Group #10: Community of Interest on the Future of Scientific Methodologies

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| Date | November 2, 2020 |

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| Participants |
| Jeffrey Vetter | Lee |
| Angie Lester - MS | Alex Aiken |
| Bruce | fac- Nami Ishihara |
| Bruce Hendrickson | Sarp Oral |
| Wahid Bhimji | Martin Foltin |
| Nathan Tallent | Sonia Sachs |
| Lee Ann Kiser | Hal Finkel |
| Rajeev Thakur | Richard Gerber |
| madeleine glick |

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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:**
Lee, Bruce Hendrickson, Lee Ann Kiser, Angie Lester - MS

**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?
	+ (2) How to scalably connect the resources? (#1)
		- (2) new(ish) interconnect technologies such as photonic interconnects can aid with data movement for higher bandwidth connectivity and flexibility for reconfiguration. Reconfiguration at runtime will still be affected by global/local questions of data transfer economics. (#43)
		- (2) How extreme can disaggregation go - are there physical limits (#2)
			* local or global disaggregation (#31)
			* (1) Moving data is expense (#36)
				+ will there be technologies to make it less so ? Currently data movement does mean compute is done near data in some cases but also still can be global - do we need workflows that allow for passing around data effectively. (Data sets seem to be outgrowing improvements in technology) (#39)

The expense of data movement, at all scales, is going to drive a lot of heterogeneity in the hardware. (#40)

* + (5) In 30 years, commercially available cloud computing will be highly mature, economically priced, and accessible through super-fast networks. As a result, DOE labs will need to reconsider whether they should host large-scale computing facilities on site as they do today, for both capacity and capability computing. Instead, an alternate role for facilities at the labs 30 years from now could be to host testbeds for exploring futuristic technologies, beyond what is commercially available at that time, perhaps in areas such as quantum, neuromorphic, and bio-inspired computing. (#5)
		- How does DOE fit into the ecosytem? Does "production" computing go to the commercial space? (#11)
		- (1) How can we continue growing compute capabilities given the constraints? (#7)
		- Can we utilize resources across cloud and the testbeds - what barriers need to be overcome? (#24)
	+ (1) Multiple technologies are needed to continue growth of capability because of power constraints (#3)
		- (2) Power constraints guarantee that there will not be a single computing or memory device: there will be a variety of compute devices and memory devices. Fundamentally people will not be able to learn to program all of this hardware "by hand" --- the software will have to be written at a higher level of abstraction than today to enable portability and the ability to target all of the different technologies. (Alex) (#4)
	+ (2) Over the next decades, what we currently consider the breakdown between computing hardware, reconfigurable hardware, and software may change. As AI drives hardware and software implementation, we will have a new set of challenges going forward. (#10)
		- what will be requirements to aim for? (#8)
	+ (2) The rate of evolution of the hardware, at least for the next decade, will actually be faster than it has been in the past. How will application development keep up? (Alex) (#12)
		- (4) Current software and workflows are ill equipped to deal with heterogeneity. (#13)
			* (1) DOE needs to focus on software for heterogeneous computing. (#9)
			* How to mix and match at runtime? HW/SW (#6)
			* Easier programming methodologies. High-level abstractions. (#45)
		- One major challenge is in the verification of hardware, both in terms of logic complexity and in terms of physical aspects of the design (power, resilience, etc.). It will be interesting to see if future technologies can make this verification process more scalable and faster. (#17)
		- Will "general purpose" computing system still be preeminent? (#34)
			* (4) How does quantum computing fit into the DOE ecosystem? (#16)
				+ there are several comments about the constraints; should we think about these more specifically regarding the technologies and methodologies and also the time scales and commercialization (#22)
	+ (1) Is there a shift for ASCR to focus on other aspects of 'advanced' (other than extreme scale) (e.g. extreme disaggregation ) - if industry is not going to tackle these. (And is industry going to tackle whats needed) (#14)
		- Great observation. Think can be combined with other similar ones. (#23)
	+ (2) How does DOE/HPC community plan for unknown or unthinkable (today) technology advances? (#15)
	+ Will DOE leadership move from leadership at scale to leadership identifying and enabling emerging technologies, then handing off to the commercial space? (#37)
		- (1) How do define leadership in 20 30 years? (#38)
* Who would develop it (basic research to advanced deployment)?
	+ DOE labs in collaboration with academia and industry. (#18)
	+ If you're talking about 30-40 years basic research should be involved, industry could change quite a bit in that time scale (#33)
	+ Who develops and maintains the tools and infrastructure needed to support usable heterogeneous/disaggreated systems? (#44)
* Who would use it and what skills would they need to use it effectively?
	+ DOE computational scientists and their collaborators in academia and industry. HPC programming skills are needed. (#19)
	+ breaking down of some hw/sw silos may be needed in skills to effectively implement the systems (#25)
	+ Will community apps, workflow, frameworks replace the Fortran/C/C++ type programmers? Julia? DSLs? AI frameworks? (#28)
	+ Will "quantum computing" facilities operate more like an experimental facility, e.g. light source? Would imply a different skill set. (#30)
	+ how do we abstract out the data movement aspects into a framework (#41)
	+ Usability is a key aspect to future systems. As software becomes more complicated, and hardware becomes more complicated, and with disaggregation and more-complicated data movement, we need programming environments that can help users more-productively make use of the systems. Otherwise, people will not be able to make sufficient use of the systems. (#42)
* When would it be expected to be in production use (N years in the future)?
	+ It is already available but will grow and become more heterogeneous over the years. (#21)
	+ Already starting now - so presumably will grow. But actually maybe over 30 years it could change to being less heterogeneous (!) (#26)
	+ it is only beginning to be available, scalability for 30-40 years will be a question, new technologies will need time to be developed and made commercial (#27)
* Where, and how widely, would it be deployed?
	+ DOE labs and commercial cloud providers. (#20)
	+ edge? (#29)
* What is the setup time and/or process for using it?
	+ What is the process for programming these kind of system of the future going to look like (see also green box) (#32)
	+ (1) how to schedule resources across multiple resources (disaggregated)? Automated workflow decomposition and resource mapping? (#35)

