Scientific Data Management Center

Presented by

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Co-Principal Investigators

DOE Laboratories

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LBNL: Doron Rotem
LLNL: Chandrika Kamath
ORNL: Nagiza Samatova
PNNL: Terence Critchlow
Jarek Nieplocha

Universities

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NWU: Alok Choudhary
UCD: Bertram Ludaescher
SDSC: Ilkay Altintas
UUtah: Steve Parker

SCIDAC

Office of Science
U.S. DEPARTMENT OF ENERGY

Scientific Data Management Center

Lead Institution: LBNL

PI: Arie Shoshani

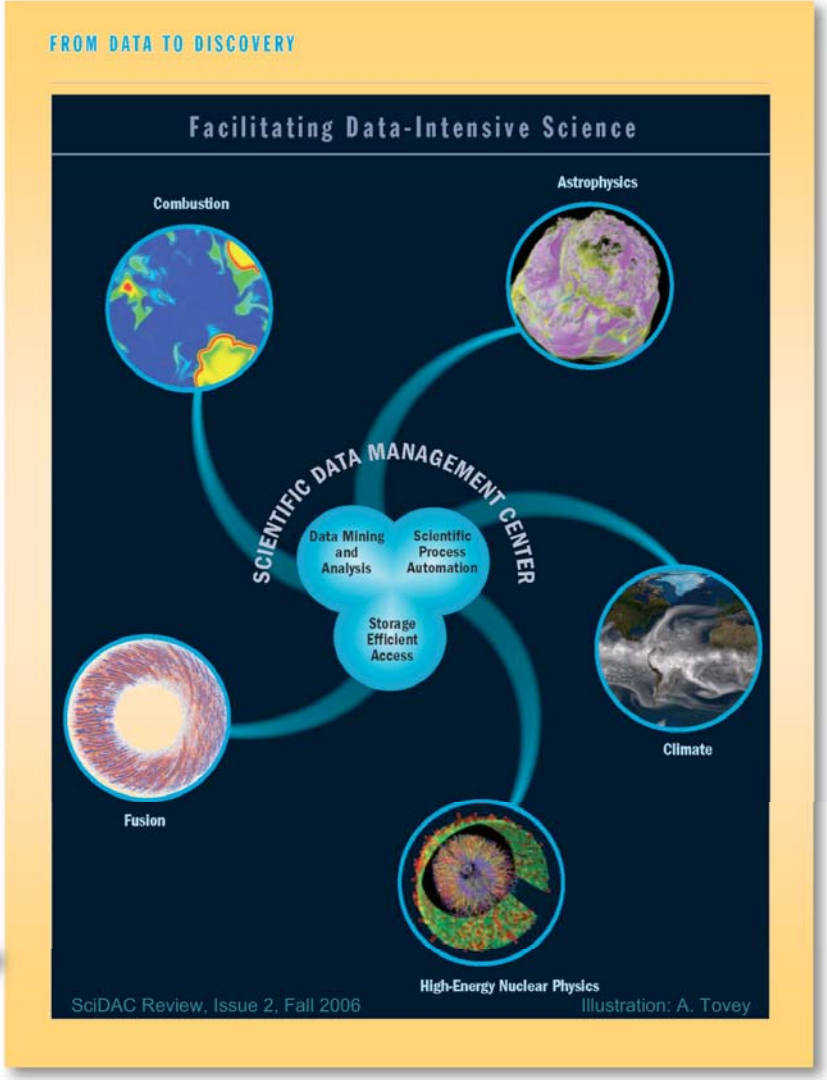
Laboratories:
ANL, ORNL, LBNL, LLNL, PNNL

Universities:
NCSU, NWU, SDSC, UCD, U. Utah

Established 5 years ago (SciDAC-1)

Successfully re-competed for next 5 years (SciDAC-2)

