Scalable Analysis Methods and In Situ Infrastructure for Extreme Scale Knowledge Discovery (LAB 14-1043)

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Project Overview

- Aims at set of research challenges in enabling scientific knowledge discovery within context of *in situ* processing at extreme-scale concurrency.
- Motivated by widening gap between FLOPS and I/O capacity.
- Focuses on new algorithms for analysis and visualization suitable for *in situ* use aimed at scientific knowledge discovery in several application areas of interest to DOE.
- Includes efforts on several leading *in situ* infrastructures, tackling research questions germane to new algorithms at scale across diversity of existing *in situ* implementations.
- Move the field of *in situ* processing to write an algorithm once and have it execute in one of several different *in situ* software implementations.

Problem Statement

- Lost science, due to widening gap between our ability to compute and save data.
- As a relatively new idea, want to promote production quality *in situ* infrastructure suitable for use at extreme-scale.
- In many cases, data analysis and visualization (DAV) algorithms need to be completely redesigned for use *in situ*.

Approach

- Algorithmic R&D for in situ DAV algorithms.
  - Design pattern abstraction of in situ DAV algorithms over various in situ execution models
- Move towards cross-infrastructure portability by normalizing access to resources and infrastructures
- Scalability and optimization for use at extreme scale and on emerging architectures.
- Direct interactions with science stakeholders and broad community engagement.

Anticipated Outcomes

- Enable new science through combination of innovative *in situ* DAV algorithms and multiple, robust *in situ* infrastructures.
- Demonstrate extreme-concurrency *in situ* capability on major DOE platforms.
- Increase lifespan of investments in *in situ* algorithmic and infrastructure R&D.

Project Participants

- Team includes representatives from the four major in situ infrastructures:
- Algorithmic R&D for in situ DAV algorithms.
  - ADIOS, Glean, ParaView/Catalyst, VisIt/Libsim
- Mixture of lab (ANL, LBNL), university (GT), and industry (Kitware, Intelligent Light)
- Science partners/collaborators: climate, materials, combustion, plasma physics, fusion

Acknowledgements

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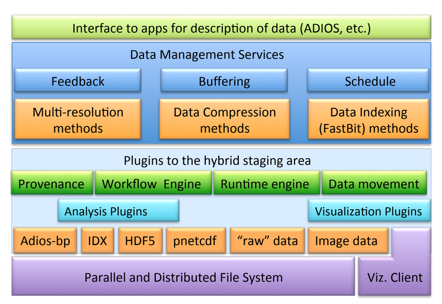
ADIOS

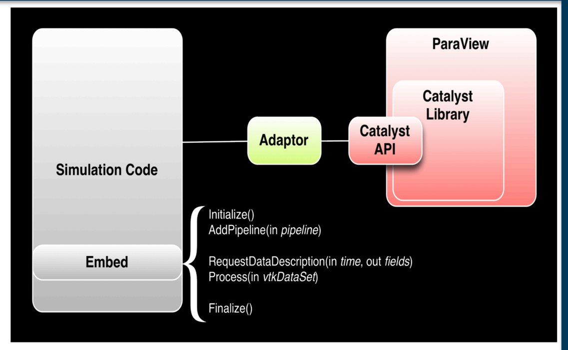
- An HPC I/O framework
  - abstracting Data-at-Rest and Data-in-Motion for High End Computing
- Similar software philosophy as Linux: there is no single owner
- Provides portable, fast, scalable, easy-to-use, metadata rich output
- Dynamically change I/O methods, even during an experiment/ simulation
- Provides multiple methods to stage data to a staging area (on node, off node, off machine)



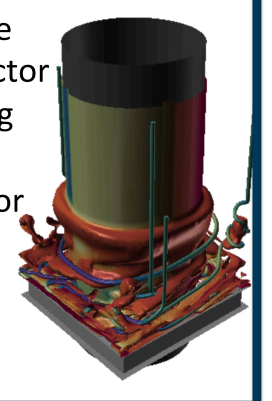
- Astrophysics
- Climate
- Combustion
- CFD
- Environmental Science
- Fusion
- Geoscience
- Materials Science
- Medical: Pathology
- Neutron Science
- Nuclear Science
- Quantum Turbulence
- Relativity
- Seismology
- Sub-surface modeling
- Weather

http://www.nccs.gov/user-support/center-projects/adios/

ParaView Catalyst



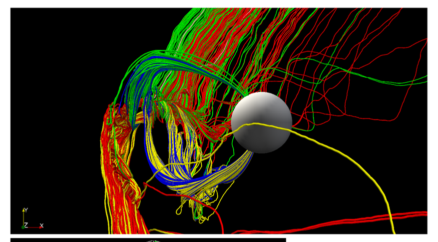
- Catalyst is a light-weight version of the ParaView server library that is designed to be directly embedded into parallel simulation codes to perform in situ analysis and visualization.
- Access to More/Richer Data
- Demonstrated scaling to 64K cores
- Codes: PHASTA, H3D, CTH, Rage, Hydra, Albany, MPAS-O, CAM5 FD, …