1.2 Breakout 2 - Implications of this Problem.

Participants: 0

**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?
	+ Local and global disaggregation ; data movement etc (#1)
		- low latency interconnect (also requires hardware and software integration to be developed) (#8)
			* photonics - both local and global (#28)
		- Tools to match data to appropriate (globally) disaggregated resources (#12)
			* also need runtime aspects to this (see below) (#16)
	+ Cloud computing and role of DoE HPC facilities (#2)
		- Integration/interoperability of DOE HPC and Cloud computing (#7)
	+ Hardware integration and software (#3)
		- programming abstractions --- how will we write code that can span the range of hardware that will be available? (#14)
		- Runtime, scheduling and workflow orchestration tools (#15)
			* Optimizing extremely disagregated resources might need new techniques (#18)
			* Higher level "natural language" type tools; or automation (#17)
				+ Validation and reproducibility approaches in these newer scenarios (#19)
		- Software and frameworks that deal with heterogeneity (#9)
		- Tools for performance characterization and mapping different problem types to different heterogeneous environments. (#10)
			* Performance portability tools and software (#6)
				+ A way to match computational/scientific problem with most appropriate type of resource(s) (#11)
		- High-level program synthesis tools (#4)
		- Compilers are a key question - can produce the hardware more easily than software tools - time to mature for sw is a decade while hardware moving faster currently. E.g. not even GPU yet and now have AI acclerators (#23)
			* Automate development of software stack (#24)
			* Big divide between local and distributed (#25)
		- does ubiquitous photonics at silicon photonics scale - does it radically enable new system design (#29)
			* need different software tools again (#30)
			* reallocate at run time - need switching (#31)
				+ reconfigurable systems (#32)
	+ DOE leadership and role of ASCR (#5)
	+ Use and integration with Quantum Computing or similar (#13)
	+ highly distributed sensor + computing large scale edge computing and their place in disaggregated heterogeneous computing environments of the future? (#21)
	+ For 'data science' how can one bring central data stores with compute distributed resources.. in a way that is as easy as a pandas data frame.. (#22)
	+ data science a field of its own - "computational statistics" (#26)
		- will it subsume all CS ? (#27)
	+ Research area: Designing (extreme disaggregated) hardware to match program rather than vice-versa (#33)
* Who is/will develop this companion technology/service?
* What skills/knowledge does the end user require?
* What are the training/support requirements?

