End-to-End Computing at ORNL

Presented by

Scott A. Klasky

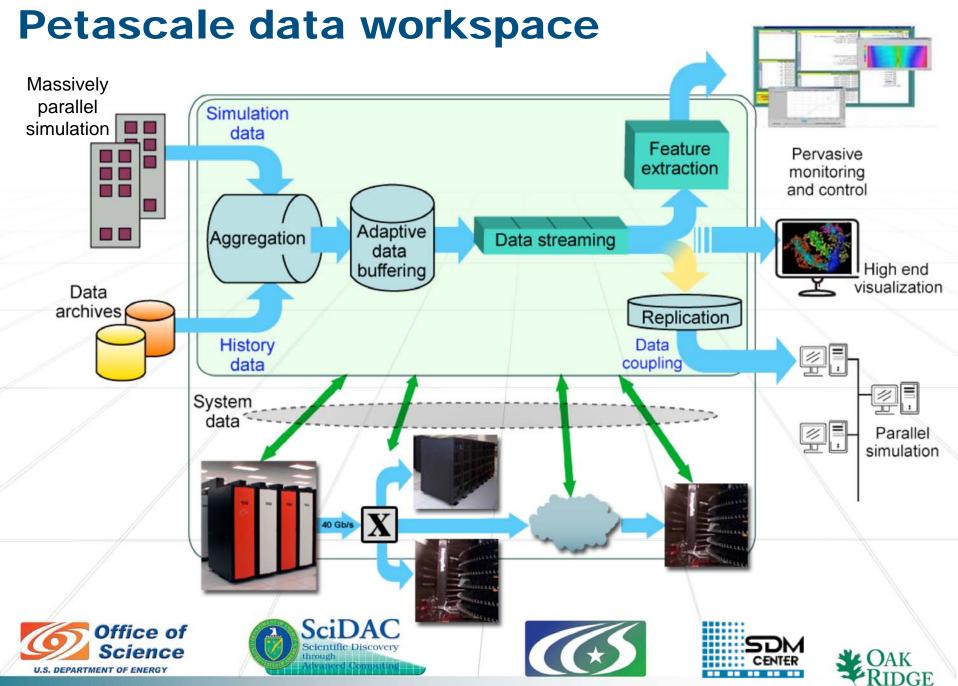
Scientific Computing National Center for Computational Sciences

In collaboration with

Caltech: J. Cummings Georgia Tech: K. Schwan, M. Wolf, H. Abbasi, G. Lofstead LBNL: A. Shoshani NCSU: M. Vouk, J. Ligon , P. Mouallem, M. Nagappan ORNL: R. Barreto, C. Jin, S. Hodson PPPL: S. Ethier Rutgers: M. Parashar, V. Bhat, C. Docan Utah: S. Parker, A. Kahn UC Davis: N. Podhorszki UTK: M. Beck, S. Sellers, Y. Ding Vanderbilt: M. DeVries

