Parallel Data Storage, Analysis, and Visualization of a Trillion Particles

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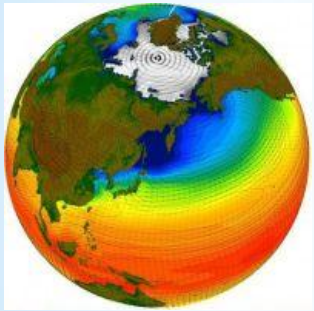
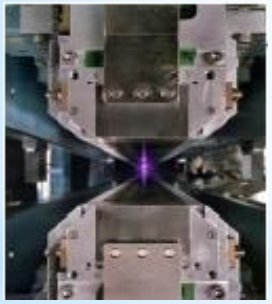
Data Explosion in High Performance Computing

- **Modern scientific discoveries are driven by data**



By 2020, climate data is expected to be hundreds of exabytes or more

LHC experiments produce petabytes of data per year



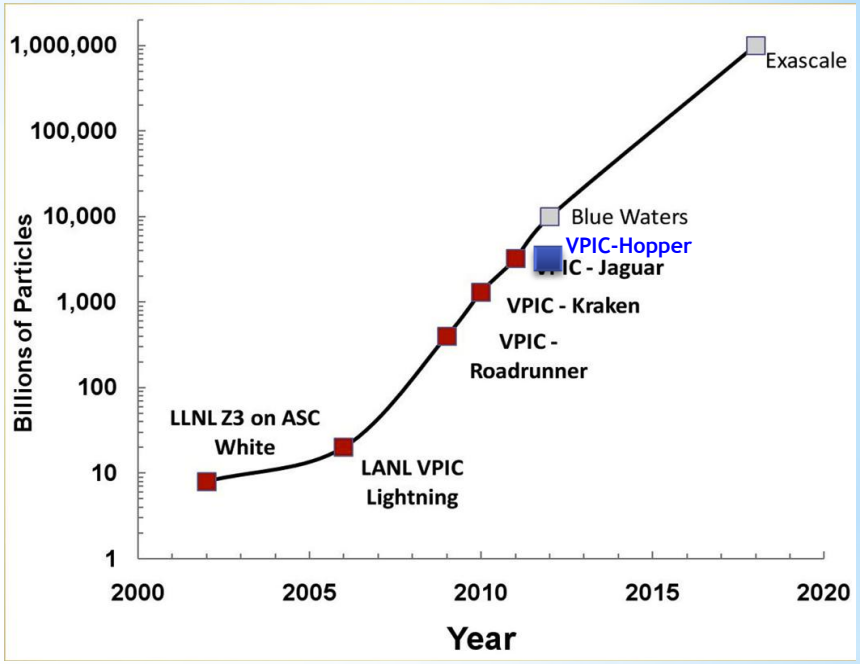
Light source experiments at LCLS, ALS, SNS, etc. produce tens of TB/day

1 Exabyte per a day (10 petabytes every hour)

- Storing, analyzing, and visualizing large data are big challenges
- VPIC is a simulation that pushes the limits of data management tools on large supercomputers