1.3 Day 1 Reflections

Participants: 0

**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.

2 Day Two - November 5, 2020

2.1 Breakout 3 - Signposts

Participants: 0

**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. [Wahid] A few of my notes from last time https://docs.google.com/document/d/1pFA3I2TlUa0v-C0jJ56-Nr5DOjJxq1U8BViTTAYjtV0/edit (See the meeting sphere for the original words)
* 3. We will have an on-demand extreme scale virtual “megacomputer” as a collection of distributed disaggregated advanced computing resources to solve dynamic and pressing societal problems. Our current infrastructure is always a result of our past planning, procurement, deployment and will always need to play catch up with the pressing needs of the challenges we as a society face today.
* 4. Vision Discussion:
[Wahid’s summary stab] Globally disaggregated computing delivering for science, incorporating diverse advanced architectures at DoE centers alongside cloud providers and edge computing at instruments, with “Higher level” workflow tools automation and compilers to dynamically and effectively exploit this infrastructure
[Are we actually asked to imagine this exists -> what would it enable]
We could put computing “everywhere” and then reconfigure whatever we needed at that moment
Agent that matches your computation to the most appropriate resource.
Understand what resources are available in the system and determine what are appropriate for a problem and configure appropriately

[Edge Computing] Balance of computing at scientific facilities / instruments and compute facilities.

Sudden provisioning of appropriate computing on massive scale to tackle a problem - e.g. track a hurricane
Could solve problems that are not possible today because we can “borrow” compute capability on demand - extreme scalability - “beyond cloud”
Whole resources on the planet - (and beyond!)
Does distribution of technology go beyond earth

We will have an on-demand extreme scale virtual “megacomputer” as a collection of distributed disaggregated advanced computing resources to solve dynamic and pressing societal problems. Our current infrastructure is always a result of our past planning, procurement, deployment and will always need to play catch up with the pressing needs of the challenges we as a society face today.
* 5. Signpost discussion
Faster than light communication!
Need for low latency /high bandwidth interconnects within campus but also wider do we need a wireless
Latency tolerant algorithms
Appropriate memory semantic model
What is the programming model ; can we have a hierarchical model
Hierarchy of abstractions
How to modify and distribute workload to ensure data locality to device (templates?)
Management at scale and provisioning - extending microservices based architecture to these diverse and distributed resources.
Security - how to make it resilient in this distributed environment.
Privacy preserving algorithms
Standards for device interfaces for a heterogeneous computing environment
DOE might be the seeder of standardization for access
Commercial bodies need to follow
International standards body might needed
Power: feasibility of designs- e.g. for optics

5 year ideas - prototype small-scale implementation of this vision
More collaborative use of edge resource and supercomputing
Solve a “grand challenge” problem on such resource

Low- Latency:
Need to reduce everything that causes latency
Compression and reduction algorithms
Data-reduction by better use of metadata
Some sort of optical communication - doesn’t have to be limited to fiber ..
Business model:
‘Incentivising’ edge resources to contribute
E.g. solar selling back power
Possible blockchain type model that allows indemnification of who contributed and compensation
AWS of the future harvesting these consumer resources and DoE could tap into this - DoE could build sw and abstractions to make this viable.

