APS UPGRADE FORUM



APS SCIENTIFIC COMPUTING STRATEGY

BRIAN TOBY Chief Computational Scientist, Senior Physicist, Group Leader Computational X-ray Science (CXS)

NICHOLAS SCHWARZ

Principal Computer Scientist, Group Leader Scientific Software Engineering & Data Management (SDM)

OVERVIEW

Drivers & Challenges Current State Strategy Notable Accomplishments Next Steps



DRIVERS & CHALLENGES



DRIVERS & CHALLENGES

New scientific opportunities drive demands for increased computing at the APS

These opportunities are/will be enabled by

- new measurement techniques
- technological advances in detectors
- multi-modal data utilization
- advances in data analysis algorithms
- and, of course, all the benefits of the APSU

And they create demand for sophisticated and large-scale

- computational resources (CPUs, storage, and networking)
- algorithms and scientific software



MAPPING OF MESO- AND MICRO-STRUCTURE IN ENGINEERED MATERIALS

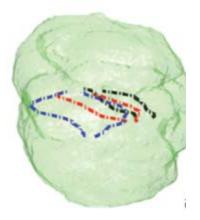
Goal: understand function and how to enhance properties of next generation atomically engineered materials

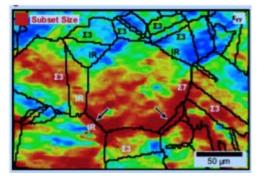
Applications: better high-performance alloys for aerospace, defense, fuel-efficient transport

Measurements: simultaneous high-energy diffraction microscopy (HEDM), ptychography, high-energy microtomography and coherent diffraction imaging (CDI)

Challenges:

- Big data transport and management (>terabytes/hour)
- Advanced algorithms: image reconstruction with internally consistent experimental artifact correction
- Just-in-time high performance computing to provide realtime feedback to experimenters
- User friendly software. Professionalize existing and new code into a supported package that runs on workstations and HPC.







RAVEN: NONDESTRUCTIVE 3D IMAGING OF INTEGRATED CIRCUITS

Chris Jacobsen, et al.

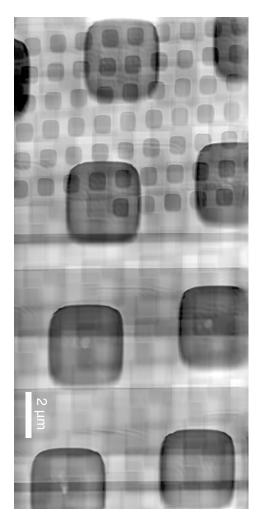
Goal: Image all layers in a 1.5 mm³ device with < 10 nm resolution (USC/Northwestern/APS proposal for RAVEN project in IARPA)

Applications: National defense & quality assurance

Measurements: ptychography, tomography & possibly elemental mapping

Challenges:

- Huge data volume transmission and management (> 1 petabyte/day!)
- Multimodal image registration algorithm development
- Large-scale HPC adaptation of codes
- Algorithm development for automated reconstruction optimization
- HPC data analysis integration into beamline workflows
- Device-library driven circuit analysis; petabyte-leve Idata interpretation and visualization





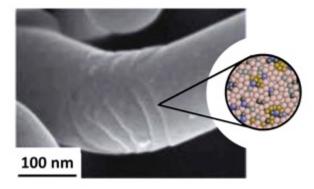
CHARACTERIZE ATOMISTIC DYNAMICS DURING PLASTIC DEFORMATION

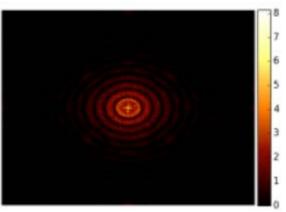
Goal: Understand how amorphous polymers and metals fail due to external stress

Applications: New hard and crack-resistant materials for transportation and other high-performance environments

Measurements: XPCS mapping combined with CDI Challenges:

- Algorithms combining dynamics from XPCS and structure from CDI
- Adaptive control of experiments to capture rare failure events
- Combined use of simulation techniques (metals: DFT or polymers: MD) with experimental data
- Large data volumes (10⁶ frames/sec XPCS 10³ CDI)







CURRENT STATE



THE APS SUPPORTS OVER 30 SOFTWARE PACKAGES

Advanced Photon Source

an Office of Science User Facility

Argonne and a playing values has suggested hade for baseding shift, while country the longity and amonto of due days. It will simplify manual track prime in \$55 for terms and w service or infrastructure for requiring the couples then days and and in into only with administrative About | Conferences | Long-Range Schedule | Publications | APS Science 2014 | APS Brochure | APS-U | APS 5-Year Facility (Strategic) Plan Search the APS Q Sinte Katharipi MACHINE STATUS BEAMLINES APS USER INFO DIVISIONS INDUSTRY SCIENCE & EDUCATION DIRECTORY a finder in the local and the state and and the tasks iteragin its Catalog of Data Analysis Software Science & Edu. special and SOFE. ingliances the lines Science & Edu, Home Development of software for visualization, analysis, reduction and simulation of x-ray experimental work has been a major COW-Onetal Coordinate Science Highlights output from the APS. This page describes a number of projects, some mature and others in initial stages that are being free Washington The just of a larger 1242-2 actively developed by scientists with the X-ray Science Division, often aided by software engineers within the AES Software Conferences project "Discovery Enginesities Hig Date," and is second to provide trail time, or new real time Services Group and sometimes in collaboration with other parts of Argonne or external laboratories. mailurity and subplus of single strend \$55. carsoting lates. (XTW is corporable for Seminars & Meetings asthurating between them tool to inclusional SAXS & BAXIS on BARD WARE Publications Note other relevant web pages: solution, thereils and fitting A set of programs BODD, WAAR date COMPANY OF eduction, Headlantics and purposi Annual Reports CONTRACT IN A Mariah-Issue · Beamline data collection packages. publics for standington. reduction, and analysis of cfl APS Upgrade party million 2 mg careering (12100) Area taken · Software Services Group software projects web page administrations that an Courses & Schools other supported on surface : Xelater Calculation of some balls that is then then TAN Control System operation in place Graduate Programs AND serves or the past quittely and he An importance sourced and data proce DAVE II, CAAS and EXPLICE I Schules in a 1977 and initialization had Kild miner probably (a 45 K, a 45 K, a 46 K) amone for how-graphy benefices. Into GSAS-2 Developmental Anglesis for one lade spectroscope and group A REA OF THE OWNER, ON THE OWNER AND with EPUD for bounding courted and with his and office data reveing, have state properties within a damage Scientific Software It butures analysis methods for elemental tratative multiplet incoded, utilizing a which provide these tion institution between and start tops, spectral, spectrum, and new suppl met arrangement from our type of to be many hade Davidsonan with spranting that some body a UPCD-matter marrie data. It operator to batch much: and and in the difference managements of Codemit, spin-infek, impeld Solid. desides are interesting OVI. Mapping in a apparettes. Displays free data as well as ar sutorials characterization info previously incoded type, office graphical Address of the Address of the Owner, Name trian hand spin acces millions parking Multiple defeats inside the constituent that a site Datum - But 2nd Colork and being developed to replace \$1078 that will be tion and adjusted to other water the property of the property date, but or parameters study. Can be used for all and active and charge tracate our take and triangents into heartfline workflines. of conclusive from materials observations of field parameters. The program solutions SAA, 3275, PDA, and 2752 spectra and to probables. the shafteness STORE Managing using a Peaker S tion baselines but want XXAPM, S-rey Meants Phys. The Manuscriptured Integling using Differenties Manhala ad the adjub follows (MIDAR) advanciatings starting and triplating (statistics mints with allows used to non-destructively image the Realists the investion of a shely useful to single price diff ance with an a real poline untig t res of prostalline materials. The performed at the methods 'Correlation' and 'Soulastaits' comput is a pit may with information about save APR. Dave spick Notes-Carlo Rate Equation ton it taiwish ask as rock his and shich an used to thak the evalution of dender in the local soil the summer which is summing the manine sta act of dams by looking for oursel appleations of a car free electro This period determines charges that une (2010). It prevides a comp ample with a error in a parametric study in mining tracking of all the electronic ists from some without impo transitions and challing by atom region of internet from the visible light tough and institutes makes of, all, and physically-makes and ADMAN SALE, WARD south diffusitive size, it is maritie of taking it matti Familyes set of images and A flat forver ME, GD of TER of Innue Ample Augh Scattering Para In Children al. MART, al. and Mich. distant of the manufactory producting or three of the The Road Spinst is a spin of WWW and and to advantation included a sill adjets that the stall angle (3) we used in AARD at periods similations of stat ne. It say pulpy other while antering data, primarily for complex, topic authors for online mainling of 2 day and wide angle scattering crowallins acherologity is one data in character the torgets naterials. Performs a masher of Munitive, spinulae reflection and worth assessibles of particles, such as inorganic stration or wrigh information whiles d another the standard or writed in and with principle adaptivations in studying listics pulpholes, organic malarales, presidua ar post-proceeding Reactions, such as ring artiflast corrections, phase relational, optima a surface barrow of countrie, designing it real dent making of sustaining from disords ring, impre-reserved, etc. the restricts elisted partners, including Standal accounts action, and manifolds the dynamical differenties hearp. The programs compare 5 ray NAVIDA Multi-prints Analysis anali angle differences, with evening of may have bet these threads on the sector acarbonies barbate. Brouge difficulture profilies halk they import/opert, maripulation, p so) includes arefering contrast solutions. Does not uis. 5 car special reflective, starting works from multi-WTB Multi-water Affaires To multiple from difference, and they have been been and engineer and engineer and engineer d Programs a prighted · Beartransconnege/ http: tion from staggards multilated sair initian it has only be taked that it data fared and making and the anglesting reduins and its interaction with samples and optical document. These status automic and therefore to grant allow he design of feamline withingson in the fait dominant 9 strain and second