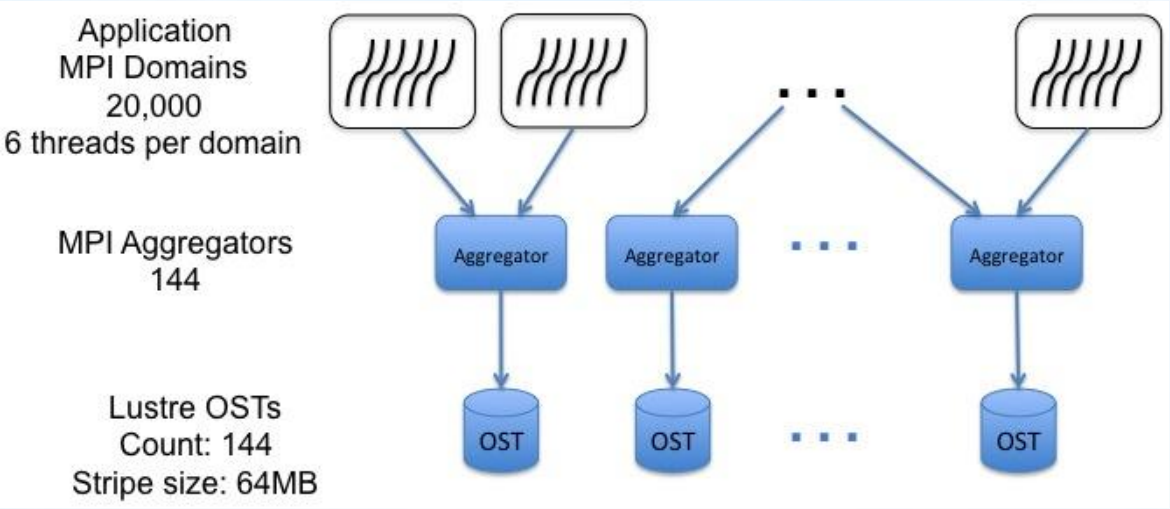
Vector Particle-in-Cell (VPIC) Simulation

- A state-of-the-art 3D electromagnetic relativistic PIC plasma physics simulation
- It is an exascale problem and scales well on large systems
- An open boundary VPIC simulation of magnetic reconnection
- NERSC Hopper Supercomputer



  - 6,384 compute nodes; 2 twelve-core AMD 'MagnyCours' 2.1-GHz processors per node; 32 GB DDR3 1333-MHz memory per node; Interconnect with a 3D torus topology
  - Lustre parallel file system with 156 OSTs at a peak BW of 35 GB/s

VPIC Trillion Particle Simulation setup



- ✧ 20,000 MPI processes using 120,000 cores
- ✧ Each MPI process writes ~51 Million (±15%) particles
  - ○ Non-uniform number of particles
- ✧ Lustre-aware MPI-IO implementation
  - ✓ MPI collective buffer size is equal to the stripe size
  - ✓ Number of MPI aggregators is equal to the stripe count
- ✧ Each particle has 8 variables
- ✧ **Particle dataset size per time step varies (30TB to 39TB)**
- ✧ **Collected a total of 400 TB data for 11 time steps**

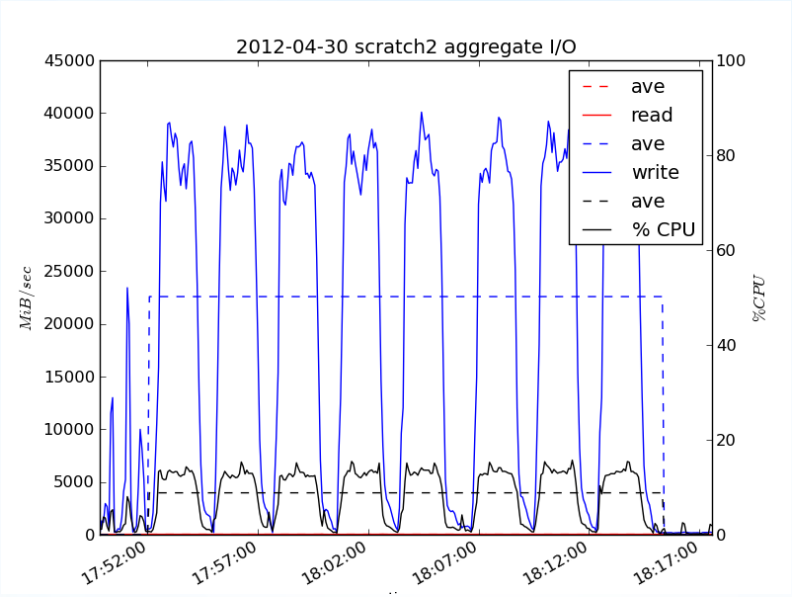
Data Challenges

- What is a scalable I/O strategy for storing massive particle data output?
  - In situ analysis works well when analysis tasks are known *a priori*
  - Many scientific applications require to store data for exploratory analysis
- What is a scalable strategy for conducting analysis on these datasets?
  - Sift through large amounts of data looking for useful information
- What is the visualization strategy for examining the datasets?
  - Display information that makes sense