Featured in Fall 2006 issue of *SciDAC Review* magazine



SDM infrastructure
Uses three-layer organization of technologies

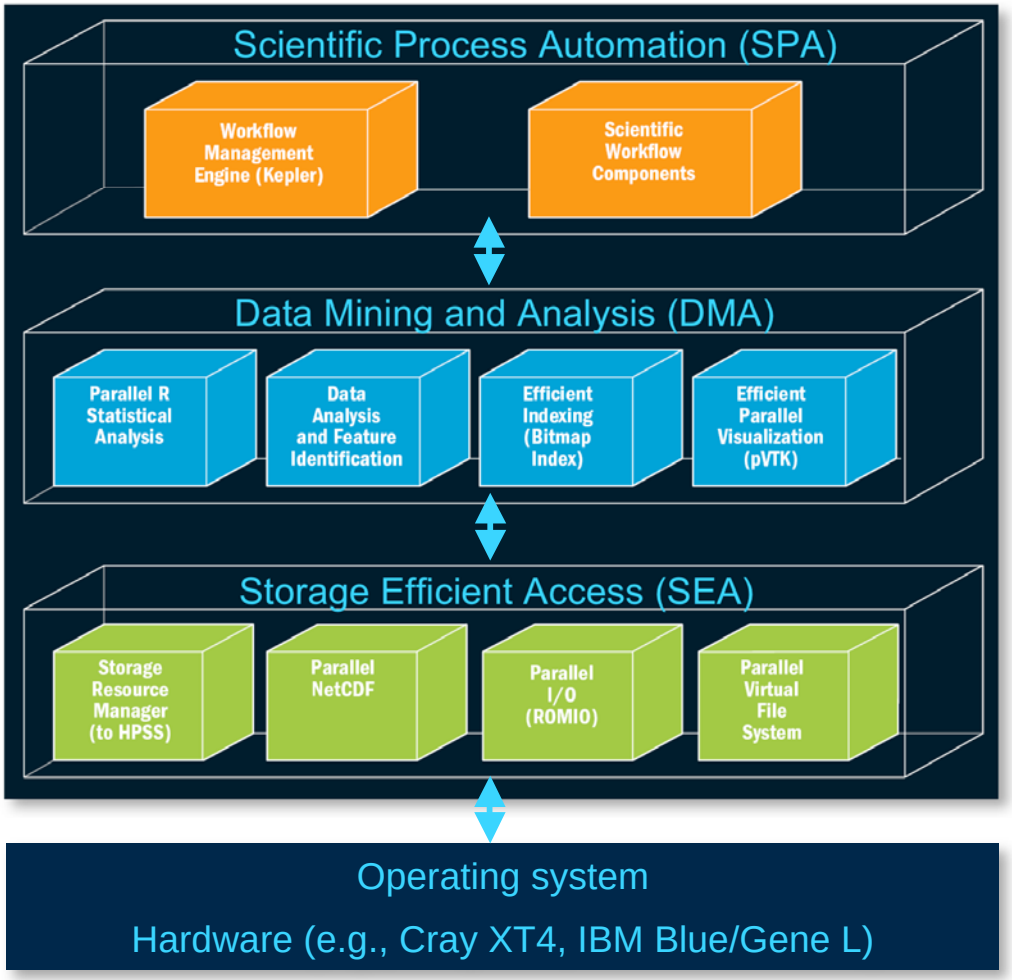
Goal: Reduce data management overhead

Integrated approach:

- To provide a scientific workflow capability
- To support data mining and analysis tools
- To accelerate storage and access to data

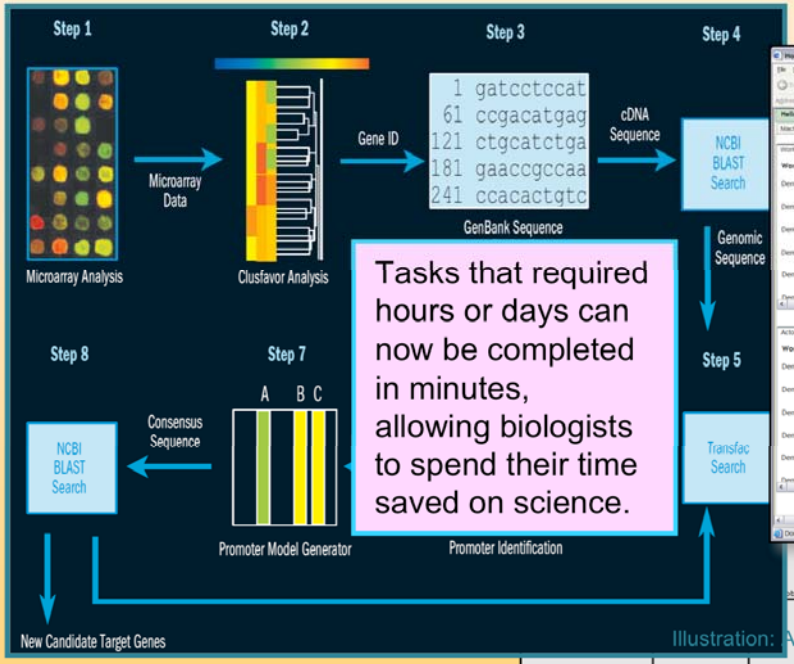
Benefits scientists by

- Hiding underlying parallel and indexing technology
- Permitting assembly of modules using workflow description tool

