Group #4: Community of Interest on the Future of Scientific Methodologies

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| --- | --- |
| Date | November 2, 2020 |

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| Arjun Shankar | Harriet Kung |
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| Dantong Yu | Dan Ratner |
| Lavanya Ramakrishnan | Dmitry Liakh |
| Josh Greenberg | Ben Brown |
| Ramana Madupu | Huolin Xin |
| Kerstin Kleese van Dam | \*fac- Nami Ishihara |
| Tekin Bicer (ANL, Computer Scientist) | Nicola Ferrier |
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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:**  
Nicola Ferrier

**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?
  + (4) A key challenge is how will all these pieces be integrated. (#27)
    - I think this is one of the key places where humans will need to stay in the loop. Which potentially poses a problem: if the "AI" designs the experiment, how will we know what needs to be checked or what to watch out for. This points to how we train scientists and users. (#68)
  + (4) Composability and dynamic configurability of autonomous facilities to address specific scientific discovery problems: - How to compose, configure and deploy an autonomous scientific discovery solution (HPC + AI + Experiment) based on pre-existing building blocks and capabilities effectively and efficiently; - How to translate the high-level description of the scientific problem into the specific design of an autonomous facility which will be able to solve that problem; - How to convert back the knowledge gained by the AI analysis into useful scientific concepts (interpretability); - How to make this automated workflow reproducible; (#13)
    - How do we combine facilities ad hoc throughout an experiment to maximize the scientific outcome? (#5)
      * Too much manual involvement required currently. We need autonomous coordination. (#30)
        + yes (#49)
  + (4) Digital twins help in the in silico planning/operations of these campaigns. A way of thinking about the forward space. (#15)
  + (3) AFs need more from users.. Hypothesis generation needs to be more rigorous. (#3)
    - Successful AFs would also likely rely on rich and smart interfaces with users, to avoid the "black box" effect and enable (i) failure / gap identification by experts, and (ii) build confidence with "regular" user. (#22)
    - How do we capture and express hypothesis in a form that is understandable to both machines and humans, how do we ensure our 'mental models' align. (#51)
  + (3) Future is inverse design. (#9)
    - This goes for me towards the experimental design tool, I want to achieve X, what do I need to do to get there. (#61)
    - Configuring and training the autonomous facility (HPC+AI+Experiment) to be able to solve the given inverse design problem. (#66)
  + (3) Integrated experimental design process from the users perspective - design experiment in sillico (optimal experimental design) incl. combination of facilities needed, how they interact, what your scientific goals is etc. This can be test run in a simulation (digital twin), which also accompany the actual experiment it self. Once tested the experiment can be resourced and executed. From the facilities perspective - automated execution of experiments, optimized resource allocation that avoids complex switches and coordinates with other facilities schedules if needed (an optimization problem) - Facilities and users need to work together during the experiment to react to unexpected occurances. (#37)
    - (1) I picture something like one github repo for an experiment+facility. All changes are tracked from day 0. (#67)
  + (2) Standardization between compute facilities (#12)
    - Also Comment 69 applies here. (#136)
  + (2) Interoperability between sub-fields. (#11)
    - Establishing data formats and access is paramount for this interoperability (#20)
    - Standardized extensible interoperability interfaces and protocols (e.g., autonomous facility microservices). (#69)
  + (2) How do we capture and express hypothesis in a form that is understandable to both machines and humans, how do we ensure our 'mental models' align. (#45)
    - symbolic regression is re-emerging recently that may help with this. (#65)
  + (1) How to map intention to the facility? (#2)
  + (1) Need to connect to the full scientific process. SciFi version: what if you could type question into google - and fully design of the experiment as output. (Incl. where to point telescope, data analysis, etc.) (#4)
  + (1) We don't know yet where the mental model breaks down? Where is the HIL issue? Abstraction failure modes, etc. are important. (#6)
    - Given the complexity of the experiments and scientific goals, there is a question is we can sufficiently express our mental models (#54)
  + (1) Lots of downtime in facilities. (#7)
  + (1) Using different facilities to solve different problems. (#10)
    - Connecting instruments to other (non-compute) instruments (neutron instrument to electron microscope or 3D printer) is as important as connecting instruments to computers (#75)