Our Tools and Techniques

- Scalable I/O strategy for storing particle data
  - H5Part: A simple API on top of HDF5 to read/write particle data
  - Search for Lustre striping optimizations
- Scalable strategy for conducting analysis on these datasets
  - FastBit: Bitmap index generation and querying software
  - Hybrid Parallel FastQuery
    - ✓ API to generate bitmap indexes
    - ✓ API to query indexed or data from different data formats (HDF5, NetCDF, and ADIOS-BP)
- Visualization strategy for examining the datasets
  - Query-driven visualization using VisIt

Performance of Writing and analyzing

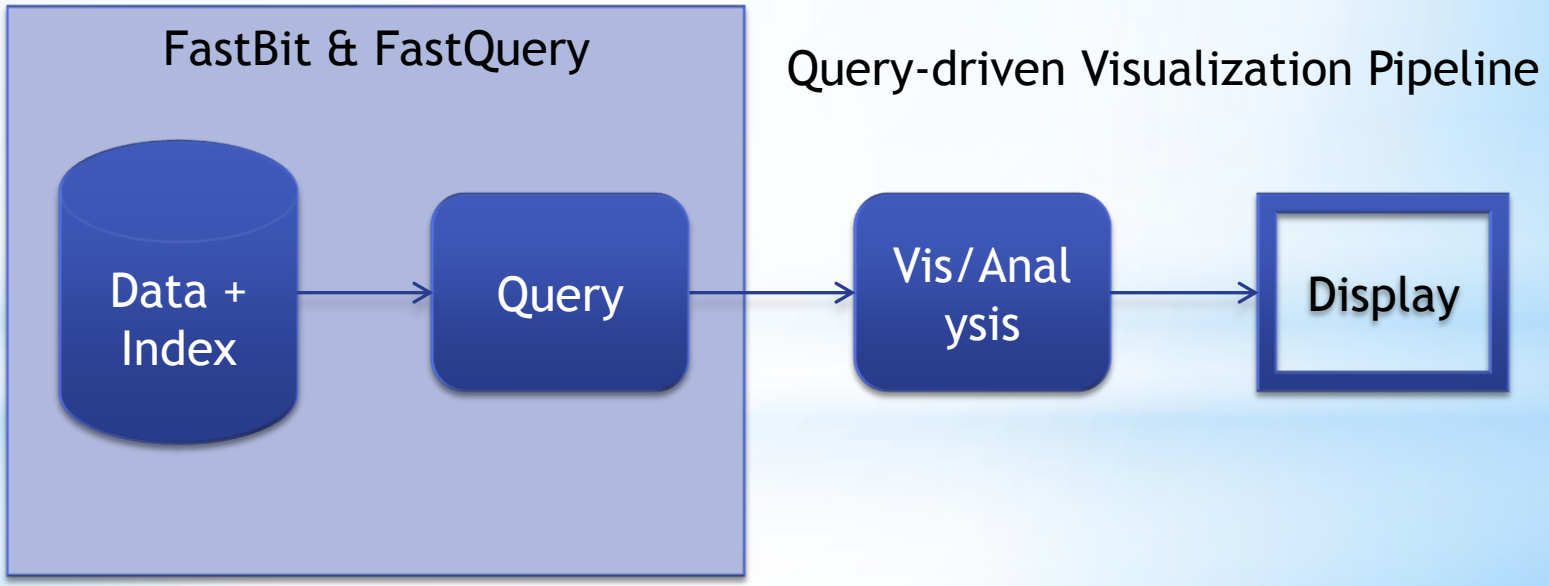


- Reached I/O peak rate in writing each variable
- Amortized I/O rate of 26 GB/s on the Lustre parallel file system with 35 GB/s peak bandwidth