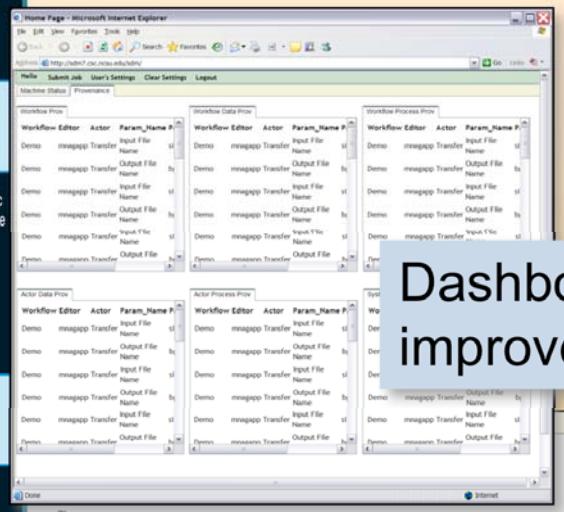


Automating scientific workflow in SPA
Enables scientists to focus on science not process

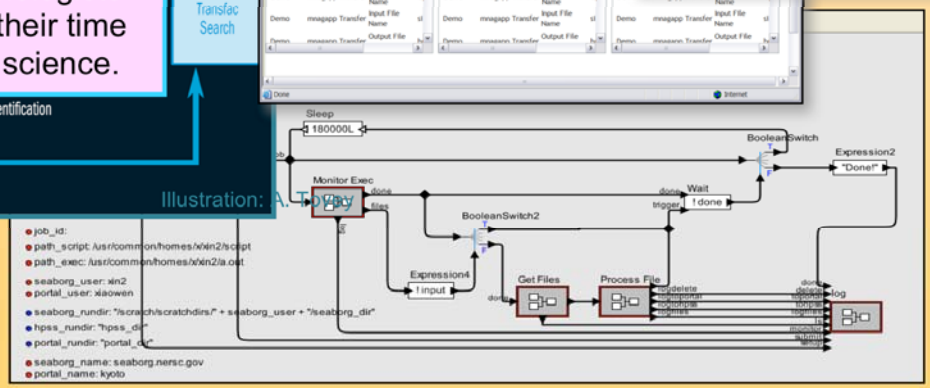
Scientific discovery is a multi-step process. SPA-Kepler workflow system automates and manages this process.



Tasks that required hours or days can now be completed in minutes, allowing biologists to spend their time saved on science.



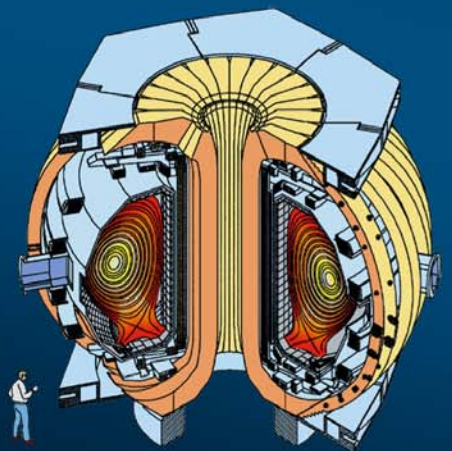
Dashboards provide improved interfaces.

