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Spreading a Rumor: The SciDAC2 Scientific Data Management Center for Enabling Technologies

(Please just call it the SDM Center)

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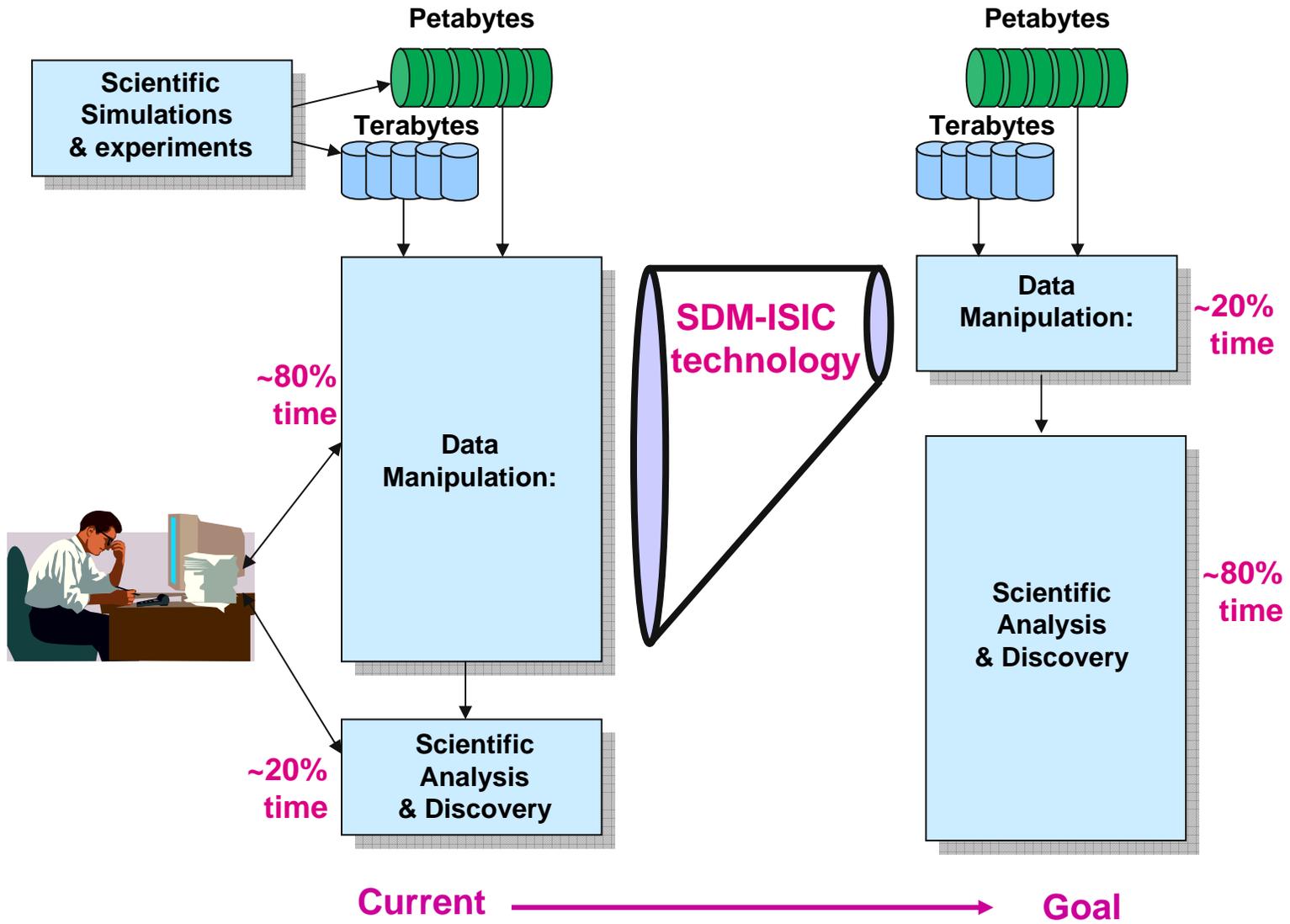
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What is SciDAC?

- Scientific Discovery through Advanced Computing
- Brings together application scientists and mathematicians and computer scientists to perform breakthrough science using the world's most powerful computing systems
(at least, that's my take on it)
- Application groups might include
 - Astrophysics, Fusion, High-Energy Physics, Climate, Biology, etc.
- Computer scientists and mathematicians might provide
 - Solvers, software component infrastructure, I/O tools, etc.