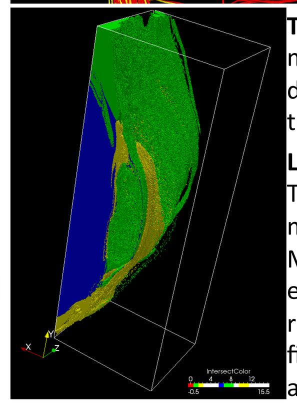


Flow around a single pin in a nuclear reactor core simulated using Hydra-TH with ParaView Catalyst for *in situ* analysis and visualization (image by P. O'Leary)

Science Story: Global Magnetospheric Simulations

Problem: Poor temporal resolution is primary obstacle in understanding magnetic reconnection related phenomena. *Post hoc* analysis results in (i) prohibitive I/O costs; (ii) "missing important science" since not all time steps are available (iii) poor time resolution limits tracking and analysis of dynamics.
Approach: Reduce the I/O costs by Identifying the magnetosphere, and applying feature detection algorithms insitu. Compact representations will be generated greatly increasing the temporal resolution while staying within physical I/O constraints
Results and Impact: Enables high resolution analysis of evolution and dynamics of the magnetosphere and features such as magnetic reconnection, flux transfer events, and Kelvin Helmholtz generated events.

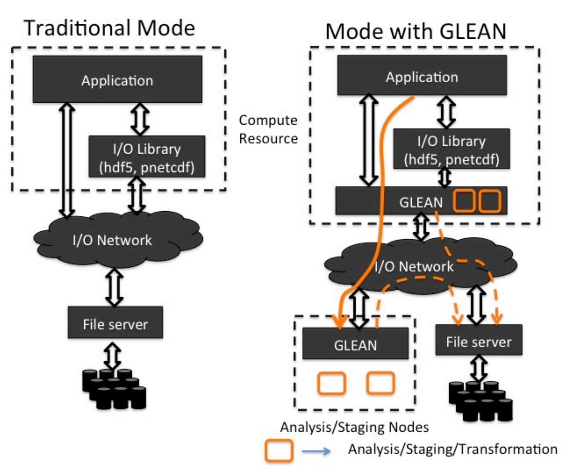




Top: Twisted magnetic fields during an flux transfer event.
Left: Topological map. The Magnetosphere is blue while reconnecting fields are green and yellow.

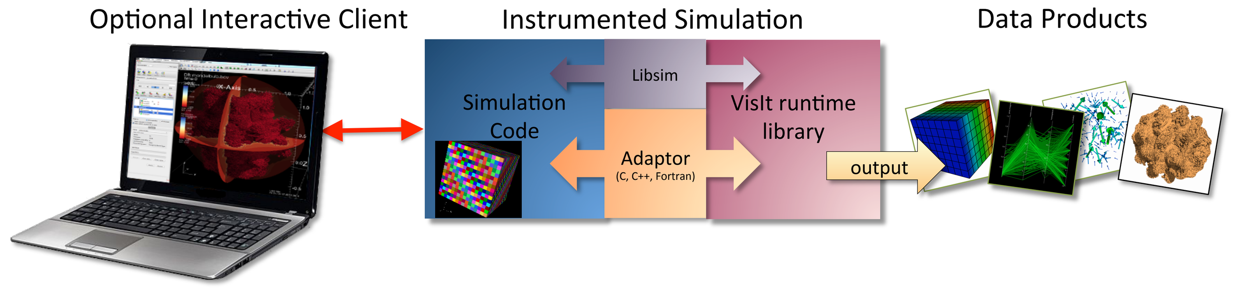
GLEAN

- Provides the functionality to enable in situ, in transit, and hybrid combinations of these to enable analysis at the right place and time
- Leverages data models of applications including adaptive mesh refinement grids and unstructured meshes
- Non-intrusive integration with applications using library interposition
- Scaled to 768K cores of the ALCF2 Infrastructure and demonstrated with FLASH, PHASTA, and HACC