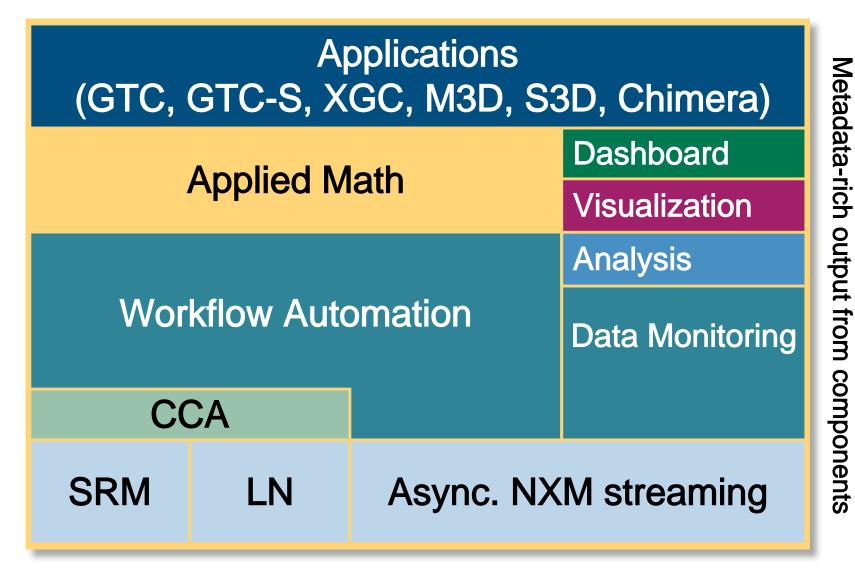






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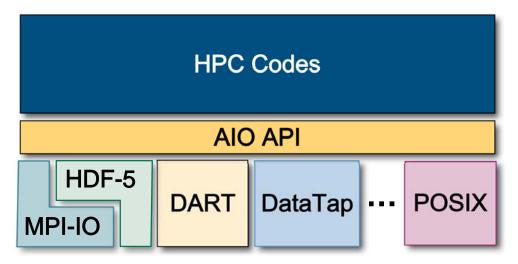
The End-to-End framework





Unified APIs for MPI/AIO (Lofstead)

- **Single**, **simplified API** capable of supporting various low-level implementations (MPI-IO, HDF5, POSIX, asynchronous methods)
- Transmits buffered data only during non-communication phases of HPC codes
- External XML configuration file describing data formats and the storage approach and parameters for each



- Implements best practices for underlying implementations
- Adds data tagging and annotation
- Enables complex inline processing with DataTap and DART (off compute node)
 - e.g., custom compression, filtering, transformation, multiple output organizations from single write, real-time analysis



Asynchronous I/O API usage example

XML configuration file:

<ioconfig>

<datatype name="restart">

<scalar name="mi" path="/param" type="integer"/>

... <!-- declare more data elements -->

<dataset name="zion" type="real"
 dimensions="nparam,4,mi"/>

<data-attribute name="units" path="/param" value="m/s"/>

</datatype>

... <!-- declare additional datatypes -->

<method priority="1" method="MPI" iterations="100" type="restart"/>

<method priority="2" method="PBIO" iterations="1" type="diagnosis">srv=ewok001.ccs.ornl.gov </method>

<!-- add more methods for other datatypes -->

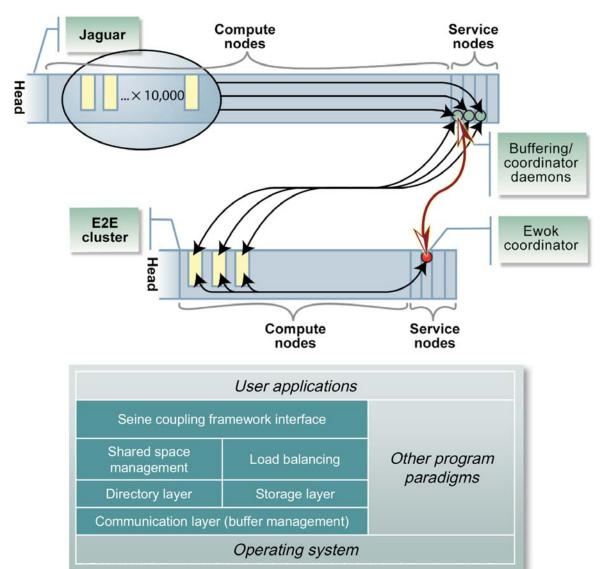
</ioconfig>

Fortran90 code:

! initialize the system loading the configuration file aio_init (100) ! 100 MB of buffer ! retrieve a declared type for writing aio_get_type (t1, "restart") ! open a write path for that type aio_open (h1, t1, "restart.n1") ! write the data items aio_write (h1, "mi", mi) aio_write (h1, "zion", zion) ... ! write more variables ! commit the writes for asynchronous transmission aio_close (h1) ... ! do more work ! shutdown the system at the end of my run aio_finalize ()



