Group #13: Community of Interest on the Future of Scientific Methodologies

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| Date | November 2, 2020 |

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1 Day One - November 2, 2020

1.1 Breakout 1 - Define the Scope of the Problem.

**The following participants have not been active:**
\*fac- Nami, Angie Lester

**Question or instruction for the discussion:**
Breakout 1 - Define the Scope of the Problem.
The purpose of this session is to lay the foundation for the next 5 sessions. That is, each breakout group will define a key piece of technology, a new device, or methodology that would have an impact on how the labs/scientists operate. The details should include answers to the questions below.

**Sticky points:**

 Top Takeaways (5 points per participant)

* What is the problem, issue, technology, device, methodology?
	+ It can be beneficial to identify the variations in the needs of the scientific community when it comes to using HPC resources. (#1)
		- I have done this for LCLS - there are over 20 individual workflows envisioned. 80% of those workflows require 5 PFLOPs or less, but the other 20% or north of 128 PF and several are in the exascale. (#4)
			* I have done this for LCLS - there are over 20 individual workflows envisioned. 80% of those workflows require 5 PFLOPs or less, but the other 20% or north of 128 PF and several are in the exascale. (#2)
		- This transcends 'HPC' and will need to encompass all forms of computing that may be usable - computing could be viewed as fungible as power in the future where the interface (plug) doesn't care how it was generated (#17)
	+ (1) Emphasis on user-friendliness: think less about how to use a beamline or how to compile code for a specific architecture and enable the scientists to interact with the data seamlessly in near real-time. (#3)
		- Shorten the time to science: allow seamless transfer of data to compute so that scientists can get answers to their science questions during their beamtime. Eventually, one hopes that this will produce smarter, better directed experiments that produce better data and better scientific results. (#7)
		- Allow users to interact with the data without requiring them to launch a large computing effort to do so (#6)
			* improved interactivity and access to compute resources. (#59)
		- more investment into software stacks that are data agnostic - and can do a task (analysis, simulation, etc) instead of having to re-invent new approaches. (#21)
		- role of digitial twins? (#46)
	+ (1) Facilities today are distinct, in almost every way, accounts, security, policies, priorities. In order to support the science of the future, facilities need to be strongly interconnected. (#8)
		- With a unified view of how one can set expectations and interact (e.g. APIs, process, inputs/outputs) (#13)
		- By facilities, I suspect we mean both ASCR facilities and BES light source facilities and other SC facilities. The experimental facilities would benefit from a streamlined interface to the computing facilities. Likewise, a more unified interface to the light sources, for example, would make it easier for data to flow back and forth between the ASCR facilities and the BES light source facilities. BES light source facilities would then be able to share data, which would enable training of better models, smarter experiments, and so on. (#38)
			* What sorts of assumptions are we making? What sorts of problems do we expect will be reduced to a problem already solved? I heard things like Federated Identity, computing reservations... (#28)
	+ (2) Self-driving facility (#5)
		- AI driven facilities: replace human in the loop decision making, at least for common operations, common problems (#9)
			* The challenges to this are both technical as well as policy related. (#12)
		- Before AI driving can take over, humans need to define the automation space and create APIs that allow "drivers" to launch compute or data acquisition in a consistent fashion (#60)
	+ (3) Seam-less integration between instrumentation/science and the machinery that must operate on the subsequent data (e.g. the processing, storage, network, and linking software). A view of the system that is data centric and scalable to whatever the discipline happens to be (#10)
		- also the role of of automation and removal of technology barriers (#19)
		- System-agnostic data analysis: scientists interact with high-level services to analyze data without getting bogged down in details of software stack, data movement protocols, etc... (#11)
	+ Here's a crazy thought: Could we develop an Alexa for the beamline? Or the computer from Star Trek? "Alexa, show me the distribution for this variable from this run" (#15)
	+ Computing needs to be both ubiquitous and accessible, but also continue to push the state of the art. How we balance these two tensions will be a key challenge. (#16)
	+ (2) Seamless data to analysis: Ability for instrumentation/science facilities to use capabilities and orchestrate seamlessly on available compute and data facilities including the resources offered as a cloud (#18)
		- Yes, users shouldn't care about where their compute is coming from, where their data is, or where it is being analyzed. All they need are the results of a science query, usually with low latency. Hiding the complexity of deciding where the computing is, how the code runs, how to move data there, etc. would greatly enable the process of getting to the heart of the science results. (#26)
	+ From an infrastructure perspective, what will be the demand on the network pipeplines for the seamless workflow that allows users to interact with the computing environment, possibly using large datasets acquired in real time? (#34)
	+ (2) Solutions need to be scalable, adaptive, end-to-end and cover the full lifecycle of the data. (#45)
		- Many capabilities are needed besides compute -- data archives, web portals, visualizations and interactive analysis. These capabilities need to be first class citizens. (#56)
		- Experiment metadata needs to be stored along data and easily queried for future retrieval (#57)
	+ (2) Policy changes are as important as technological developments in this area. (#58)
		- (1) For the 10-20 year time scale, it's worth considering how the changing HPC architecture will influence the workflow. (#14)
			* How can authors of high-level workflows and data analysis services tap into different platforms? Do we expect a generalization of technologies like containers? (#22)
		- (1) In 20-30 years, can we expect new user facilities with different kinds of challenges? For example, networks of subsurface sensors which may deliver intermittent/noisy data but require real time processing. This type of applications may appear in earthquake monitoring or geothermal/energy storage facilities. (#47)
			* One can imagine that instead of a fixed-size compute reservation, the sensor network is linked to a long-lived allocation of compute resources that scales up/down in real-time according to the data velocity. This requires a different way of thinking about machine time (cloud-like utility model) and non-traditional scheduling (#54)
* Who would develop it (basic research to advanced deployment)?
