Community of Interest on Future Scientific Methodologies

A Curated Unconference

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Envisioning the Future of Computing in DOE/SC

March 2020 – Charge from ASCR AD to run a workshop in May 2020 on the Future of Computing in the DOE/SC complex

Co-chairs identified and organizing committee quickly established

In-person meeting delayed several times and finally run as a virtual meeting in November 2020

The challenge was to get the community to speculate on possible futures while grounding them in today's reality

Meeting the challenge

"It's tough to make predictions, especially about the future" – *Yogi Berra*

Some definitions:

- **Speculation**: The forming of a theory or conjecture without firm evidence – *Oxford Languages*
- **Unconference**: A meeting where the agenda is created by the attendees at the beginning of that meeting
- **Curated Unconference**: Topics and structures are collected by potential participants prior to the event
- **Vignette**: A brief evocative description, account, or episode – *Oxford Languages*

Vignettes – the key insight

Imagine it is 1900 and you are invited to a major national conference to discuss the future of the U.S. transportation system. Presentations and discussions focus on trains, steam, and the need for coordinated time. Near the end of the conference, you stand up and state “The future of transportation will be linked to the AIRPLANE!”

This vignette was used to motivate the attendees to speculate about potential futures, unconstrained by ‘how we get there’ while grounded by ‘their experience and knowledge’.

Meeting structure

- The meeting was originally planned for in-person
  - Pivot to Zoom was a challenge for an unconference
- Format was small groups led by facilitators from the community
  - BetterMeetings provided professional facilitation, advice, and training
  - ORISE provided logistical support for Zoom and a data collection tool
- A pre-meeting process was used to gather ideas for the groups
- Unconference was held over three days in November 2020
  - Spacing allowed for some modest course corrections based on feedback
  - Roughly 150 participants per day in 15 groups
  - Each group engaged in structured activities: brainstorming, collecting information, voting on ideas
  - At end, the facilitators summarized the group work as a vignette

Keys to success: Curated Topics

Tomorrowland Vision

- What technological advance could cause a dramatic shift in how science is conducted?

Interfaces of the Future

- How will scientists and computer-based agents interact, communicate, and change facility operations (self-driving), and workforce training and development?

Computing Facilities of the Future

- How will scientific data be generated and managed in a global computation fabric?

Future Scientific Methodologies

- How will DOE user facilities work in concert to undertake multidisciplinary challenges?

Future Missions

- How will scientific discovery and societal imperatives change the mission of DOE?

Illustrative vignettes

Tomorrowland Vision: What technological advance could cause a dramatic shift in how science is conducted?

A climate scientist reviews the latest kilometer-resolution continental carbon flux data from the North America Eco Fabric. The millions of powerful fingernail-sized sensors, artificial intelligence (AI) chips, and wireless devices—costing pennies and consuming milliwatts—that make up the fabric are the result of recent neuromorphic computing breakthroughs at the national labs. It looks like the new microbes that she seeded in the tundra had reduced methane emissions by 90%!

Interfaces of the Future: How will scientists and computer-based agents interact, communicate, and change facility operations (self-driving), and workforce training and development?

Before retiring for the night, the nano-materials scientist explains to the smart self-driving facility (SDF) his idea for a new super-efficient and environmentally friendly catalyst. The SDF immediately starts to translate his expressed goals, intent, and strategies into autonomous exploration. The routine setup and troubleshooting steps that used to consume so much time between successive phases of discovery on different experimental apparatus are no longer his concern: They execute silently behind the scenes, refining his hypothesis while he sleeps.

Moderators' Session Roadmap

General Phases and Duration

Coming Together	Idea Generation	Deciding & Concluding
20-25 min	30-40 min	10 min

Specific Steps for 90-minute Sessions

Use these as a guide but allow for more or less time as you feel benefits your group.