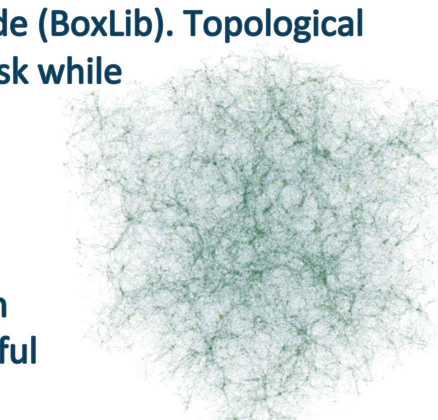
VisIt Libsim

- Libsim is a lightweight library that enables simulations to dynamically load VisIt's runtime library, which performs data analysis and visualization in situ using data directly from the simulation. VisIt runtime library has scaled to 98K cores.
- Libsim supports interactive and batch-only operation.
- Codes: Ale3D, Mercury, Kull, Nek5000, Kestrel, FUN3D,…



Science Story: Cosmology (Nyx)

Problem: *Post hoc* halo finding in cosmology simulations, i.e, identifying stars, galaxies, etc. : (i) Results not available to influence physical simulation model; (ii) "Miss important science" in time steps not available for analysis.
Approach: *In situ* halo finding in Nyx (BoxLib) code (BoxLib). Topological methods save reduced data representation to disk while supporting interactive exploration by changing parameters after simulation run. Use identified halos to set simulation boundary conditions or change physics model.
Results and Impact: Enable use of halo detection results within simulation, necessary for meaningful simulations. Support analysis on greatly reduced data representation. Avoid "missing important events/science."



Volume rendered density distribution in cosmological simulation. Halos are regions of locally higher density

Tech objectives/plans:

Characterize and abstract the parallel algorithmic patterns, implementation patterns, and in situ executions patterns of *in situ* analyses for various science applications

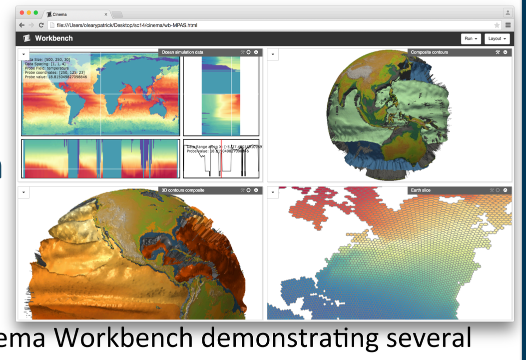
Science Application (Code)	Analysis Operation/Stage	Parallel Algorithmic Patterns	Implementation Patterns	Execution Patterns
Materials (LAMMPS)	**Stage 1**: Projection onto grid	Task parallelism (some dependency between tasks, e.g., distributing particles to proper voxels)	BSP	*In situ*
	Stage 2: Isosurfaces	Data parallelism (Marching cubes)	SPMD	Likely *in situ*
	Stage 3: Spectral computation (FFT)	Geometric decomposition, communication intensive	BSP	In transit
Cosmology (Nyx): Halos Materials (Chombo): Carbon sequestration, possibly batteries Local-global topological descriptor computation	**Stage 1:** Compute local descriptor on each grid	Task parallelism, no communication necessary	BSP	Depends on descriptor: Merge Tree (MT): *In situ;* Reeb graph: in transit *or in situ;* Time-varying MT/Reeb spaces*: in transit*
	Stage 2: Compute global-local representation of topological descriptor	Task parallelism, communication intensive	BSP	Depends: MT: *in situ, possibly in transit, RG: in transit* *Time-varying:* in transit
	Stage 3: Perform analysis operation based on topological descriptor	Task parallelism, minimal to moderate communication	BSP	(same as above)

Cross infrastructure portability by normalizing the access to data and system resources

Science Application (Code)	Simulation View	In Situ Infrastructure View		Analysis View
Materials (LAMMPS)	Particles data with interleaved Variables	ADIOS	Groups of 2D and 1D arrays	Polymers Structures: Projection of particles on a 3D grid Thresholding: De-interleaved variables
		Catalyst	vtkUnstructuredGrid	
		GLEAN	Multidimensional arrays with interleaved variables	
		Libsim	Point mesh/ vtkPolyData	

Science Story: Climate (ACME)