	+ Investment is needed from all offices, from basic research, to applied research and facility deployment. (#20)
	+ AI research is needed to help automate driving experiments at facilities. (#23)
	+ More cross-agency cooperation as we see in some areas of Science - since the solutions for one flavor of instrument (e.g. telescope) may apply to others that share common components (location, staff, computing, storage, etc) (#24)
	+ longer time scales than just the life of a project - the data usefulness doesn't stop when the project stops. Example: cosmological simulations may have usable lifecycles that go beyond a 5yr funding run - but what happens when the 5 years is up? Where does the data live long term so that it remains useful for future use cases (both anticipated, and non-anticipated) (#27)
		- Data storage infrastructure that is distributed, allows for data cataloging and discoverability. (#52)
	+ Basic research into workflows and the appropriate APIs are needed. (#30)
		- and the building of a common set of 'solutions' for similar workflows over time. There is a lot of opportunity for re-use at all technology layers (compute, storage, networking, software) (#53)
			* (1) Coordination across the various offices of science, with an eye towards building blocks that might be used by multiple science disciplines/collaborations. Too many customized solutions are being built now that cannot be leveraged across the various offices leading to silo'ing of solutions. (#31)
	+ Research in edge computing -- how the definition and concept of a supercomputer may need to change (#32)
	+ Optimized hardware architectures for a variety of applications and use cases. Middleware and software so end users do not have to be computing experts. (#40)
	+ (2) Policies would be needed to encourage scientists to share data. In some disciplines, data is open and published, but in others, it is closely guarded by the groups that generated it. Likewise, in order to analyze some data or understand how to use it, one must have metadata to provide the appropriate context. (#44)
		- Beyond policy - making it easier just to store and publish data long term. Right now there is a patchwork set of solutions for doing this, and data that may be useful can easily go 'dark' if it has no home. We offer allocations for compute that come with storage, why can't we just have storage allocations that come with an easy to use system for publishing/sharing/cataloging data? (#55)
	+ (1) Need strong long-lasting collaborative partnerships between experimental facilities and ASCR computing and networking facilities. (#50)
* Who would use it and what skills would they need to use it effectively?
	+ (2) Ultimately, end-users will be domain scientists with knowledge of certain analysis methods. They should not, however, require any in-depth knowledge of hardware architectures or details of storage and data movement (#29)
		- Removal of technology barriers for users is very important. The future ecosystem should be seamless and highly usable. (#33)
	+ (2) To use a car analogy - a car's driver shouldn't have to understand how an engine works to be able to operate a car a safely (different sets of knowledge/skills). If we want scientific users to be the most productive, the most time/effort should be put into hiding technical details and providing usable solutions for the common use cases. There will always be corner-cases, but providing a simple and easy to use mechanism to 'do science' is paramount without having to need to know all the goo underneath (#35)
		- This implies an investment in optimized computing libraries and middleware. If we want the US to continue to lead on developing new and faster hardware architectures, there must be optimized libraries end users can build applications on if there will be of use for end users. (#37)
* When would it be expected to be in production use (N years in the future)?
	+ staged availability is better, as it would allow for the middle generations to prepare the next generation (and next next generation ...) for eventual operation. As it stands right now, there is an incredible amount of time / effort sunk into teaching scientists (and IT staff) the 'right way' to do things. A lot of that is sunk cost on systems that may not be around forever (#36)
	+ (1) prototypes exist today that are intended to discover use cases and focus basic research on gaps. This should lead to production services between some instruments and computers in the next 5 - 10 years. Complex wide federation to follow? (#39)
	+ It will be a gradual ramp up. Some capabilities are coming soon, federatedID, improved queing and interactive capability, shared data endpoints (globus), an upgraded network ESnet5, and portability across facilities (containers). Other capabilities will take more research and investment - including AI to control experiments, seamless APIs for facilities, distributed filesystems and metadata, advanced edge computing. (#48)
* Where, and how widely, would it be deployed?
	+ Coupled facilities would be used by nearly all facility users of Office of Science facilities. (#25)
	+ There is a need for high-level orchestration APIs to expose facilities to scientists or other automation software uniformly. These orchestrators would be deployed across the complex and interact with lower-level system services, which encapsulate local storage and computing details (#41)
	+ (3) Computing and storage should become more ubiquitous (via networks) and fungible when possible. This won't make sense everywhere (tops of mountains, the South Pole), but where infrastructure exists there shouldn't have to be open questions about 'where will I compute or store'. The golden ring will be linking the experimentation site to a more or less abstracted layer that facilitates the technology needs through a common software layer. This will eliminate the need to worry as much about having to prepare/create a set of code for each system and allow faster 'idea to implementation' (#42)
	+ Today, data management policies are unique to the instrument and access to data and analysis resources varies often among apparatuses within a single facility. (#61)
	+ BES funding of computing is not incentivized to promote collaborative, facility-wide, light-source-wide data management and computing solutions. (#62)
	+ Policy to support full end-to-end infrastructure, monitoring, troubleshooting. (#63)
* What is the setup time and/or process for using it?
	+ Ideally, end users would not have to set anything up or learn any new process for using coupled/linked facilities. (#43)
	+ If a new experiment / facility is about to come online, the ideal questions to ask should revolve around data volumes, the time scales they are produced, and the expectations the scientists / end users have on availability of the data. The answers to questions like that will help steer toward the kind of compute (HPC, HTC, cloud), location of compute/storage (if resources are not allocated in a uniform way), as well longevity and growth pressure. (#49)
	+ (1) The timeline for a fully realized facility of the future may be long due to needing to expand existing infrastructure and methodologies to enable edge, self-driving facilities, federation, etc. (#51)