Asynchronous petascale I/O for data in transit

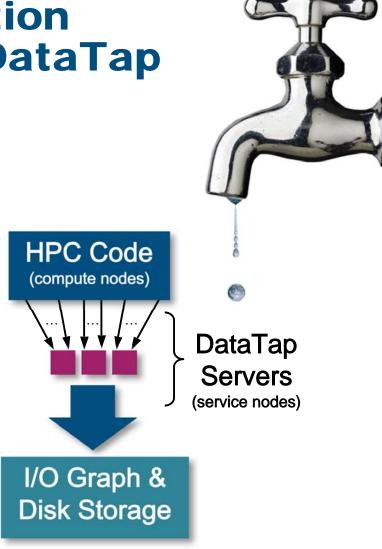


- High-performance I/O
 - Asynchronous
 - Managed buffers
 - Respect firewall constraints
- Enable dynamic control with flexible MxN operations
 - Transform using shared-space framework (Seine)



Lightweight data extraction and processing using a DataTap and I/O Graph

- Adding a DataTap to an HPC code reduces I/O overhead tremendously.
- Rather than writing directly, the client HPC code notifies the DataTap server to read data asynchronously when resources are available.
- The DataTap server scheduler manages data transfer to reduce I/O impact:
 - Guarantees available memory and egress bandwidth consumption does not exceed a user specified limit. Other considerations, such as CPU usage, are also possible.



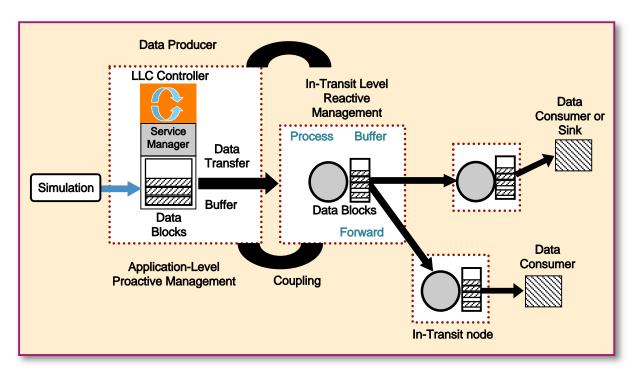
 The DataTap server is the gateway to I/O graph processing for storage to disk or additional processing--even on another cluster.



Data streaming and in-transit processing

Requirements

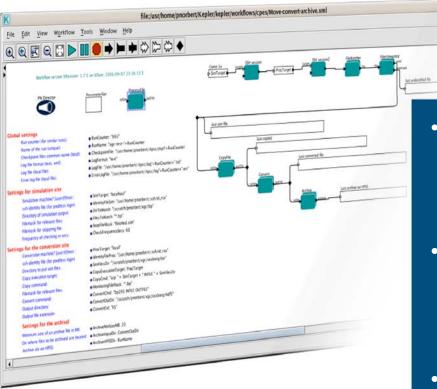
- High-throughput, lowlatency transport with minimized overheads
- Adapt to application and network state
- Schedule and manage in-transit processing
- Approach Cooperative self-management
 - Application-level data streaming
 - Proactive management using online control and policies
 - In-transit data manipulation
 - Quick, opportunistic, and reactive



- Experimental evaluation
 - ORNL and NERSC -> Rutgers -> PPPL
 - Adaptive in-transit processing reduced idle time from 40% to 2%.
 - Improved end-to-end data streaming -
 - Reduced data loss.
 - Improved data quality at sink.