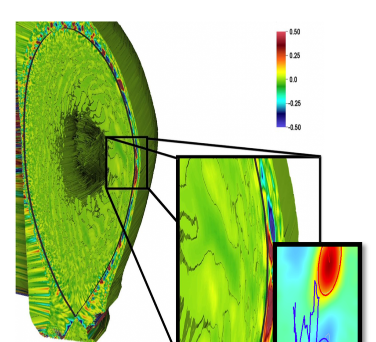
Problem: Achieve optimal performance for production of Community Earth System Model (CESM) diagnostics (analysis and visualization) at DOE Leadership Class Facility Computers scale.
Approach: Implement *in situ* frameworks for CAM-SE and MPAS-O simulation codes. Explore down-sampling techniques and statistical analyses to enable exploration and discovery of LCF-simulations.
Results and Impact: Enable climatologist to produce scalable diagnostics within MPAS-O and CAM-FD. Down-sampling techniques with ParaView Cinema significantly reduce data while preserving important simulation elements and offer as much flexibility as possible for post-processing exploration.



Cinema Workbench demonstrating several approaches for exploration visualization of *in situ* produced MPAS-O data products.

Science Story: Fusion

Problem: Identify transient features known as blobs that could cause disruption of confinement of fusion plasma.
Approach: Perform in situ feature extraction and in transit analysis to reduce overall analysis time.
Results and Impacts: Developed a feature extraction algorithm based on an outlier detection approach; demonstrated the viability of such an approach at SC'14 conference. Enable scientists to accelerate the detection of spatio-temporal features in streaming data that can be described with conjunctive or disjunctive range predicate style conditions.

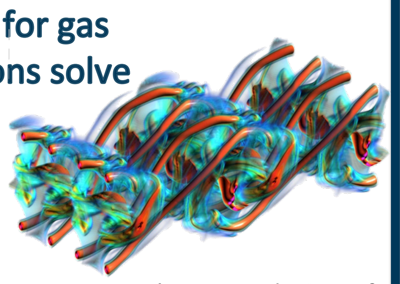


Blobs in fusion reaction (source: EPSI project)

Blob trajectory

Science Story: Turbulent Mixing and Combustion

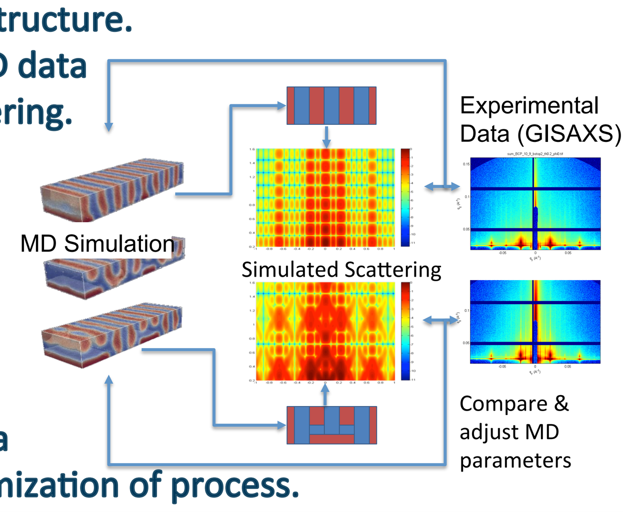
Problem: The LESLIE3D code is used in design studies for gas turbine combustors and rocket engines. The simulations solve large eddy simulations of complete real geometry with chemistry and Lagrangian droplets for liquid to gas phase changes and combustion.
Approach: Implement in situ including in transit methods, use feature detection methodologies to automatically explore salient flow features such as flame fronts and turbulent vortex cores.
Results and Impact: Enable scientists and engineers to more readily analyze the effect of system design variations such as mixer shapes and system pressures resulting in increased throughput of the total number of simulations achievable for any given design study.



Volume rendering of the vorticity field from a temporally mixing jet simulation from LESLIE3D. Hot colors (red) represent high regions of vorticity, cool colors (light blue) are low regions of vorticity

Science Story: 3D Structure of Block Co-Polymers

Problem: Determine 3D structure of block co-polymers. Scattering data will provide insight but analysis tools need to be developed to interpret the experimental data (detector images). *In situ* approach will enable on-the-fly analysis to study the evolution of 3D structure.
Approach: Develop methods to use 3D data from MD simulation to simulate scattering. Compare with experimental data. Iterate to modify parameters until scattering patterns match.
Results and Impact: Enable scientists to study 3D structure as a function of materials and processing parameters. Methods for analysis of scattering data useful for other users of GISAXS. Optimization of process.



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