  + Sub-fields get connected over time and work with each other. (#14)
  + (1) A tool that knows all the past literature and makes expert recommendations. (#16)
    - Is there a risk then to miss creative thinking / design, and end up in "closed" loops of repeating what has been done before ? (#34)
      * I think it can be helpful in identifying things that have already been done, or areas where scientific opinions clash. However, yes there is a risk in saying I don't pursue this further as other have already done this or have already failed. On the other hand it could lead to more rigorous testing of hypothesis before the real work starts. (#64)
  + (1) The problem is that data complexity and nuance of science challenges (for discovery) is hindered by lack of precision in experimental design and operation. We need systems that carry us forward from the design phase into the execution phase of expt.'s. (#17)
    - The methodology will likely involve whatever the future version of AI. Each aspect of an experiment --- hypothesis generation, simulation (theory), operation (data-taking), analysis --- will benefit from something like AI for increased automation. (#25)
      * (1) Yes, and uncertainty quantification/checking would be important. What if the AI model is wrong? Who will discover it? How will it be fixed? (#31)
        + Does this become a key skill / expertise that is needed in each AF, i.e. a domain-expert who also understands AI and can identify and fix these instances ? (#42)
  + (1) Scientist kick off the question.. intelligent machines will iterate and pose new questions. (#76)
  + (1) Can we refine/define self-driving better? What is self-driving vs. assisted driving? (#77)
  + (1) What feedback to give the human? (#81)
    - (1) We should be working in earnest with socio-tech-anthro processes.. we know less about the narratives. Mental models mapping. (#82)
  + Tool can tell us what the gaps are. (#8)
  + What is the role of the researcher if the labs are self driving? Self driving cars will not have drivers, just passenger. (#23)
  + Tried to respond to #5. One subcategory of #5 is the integration with compute facilities with experimental facilities to enable autonomous experimentation. (#63)
  + what are the implications for funding competitions? will program managers look for a score out of the experiment design software? (#71)
    - Yet to map intuition to facility operations. (#1)
  + self-driving is part of training (#87)
    - Given the complexity of the experiments and scientific goals, there is a question is we can sufficiently express our mental models (#135)
  + Instead of pyramid, circle metaphor (#142)
  + We need probabilistic symbolic languages. (#144)
  + Digital Twin can be used as a portal into the real twin. (#145)
  + Augmented reality, virtual reality can be companion technologies (#154)
* Who would develop it (basic research to advanced deployment)?
  + This will need to be collaboration between research, user facilities, HPC facilities, and vendors who provide hardware and software. (#19)
  + (1) Academia + DOE labs - joint targeted teams of computational and domain scientists. (#21)
  + Need experts in "autonomy design" (#28)
  + Vendors would develop operational versions of the initial prototypes. (#32)
  + domain scientists should work closely with computer scientists, because design will need to happen in silico. Imagine having a github repo for a full scientific experiment --- after it's designed --- the same repo would run the operations and then the analysis. (#35)
  + Individual domains will likely develop the prototype platforms. (#38)
    - after individual domains, then domains may federate into larger consortiums. (#70)
  + Students should be heavily involved. Cultural change is critical for adoption. (#39)
  + we may want to partner with social scientists to optimize usage for scientists/engineers. (#43)
    - And UI specialists as well for accessibility (#48)
  + Delegate more mundane tasks and some expert tasks to AI (#56)
  + Need to close the loop.. with AI assistants. (#74)
  + sociological/psychological study of what scientist decision making really looks like, how can AI replicate or assist with this (#80)
  + Need a lot of training of new users. Self-driven would help it. (#84)
* Who would use it and what skills would they need to use it effectively?
  + Current user-facility users, some demographic of people who don't know they could benefit from a user-facility (#18)
  + Skills required: maybe less detailed knowledge of HPC resources than before (tech abstracts away-- or AI decides-- the complex parts) (#24)
  + The success of this would depend on if we can deploy it such that it is easy to use for a new student/postdoc/faculty. Required skills should be minimal i.e., users should be able to focus on their domain science. (#26)
  + Experiment teams would use this for preparing proposals. (#40)
    - Does the typical proposal path then changes, with a 2-step process, e.g. pre-proposal selection based on topic, then a phase of AI-driven experimental design before full proposals are evaluated ? (#53)