Workflow automation





- Automate the data processing pipeline
 - Transfer of simulation output to the e2e system, execution of conversion routines, image creation, data archiving
- And the code coupling pipeline
 - Check linear stability and compute new equilibrium on the e2e system
 - Run crash simulation if needed
- Using the Kepler workflow system
- Requirements for Petascale computing
 - Easy to use

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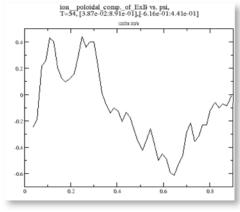
- Dashboard front-end
- Autonomic

- Parallel processing
- Robustness
- Configurability



CPES workflow automation

- NetCDF files
 - Transfer files to e2e system on-the-fly
 - Generate images using grace library
 - Archive NetCDF files at the end of simulation
- Proprietary binary files (BP)
 - Transfer to e2e system using bbcp
 - Convert to HDF5 format
 - Generate images with AVS/Express (running as service)
 - Archive HDF5 files in large chunks to HPSS
- M3D coupling data
 - Transfer to end-to-end system
 - Execute M3D: compute new equilibrium
 - Transfer back the new equilibrium to XGC
 - Execute **ELITE**: compute growth rate, test linear stability
 - Execute M3D-MPP: to study unstable states (ELM crash)

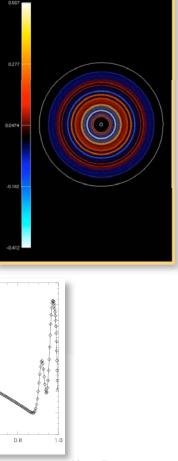


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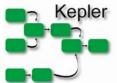
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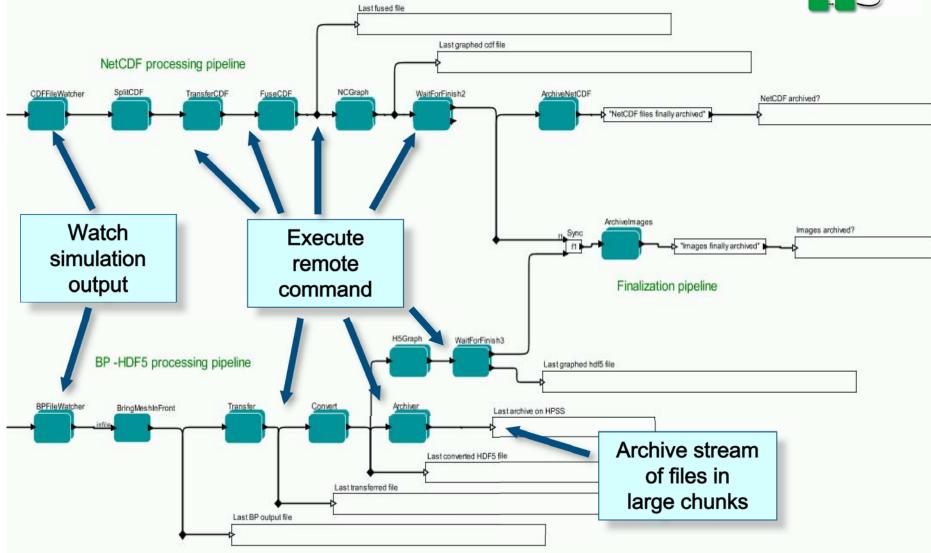






Kepler components for CPES





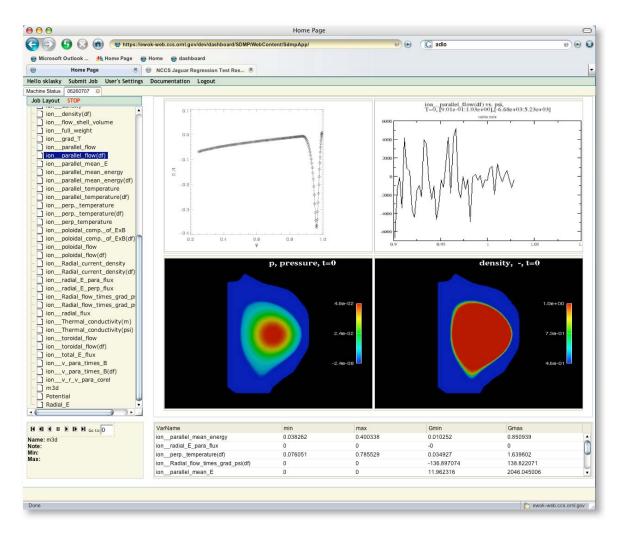


Kepler workflow for CPES code coupling

Combines data from

- AVS/Express,
- Gnuplot,
- IDL,
- Xmgrac.