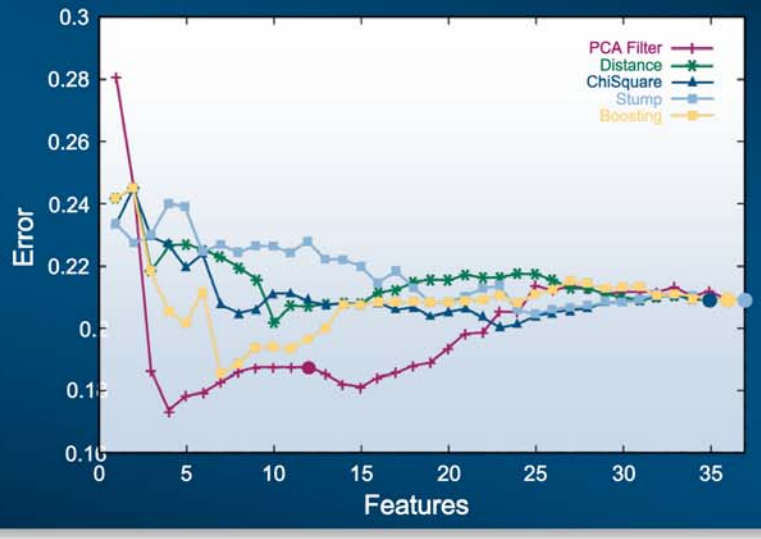


Execution monitoring (provenance) provides near real-time status.

Contact: Terence Critchlow, PNNL (critchlow1@pnl.gov)

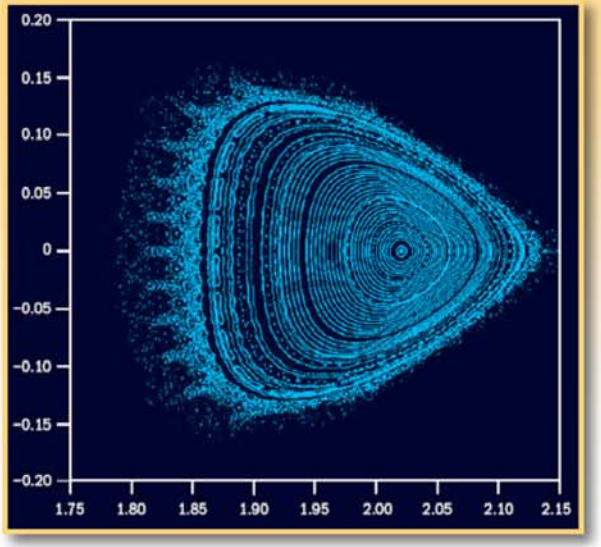
Data analysis for fusion plasma





Feature selection techniques used to identify key parameters relevant to the presence of edge harmonic oscillations in the DIII-D tokomak.

Plot of orbits in cross-section of a fusion experiment shows different types of orbits, including circle-like "quasi-periodic orbits" and "island orbits." Characterizing the topology of orbits is challenging, as experimental and simulation data are in the form of points rather than a continuous curve. We are successfully applying data mining techniques to this problem.



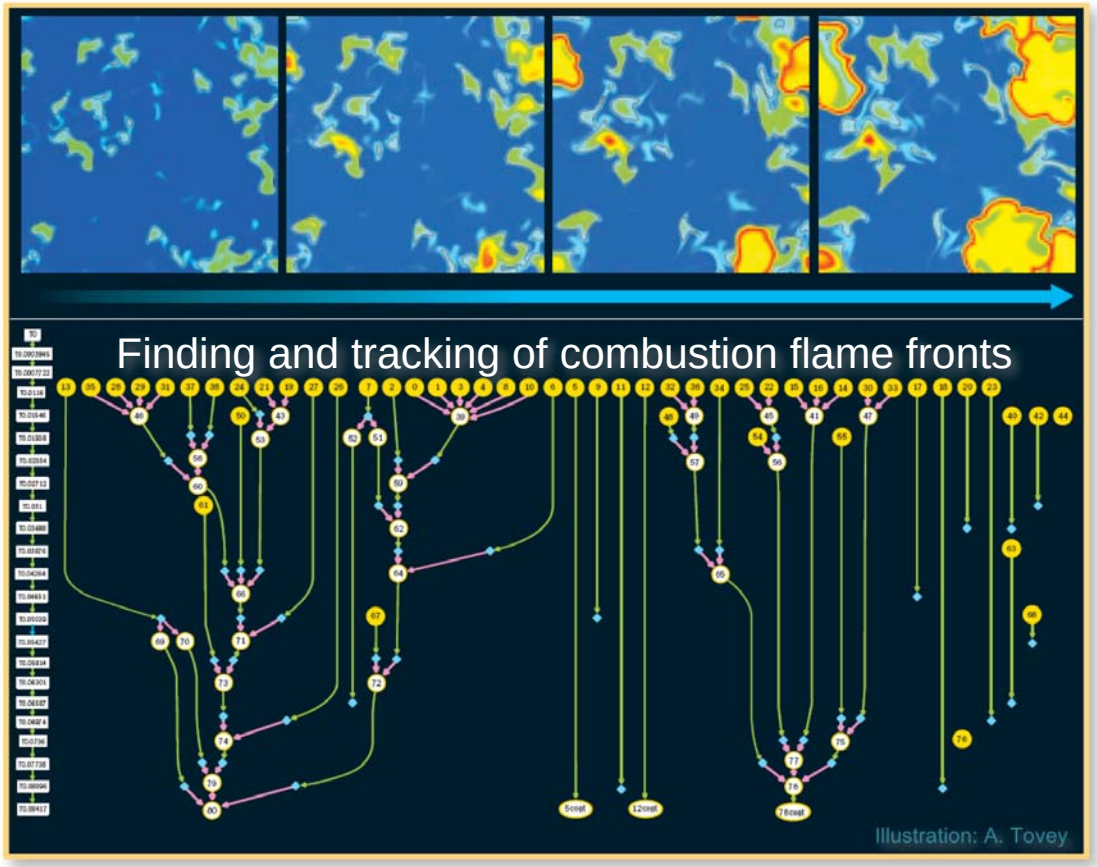
Contact: Chandrika Kamath, LLNL (kamath2@llnl.gov)