  + Should all users be proficient in basic programming? (#44)
  + AI as seen in (AlphaZero, etc.) will have map the intuition + intention to "adjust" the self-driving facility. (#47)
  + Need hypothesis generation.. on steroids. (#85)
  + Need to express the question.. and be receptive to the self-driving facility's advice. (#86)
* When would it be expected to be in production use (N years in the future)?
  + I think this is a continuum. We will see increased capabilities of self-driving in the coming years. Full self-driving will likely be in the 20-30 year time frame. (#29)
  + guess for cosmology/astronomy: 5years: small home telescopes; 10years: prototype on a major scientific facility; 20 years: a full experiment has been designed; 30 years: federation of instruments (#52)
  + i think it's a little like legos: some bricks can be automated now/very soon and other bricks will take longer. (#55)
    - Any speculation on what the first bricks will be and which will come later..? (#58)
    - Agreed, at least for biology it seems like some parts (e.g. data pre-processing, standard analysis) will be automated relatively soon, while other (experimental design, work across user facilities) would be further in the future (#60)
* Where, and how widely, would it be deployed?
  + It will be deployed at all DOE facilities. (#33)
  + ideally similar deployments at all DOE facilities in order to standardize setup. this allows users to move more freely between facilities. would also provide redundancy and make it easier to switch to other facilities if primary facility goes down. (#46)
  + All the way from individual laboratories to billion-dollar facilities. (#50)
  + Needs a way to permeate across facilities. (#72)
  + At a very wide-scale deployment level (i.e., enough resources and hard enough problem), AI may be able to scan the literature to generate new ideas. (#79)
* What is the setup time and/or process for using it?
  + Iterative setup procedure- self-driving pieces added every ~1 year, users/scientists/sys admins adjust, new self-driving piece added, adjustment, etc (#36)
  + User will have a short training period - maybe a 30 min youtube video to get themselves setup to use the facility. (#41)
  + Virtual synthesis of samples can be coupled with characterization. Users may only need to supply recipes. (#57)
  + easy to use like a mobile applications. (#59)
  + One question is whether international users will be easily accommodated -- will this make research a more global enterprise? (#62)
  + How can this be extant all along.. influencing the new ay science is done. (#73)
  + The process should include measuring all outcomes - failures and intended/unintended byproducts are often useful. (#78)
  + important to remember that AI won't be able to solve everything and likely won't be as creative or innovative as humans (#83)
  + Realistically, transition to autonomous research will be via incorporation of AE elements in existing workflows. Removing human-limited bottlenecks one by one, as determined by product of technology availability, cost, and perceived efficiency increase. (#153)
* Summary and notes
  + V0: The future of automated facilities closes the loop on scientific experiments with end-to-end design-to-execution, and which enables scientific discovery. (#137)
    - Human mental models and intention/intuition will be mapped. (#139)
    - needs to include something about digital twin, maybe (#140)
  + The future of (autonomous/self-driving/?) facilities ... (#138)
  + Human is adjudicator - machine suggests (#141)
  + V1: The future of self-driving facilities closes the loop on scientific experiments with end-to-end design-to-execution, in silico-to-in vivo, enabling accelerated scientific discovery. (#143)
    - This system will prioritize, optimize, and control its trajectory. Offer new hypotheses and explore them - potentially informing the human to change goals. (#155)
      * [Coordination, logs, multiple facilities - coscheduling] (#156)
      * Will science be automated itself? (#157)
  + Role of digital twins (#146)
  + Assistance with hypothesis generation (#147)
  + Using inverse design (#148)
  + Composability of various AI/automated pieces (#149)
  + Key question: how will this be integrated? (#150)
  + Both theory and experiment give incomplete representation of reality. Theory has full access to all degrees of freedom, but has different levels of abstarction and precision. Experiment can be subject to latent variables, confounder effects, and observational biases. Hence, big problem of AE is how to integrate two imperfect representations of reality in such a way that there factors partially compensate, rtaher then magnify each other (#151)
  + Secondly, from practical perspective, we should always consider the interplay between precision and latency of computation (this is where edge computing can help!), and veracity of th emodel (no need to go for more complex/precise model if experiment has uncotrollable parameters) (#152)