Parlow: X-me prois-active A proton of prilling in computing the standing@.dependence for a car and and description. The orbital car be around Strength Into (127) Instead Pythons contained (for these factors of sharepring) of the s

possible differenties asingle instantion or in the local distance in the second second





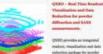


tone in 20 determines per width's tand in printers algos able has signs firm unto NARS and WARS due to their effectuals. Niks includes such data distant in prime trained, to intrastive or function of cloning angle - suitable for most of the data products programs in a linear i

and WANTS

our calledge in a bullet

deni). It can also be used for graving incidence generates \$400 or \$40.00.



COURT aircritics on integrated realiset, visualization and date relation parkage for preside difference and lock? ent. It's matting up

they will a Bullin Hourt for panel simular hat has also been used to methantics marCO, martal, and Plana data. A major focus of the opplication is that it on authors also there are a substituted to a set that a sharing in and time or the

and store \$100 % Married root, Supplying

raits length-wale dependent do preserves for the ascepte laring protont, by sting the time some arrive of all area determs incases. To effore paration in real-time, the Hadrog Maple perities is required to depice this to a

All had impled aroung a

beniative imageding (30PC) to a mealing side on to and in prove data troupedire of the preservity of the represent such as small angle to inconsistion, graphy incidence or under th



respond space. Provide th sense for limits at martional and through the map. The input he proceeding of this data and over a range of diffractmenter angle

Pathene (TTTR)

territorial territoria prick and multi-stars effectives test in a to tion Their sub-shares of

and a rap differential topography), initiation a rap free he FUT disks and presides a line other beloful lasts for a one energy optics and



SCIENTIFIC SOFTWARE

The APS has a wealth of beamline scientist-generated software

- Highly heterogeneous
- Few packages developed to professional software engineering standards
- Very little is supported to professional standards (regular) releases; packaging; user support...)
- \rightarrow All XSD groups have unmet software needs some very extensive
- \rightarrow Migrating existing codes to HPC can be very difficult
- → Some of the most challenging/exciting scientific and computational challenges will require significant effort from teams of experts



Catalog of Data Analysis Software

Development of software for visualization, analysis, reduction and simulation of x-ray experimental work has been a major output from the APS. This page describes a number of projects, some mature and others in initial stages that are being actively developed by scientists with the X-ray Science Division, often aided by software engineers within the AES Software Services Group and sometimes in collaboration with other parts of Argonne or external laboratories.