Allows us to monitor the weak code coupling of XGC0 (Jaguar) to M3D-OMP (ewok) to ELITE (ewok) to M3D-MPP (ewok).

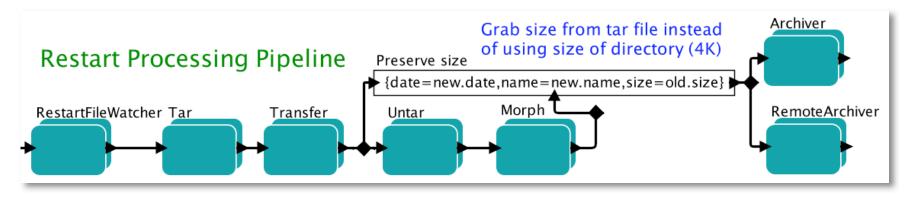




S3D workflow automation

- Restart/analysis files
 - Transfer files to e2e system
 - Morph files using existing utility
 - Archive files to HPSS
 - Transfer files to Sandia
- NetCDF files
 - Transfer files to e2e system on-the-fly
 - Generate images using grace library and AVS/Express
 - Send images to dashboard system

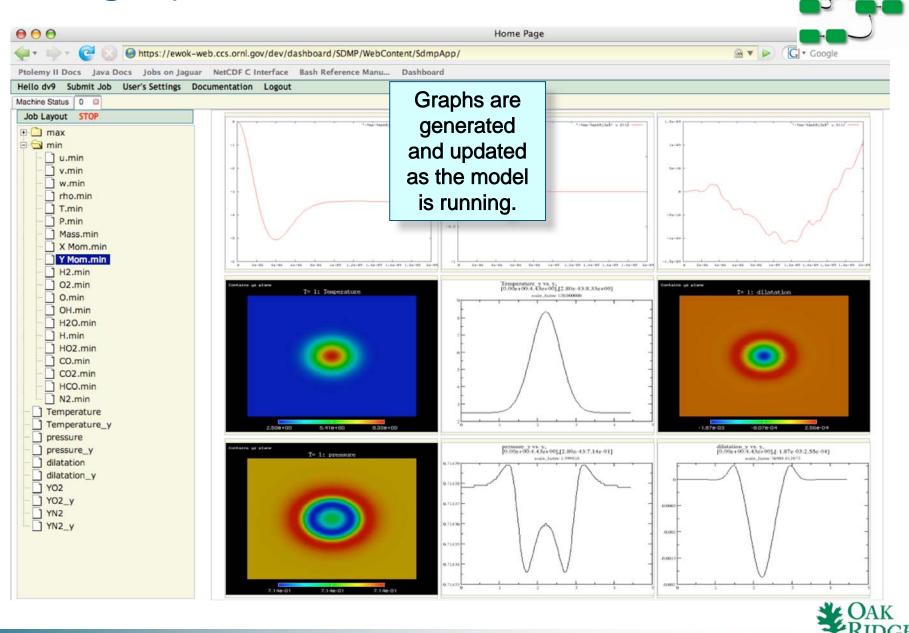
- Min/max log files
 - Transfer to e2e system at short intervals
 - Plot with gnuplot
 - Send to dashboard for real-time monitoring