Searching and indexing with FastBit
Gleaning insights about combustion simulation

Searching for regions that satisfy particular criteria is a challenge. FastBit efficiently finds regions of interest.

About FastBit:

- Extremely fast search of large databases
- Outperforms commercial software
- Used by various applications: combustion, STAR, astrophysics visualization



Collaborators:

SNL: J. Chen, W. Doyle

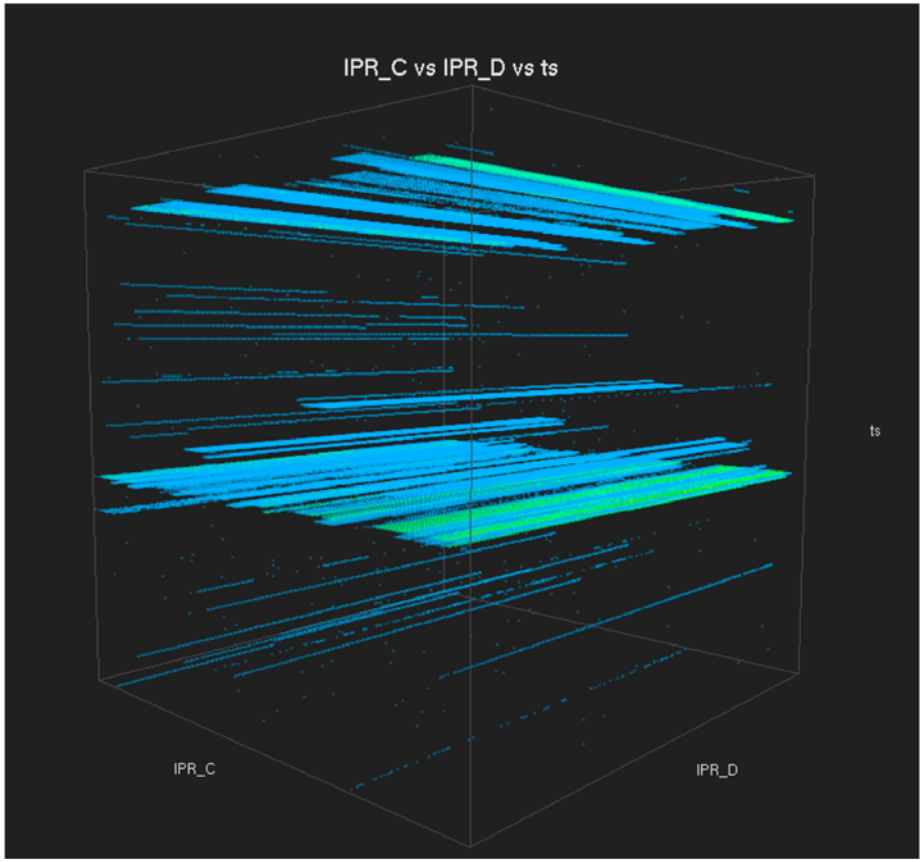
NCSU: T. Echekki

Contact: John Wu, LBNL (kwu@lbl.gov)

Data analysis based on dynamic histograms using FastBit

Conditional histograms are common in data analysis.
FastBit indexing facilitates real-time anomaly detection.