Note other relevant web pages:

· Beamline data collection packages.

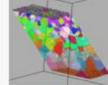
+ Software Services Group software projects web page

Imaging

HiSPoD; undulator white-beam diffraction analysis software

HiSPoD is a Matlab@ program, developed for simulating and analyzing undulator white-beam diffraction patterns. It is particularly useful for single-pulse diffraction patterns and where an area detector is not perpendicular to the beam and the transmission beam spot may not fall on the detector

LaueGo



Provides a convenient means to view and analyze 1D, 2D, and 3D spatially-resolved diffraction data. It is capable of taking a multi-Terabyte set of images and automatically producing a view of the strain or orientation throughout a 3D volume. It can analyze either white or monochromatic x-ray data to obtain the orientation or strain information within an inhomogeneous material

MANTIS (Multivariate ANalysis Tool for Spectromicroscopy) is a Python-based open source analysis code that uses a number of multivariate statistical analysis and classification techniques to find the dominant spectroscopic themes within a dataset.

MANTIS: Multivariate Analysis Tool for

Spectromicroscopy





COMPUTING INFRASTRUCTURE

Today: very little beamline computing is done on centralized systems (ALCF & LCRC); most HPC use is in storage ring/accelerator simulation

- The APS has a small cluster (Orthros: 53 nodes, <1000 cores; ~250 Tb) serving 3 beamlines (and APSU).
 - Orthros nodes are configured for and allocated directly to beamlines and are idle when not required
- Significant additional computing done on beamline workstations.

→ Computing demands are only going to grow, and are beyond the means of the APS to manage



CHALLENGES OF SHARED RESOURCES

Scheduling: Much APS computing falls in the category of "weather forecasts" (no value if too late); reserving nodes will not scale

Challenge to CLS: develop preemptive scheduling approaches for LCRC & ALCF

Latency: Must move large amounts of data

- Adaptation of ESNet DMZ concept intracampus to allow firewall-free transfers
- Longer range: algorithms for initial data reduction at beamlines, reducing network footprint

Support: APS runs 24/6; CLS runs best effort from 7 pm to 7 am

Need to work out an out-of-hours support mechanism



STORAGE MANAGEMENT AND INFRASTRUCTURE

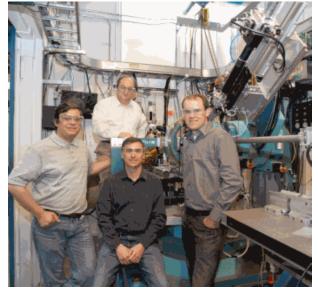
- The APS is currently producing ~2 Petabytes of data/year
- Data from XSD beamlines must be provided to users for archiving
- Beamline scientists need to stage, migrate, clean up and catalog large volumes of data
- Data typically stored in vendor-supplied image formats; lacks metadata & provenance
- Limited on-line storage



BEAMLINE OPERATION SOFTWARE

Most APS beamlines have developed their own versions of user interface/controls

- Idiosyncratic; often not "user-friendly"
- Beamlines need combination of GUIs and scripting; software is continually being adapted





STRATEGY



APS SCIENTIFIC COMPUTING STRATEGY

Scientific drivers coupled with technological advances make scientific computing a priority for the facility.

- All techniques at the APS will benefit from advances in this area.
- It's important to note that without the application of advances in this area, we won't be able to fully realize the scientific benefits of the APSU.

