Scalable Data Management, Analysis and Visualization of Particle Accelerator Simulation Data

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High-performance Query-based Analysis and Visualization

Science Problem:
- Simulations of particle acceleration processes require the use of large numbers of particles, making analysis and visualization challenging task.
  - Simulations of electron-LINACs for a proposed next-generation x-ray free electron laser (FEL) at LBNL require >10⁶ macroparticles to control macroparticle shot noise and avoid overestimation of the microbunching instability.
  - Magnetic reconnection processes are initiated in the small scale around individual electrons but eventually lead to large-scale reconfigurations of the magnetic field, e.g., in the Earth’s magnetosphere. Detailed modeling of electron motions in large-scale fields requires the use of >10¹⁰ macroparticles.

Simulation Codes:
- Impact-T, Impact-Z, VPIC

Solution:
- I/O: Integrated H5Part with the Impact and VPIC simulation suite, enabling high-performance parallel data write and storage of large particle data sets.
- Data Management: Developed FastQuery, making distributed, hybrid parallel (MPI+pthreads) index/query technology based on FastBit accessible to scientific file formats enabling:
  - Fast generation of indexes (256s for 1 billion particles using 10,000 cores) and evaluation of data queries (Fig. 1).
  - Repeated, complex, large-scale query-based analysis of massive datasets, which would otherwise be impractical with respect to both time as well as computational cost (Fig. 2).
- Visualization: Integrated FastQuery with the parallel visualization system VisIt for fast, query-based data exploration.

Application Example I: Query-based Beam Diagnostics for LINACs
- Use advanced queries to identify and quantify the extend of the halo of particles beam with Warp

Application Example II: Magnetic Reconnection
- Combine query-based data analyses and cross-mesh field evaluation to study the relationship between particle subsets of interest (scattered data) and the magnetic/electric fields (structured data)
  - Study the global and local distributions of accelerated particles to investigate, e.g., the spatial localization patterns of particles (Fig. 3)
  - Compare accelerated particles with different principle motion with respect to the magnetic field to study the alignment of accelerated particles with the magnetic-field (Fig. 4a,b)

In Situ Visualization and Analysis using Warp and VisIt

Science Problem:
- The available I/O bandwidth and data storage capabilities are decreasing relative to computation, making in-situ visualization and analysis indispensable.
- The current approach for in-situ visualization and analysis using Warp has several limitations:
  - The legacy system OpenDX is no longer supported.
  - Visualization is performed by a single compute core.
  - The data often needs to be reduced for the visualization.

Solution:
- Couple general purpose, state-of-the-art in situ technology using VisIt with Warp
- Using VisIt for in-situ data analysis and visualization:
  - Enables in situ processing of the complete data in parallel,
  - Makes new advanced analysis capabilities accessible to Warp,
  - Avoids reduction and communication of data for the purpose of visualization as the data can be processed in place.

Automatic Beam Detection for Laser Plasma Accelerator Simulations

Science Problem:
- Develop new compact, high-quality accelerator technology based on laser-plasma acceleration.
- Datasets are extremely large, heterogeneous and of varying spatial and temporal resolution.
- Particle beams are small (<1% of the data) and beam formation and acceleration are highly complex processes.
- Diverse physical settings, including single laser pulse and multiple colliding laser pulse accelerator designs (Fig. 5).

Simulation Code:
- VORPAL

Solution:
- Integrate high-performance data query with the visualization and analysis to accelerate beam detection and selection enabling:
  - Fast tracing of particle over time within seconds rather than hours.
  - Analysis of even large 3D laser plasma particle accelerator simulations.
- Develop advanced algorithms for automatic detection of particle beams and their sub-structures based on the full temporal particle traces enabling:
  - Automatic detection of all particle beams and subtle temporal beam substructures not easily detected otherwise.
  - Efficient processing of large numbers of particle datasets.
- Link automated analysis with the visualization enabling:
  - Effective exploration of the space of particle features,
  - More accurate and efficient analysis of particle beams and beam substructures then previously possible.

Fig 1: Time for querying 1 trillion particle dataset with different number of cores.
Fig 2: Number of halo particles per time step and halo query at timestep 20 (inset) of an IMPACT LINAC simulation.
Fig 3: Plot showing all energetic particles in a trillion electron VPIC simulation colored by UPar.
Fig 4: Comparison of the spatial distribution of particles with positive (left) and negative (right) UPar values in a trillion electron VPIC simulation.
Fig 5: Single laser pulse and multiple colliding laser pulse.
Fig 6: Example in situ visualization of Warp simulation using VisIt’s ibeam simulation interface.