1.2 Breakout 2 - Implications of this Problem.

**The following participants have not been active:**  
b, Ben Brown, Nicola Ferrier, Josh Greenberg, \*fac- Nami Ishihara, Sergei V. Kalinin, Ramana Madupu, Robinson Pino, Kate Shattuck, Huolin Xin

**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?
  + (6) Reproducibility, replay (#21)
    - Data infrastructure needs to accommodate the recording of autonomation, AI inputs/outputs for reproducibility. (#57)
    - Everything should be under version control (#67)
  + (5) Realtime feedback of data and results of decision-making to self-driving system (#28)
  + (4) Explainable AI for trustworthy decisions made by ML/Self-Driving Robots (#2)
  + (4) Digital twin - need to do simulation well, need to know what happened in the real system. Need to trust it. Theory to model the physical system. E.g., complexity in biology. (#3)
    - How do we establish trust in a digital twin? (#63)
  + (4) Compute resources being available when its needed. (#16)
    - May mean some compute resources are set aside for this real-time/interactive use. Different than traditional HPC metrics success metrics like high system utilization. (#64)
  + (1) Abstraction and interpretation of experimental measurements/computational outputs needs to be automated. (#1)
  + 1. Interplay between latency and veracity of the calculation. 2. What confounding factors/completeness. (#10)
  + (2) Optimal experiment design under uncertainty. Instrument errors. Choices of methods. Initial plan - and how to optimize the plan as we are moving forward. (#12)
  + (2) trade off between exploration and execution, and exploitation (maximize current benefit). (#13)
    - (1) in RL, it tends to be framed as exploration vs. exploitation. (#14)
  + (3) Need to have a lot of sensors, lots of machine-to-machine communication. New wireless technologies. (#15)
  + (2) 24x7 instruments uptime. Reliability/availability. (#17)
    - How do we define reliable? Some set of unit tests or integration tests that run periodically? (#66)
  + (2) Virtualization technologies.. containerization - move it to instruments. Into workflows, microservices arch, interoperable components. (#18)
  + (3) Security - if we have these type of facilities controlled and steered by computer systems, how do we ensure they operate securely, safely and cannot be hijacked by outside players (open campus) (#19)
  + (1) Need to adapt this capability to another campaign easily. Versatility. (#20)
  + (3) Encode decision-making rationale, explainability methods. (#22)
    - Encoding the causal chains in the facility will be very important. (#23)
  + Implications and consequences of the experiment. (#24)
  + (3) Augmented/virtual reality will be a need. Still need guidance from domain scientist. (#25)
  + (1) Tracking sensor configuration and experiment design is vital. (#26)
    - Storing a log of all the system data will help reproducibility and increase trust in this self-driving system. (#56)
  + (1) sociological understanding of human interactions with machines scientific creative process (#27)
  + (3) Hypothesis generation, constraint by physical laws, prioritized - selecting those that propose feasible directions parallel, synergistic or orthogonal to what the scientist is currently pursuing (#32)
    - the current scope of ken (i.e., where existing physical laws apply) may over-restrict the search space for new knowledge --- e.g., Newton's vs. Einstein's gravity. How do we deftly tow that line so that we don't exclude real discovery space? (#43)
  + (1) re exploration vs exploitation --- new understandings of epistemology and how to explore the space of what is not known. (#34)
  + (2) Encapsulating verified building blocks for better integration testing (going beyond unit testing) will be vital. (#69)
  + (1) Data substrate. (#70)
  + Predicting consequences of decisions (#71)
* Who is/will develop this companion technology/service?
  + Lab staff will develop initial prototypes, and transition to vendors. (#30)
  + The companion technologies will be developed by vendors, large collaborations, and lab staff (#31)
  + New methods will be sourced from academia and labs (e.g., to compactly represent experiments). (#33)
  + Orchestration workflow managers and virtualization technologies will likely have a lot of R&D input from DOE labs, in collaboration with Industry and Academia. (#37)
  + Government solicitations and funded centers will drive new capabilities - tracking provenance, building better reliability. (#38)
