the main part of information is carried by only a **small fraction of reflected radiation**

➢ in situ analysis **extremely useful** in this case

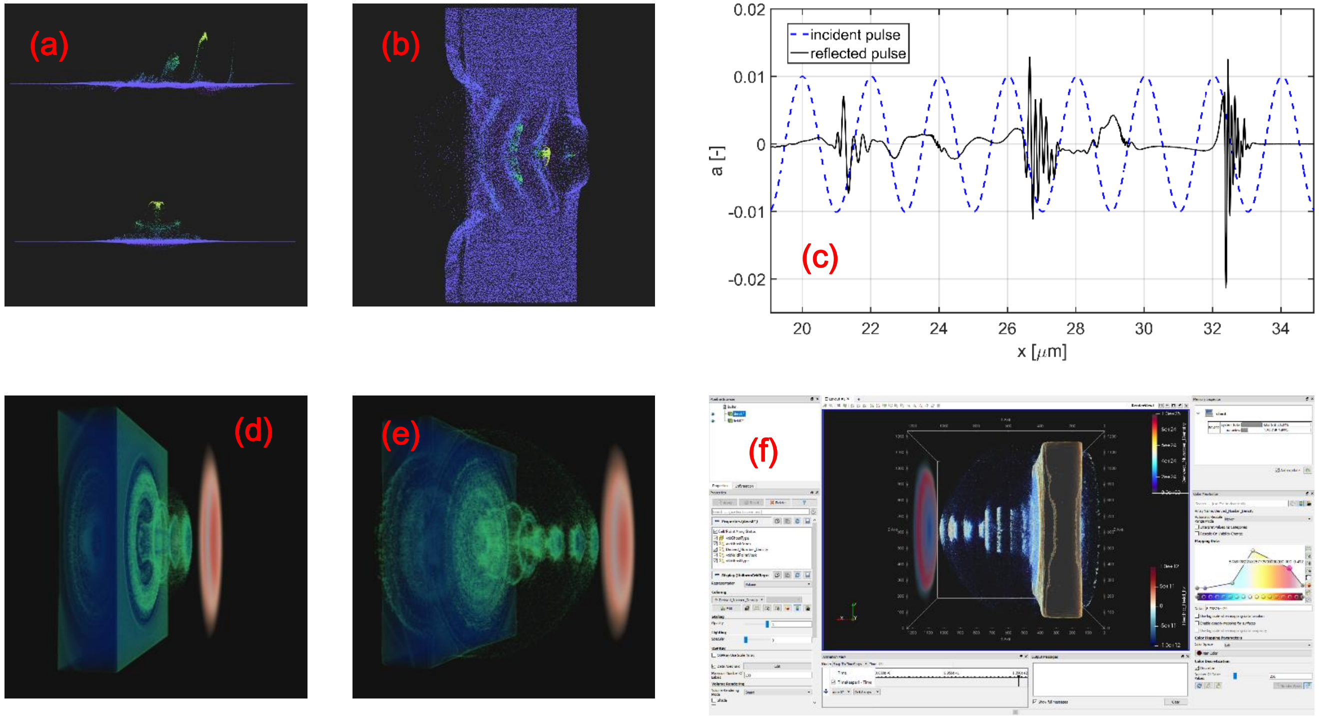

Figure 2: **(a)**, **(b)** Rendered images of the phase space. **(c)** Plot over line filter applied on the incident and reflected light. **(d)**, **(e)** 3D laser-plasma interaction displayed using volume rendering. **(f)** Electron density and laser electric field showing the formation of plasma mirrors in the interactive mode using *ParaView* GUI.

Examples...