  - 10 minutes to index 30TB data and 3 seconds to query highly energy particles with FastQuery

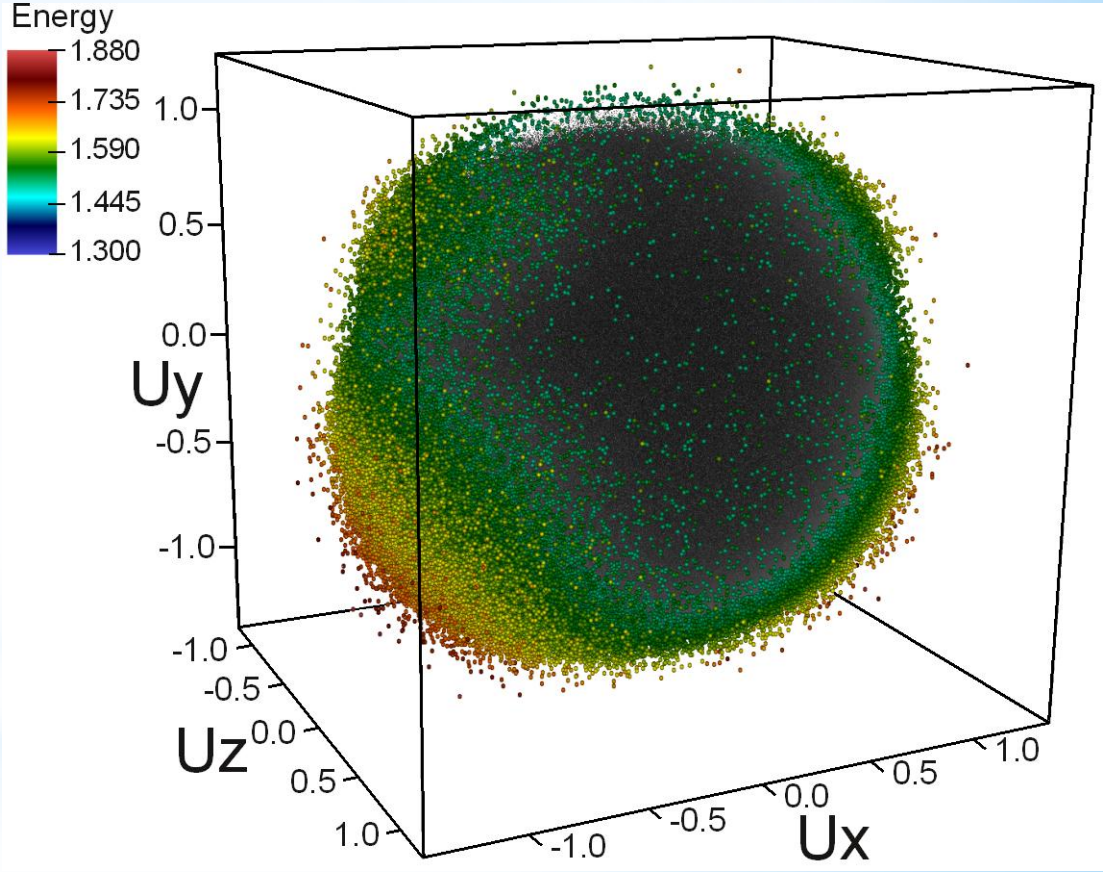
Query-driven Visualization

- Reduced the number of particles before rendering by down-selecting the scientifically interesting features
  - Highly energetic particles in this case
- New feature: Cross-Mesh Field Evaluation (CMFE)
  - Correlate particle data with the underlying magnetic field data