  + Multi-disciplinary teams: We will need a close collaboration - co-design - between domain scientists, facilities scientists and computer science, integrating staff from leading edge research to engineering to evolve from first concepts to operational technologies. (#41)
  + Will the development of these automated systems be done in a collaborative fashion similar to what we have now (e.g., scientists + industry in some interplay that is limited to them), or will collaborations need to look different to accomplish this? (#50)
  + Technologies should be general and not specific to one facility or center. Users can expect same technology/interface in other places. (#54)
  + The facility operators will define the appropriate self-driving behavior and teach the self-driving systems with behavior clone, inverse imitation learning. (#58)
  + Explainability is related to domain knowledge and involves domain science models, equations, and simulation in every step to build a trustworthy self-driving system. (#65)
* What skills/knowledge does the end user require?
  + Users need to be able to quantify targets/objectives, and possibly perform simple coding. (#29)
    - Need new computer science tools to map mental models to objectives, to hypothesis, to execution/experiment "plans" (#42)
  + End user needs some awareness of the strengths and weakness of the self-driving decision making. For example, in self-driving cars, drivers are aware that white objects may fool the car into making an unsafe decision. (#35)
    - How should this assistant be by the scientist's side? AR/VR-type tech? (#45)
    - The user needs to be aware of approximations and assumptions to steer correctly (#47)
  + End users should be mainly focused on the science objectives. However, we will need users to also have understanding on how to interact with the models that are self-driving! (#36)
    - Is there a danger of users knowing too little to e.g. validate results, see if things go wrong? (#49)
  + Providing some kind of a "Virtual Research Laboratory" interface to end-users would help adoption and facilitate productivity. (#46)
    - Yes - the abstraction of a VRL can also hide how underlying "multi"-facilities are coming together for the scientific question. (#52)
  + User should not be on "autopilot" themselves. User should always be evaluating and thinking critically about every AI decision. (#48)
    - What if there could be a system where autopilot is possible? (#53)
  + One could think of the end User as someone who doesn't need to know anything except their science, and then the facility operators could be thought of as the team that ensures the output's fidelity. (#55)
    - perhaps the user could choose their level of direct involvement, which may have a correlation with the fidelity of the outcome. (#60)
  + This raises the interesting question where the users wants and needs to interact/ steer the autonomous experiment. There may be measurement experiments that can largely run on their own with little intervention, thus the user needs to know less. On the other hand for exploratory experiments the user will need to be much more hands on and therefore needs to understand much more of the inner workings of the system. (#59)
  + End users with domain knowledge will ultimately determine the quality of autonomous systems and evaluate the consequence and results. (#68)
* What are the training/support requirements?
  + System should provide overview dashboard that displays system health (green, yellow, red) for each component. User should be able to report issues in some automated way. (#39)
  + Training/support might itself be AI driven ( e.g., chat bots etc). But the training will shift to helping users interact better with the systems. (#40)
  + System should provide clear interface with easy to understand visualizations, plots, and system state information. Users should be trained in how to understand this. (#44)
  + Scientists of all types will need to understand the implementation and limitations of AI (#51)
    - Enough training to avoid misusing Autonomous Facilities as expensive black boxes without any scientific judgement on what they produce. (#62)
  + Training.. methods to design the software must be tightened up. (#61)
* Summary from Breakout 1
  + Human is adjudicator while machine suggests (#4)
  + Role of digital twins (#5)
  + Assistance with hypothesis generation (#6)
  + Using inverse design (#7)
  + Composability of various AI/automated pieces (#8)
  + How will all this be integrated? (#9)
  + Vision statement V1: The future of self-driving facilities closes the loop on scientific experiments with end-to-end design-to-execution, in silico-to-in-vivo, enabling accelerated scientific discovery (#11)