Participative Process:

- Current landscape
- Technique-by-technique assessment (short- and mid-term needs / overlaps)
- Anticipated technological advances
- APSU first experiments (long-term)



APS SCIENTIFIC COMPUTING STRATEGY

Facility-wide strategy to meet these demands: APS Scientific Computing Strategy.

- Prioritization
- Strengthening / aligning internal resources
- Collaboration

Address Four Areas:

- 1. Scientific & Data Analysis Software
- 2. Data Management & Distribution
- 3. Computing Infrastructure
- 4. Beamline Operation Software

Do all of this with foreseeable budgets.



PRIORITIZATION

Prioritize what's most important to the APS (we can't do it all):

- Primary focus is on APSU enabled and improved techniques
- Improvements that have a facility-wide impact
- Support existing / successful user programs
- Consider initial and ongoing costs, and funding sources

Participative, iterative, *living* process – regular review and discussion

Appendix A – Projects and Priorities

Table A.1 Scientific Software & Data Analysis

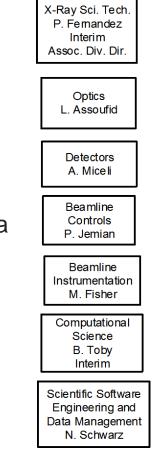
Project	Completion	Funding	Priority	Details	Effort	Ongoing Effort / Year
HPC enabled real- time correlation toolkit	2017	APS Operations / CLS	Mission Critical	Development of an HPC enabled application for real-time photon correlation analysis of time-resolved datasets (e.g. XPCS, surface-XPCS, etc.).	2 FTE	0.25 FTE
HPC enabled real- time XAS analysis toolkit	2018	APS Operations	Mission Critical	Development of an HPC enabled application for real-time analysis of x-ray absorption spectroscopy datasets (XANES, EXAFS, XFM).	3 FTE	0.25 FTE
Ultrafast time- resolved imaging with large-scale MD modeling	2018	LDRD	Mission Critical	Integrated ultrafast time-resolved imaging with large-scale molecular dynamics modeling for in situ data analysis and visualization of energy transport.	2 FTE	
Multimodal imaging of materials for energy storage	2018	LDRD	Mission Critical	Integration of multimodal data from x-ray and electron microscopies in order to understand the interaction of materials at multiple length scales from nang to micro.	2 FTE	
HPC enabled real- time CDI analysis toolkit	2019	APS Operations	Mission Critical	Development of an HPC enabled application for real-time x-ray coherent diffraction imaging datasets (CDI, <u>Ptychography</u>).	2 FTE	0.25 FTE
HPC enabled real- time x-ray scattering analysis toolkit	2019	APS Operations	Mission Critical	Development of an HPC enabled application for real-time reciprocal space analysis of x-ray scattering datasets (SAXS, WAXS, HEDM, XPD).	2 FTE	0.25 FTE
Microstructural Imaging using Diffraction Analysis Software (MIDAS)	Ongoing	APS Operations / Industrial Partner / AFRL	Mission Critical	Development and maintenance of a suite of analysis tools for different modalities (near-field, far-field, and very-far-field) of high energy diffraction microscopy (HEDM)		1 FTE
TomoPy	Ongoing	APS Operations	Mission Critical	Package, maintain, and support the TomoPy reconstruction toolkit.		0.5 FTE
General purpose analysis workflow toolkit	Ongoing	APS Operations / CLS	Mission Critical	Leverage best-in-class workflow tools for use at APS beamlines.	2 FTE	0.5 FTE
General purpose	Ongoing	APS	Mission	Development of algorithms for	2 FTE	0.5 FTE



STRENGTHEN / ALIGN INTERNAL RESOURCES

Two groups dedicated to scientific software:

- Computational X-ray Science (CXS)
 - 3.5 FTE
 - Algorithm development and external collaborator coordination
 - X-ray scientists and applied computational scientists
- Scientific Software Engineering & Data Management (SDM)
 - 8 FTE
 - Software creation and maintenance, HPC development, and data management
 - Software engineers
- Aligned within a cohort of support groups, including Beamline Controls, Beamline Instrumentation, Detectors, and Optics: Build partnerships with scientists
- Very modest staffing increases





COLLABORATION

Leverage the broader community for expertise and effort. We won't achieve all that we need with only what we have internally.