SDM Center: Reducing Data Management Overhead

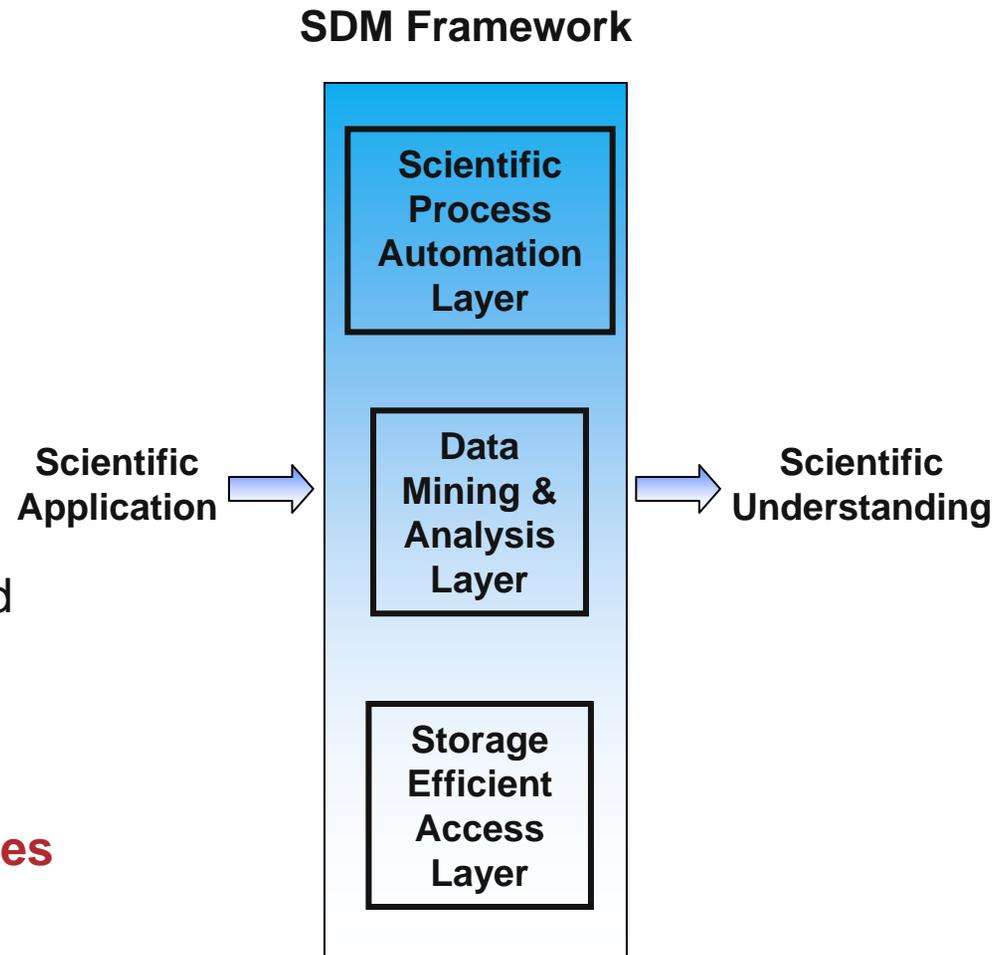


Participating Institutions

- Lawrence Berkeley National Laboratory
 - Arie Shoshani (PI), Doron Rotem
 - Argonne National Laboratory
 - Rob Ross, Bill Gropp, Rajeev Thakur
 - Lawrence Livermore National Laboratory
 - Terence Critchlow, Chandrika Kamath
 - Oak Ridge National Laboratory
 - Nagiza Samatova, Jeff Vetter
 - Pacific Northwest National Laboratory
 - Jarek Nieplocha
 - Northwestern University
 - Alok Choudhary
 - North Carolina State University
 - Mladen Vouk
 - University of Utah
 - Steve Parker
 - University of California at Davis
 - Bertram Ludaescher
 - San Diego Supercomputer Center
 - Ilkay Altinas
-
- Expertise in a wide range of I/O and data management technologies, from wide-area data movement, to data analytics, to automation of workflows, to I/O middleware and parallel file systems

Proposed Approach

- Use an integrated framework that:
 - Provides scientific workflow capabilities
 - Supports data analytics tools
 - Accelerates data storage and access
- Simplify data management tasks for the scientist
 - Hide details of underlying I/O and indexing technologies
 - Permit convenient assembly of workflows
- **Focus on leadership class machines and associated applications**



SDM Center Impact

Astrophysics:

High speed storage technology, parallel NetCDF, parallel VTK, and ASPECT integration software used for Terascale Supernova Initiative (TSI) and FLASH simulations