								
Arriving Getting settled	**Intros** Who's in the room? 1 min intros	**Recap** What have we already done?	**1st Thoughts** Each person shares initial thoughts for 1 min.	**Brainstorm - Part I** Everyone quietly enters their own ideas in Meeting Sphere.	**Break**	**Brainstorm - Part II** Open, facilitated discussion; also continue to enter group/personal thoughts in Meeting Sphere. (Make sure someone is typing in the group's thoughts.)	**Voting** Choose top ideas in the Meeting Sphere boxes; discuss, time permitting.	**Wrap-up** Record your thoughts.
5 min	**10 min**	**5-10 min**	**5-10 min**	**10 min**	**5 min**	**15 min**	**5min**	**5 min**

Day 1	
Identify new technology or methodology	Implications and possible consequences

Day 2	
Signposts or milestones of progress	Signpost plausibility; programs to be run

Day 3	
Pitfalls and roadblocks preventing the goal	Identify the keys to ensure success

Leadership team

- Amber Boehnlein (JLAB)
- Ian Foster (ANL)

- Jim Ahrens (LLNL)
- Joshua Elliott (DARPA)
- Kjiersten Fagnan (LBNL)
- Nicola Ferrier (ANL)
- Dan Ratner (SLAC)
- John Shalf (LBNL)

Rich Carlson (DOE, ASCR)

Facilitators

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Outcomes

Final report to be posted after DOE review

Contents

Nine scenarios for possible futures

Smart self-driving facilities automate experimentation	Experimental facilities are automated, scaled, and enriched with AI to the extent that they can work as collaborative partners with researchers.
A representative workforce turbocharges the labs	New practices allow DOE labs both to recruit and retain a broader range of talents and to flourish in an era of decentralized, collaborative work.
The theory machine transforms science	Construction of a universal theory machine means that a global knowledge map rapidly ingests new data and findings.
Linked facilities form a discovery cloud	Seamless, petabyte-per-second integration of all DOE facilities into a unified whole enables science at unprecedented scale and speed.
New missions drive new modes of working	A focus on societal grand challenges drives increasingly ambitious, multi-disciplinary, and integrated team-based science.
A universal data service make all data easily accessible	Online access to all data and the automated maintenance of organizing maps create a universal library of known facts, exploratory principles, and hypotheses.
Science in a world of purpose-built computers	Computational power is enhanced by orders of magnitude because scientists can rapidly design and create customized computer systems to solve specific problems.
Every system has its doppelgänger	Ubiquitous availability of digital twins for both research tools and the objects of research reduce the cost, time, and risk associated with experimental campaigns.
Delphi: The universal knowledge map	AI methods capable of interpreting the scientific literature make predictions of future developments possible.