1.3 Day 1 Reflections

Participants: 1

**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.



* 1. Day 1 notes are posted in Breakout1 ("Summary and notes"). Group reviewed Day 1 summary and notes. Communication between facilities bubbled up (co-scheduling - maybe only 5 years out, not 30 years out). Exploration vs. measurement -- exploration is farther out.
* 2. Implications: Need to discuss ethical framework

2 Day Two - November 5, 2020

2.1 Breakout 3 - Signposts

**The following participants have not been active:**  
Ben Brown, Josh Greenberg, \*fac- Nami Ishihara, Nami Ishihara, Sergei V. Kalinin, Harriet Kung, Ramana Madupu, Robinson Pino, Dan Ratner, Kate Shattuck, Huolin Xin

**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)

* Unsorted (1)
  1. 2. V1: The future of self-driving facilities closes the loop on scientific experiments with end-to-end design-to-execution, in silico-to-in vivo, enabling accelerated scientific discovery.
     + Comments
     + This system will prioritize, optimize, and control its trajectory. Offer new hypotheses and explore them - potentially informing the human to change goals. (#3)
       - [Coordination, logs, multiple facilities - coscheduling] (#4)
       - Will science be automated itself? (#5)
     + Near term (5-10 years) should be able to automate a individual tasks (#12)
     + Self-driving facilities will include both large laboratory facilities as well as automated field sites operating in coordination (10 years) (#17)
     + Simulations will need to be advanced enough to produce high fidelity data indistinguishable from real experimental measurements (15 years). (#23)
     + Continuous interaction of computational and experimental facilities throughout the experimental design, execution and optimization (#71)
* Workforce - 5-10 years; Initiate buy-in from community (Social exercise). (6)
  1. 26. Socialize/familiarize scientists with a new way of conducting experiments.
  2. 51. Next 1-2 years: Build engineers trust: AI in facilities is there to help reduce Mean time to Repair (MTTR), reduce failures and automate fault tolerance
  3. 28. Workforce development/training for scientists in an automated facility (5-10 yrs)
  4. 89. workforce development: traffic controller vs chef
  5. 9. How will smart facilities will change workforce? Do beamline scientists become obsolete?
     + Comments
     + Scientists will still drive improvements of the self-driving technology (#11)
  6. 27. Need input from facility users about which self-driving technologies would be most useful for them (i.e. beam calibration, data analysis, experimental design advice)
* Ethics, Fairness, Social, Human Issues; 20-30 years; Hard (science needs to take this up) (4)
  1. 7. Ethical framework needs to be in place
     + Comments
     + Control / Verification of self-driving facilities will likely need scientists to be familiar with AI functioning, at least in terms of potential flaws and blind spots, and how to make their "learn" efficiently. (#8)
     + Data stewardship framework needs to be in place (perhaps separate milestone) (#21)
  2. 16. Fairness is a key thing in the self-driving facility.
     + Comments
     + Need to make sure resources are allocated fairly (#59)
     + to be merged with 60 (#99)
  3. 60. FAIR is a big concern - who allocates resources? who gets priority.
  4. 76. Can an autonomous facility lower quality of science output? by optimisation of concurrent goals and requests
* Security - 5-30 years; Medium (4)
  1. 69. Cybersecurity of the automated facilities and associated data repositories must be addressed (10-15 yrs)
  2. 86. Cybersecurity of these sites.
     + Comments
     + can be removed. 69 address this point (#98)
  3. 101. Trustworthiness is listed in Experimental verification area.
  4. 116. Physical security of changing experiments of HIL
* Data, Logging Trail - 5-10 years; Easy - necessary backplane. (5)
  1. 22. Data stewardship framework needs to be established (5-10 yrs)
  2. 41. Well curated library of data across experimental systems available (in the cloud?) to broad scientific community (10 yrs)
  3. 45. Availability of data across facilities, anonymization capabilities, policies for data sharing (5 years)
  4. 47. Data backplane for system state - 10 years.
  5. 72. Quality of information
     + Comments
     + Help collect "right" data, help analyze data more quickly and more effectively (#74)
* Simulations, Digital Twin - 5-20 years; Medium but a key building block. (Hard in Bio) (5)