Security / resilience:
Allow private compute contributions through encoding of the data and operation on that data. Research exists - not unresolvable. (e.g., homomorphic encryption)
* 6. Google doc is primary source now : https://docs.google.com/document/d/1pFA3I2TlUa0v-C0jJ56-Nr5DOjJxq1U8BViTTAYjtV0/edit

2.2 Breakout 4 - Signpost Plausibility

Participants: 0

**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. Plausibility

5 year ideas - prototype small-scale implementation of this vision
More collaborative use of edge resource and supercomputing
Solve a “grand challenge” problem on such resource

Address need for tools for workload orchestration on heterogeneous resources
Going beyond current k8s or grid specification
Automatically find place for different components
Current approaches are essentially sophisticated batch scheduler.. Doesn’t inspect task and optimize for data locality.
Need to decompose workloads.
Scavenge resources
Was some work on creating virtual supercomputer - didn’t tackle problem of different latencies.
Faster (than light) communication / low-latency goal
Can come after the workflow piece; but don’t leave too far in the future
can change capability e.g. move I/O to memory like semantics
Disaggregating memory from compute
Existing projects with photonics
Enables new optimizations - eg. large pool of memory distributed on different devices but accessed through low latency interconnect for precomputed results.
Integrated photonics directly on the asic
Questions of flow control and protocols and interfaces - potentially interdisciplinary and a blocker
More work needed

Smarter memory
Doing compute without having to transfer back to computing device .
Eg. AI accelerators - possible single device
Frameworks and compilers and software paradigm needed
Have seen abstractions eg. in matlab
Code generation
Important to partition problem to exploit data locality even with advanced interconnects

How are the incremental vision of integrating DoE edge-computing and HPC be leveraged as a foundation of something more disruptive hive “metacomputer” vision
Existing projects on optical compute to memory and storage
Currently expensive and barriers to commercial success
Going beyond a single machine room - gets beyond the hardware
Practical examples in high-energy physics and biology - currently take latency hit in moving off instrument for collaboration access; data structures designed for sharing rather than individual analysis
Edge computing has a couple of meaning of both on-instrument “trigger” like and as well as computing at science facilities
Software defined architectures - could work with microservices, in partitioned larger compute ..- need lightweight virtualization - e.g. used in aeronautics
People looking also in software defined networking for photonics
Federated computing - e.g. for distributed swarm AI learning (can’t have all data in one areas)

How would this change science facilities - e.g. making experimental facility 10% more efficient then huge win. E.g. running simulations while experiment running
Might mean compute resources close to the science facilities.
Does degradation have a role to play - should we have centralized resource.
Reliability - When one microservice dies another starts up
* 2. Time line excel sheet https://docs.google.com/spreadsheets/d/140xTjUmH6IsfsSJhk\_Yb7MJI0piAAwFaaIAYJIy2c7s/edit#gid=0

3 Day Three - November 10, 2020

3.1 Breakout 5 - Pitfalls and Roadblocks

Participants: 0

**Brainstorm question or instruction:**
Breakout 5 - Pitfalls and Roadblocks
Detailed discussions on identifying pitfalls and potential roadblocks. If possible, list in rank ordering. o What could prevent the technology/service/device from being developed (funding, materials, policies, researchers, operations staff, etc.)? o How will progress be measured/evaluated? o How will lack of progress be measured/evaluated? o Who will decide if progress is being made? o What are the consequences of not engaging in this area?

**Sticky points:**

 Top Takeaways (5 points per participant)

3.2 Breakout 6 - Keys to Success

Participants: 0

**Brainstorm question or instruction:**
Breakout 6 - Keys to Success
Identify who needs to be engaged, research communities, domain science communities, staff, management. Identify needed skills and knowledge (give examples) o What benefits would society obtain? o What benefits would the science/research community obtain? o What research communities need to be involved? o What domain science communities need to be involved? o What staff and management communities need to be involved? o What kind of management structure is required? o How broadly will this impact society and/or the science community?

**Sticky points:**

 Top Takeaways (5 points per participant)