1.2 Breakout 2 - Implications of this Problem.

**The following participants have not been active:**
\*fac- Nami, Justin Whitt

**Question or instruction for the discussion:**
Breakout 2 - Implications of this Problem.
Each group will now develop a list of issues and implications for the issue/technology/community they settled on. There are lots of implications for how a technology can be used, or further developed.

**Sticky points:**

 Top Takeaways (5 points per participant)

* What other/companion technologies, services, software/hardware must also be developed and deployed?
	+ Open-source software is key: common tools needed to integrate facilities (#1)
		- Timescale to implement adaptation of new software in user communities. May consider wrappers for existing software in the near future and lower level software development in the longer term. (#3)
	+ (1) Well defined services with APIs (#2)
	+ (1) Flexible, easy to use orchestration and workflow technologies (to build on the comment on APIs) (#4)
	+ while an older approach, adhering to the concept of the 'narrow waist' in design that allows for maximum flexibility for development on the tops and bottoms of components. (#5)
	+ (1) I am unsure if federated identity has been mentioned before, and if it is something worth calling out. It is well recognized as a gap. (#6)
		- and coupled with this is just the cyber-sec posture altogether. In part 1 we argued for ubiquity which is both a technology solution and a policy challenge. Keeping it all safe (when we we want to give everyone access, wherever) brings many new situations that are social and technical. (#7)
	+ 'people' will be an important component over all of this beyond just the raw technology. Making things seamless implies there will be experts in place to walk people through how to do things, or to make the necessarily linkages. (#11)
	+ (5) Expansion of the definition of a supercomputer -- can ESnet be more tightly coupled to experimental facilities and edge computing? (#13)
		- Ability to port jobs seamlessly from one facility to another in the event of an emergency (#15)
	+ (1) Highly optimized middleware and software will be required in order to hide complexity from users. (#14)
	+ (1) Distributed storage and filesystems with data accessible across sites. (#16)
		- storage allocations that outlive the 'experiment' life cycle (#21)
		- ability to track use over time - so that poplar items can be replicated and shuffled to where they are needed (e.g. caching) vs. non-popular things can remain available, but not consume high-performance resources (#22)
	+ (2) Robust, descriptive and searchable metadata stored with the data (#17)
		- and the ability to 'search' in a unified location, and be confident that you can locate what you want (wherever it may be) (#20)
	+ Adaptable workflows (AI for workflows), automatically generated metadata. (#18)
	+ (1) End to end monitoring of workflow. Where is the bottleneck? What is performing well and what isn't? (#28)
* Who is/will develop this companion technology/service?
	+ (2) Funding for compute/network technologies associated with large user facility grants (#8)
		- If we do not adopt this approach, data goes unanalyzed thus seriously delaying scientific discoveries, and not taking advantage of the money invested in building the facility (#9)
	+ (1) Supporting the science complex is something that should be addressed across agency boundaries where possible. Different agencies (e.g. DOE, NSF, NOAA) all have similar workflows and science goals - thus they should be approaching how to streamline and efficiently deploy storage, compute, software, etc (#12)
	+ working with the underlying educational providers (e.g. universities, etc) to better articulate what skills are needed for the workforce of tomorrow. A lot of time is spent re-training the next gen for the workforce, because they don't have the base set of skills. (#23)
		- This is probably more suitable for the yellow card (#33)
	+ (2) More collaborative software efforts, and the funding models that support this would bring the community together to develop common solutions and software adopted by a broader community (#25)
		- There needs to be a better incentive structure for developing useful software and open-sourcing tools to be shared among research groups. GitHub stars, literature citations, ... (#26)
	+ (1) SC level policy implementation to address issues/failures that encompasses SC user facilities and ASCR facilities (#30)
* What skills/knowledge does the end user require?
	+ The end-user may not have knowledge of the full end-to-end workflow complexity especially when it relates to data and compute performance outside their domain of expertise. (#10)
	+ (3) We should allow the scientists to focus on the science when possible. The best approach would be to ensuring that the science requirements can be properly articulated to the subject matter experts in the tech fields (networking, storage, software, compute) so that they can 'implement' in a manner that doesn't require as much bottom up training. (#24)
	+ Scientists should be trained in forward-thinking data management systems for archiving data and metadata, and making it searchable across the complex. One group's "garbage" may prove valuable to another effort (#27)
* What are the training/support requirements?
	+ Software training to develop new generations of codes in new architectures. These developments need to take place within user communities who understand the science/application the most. (#19)
	+ (3) Cross-facility support staff who can tell where a complex workflow spanning multiple physical sites has failed or has problems. Deeper connections between the facilities. (#29)
		- In a highly distributed environment, logs and error messages need to "bubble up" from various systems and be tracked as metadata for a particular analysis task. (#31)
	+ working with the underlying educational providers (e.g. universities, etc) to better articulate what skills are needed for the workforce of tomorrow. A lot of time is spent re-training the next gen for the workforce, because they don't have the base set of skills. (#32)