- Example of finding the number of malicious network connections in a particular time window.
- A histogram of number of connections to port 5554 of machine in LBNL IP address space (two-horizontal axes); vertical axis is time.
- Two sets of scans are visible as two sheets.



Contact: John Wu, LBNL (kwu@lbl.gov)

Parallel input/output
Scaling computational science

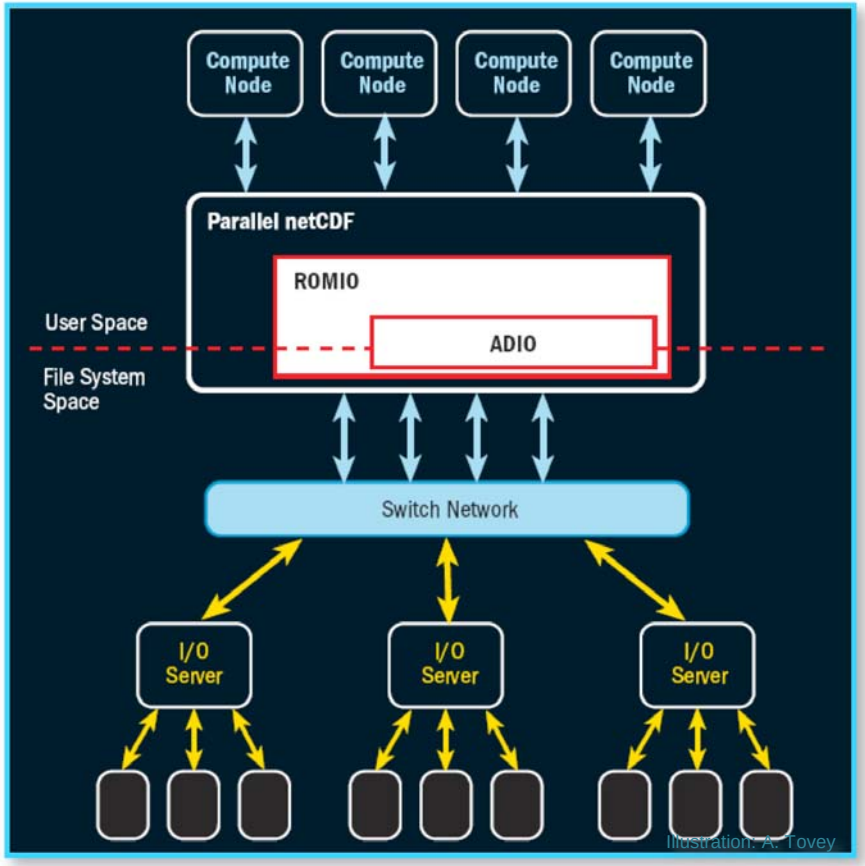
Orchestration of data transfers and speedy analyses depends on efficient systems for storage, access, and movement of data among modules.

Multi-layer parallel I/O design:

Supports Parallel-netCDF library built on top of MPI-IO implementation called ROMIO, built in turn on top of Abstract Device Interface for I/O system, used to access parallel storage system

Benefits to scientists:

- Brings performance, productivity, and portability
- Improves performance by order of magnitude
- Operates on any parallel file system (e.g. GPFS, PVFS, PanFS, Lustre)



Contact: Rob Ross, ANL (rross@mcs.anl.gov)