Tony Mezzacappa – ORNL, Mike Zingale – U of Chicago, Mike Papka – ANL

Scientific Workflow

John Blondin – NCSU

Doug Swesty, Eric Myra – Stony Brook

Climate:

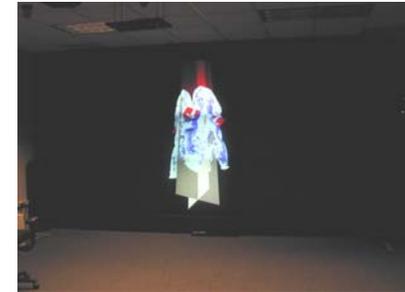
High speed storage technology, Parallel NetCDF, and ICA technology used for Climate Modeling projects

Ben Santer – LLNL, John Drake – ORNL, John Michalakes – NCAR

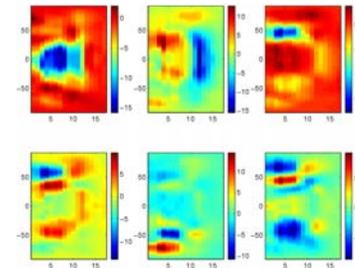
Combustion:

Compressed Bitmap Indexing used for fast generation of flame regions and tracking their progress over time

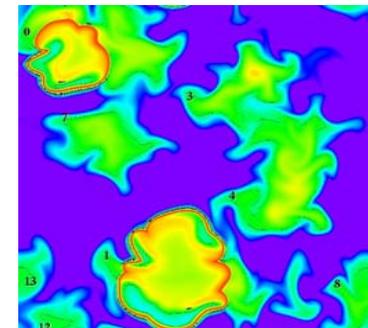
Wendy Koegler, Jacqueline Chen – Sandia Lab



ASCI FLASH – parallel NetCDF



Dimensionality reduction



Region growing

SDM Center Impact (cont'd)

Biology:

Kepler workflow system and web-wrapping technology used for executing complex highly repetitive workflow tasks for processing microarray data

Matt Coleman - LLNL

High Energy Physics:

Compressed Bitmap Indexing and Storage Resource Managers used for locating desired subsets of data (events) and automatically retrieving data from HPSS

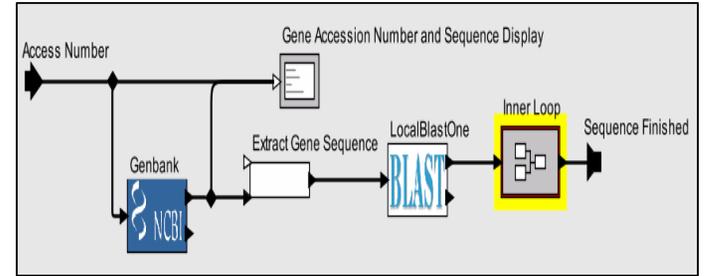
Doug Olson - LBNL, Eric Hjort – LBNL, Jerome Lauret - BNL

Fusion:

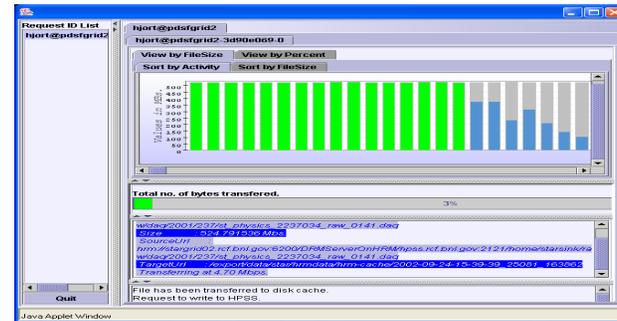
A combination of PCA and ICA technology used to identify the key parameters that are relevant to the presence of edge harmonic oscillations in a Tokamak