1.3 Day 1 Reflections

**The following participants have not been active:**
Bruce, Angie Lester, Line POuchard

**Brainstorm question or instruction:**
Day 1 Reflections
This area is for the Moderator to note key discussion points to summarize what was accomplished in Day one. Remember that day one is focused on Identifying a new technology or methodology and identifying the implications and possible consequences of it. The moderator can populate this individually at the end of the day or request input from the group here.

* 16. Unified Vision (summary)
There is a fabric integrating compute, networking, and storage services with producers of data from experimental and observational facilities across the Office of Science complex. This covers the full lifecycle of experimental, observational, and simulation data. Everything from experiment design, simulation/modelling, data reduction/processing, analysis/viz, and sharing/dissemination of data is facilitated by the "fabric":

1) Petabytes per Minute flow from computing, experimental, observational facilities (and highly distributed sensors) onto the fabric
2) A high-speed network links the experimental facilities, edge devices, clusters, super computers, and experimental facilities, blurring the edges between one system and the next
3) A distributed data warehouse with distributed cacheing infrastructure enables \*rapid\* query and retrieval of data across the complex without any concern for where it physically lives. The warehouse takes care of long term storage / FAIR data access / availability and durability of data / rich queries by metadata
4) The fabric is seamlessly accessible across the DOE through uniform auth/protocols/portals

Self-driving facilities enable scientists across the complex to programmatically access experimental data and computing through seamless interfaces for scientific discovery.

Computational agents can "subscribe" to data feeds with known/standardized structure on the fabric (e.g. tags = ["band\_gap", "perovskite"]), and perform pattern-detection/experiment steering on the fly.

Experimental facilities and highly connected, configurable, and automated scientific instruments and sensors have their own standardized APIs. Computational agents can autonomously design and submit interesting follow-up experiments based on the data feeds they are receiving. Humans only "tap in" where they have time / find interesting.

The landscape of compute hardware is incredibly diverse, with a variety of CPU architectures, accelerators, quantum computers, etc... sitting on the same "fabric". A highly-developed stack of Middleware and protocols enables data and compute to flow from "high-level" scientific scripts down to optimized low-level implementations. One kernel might map onto 18 CPU cores in Iowa or a quantum computer in Viriginia and the end-user doesn't really care!

On top of the lower-level abstractions and middleware, a rich set of science domain-specific libraries are built suiting the needs of diverse SC user audiences.

This fabric facilitates push-button analysis to end users in BES facilities: data movement, deployment of computing operations, and generation of results is transparent to the end user. If many FLOPs for a particular task are required (e.g. digital twin simulation), the needed resources "spin up" and link to the experiment in real time, without any user concerns of authentication, data movement, software environment, etc...
* 1. Self-driving automated AI driven facilities
* 2. Automated digital twin experiments run simultaneously at different sites
* 3. Ability for scientists to tap into data streams coming from experiments
* 4. An integrated and seamless computing experience for users throughout the Office of Science complex, extending the concept of what a supercomputer is to include edge computing and ESnet
* 5. New computing architectures will challenge ease of use
* 6. key concept: abstractions
* 7. Vision (Misha): fully-automated experimental science facilities enable researchers to programmatically control and "queue up" experiments with ease

Petabytes per minute worth of data from simulations and experiments flow through ESNet into a distributed data warehouse

Users belonging to any institution can instantly query and visualize datasets moments after they're collected, or "subscribe" to data events with particular characteristics (e.g. anything with "Xray-scattering" and "perovskites" or "DFT" and "band gaps") and feed them into their own models running locally

At the same time, autonomous RL agents running in DOE data centers around the country "subscribe" to the data feeds, identify patterns in the noise, and design NEW follow-up experiments to generate further data. The computational researchers use the "experimental facility" APIs to drive the work in a closed loop.

Hence, there are "loops" between computational agents, simulations, and live experiments distributed all over the DOE complex, with humans tapping in, intervening, controlling priorities, wherever they deem interesting.