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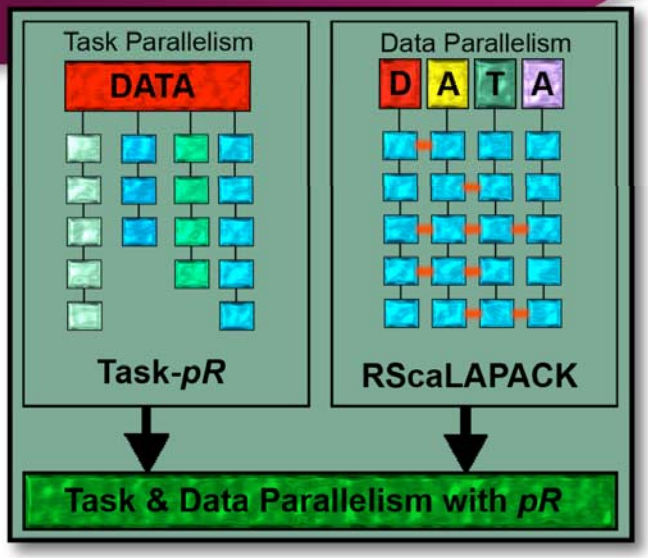
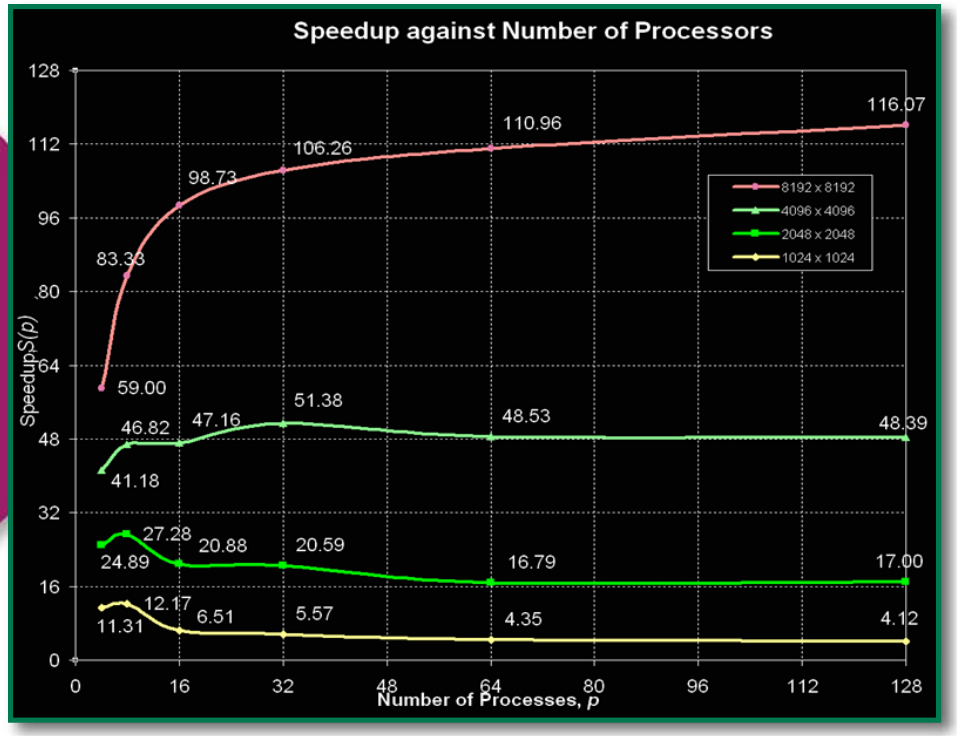
Parallel statistical computing with *pR*

Goal: Provide scalable high-performance statistical data analysis framework to help scientists perform interactive analyses of produced data to extract knowledge





- Able to use existing high-level (i.e., *R*) code
- Requires minimal effort for parallelizing
- Offers identical application and web interface
- Provides efficient and scalable performance
- Integrates with Kepler as front-end interface
- Enables sharing results with collaborators

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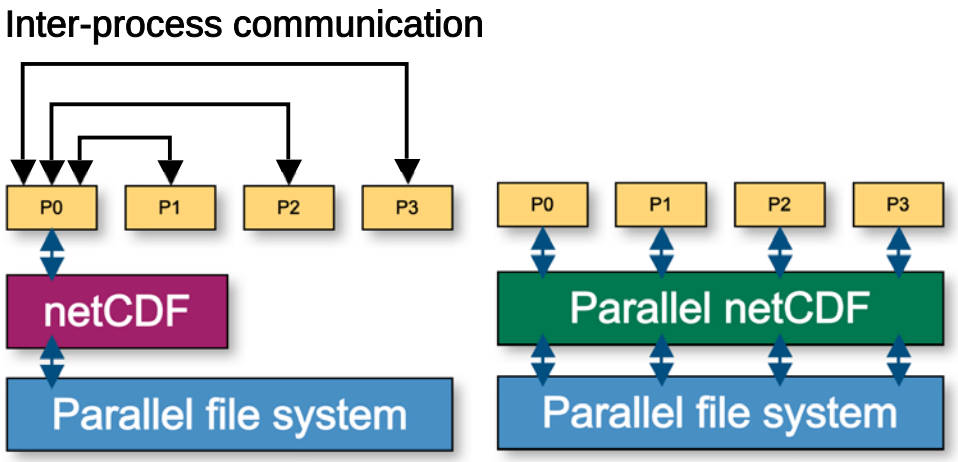
Speeding data transfer with PnetCDF