Kepler

S3D graphs on the dashboard

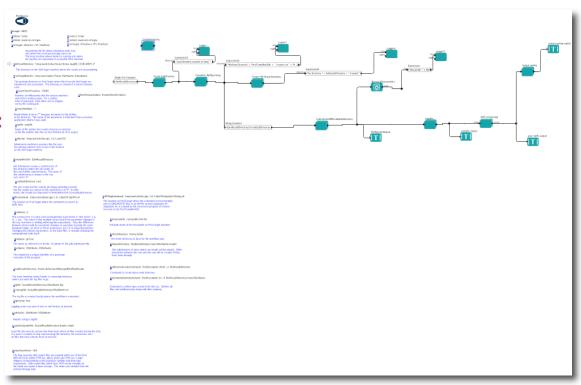


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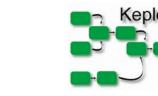
GTC workflow automation

- Proprietary binary files (BP)
 - Convert to HDF5 format
 - Generate images
 - With custom processing programs (bp2h5-png)
 - With connection to VisIt
 - Archive files in HPSS
- Key actor: ProcessFile (N. Podhorszki)
 - Check-perform-record checkpoint pattern
 - Operates on a stream of operands (remote files) in a pipeline of processors



 Logging and error logging of operations provided within the component; just configure for location of log files





Simulation monitoring

- Simulation monitoring involves the successful integration of several sub-tasks:
 - Monitoring of DOE machines
 - Visualization of simulation data:
 - graphs, movies, provenance data, input files etc.
 - Database integration and High Performance Storage System:
 - Annotating images and runs
 - taking e-notes and maintaining an e-book
 - High-speed data delivery services
 - Workflow system that pieces these tasks together
 - Check machine status and queues
 - Submit job through dashboard and workflow
 - Visualize simulation data from provenance information to output files and graphs
 - Analyze data
 - Keep notes on runs
 - Download selected information or move to specific storage

Scientist with limited knowledge about dashboard technology

Interact with workflow



Machine and job monitoring

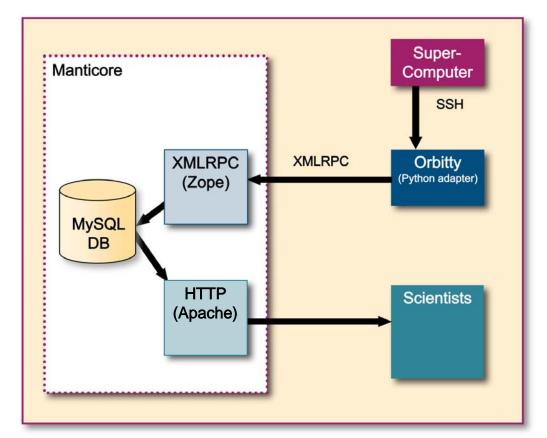
- Back end: shell scripts, python scripts and PHP
 - Machine queues command
 - Users' personal information
 - Services to display and manipulate data before display
- Dynamic front end:
 - Machine monitoring: standard web technology + Ajax
 - Simulation monitoring: Flash
- Storage: MySQL (queue-info, minmax data, users' notes...)