The compute infrastructure is highly diverse, with a variety of CPU architectures, accelerators, quantum computers, etc... sitting on the same fabric. Layers of abstraction enable scientists to write "high-level" programs with minimal detailed knowledge of the hardware or implementation details. There are teams focused in 1) hardware-specific implementations and optimizations, 2) design of APIs and middleware, 3) higher-level libraries focused in specific domains
* 8. Vision: Develop a computational fabric that covers the full lifecycle of the data generated at the BES (or other) facilities. Facilitie everything from experiment design, simulation/modeling, data reduction/processing, analysis and interpretation, and sharing/dissemination of data.
* 9. Vision: Push-button experimental analysis that automatically moves the data, selects appropriate compute, and generates results.
* 10. Katie: Vision statement: Self-driving facilities that enable scientists from across the DOE SC complex to programmatically access experimental data and advanced computing through seamless interfaces for scientific discovery
* 11. Vision: Develop a computational fabric that covers the full lifecycle of the data generated at the BES (or other) facilities. Facilitie everything from experiment design, simulation/modeling, data reduction/processing, analysis and interpretation, and sharing/dissemination of data.
* 12. Jason Vision: The 'superficiality' of the future is roughly a 'cradle to grave' view of all aspects of scientific innovation. Starting at the experimental source - instruments/sources of data should be able to 'plug in' to the scientific back-plane in a unified way. That can/should be a high speed networked infrastructure, and intelligent software, that links all other resources. Resources that an instrument needs are roughly: long term storage and ability to share with others/move to where the data is most needed transparently, analysis/computational capabilities of a variety of types that can operate on the data (of an type/format) using a common language that is understood by all, and a set of policies that facilitate the use of these items. There is glue that holds it all together in form of software with well known/understood APIs that offer abstractions that facilitate growth and expansion and unburden the user from having to be an expert in any one piece of the infrastructure beyond their science. The end goal is being able to unburden the end user from having to worry about choices of 'how' computation/storage/data movement is accomplished, but rather provides an interface that can be easily interacted with to accomplish the end goals of data handling/manipulation.
* 13. On the BES facilities/user side, push-button, easy and transparent access to a data analysis resource (computing, network, data movement/storage), the ability to use large scale real-time computing for simulation (to feed an experiment while it is running and also for post-analysis), training of AI/ML, updating of AI/ML running in an experiment edge computing layer, and real-time feedback for users and/or AI/ML driven experiments. The goal should be to reduce the time to scientific insight and allow the users to focus on science, not the computing aspects of an experiment.
* 14. Vision (Sash) 1. Develop middleware and software to leverage the benefits of new computing architecture with applications suitable for different science needs of a versatile SC user group; 2. Create an interconnected ASCR compute/network facility with one interface; 3. Anticipate the growth in hardware and data in the experimental/observational facilities and provide a compute/network platform for these facilities, better integrating the broad SC user community
* 15. Vision: The premier research network in the world for open science that leverages highly connected, configurable, and automated scientific instruments and sensors, high performance computers, and curated data to accelerate learning that spans instruments, domains, and federal sectors to allow researchers to answer burning scientific questions by interrogating tightly coupled physical and digital worlds.

2 Day Two - November 5, 2020

2.1 Breakout 3 - Signposts

**The following participants have not been active:**
Angie Lester, Line POuchard

**Brainstorm question or instruction:**
Breakout 3 - Signposts
What we are looking for is technology or social trends that would give us clues that we are on the right track. o How would precursor technologies/services be identified? o What are the precursor technologies/services? o Is there a rank order for when specific technologies/services need to be available? o What DOE or Lab policies need to be in place now, in 5 years? o What facilities need to be in place now, in 5 years?

**Sticky points:**

 Top Takeaways (5 points per participant)

* 1. Some thoughts to get started: 1. Combined computing facility, 2. More clear interface with other SC user facilities, 3. Address the issue of changing computer architecture in the 10-20 time scale, Sash
* 2. Vision: Develop a computational fabric that covers the full lifecycle of the data generated at the BES (or other) facilities. Facilitie everything from experiment design, simulation/modeling, data reduction/processing, analysis and interpretation, and sharing/dissemination of data.
	+ Comments
	+ What you need to get there: Smarter, faster, better algorithms (AI/ML), scalable software libraries that can run on any architecture within the ASCR facilities, workflow and orchestration tools, seamless on-demand computing from the "blob" of ASCR facilities, adaptable network to interconnect all of this, discoverable data repositories (#3)
* 6. Early signposts: within the next 5 years Federated Identity between SC facilities will need to be ubiquitous
* 7. Network Related Signposts/Milestones:

 - Capacities that are orders of magnitude greater (e.g. 100Gbps today, 1Tbps in the 2-5 year mark, potentially Pbps in the future).

 - Ability to reserve allocations on a point to point (or multipoint) basis to ensure real-time requirements between resources

 - Adaptive networking protocols that are resilient to the current conditions, and responsive to the use cases

 - Ubiquitous capacity to all locations (domestic, International, and interstellar)

 - Well defined APIs/Usage models to link the underlying network resource, via software, to the overarching use cases (instruments, compute, storage)

 - Innovation unconstrained by location - being able to effectively use the components connected to a network without having to worry where they may exist
* 30. Mid-term sign-post: Integration of data services in the network to enable sensing, edge computing, caching and other services needed to enable seamless connections of various large and distributed facilities
* 8. Mid way sign post: Distributed and seamless data access available across all facilities (not data duplication, but metadata access from everywhere and fast transfer via ESnet)
* 9. an intentional approach to data curation
* 10. Early-ish signpost: APIs into computing facilities and exeperimental that facilitate scheduling of resources, real-time access, ability to query resources and interactivity at scale.
	+ Comments
	+ Finding early user cases and teams to partner with (#31)
* 11. Mid way sign-post: Ability to do an automated digital twin experiment
	+ Comments
	+ Requires -- seamless view of data at multiple site, descriptive and searchable metadata, (#32)
* 12. early-ish signpost: a highly configurable hardware and software infrastructure that allows the connection of varied service providing end points (instruments, sensors, computers, storage, portals, etc.).
* 13. Mid way sign posts: Sophisticated AI to be able to drive and control experiments at facilities and to determine what experiment or parameters to change
* 18. BES facility signpost: Transparent data analysis capable of analyzing data at its natural production rate that can feed AI/ML algorithms the information needed to effectively drive experiments.
* 14. Mid way: A burning scientific question that demonstrates the need for this future ecosystem and drives collaboration that spans communities and federal sectors.
* 15. Data Movement & Locality Singposts/Milestones:

 - Intelligent, efficient, and transparent staging of data where it is needed.