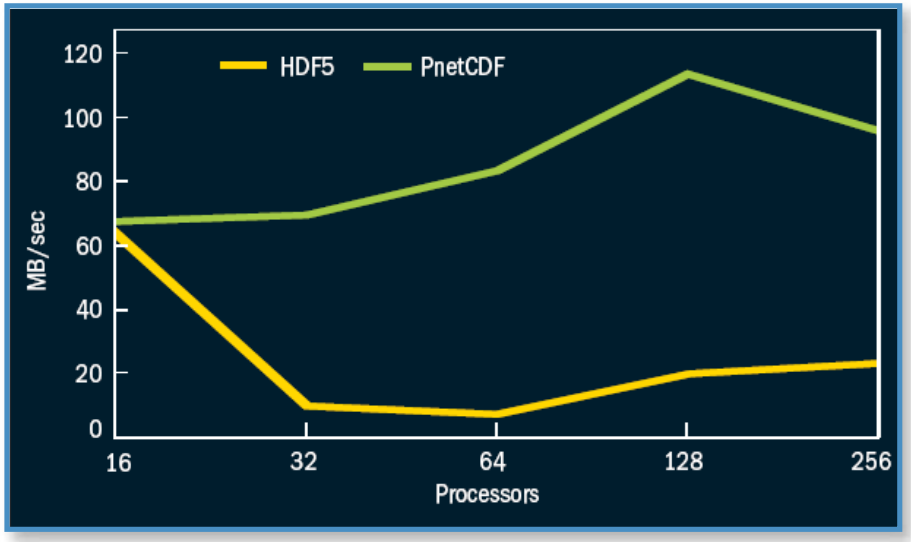


Enables high performance parallel I/O to netCDF data sets.

Achieves up to 10-fold performance improvement over HDF5.

Early performance testing showed PnetCDF outperformed HDF5 for some critical access patterns.

The HDF5 team has responded by improving its code for these patterns, and now these teams actively collaborate to better understand application needs and system characteristics, leading to I/O performance gains in both libraries.



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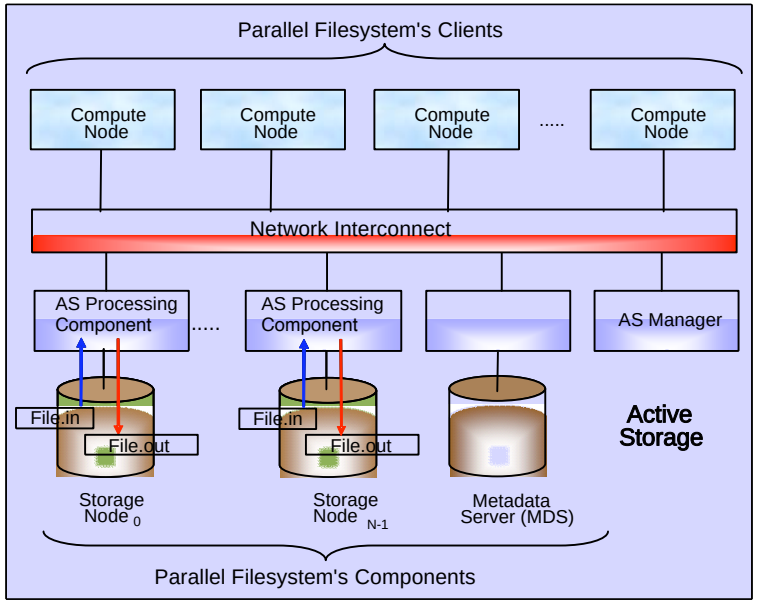
Active storage

- Modern filesystems such as GPFS, Lustre, PVFS2 use general purpose servers with substantial CPU and memory resources.
- Active Storage moves I/O-intensive tasks from the compute nodes to the storage nodes.
- Main benefits:
  - local I/O operations,
  - very low network traffic (mainly metadata-related),
  - better overall system performance.
- Active Storage has been ported to Lustre and PVFS2.



Active Storage enables scientific applications to exploit underutilized resources of storage nodes for computations involving data located in secondary storage.

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