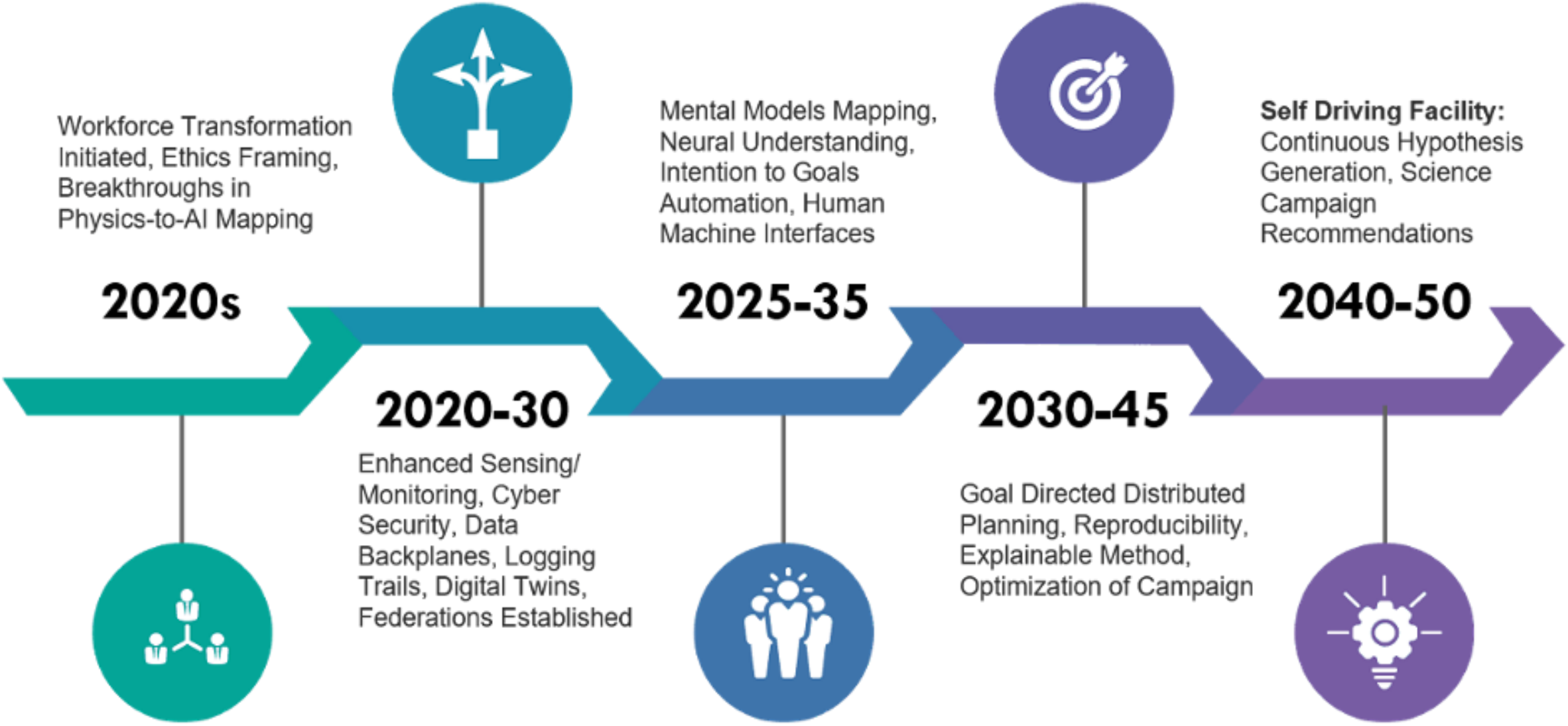
Smart self-driving facilities automate experimentation

In 2050, advances in automation and AI allow tasks that previously required extensive, time-consuming human labor (e.g., synthesizing materials, configuring and managing experiments) to proceed without direct human engagement.

A nano-scientist lets the facility drive. *Jane, a nano-materials electron microscopist, hits send on her latest nano-material design, dispatching it to the smart self-driving facility (SDF) along with a high-level statement of what she wants to know. The SDF immediately begins translating her goals, intent, and exploration into an autonomous exploration program. The mundane procedural steps between successive phases of discovery at the set of microscopes are no longer her concern—all are executed silently behind the scenes by the instruments, data backplanes, and control loops. Bits fly between sensors, AI inferencers, and the massive physics-informed AI trainers that pull in the sum of all knowledge from science corpora. Analysis suggests that the atomic defect patterns require a higher resolution probe with a different modality to explore a new catalysis action. Jane, impressed by how the SDF has expanded upon her ideas, approves the new plan with suggestions for further improvements.*

The sample is moved automatically to a beamline and queued along with parallel campaigns. With upgradeable AI packed into robotic interfaces, the SDF makes autonomous decisions on the configuration of the microscope and sends a cross-facility and inter-organization request to its sister facility in the federation to establish a distributed plan for the next phase of the campaign.

Potential signposts for self-driving facilities



From speculation to reality

- Unconference participants were asked to **speculate** (to “form a theory or conjecture without firm evidence”)
- The process spurred much creative thinking by an eclectic group on new ways of working, and implications for the labs and society
- The material captured for each of the nine “scenarios for possible futures” could form the basis for more focused BRN activities

Lessons learned

- This was not an easy process! It was hard, and a lot of work
- Participants seemed to enjoy this opportunity to engage in such forward-looking conversations, unconstrained by need for BRNs
- The substantial preparation, and assistance of external facilitators, helped a great deal
- While conversations ranged widely, and not all proved "productive," the process identified areas that could be pursued further