 - Software/hardware Tools that are capable and pluggable with instruments, storage and compute

 - Adaptive protocols that perform well despite network conditions or use cases

 - Security 'built in' to the use cases by default - e.g. integration on an end to end basis with whatever authentication, encryption, or other policy considerations that are needed

 - Tools that can scale with the data definition that is being manipulated (e.g. experience is the same for small and large volumes)
* 24. Identify distributed storage solution and mechanisms for data movement across the fabric of interconnected facilities.
* 16. Mid way sign post: Data provenance tracking mechanism
* 17. Early signpost: Updated policies and metrics for ASCR HPC facilities that expand the definition of 'capability' from only compute jobs that use a large number of nodes, to compute campaigns that utilize other unique capabilities such as tight coupling between experimental facilities or large amounts of data processing.
* 19. Idea: Develop middleware and software to leverage the benefits of new compute architecture with applications suitable for a diverse community of SC users.
-Short term signpost: Identify and assess the granualrity of existing user workflows. Group these different workflows with different science objectives into categories that have similar compute/network/data needs.
- Midterm signpost: For each of these groups, create middleware and software in collaboration between computer scientists and scientists from the user communities.
- Long term sign-posts: Use these platforms/hubs to build algorithms/codes that leverage future computing/network technologies and data processing techniques
* 20. mid-sign post: Policy: Agreement on how staff across facilities with handle support and trouble shooting
* 21. Early signpost: Prototypes to explore the solution space for particular workflows, drive new use cases, and demonstrate what's possible.
* 22. Mid way sign post: Highly optimized middleware/software for advanced and emerging architectures such that complexity is abstracted from end-users.
* 23. Software/API Abstraction Singposts/Milestones:

 - Training/education for SMEs on a given technology component such that they can fully understand the nuances of the technology, and expose a unified view to the 'layers' above to abstract away the nuances (ex: instrument wants to store data, uses API that figures out the best location to do so, way to stream across a network, way to stripe/divide among the storage resources, and catalogue/categorize so it can be found)

 - Updating the technology without changing the abstraction (hour-glass of common APIs)

 - Cross-agency adoption for common components (e.g. standards for data movement, data description)

 - Universal mechanisms to interact with a resource (e.g. a common way to store, analyze, simulate, locate)

 - Sensible cybersecurity posture and expectations

 - Identify management that is deeply ingrained, and well understood, across the entire mechanism
* 25. File management/data management tools to track data creation, movement, archiving, provenance
* 26. Idea: Create an interconected ASCR compute/network facility with one interface.
-Short term signpost: Identify policy implications, develop new policy.
-Midterm signpost: Develop and deploy federated ID.
-Long term goal: Incorporate the implications for the integrated system for future development and deployment of next generation large projects.
* 27. Transparent Data Access and data sharing: unformly implement FAIR data principles to metadata collection in order to capture data provenance
* 28. Idea: Anticipate growth in hardware/data needs in experimental/observational communities.
-Short term signpost: Identify the areas of growth in the various user facilities and curate a list of technological advances (e.g. data size and format, compute needs). Also identify gaps in the current HPC/data processing with these advances.
-Midterm signpost: Bridge the gap on the computation/data side in parallel with the technological development.
-Long term goal: A new user technology should be ready to be able to use the compute/network resources as soon as it comes online.
* 29. Computational Signposts/milestones:

 - Unified (via libraries, APIs) to interact with computation resources. Simplifies architectures, interconnects, localities (HPC vs. HTC)

 - Scheduling / finding resources on several potentially conflicting axes. Example: 'when' it is needed, 'where' it is available, 'what' type it may be, 'how' the choice may positively or negatively input others, and 'who' (what?) constraints may exist based on other components like storage, instruments, and networks.

 - Proper cyber posture (auth, policies) that are unified across the complex

 - Integrated accounting / measurement of all aspects
* 33. Dynamic orchestration of workflow components

2.2 Breakout 4 - Signpost Plausibility

**The following participants have not been active:**
\*fac- Nami, Angie Lester, INder Monga, Line POuchard

**Brainstorm question or instruction:**
Breakout 4 - Signpost Plausibility
Now that we have the list of signposts, the groups need to consider how plausible they are and what DOE needs to do to either ensure they happen or the implications of them not happening. o Who is actively working on these precursors? o When would these precursor technologies/services be needed? o What active or pending research programs need to be in place now? In 5 years? 10? o What existing or planned facilities need to be in place now? In 5 years? 10? o What software services or capabilities need to be in place now? In 5 years? 10? o How successful has the community been in meeting previous goals?