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wok jaguar 120614 Thu Aug 16 08:57:11 2007 Right click to edit. showq showbf jaguar 98758 Wed Jun 27 14:03:09 2007 bad input data Active Eligible Blocked jaguar 98108 Tue Jun 26 09:54:26 EDT bad input data Jobb Vactive sime issue risme showig 15:07:35 scellent XGC run showing 22932 sugyarma 128 13:52 Tue Aug 16 15:07:35 gaguar 98108 Tue Jun 26 15:12:15 2007 good nun, high beta jaguar 98108 Tue Jun 26 09:54:40 EDT good nun, high beta good nun, high bet	e00613.20080.0 s00613.20078.0 s00613.20075.0 s00509.20204.0 s00509.20203.0 s00509.20203.0 s00509.20198.0 s00509.20198.0	 m3dp initp6 jet_0.25km SP s00613.ner driver_scr ak_au_10i s3dHCCI s00601.ner 	u5881 ykanai cmeakin bjulia jxcao matsui vardha stsriniv mhuda	4 10 64 12 8 1 14 1 2	16 16 16 16 16 16 16 16	03:05:06 8/16 04:52:07 8/16 08:35:46 8/16 19:51:30 8/16 00:45:51 8/16 11:12:53 8/16 11:12:53 8/16 44:26:22 8/16 04:46:20 8/16 19:01:13 8/16 12:56:44 8/16	11:34 09:21 09:05 08:20 00:10 00:46 08:56 04:42 07:30 11:25	60201 22472 60301 19121 60301 19121 60301 19120 60301 19177 60201 16716 60201 12471 60201 12471 60201 12471 60201 12471	5.0 hhh 5.0 lrfpl5n 2.0 daton00 5.0 marilani22 4.0 a4 5.0 job_16_2 9.0 SidePre 4.0 si87_300 3.0 si87_200 2.0 si87_100	kclau u2230 yop demst mtiago nemeth alberto alberto alberto	 Nodes 1 6 1 1 32 4 4 1 1 1 1 	Tasks V 8 3 0 1 0 1 0 8 7 8 8 8 8 8 8 8	WClock Stime 4:02:11 8:8:08:3 8:16:25 8:8:08:3 8:14:25 8:8:08:2 8:14:25 8:8:08:2 9:12:36 4:12:22 sklasky showsta	31 45 52 52 51 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	There Were I	No Results fo		iame No	odes	Req U		
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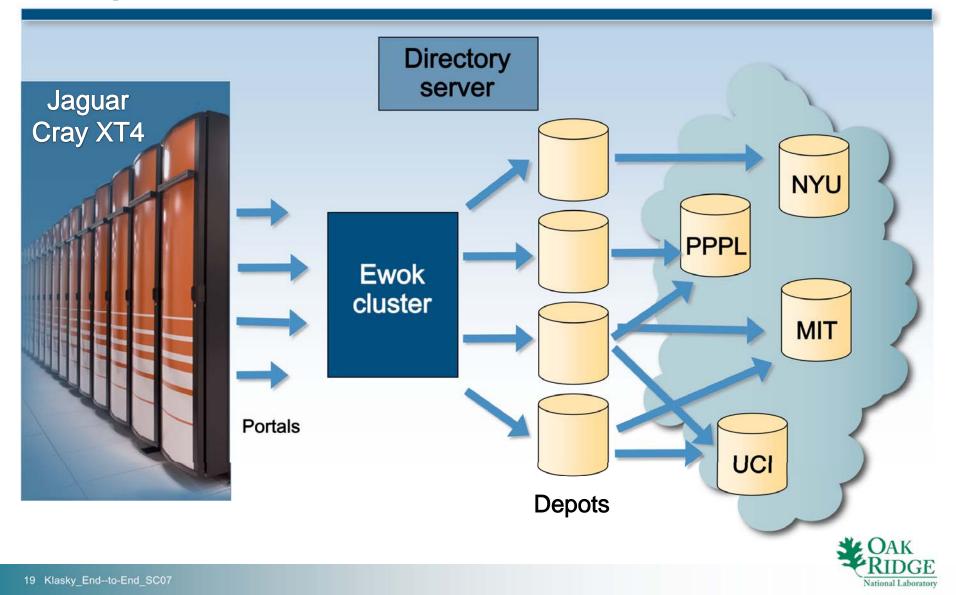
Provenance tracking

- Collects data from the different components of the W/F.
- Provides the scientist easy access to the data collected through a single interface.
- APIs have been created in Kepler to support real-time provenance capture of simulations running on leadershipclass machines.





Logistical networking: High-performance ubiquitous and transparent data access over the WAN



Data distribution via logistical networking and LoDN

- Logistical Distribution Network (LoDN) directory service adapted to run in NCCS environment:
 - User control of automated data mirroring to collaborative sites on per file or (recursive) per folder basis.
 - Firewall constraints require mirroring of metadata to outside server.
- User libraries enable program access to LN storage through standard interfaces (POSIX, HDF5, NetCDF).
- User control over data placement and status monitoring will be integrated with dashboard.
 - Download of data to local system for offline access.



Contact

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