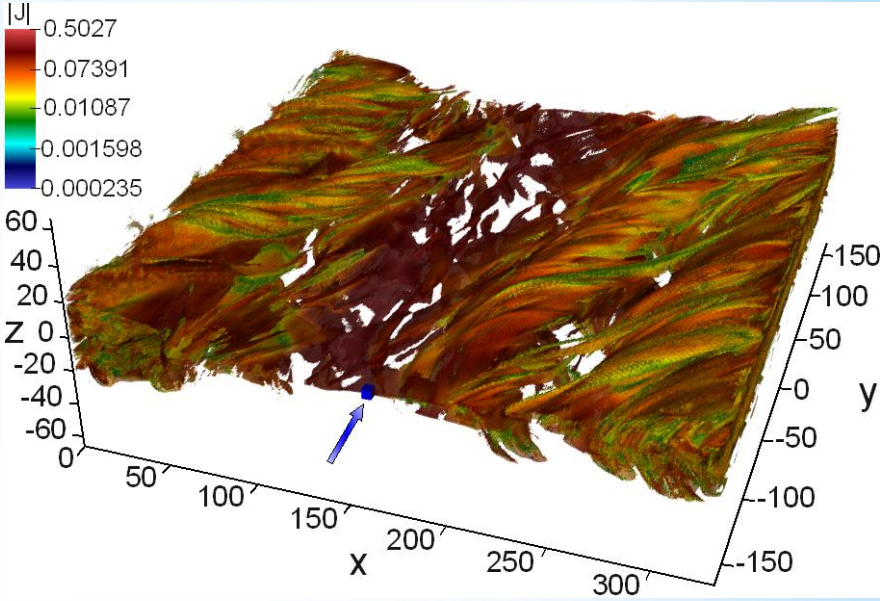
Query-driven Visualization

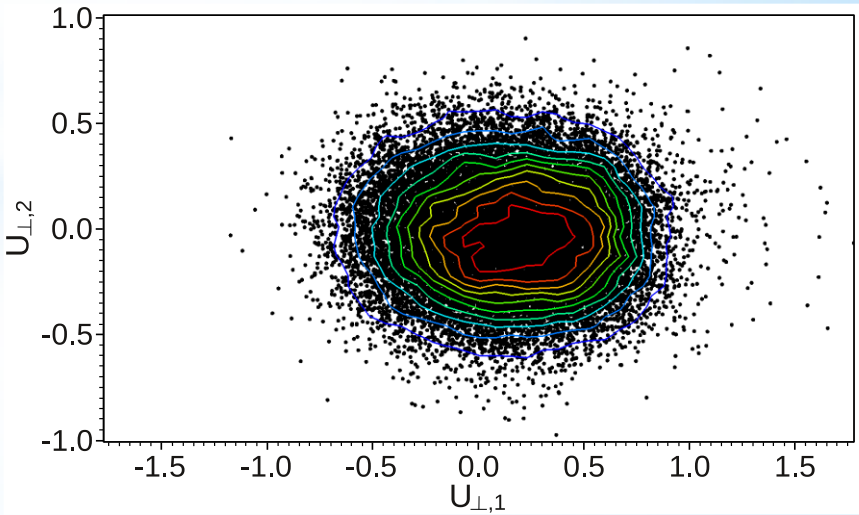
- Showing all the particles with ‘Energy > 1.3’ in gray and those with ‘Energy > 1.5’ in color
- 164million particles with Energy > 1.3 and 424,000 particles with Energy > 1.5



A science principle visualized for the first time

- The X-line, where magnetic reconnection happens
- Particle distribution of Uperp1 vs. Uperp2 in the vicinity of X-line
- The lack of cylindrical symmetry about the local magnetic field, called Agyrotropy
- This confirms the expected signature of the reconnection site in collisionless plasma





Conclusions

- Addressed the data management and analysis challenges posed by a highly scalable plasma physics simulation
  - Storage: 26 GB/s
  - Indexing: 10 minutes to index 30TB data file
  - Querying: ~3 seconds
- Demonstrated that exploratory analysis can handle challenges posed by large data
- Using query-driven visualization approach, application scientists explored and gained insights from massive particle datasets for the first time
  - Several of the phenomena visualized in this study have been conjectured about, but the capabilities developed here can unlock the scientific insights in unprecedented data volume

Thanks!

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