**Sticky points:**

 Top Takeaways (5 points per participant)

* 1. Policy related topics:
\* Need: more cross ASCR and SC facility investment in projects, workflows, and collaborations to incentivize and accelerate progress in this area.
\* Need: adjust policies and metrics for ASCR HPC facilities to align with goals supporting workflows from experimental facilities. (not just large jobs)
\* Need: Incentives to support crossfacility workflows, support and trouble shooting
\* In progress: Rich Carlson's DCDE work on Federated Identity for SC facilities -- team that is looking at Fed Identity policy and technology questions
\* In progress: Policy questions related to integrated facilities as part of Ben Brown's Integrated Research Task Force
	+ Comments
	+ A batch job queueing system is likely not the only way forward. To integrate well with bursty needs of experiments, we may consider other ways of accounting for resource usage and time sharing (e.g. a cloud utility model for some fraction of a system) (#12)
	+ Policy implications for security issues (#13)
	+ Policy on coordinated growth between user facilities and a combined ASCR compute/data/network facility (#14)
	+ A word on funding opportunities in computing at BES light sources. It was mentioned that HEP tends to be more curious about R&D in this space than the light sources. This is a direct result of how they are funded. Most of the development in the BES space is carved out of operations funding at the light source facilities. Very little is explicitly allocated to computing, unlike HEP. To make the leap, the BES facilities either need a large project to help boos their capabilities or we need to change the funding model to be more HEP like and specifically allocate funding for computing and data analytics. (#20)
		- This can be mentioned in topic 11. (#21)
* 2. Policy related topics: Super APIs
        \*Work to develop APIs that enable the pieces of the ecosystem to work together needs to begin now and should be developed as part of or in concert with specific prototypes to enable these workflows with input from users, facilities, and technology providers.
        \*These APIs must support configurability of a integrated fabric of varied instruments and sensors, computers, networks, and storage and a broad range of use cases that include analysis and visualization of data, real-time feedback, digital twins, etc.
        \*The APIs must serve as an abstraction for underlying and overarching technologies allowing them to be changed with our requiring major changes throughout the stack.
        \*When appropriate APIs should be standardized to allow broad adoption across workflows, communities and federal agencies.
        \*2-3 years: Develop prototypes that connect facilities and enable new workflows requiring instruments and analysis of data (ML/DL, tighter coupling of experimentation and simulation, real-time feedback loops). Established working groups to identify commonality and share experiences around prototype APIs
        \*5 years: Established standards for common APIs, Hardened APIs to support increased automation and intelligent analytics.
	+ Comments
	+ Work to develop APIs that enable the pieces of the ecosystem to work together needs to begin now and should be developed as part of or in concert with specific prototypes to enable these workflows with input from users, facilities, and technology providers. (#4)
	+ These APIs must support configurability of a integrated fabric of varied instruments and sensors, computers, networks, and storage and a broad range of use cases that include analysis and visualization of data, real-time feedback, digital twins, etc. (#6)
* 3. What existing or planned facilities need to be in place now? In 5 years? 10?

-Collaborative nodes: These facilities will act as hubs for direct collaboration between computing facilities and SC user communities. The facilities, likely virtual, will identify and categorize the computing/data/networking needs for user communities and act as brokers between high level workflows and architecturally diverse computing ecosystems.
                -5 years: Optimize user workflows with diverse scientific applications but similar compute/data/network needs.
               -10 years: Serve as the primary conduit for communication between user facilities and computing facilities for synchronous growth. The collaborative nodes will communicate the future needs of the user facilities to the ASCR facilities and notify the user community about the changes in the computing environment and how to leverage these changes to make new scientific discoveries that were previously untenable.
-Computing and user facilities: These are the existing facilities. They will incorporate input from the collaborative nodes for future growth plans.
	+ Comments
	+ Collaborative nodes to act as brokers between high-level workflows and architecturally diverse computing resources (#9)
	+ Linked to higher-level meta-facility APIs ("find me any resource for training a 200 GB tensorflow model with data streaming at 5 Tbps from LCLS") and lower-level facility APIs ("query idle nodes; launch container X and allocate N TB of buffer storage") (#10)
* 5. Auth & Cybersecurity

Now: early-adoption of FedID and gathering user/facility feedback from across the complex. Workflows that involve analysis of data from BES facilities on supercomputers exist TODAY and we should be focused on taking the patchwork of ad hoc schemes for Auth and data movement and trying to converge on some broadly usable standards.

5 years: Access to resources via FedID is supported at least in a "secondary" capacity by most BES and ASCR facilities. Discussions around a universally-accepted transport layer and how it will manage authentication/encryption, where certificates live, etc... need to begin