Keith Burrell - General Atomics

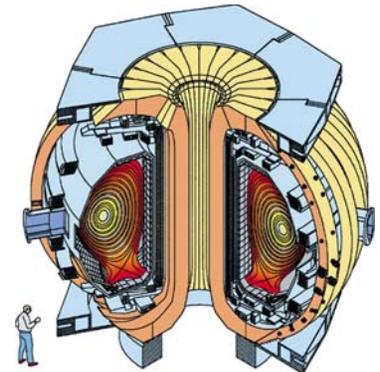
Scott Klasky - ORNL



Building a scientific workflow



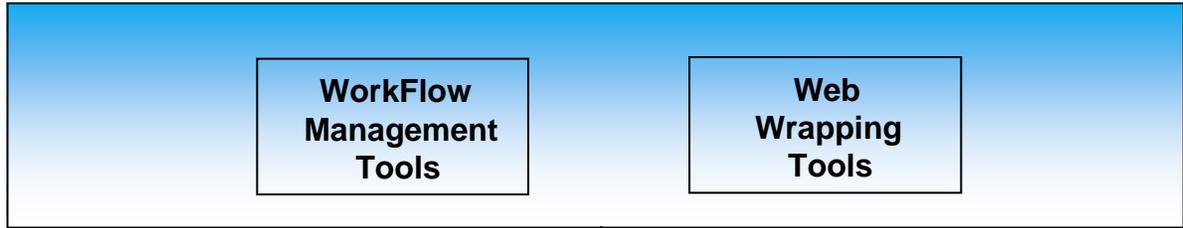
Dynamic monitoring of HPSS file transfers



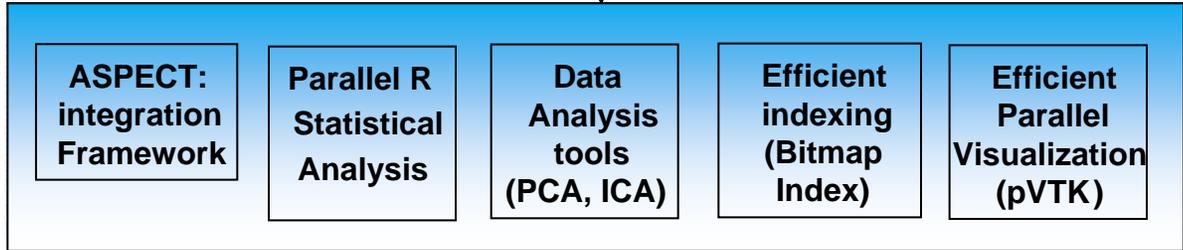
Identifying key parameters for the DIII-D Tokamak

Technology Details by Layer

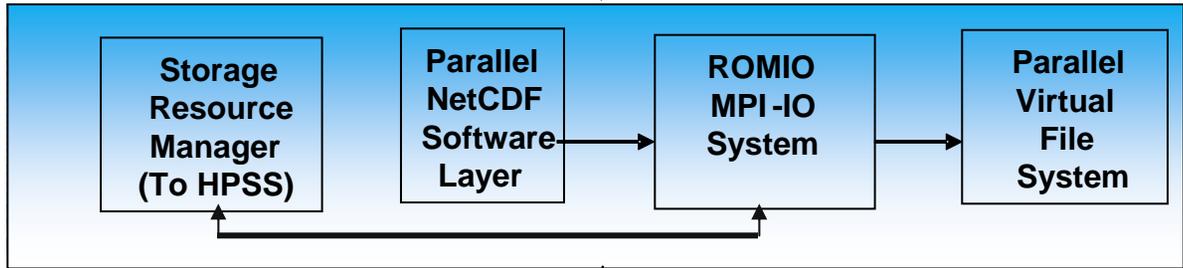
Scientific Process Automation (SPA) Layer



Data Mining and Analysis (DMA) Layer



Storage Efficient Access (SEA) Layer



SDM Storage Efficient Access (SEA) Layer



- This layer is the most relevant to the HECIWG IO and FS
- Break up I/O support into multiple layers with distinct roles:
 - **High level I/O library** maps app. abstractions to a structured, portable file format (e.g. HDF5, **Parallel netCDF**)
 - **Middleware layer** deals with organizing access by many processes (e.g. **MPI-IO**, UPC-IO)
 - **Parallel file system** maintains logical space, provides efficient access to data (e.g. **PVFS**, GPFS, **Lustre**)
- Argonne, Northwestern, LBNL, ORNL, and PNNL active in this layer

The SDM Center and You

- Stages in technology development
 - Research → Prototype → Product → Infrastructure
 - Technology starts off as research ideas
 - Technology becomes "infrastructure" when sites start installing it by default
 - *Happens when use in applications hits a certain critical mass*

- Primary role of SDM center: Prototype → Product
 - Apply technologies that have been prototyped
 - Fill gaps in I/O software stack on leadership class machines
 - Make application groups aware of these products and their uses

- SDM center might be helpful to HECURA I/O researchers by
 - Identifying critical needs on leadership class machines
 - *Possibly low-hanging fruit?*
 - Connecting you with SciDAC application groups with relevant I/O needs
 - *Your research might provide revolutionary capabilities*
 - Aiding in integration of prototypes into products
 - *Wider distribution of software often uncovers new challenges...*

SDM Center Contacts

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