  1. 35. Have Digital Twin models available to train and test the AI before onboarding to the facility
  2. 38. Will digital twin be the precursor to the self-driving facility and allow the digital twin of human to be part of the augmented facility?
  3. 68. multi-fidelity simulations of every aspect of experiment.
     + Comments
     + Small scale digital twin (#80)
  4. 65. Digital twin - remote inter-personal interactions - improved "telepresence"
  5. 70. ML/AI: need to tune to specific applications (quickly) - 5 years task: emulator of data. Need emulator for simulation to "test" methods before using facilities.
* Policy - 1-5 years/flexible/agile; Easy but sociologically hard. (7)
  1. 10. Will facilities compete? Will facilities share this technology?
     + Comments
     + The necessary infrastructure, interfaces, and technology will likely to be shared and developed collaboratively. (#15)
  2. 29. Address funding paradigms for competing auto-designed experiments
  3. 81. Democratization of facilities across DOE labs. Current strong coupling with local /physical resources. Analogous to "cloud computing" may have facilities to run experimental capabilities - but don't have to think about where it is run. Will science be done differently ? Policiies will need to change. 20-30 years
     + Comments
     + Data sharing between facilities is key (#88)
  4. 104. Scope of the requests and priorities in evolution of the facility management.
  5. 105. Data sharing and dissemination policy, transparency.
  6. 107. Enforcing and encouraging portability.
  7. 108. More seamless integration between different offices with DOE Office of Science
* Automation/Robotics - 5-30 years; Medium - key component. (10)
  1. 49. Automate all mundane tasks, delegate grunt work to AI (5 years)
     + Comments
     + Yes! Will also make experiments more robust to human error. (#52)
  2. 18. Single experiment to demonstrate self-driving technology at smaller scale before moving to facility scale ~10 years
  3. 77. Ability for different AI models to interact with each other effectively and safely, learning from each other and negotiating with each other. - 5-10 years
     + Comments
     + Also interaction with humans, experimental equipment, compute facilities. (#79)
  4. 58. should be able to collect the most relevant data from an experiment - 5-15 years introduce robots into beamlines/facilities to remotely perform experiments for domain scientist (set up experiment, increasing level of autonomy until domain scientist and beam line scientist have minimal input). ultimately domain scientist wants to collect data at nano time scale - system should determine modality, set configuration parameters, position sample, and collect relevant data (setting optimal parameters for experimental configuration) and provide data to domain scientist - this is 15-30 years. Decisions might require HPC - eg. to explore large configuration space. Some robot interaction is already started. Need to ensure safety with remote operation.
  5. 46. Objective function for instruments mapped to physical operation protocols - 25 years.
  6. 19. Automated construction of materials for experiment (30 - 40 years)
     + Comments
     + of material for experiment -> experiment themselves? (#48)
  7. 57. Self evolving facility in anticipation of future problem to solve
  8. 78. How will an autonomous facility capitize on "error" or "unexpected" - e.g. pencillum discovered as a "lab accident"
     + Comments
     + YES! and electricity has not be discovered by research on candles. (#109)
  9. 106. Control feedback mechanisms and autonomous experimental steering
  10. 113. Also in Monitoring and sensors: Systems level automation - so need more monitoring - (for success/failure).
* Federation between facilities/Facility configuration - 5-10 years; Easy (sociological issue). (13)
  1. 1. Technology/federation that allows facilities to exchange information to maximize scientific benefit and minimize experimental campaign time
     + Comments
     + Requires establishment of data standards applied across facilities to facilitate information sharing (#13)
     + Data infrastructure to allow capture, store, search of data (5 years) (#14)
     + Security and intellectual property in the facility and originator. Share knowledge rather than share raw data. (#25)
     + Reproducibility semantics (#42)
  2. 24. Federate self-driving experiments into one interacting framework (20 years)
  3. 82. Structural change in DOE policies to encourage collaboration between similar labs/facilities across the DOE complex