10 years: Universal adoption of FedID. By this point, a comprehensive hierarchy of DOE resources, user access levels and permissions, and administration tools is established. This Auth / permissions system is easily integrated with new Cross-facility APIs, which have settled on broadly usable abstraction layers for data transport and security.
* 7. 6. Automation and seamless access:
Need: research into scheduling: co-scheduling compute, data and bandwidth, API abstractions for submitting jobs into schedulers, ability for real-time scheduling while keeping system utilization high
Happening today: All ASCR HPC facilities are looking into facility integration, whether it is data access between facilities, portability between facilities.
Need: research into distributed filesystes, data management, curation and archiving that will support integrated facilities.
Need: Robust AI research program both to advance the way data is analyzed/filtered at experimental facilities as well as research into how AI can help facilities guide experiments and generate hypotheses
Need software development and research into composable and resuable workflow elements
* 8. Data Management related topics:
\* Need: Federated ID between SC facilities
\* Need: Transparent data access and data sharing, distributed and seamless data access available across all facilities (e.g. metadata access from everywhere and fast transfer via ESnet)
\* Need: Identify distributed storage solution and mechanisms for data movement across the fabric of interconnected facilities
\* Need: Intentional approach to data curation, uniformly implemented FAIR data principles to metadata collection to capture data provenance
\* Need: File management/data management tools to track data creation, movement, archiving, provenance
\* Need: Data Movement: intelligent, efficient, and transparent staging of data where it is needed. Adaptive protocols that perform well despite network condition or use cases. Tools that scale with data definition that is being manipulated
\* In Progress: XSWAP, ESnet, ECP…
\* In 5 years: Fed ID, Data provenance tracking mechanism, prototypes to explore the solution space for particular workflows, drive new use cases, demonstrate what’s possible. Hardware infrastructure to make “last mile” connection between EsNet and facilities. Software APIs to handle data movement in the last mile.
\* In 10 years: A highly configurable hardware and software infrastructure that allows the connection of varied services providing end points (instruments, sensors, computers, storage, portals, etc). Identify distributed storage solution and mechanisms for data movement across the fabric of interconnected facilities.
* 11. What active or pending research programs need to be in place now? In 5 years? 10?
- Now: Rich Carlson's DCDE work on Federated Identity for SC facilities. Ben's Integrate Research Task Force
-5 years: Instrument to compute integration, direct integration of compute funding for light source grants.
-BES AI/ML for SUF's award
- DISCUS project
- ECP ExaFEL
	+ Comments
	+ BES AI/ML for SUF's Awards (#15)
	+ BES light source proposed DISCUS project (or something like it) resembles what we have talked about. (#16)
	+ ECP ExaFEL (#17)
* 18. Networking related topics:

Now-10:
 - multiple 100s of Gbps wide and local area networking
 - Experimentation in bandwidth reservation
 - Experimentation with next-gen transport protocols (BBR, etc)
 - Facility to facility capacity increases
 - Emerging 'network APIs' to allocate resources

10-20:
 - Ubiquitous Capacity of 1Tbps
 - Manually and guided scheduling of large flows between resources
 - Plugable dynamic networking protocols that facilitate large flows and use cases
 - End-system direct connections to scientific networking back-plane/network
 - User-controlled network slices via well defined APIs

30+:
 - Ubiquitous Capacity of Pbps
 - Dynamically/automatically allocated bandwidth based on usage of resources (instruments, storage, compute)
 - New networking paradigms beyond TCP/IP
 - Ubiquitous networking (domestic, international, interstellar.
 - Full data abstractions to interact with infrastructure connected to networks
	+ Comments
	+ Quantum network/wireless (#19)
* 22. Data Movement and Locality topics:

Now-10:
 - Measurement/monitoring to indicate bet approaches to migrate and place data sets, and made available to operations teams
 - Improved streaming and bulk data movement tools that can be easily integrated with other members of the workflow/software/middleware stack.
 - Unified way to manage federated identify across a network between different storage systems

10-20:
 - Intelligent caching and placement routines that can automatically understand access patterns for data sets.
 - Seamless integration between the data movement hardware, software and storage systems - remove the need to have to choose which tools to use.
 - Easily pluggable cybersecurity/privacy policies that link the data movement tools and the storage systems

30+:
 - Dynamic and automatic data placement based on ML/AI that consumes measurement/monitoring data to better influence choices of data locality
 - Fully automated transfer of data between storage locations, that integrates with the computational (analysis, simulation) portions of the workflow
* 23. Seamless access to computing: combined computing facility
\* Need Distributed and seamless data access across facilities
\* Need Facility APIs
- APIs into computing facilities and experiments that facilitate scheduling of resources, real-time access, ability to query resources and interactivity at scale.
- Create and interconnected ASCR compute/network facility with one interface
- 5 year: Identify policty implications, develop new policy
- 5 - 10 year: Develop and deploy federated ID
- 10+ years: Incorporate the implications for the integrated system for future development and deployment of next generation large projects.
- Address the issue of changing computer architecture in the 10 - 20 timescale
- Need clear interfaces with other SC user facilities
- Develop a computational fabric that covers full lifecycle of the data generated at SC facilities
- Facilitate experiment design
- Simulation/modeling
- Data reduction/processing
- Analysis, interpretation
- Sharing/dissemination of data
- Enables: transparent data analysis capable of analyzing data at its natural production rate that can feed AI/ML algorithms the information needed to effectively drive experiments.
- Dynamic Workflow and Orchestration Tools
- Anticipate growth in hardware/data needs in experimental/observational communities
- work to develop a roadmap
\* 5 years:
- Prototypes to explore thes olution space for particular workflows, drive new use cases, and demonstrate what’s possible.
\* 10 years:
- Highly optimized middleware/software for advanced and emerging architectures such that complexity is abstract from end-users
- highly configurable hardware and software infrastructure that allows the connection of varied service providing endpoints (instruments, sensors, computers, storage, protals, etc).
	+ Comments
	+ Additional points: (#25)
	+ - Computational signposts/milestones: - unified (via libraries, APIs) to interact with computation resources. Simplifies architectures, interconnects, local (HPC vs. HTC) - Scheduling/finding resources on several potentially conflicting axes. - Proper cyber posture (auth, policies), unified across the complex) - Integrated accounting/measurement of all aspects. - Dynamic orchestration of workflow components. (#26)
* 24. Early signposts: within the next 5 years Federated Identity between SC facilities will need to be ubiquitous