ANL – ALCF/CLS/MCS

 The APS has the unique advantage of worldclass computer science and leadership hardware on-site

BES Facilities Computing Working Group

- Facility Directors' call to develop collaborations
- Avenue to collaborate with other BES SUFs

CAMERA

Three areas of interest/overlap with APS: Tomography, Ptychography, GISAXS

Scientific Staff & User Base

Often the main drivers of innovation





SCIENTIFIC SOFTWARE

Algorithm development and software creation

- Aim to provide near real-time feedback that can inform experiment steering
- Interpretation and visualization of large and complex data streams that are beyond unaided human comprehension
- Combined simulations and multimodal data to extend understanding for currently intractable scientific problems

Focus on techniques in support of science enabled by the APSU

 High-energy, multi-modal, microscopy, fluorescence, scattering, coherence imaging, time-dependent

Approach

- Open source
- Graded
- Select high-impact APS packages will be maintained for broader community use (as distributable packages or as software-as-a-service (SaaS)), such as TomoPy



DATA MANAGEMENT & DISTRIBUTION

Expect an order of magnitude increase in data volumes and rates over the coming years, and at least two orders of magnitude increase post-APSU.

Facility-wide tools that provide:

- Automated data transfer (e.g. Globus Services)
- Data ownership
- Metadata cataloging
- Provenance tracking
- Electronic notebook (e.g. OLog)
- Apply best-in-class tools to APS beamline and workflows.
- Prioritizing beamlines based on highest current and anticipated data rates/volumes.
- Work closely with Argonne computing expertise.
- APS provides systems integration.



COMPUTING INFRASTRUCTURE

A multi-order of magnitude increase in required computing power is anticipated over the coming years.

Tiered Approach

- Beamline local resources used when sufficient
- APS operated compute cluster for current mid-range problems
- Shared (LCRC/ALCF/NERSC) resources for most demanding requirements

Continually review costs of internal vs. externally managed resources to ensure the most efficient use of resources.



BEAMLINE OPERATION

The APS wants to provide intuitive yet flexible beamline operation software in order to maximize beam time efficiency.

- Common core of beamline alignment, calibration and experiment operation tools
- Automation elements, e.g. alignment, mail-in, or robotic operation

Due to foreseeable budgets, the APS will *not* devote significant resources to improving beamline operations software for existing beamlines.

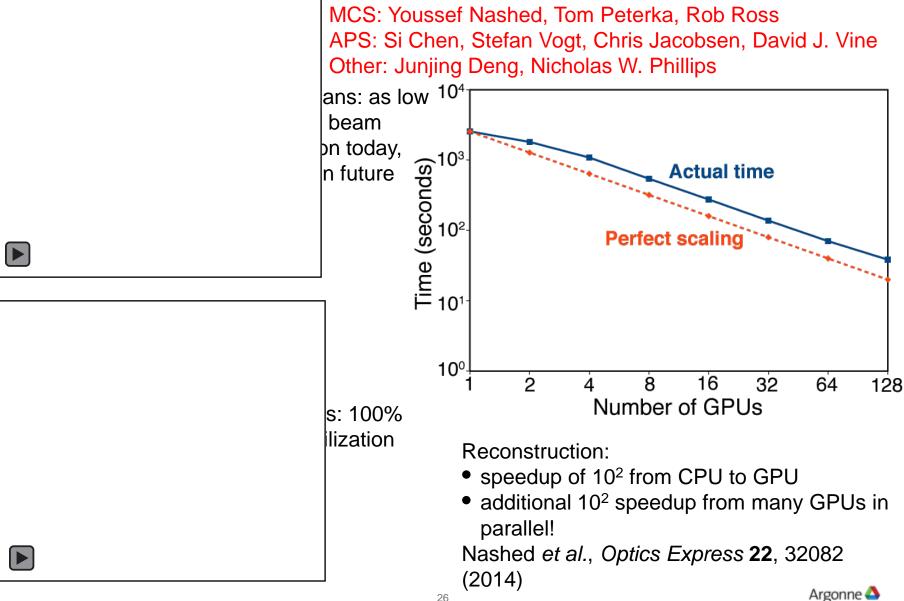
 Development projects to create new or improved beamlines (funded by the APSU or Operations) should properly budget beamline operation software as a part of the overall project.



