Exploring fusion science with SDAV’s technologies

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**Gyro-Particle Simulations**

XGC, GTS, GTC-P

Large-scale I/O with ADIOS

Objectives:
- Fast, adaptable, and scalable I/O codes across all platforms
- Unified I/O framework to hide I/O complexity from users and manage individual I/O methods. Framework handles both file and stream processing.
- Non-contiguous parallel file format, highly scalable and resilient for large scale simulations.
- Support streaming methods: DataSpaces, DiMES, Flexpath

Impact:
- E.g., XGC-1, 200k cores on Jaguar, 2TB checkpoint data to write: original parallel I/O >1 hour, ADIOS ~1 min.
- Resilient for large scale simulations.
- Example: XGC-1, 200k cores on Jaguar, 2TB checkpoint data to write: original parallel I/O >1 hour, ADIOS ~1 min.
- Code coupling with memory-to-memory data transfers & in situ visualization using staging methods (see other columns)

**Energetic Particles**

GTC, M3D-K

FastQuery: Finding Regions of Interest with Complex Mesh

Objective: locate regions of interest based on user specified range conditions.

Example: a regions of special interest in a fusion simulation data might be regions of space with extreme high electromagnetic potential. The illustration shows each connected region in GTC with a different color.

Impact: improves speed of locating spatial features hundreds of times

**Scibox: Online Sharing of Scientific Data via Cloud**

Objectives:
- A cloud-based write/read ADIOS method with data reduction
- Support partial object access in cloud
- Reduction functions are implemented using C-on-Demand, a dynamically-generated subset of C

Impact:
- Speed up sharing scientific data over the cloud.
- An order or magnitude faster read speed for analysis code of GTS output

**Magnetohydrodynamic codes**

M3D, Pixie3D, NIMROD, Siesta, VacField

Parallel vector field analysis in VisIt

Objectives:
- Enable scientists to understand the nature of velocity and magnetic fields in large scale simulations.
- Flexible, scalable framework for computing integral curves.
- Research algorithms for efficiently computing integral curves on large scale parallel computing platforms.

Impact:
- Production tools that provide scalable, parallel methods for computing integral curves which are the basis for fieldlines, streamlines, and pathlines.
- Multidisciplinary usage, e.g., astrophysics, fusion, radiation transport.
- Techniques deployed in VisIt and have become the foundation for building more complex analysis and visualization tools: Poincare plots and Finite Time Lyapunov Exponents (FTLE)

**Range Based Queries**

Objectives:
- Enable scientists to query large scale simulations to find "interesting" particles
- Develop a framework to utilize fast indexing schemes such as FastBit

Impact:
- Production tool in VisIt providing an interactive environment.
- Temporal range queries on multivariate data for finding correlations between variables.
- Multidisciplinary usage, e.g., biomass, fusion.

**Advanced Visualization Techniques for Fusion Data**

Objectives:
- High speed and high fidelity rendering design for visualizing 3D field data from tokamak simulations. (Left Image)
- Data decomposition techniques for addressing the complexity of data to study different aspects of the physics. (Right Image)

Impact:
- Enables scientists to better validate their simulations and to better communicate with others their data and findings.

A range query over 50 time steps for 500K particles in GTC using two variables, resulting in 8 particles with their paths shown. Color of particles is based on being passing (green) or trapped (red).
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**DataSpaces for In Situ / In Transit Data Staging and Analytics**

**Objectives:**
- Combine in-situ/in-transit data analytics execution to move the analytics closer to the data, reduce data movement costs, mitigate disk IO costs, and accelerate the data to insights process.

**DataSpaces**
- Semantically-specialized virtual shared space abstraction with geometry-based queries.
- Asynchronous coordination and interaction.
- In-situ/in-transit mapping, scheduling and execution

**Impact:**
- A novel scalable approach to effectively transform large-scale simulations data into insights.
- ADIOS/DataSpaces is a production tool providing scalable memory-to-memory data transfers
- Used in EPSI project for coupling fusion codes.

**FlexPath Messaging**

**Objectives:**
- Efficient execution of parallel I/O pipelines
- Data staging methods for running analytics and visualization
- Data streaming and the online QoS control of such data streams
- Aggressive use of source-based data reduction and filtering
- Convenient ways to carry out remote data visualization

**FlexPath**
- An event-based messaging middleware
- Active messaging provides a publish/subscribe paradigm
- Built on top of the EVPath event-based messaging layer
- C-on-Demand: users can create and deploy data conditioning plug-ins that can perform filtering and transformation operations on live data streams

**Impact:**
- Allows for decoupling of interacting components
- Ability to customize data streams
- Improved fault management
- Enable in situ analytics (histograms, sorting, range queries) for GTC and GTS.

**Data Compression**

**Objectives:**
- Robust and parallelizable compression library that improves over widely used classical wavelet transform.

**Impact:**
- Four-to-five times storage reduction on over 20 different datasets from applications (XGC, SSD, GTS, GroundWater, GCRM) with 0.99+ correlation and 0.01-normalized point-by-point error.

**Tight-coupling of Fusion Codes for Exascale Computing**

**Problem:**
- Goal is a mathematically tight kinetic-kinetic coupling in XGC, to extend the first-principles full-f simulation to experimental time scale

**Objectives:**
- Development on extreme scale in-memory data management, analysis, and visualization (as well as the state-of-the-art applied math) is desperately in need

**In transit Analysis and Visualization**

**Objectives:**
- Allow for concurrent analysis and visualization tasks
- Memory-to-memory transfers
- Asynchronous stepping (simulation is running free from analysis)

**Impact:**
- ADIOS/DataSpaces is a production tool that provides scalable memory-to-memory data transfers using file I/O
- Used for Pixie3D’s non-scalable analysis (PixPlot) and interactive visualization with ParaView

**Graph of data transfers**

1) Inter-node coupling data transfers (over networks) is minimized
2) Intra-node coupling data transfers can be performed using more efficient shared memory

**Locality-aware placement of coupled region processes on Cray XT5 12-cores using DataSpaces (IPDPS 2012)**