NOTABLE ACCOMPLISHMENTS



PTYCHOGRAPHY RECONSTRUCTION



MAGELLAN CLOUD RESOURCE FOR XPCS

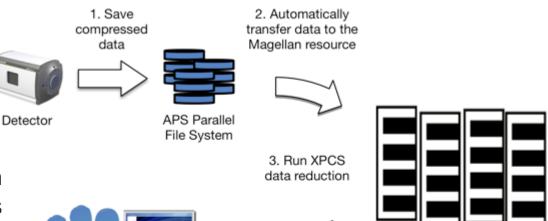
Magellan

- ANL cloud computing environment
- ~ 1,000 node resource
- Virtualized environment
- Maintained by CLS

XPCS

- XPCS multi-tau Hadoop system set up and running on 10 nodes
- Fully integrated into the XPCS workflow pipeline at 8-ID-I
- In production use this run

APS: Collin Schmitz, Ben Pausma, Faisal Khan, Suresh Narayanan CLS: Ryan Aydelottt, Dan Murphy-Olson





 Automatically transfer data back to the APS



Magellan

5. APS Users view output

visualizations and may adjust

experiment parameters

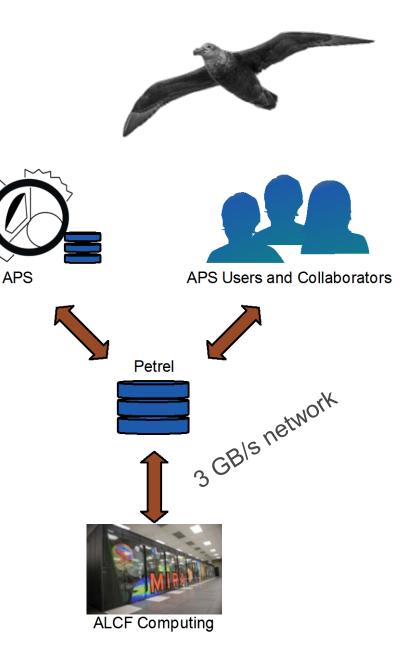
PETREL DATA SERVICE

The APS is collaborating with Argonne's CLS directorate and the Globus Services team to prototype a new data management and distribution service.

- High-speed, high-capacity data store
 - 1.7 PB total storage
 - 100 TB project allocations
- Project-focused, self-managed
- CLS provides the hardware infrastructure
- Globus Services provides the software
- APS provides integration



Re new results of the second s	Petrol Project Owners Man - Source -
--	--





EXTREPID

- Repurposed storage from Blue Gene/P Intrepid
- 1.7 PB
- Administered by APS
- Hosted by ALCF/CLS
- Online in the coming months





USE OF LARGE SCALE COMPUTING RESOURCES





NEXT STEPS



NEXT STEPS

- Continue to catalog and enumerate all computing needs
- Use APSU's first experiments as a starting point:
- Start developing aligned 5-year and 10-year roadmaps
 - Machine timeline
 - Beamline/technique timeline
 - Detector/beamline hardware timeline
 - Computing hardware timeline
 - Software timeline
 - Algorithm/math timeline



NEXT STEPS

Computing is critical to the scientific success of the APS after the APSU project completes.

Our computing needs must be addressed before the APSU completes.

Strategy Document: <u>https://www1.aps.anl.gov/X-ray-Science-Division/XSD-Strategic-Thrusts</u>

Thoughts and comments are very welcome!



WE START WITH YES. AND END WITH THANK YOU.

DO YOU HAVE ANY BIG QUESTIONS?



www.anl.gov