  4. 40. Facilities agree on data sharing strategies (federated logins) for monitoring dashboards for real-time data across all facilities
  5. 31. Standardization of sampling methodologies, metadata schema and logistics (5-10 yrs)
     + Comments
     + Maybe more important is the quality of data, how to quantify the quality of data ? (#54)
  6. 34. Facility designs/laboratory space configured for modular and rapid deployment of next generation instrumentation and workflows (5 yrs)
  7. 62. Self-driving facilities include both laboratory facilities as well as automated mobile field sites operating in coordination (10 years)
  8. 85. facilities can adapt to technology changes. Accommodate autonomous mobile field sites.
     + Comments
     + Need to think outside traditional "beamline". Other facilities like JGI have a very different set of needs. Need to be able to accommodate these diverse scientific fields. (#87)
  9. 110. Interoperability of models and configs
  10. 114. Cloud nanocenter
      + Comments
      + Use 5 DOE nanocenters as case study for federation (#115)
  11. 120. see #83 in HMI: User level: Need automated workflow to communicate intent of scientist. Want semantics across different labs/facilities. Need policy and social structure changes for how science will happen.
  12. 127. Design of next generation of facility.
  13. 128. Robotics: for labs there are commercial solutions but for some tasks (such as field sites for BER), there needs to be effort for a more general manipulation
* Human Machine Interface - 10-30; Hard (mental models) - necessary. (14)
  1. 6. Establishing a "Virtual Research Laboratory" interface and extending necessary virtualization technologies.
  2. 64. The scientists can interact with the facilities from their home as if they were there in person - 15 years
  3. 36. need natural language interface or new mental models to communicate with. the facility - "need a better battery" must be translated into achievable tasks. Humans communicate with a lot of assumptions
     + Comments
     + Yes absolutely (#55)
  4. 33. Need intelligent system paradigm to support Machine to machine, facility to facilitate, and human-facility interactions
     + Comments
     + How does human be part of this (safely) (#63)
  5. 83. User level: Need automated workflow to communicate intent of scientist. Want semantics across different labs/facilities. Need policy and social structure changes for how science will happen.
     + Comments
     + Need the right amount, the right kind, the right format of data. Most likely need a LOT of data for AI. (#84)
  6. 112. Surprises need to be made visible to a human
  7. 117. Tracking the new needs of humans as facilities get better.
  8. 118. Different support whether we are pursuing a measurement or an exploratory experiment
  9. 119. Integrating AR, VR, and telepresence
  10. 121. Human v. Machine - will there be conflict
  11. 122. Ability to detect cognitive depletion in the scientist driving the experiment - 5 years to some extend
  12. 123. Especially in late night, low oxygen, or other stressful or difficult situations
  13. 124. Dealing with observational biases?
  14. 126. these are timelines for when a machine/algorithm would replace a human.  
        
      Near term: sensor arrays to monitor and feedback systems to correct  
      medium term : interpreting output from inference  
      long term: hypothesis generation
* Monitoring and Sensors - Evolves to more intelligent systems: 5-20 years; Easy but important. (6)
  1. 56. Virtual experimental facility monitoring - ability to monitor, maintain, coordinate and intervene remotely and autonomously - 5 years
  2. 37. Need to address AI driven experiment safety, damage, equipment failure concerns (think of GIFs of robots doing silly things)
  3. 66. engineering controls: foster culture where people tie in their instruments
  4. 67. high-density sensor arrangements for monitoring facility and instruments.
  5. 111. Systems level automation - so need more monitoring - (for success/failure).
  6. 125. Self-healing facilities or self-maintaining.
* Hypothesis generation and execution - 10-40 years; Hard but most impact! (8)
  1. 75. Can autonomous facility lead to poor science? May optimize for,, say, throughput rather than quality.
  2. 53. The system suggests the best set up and execution for my experiment to allow me to collect the most relevant data for my challenge - 5 years
  3. 32. The system can suggest an optimized set of experimental methods to me for a well specified challenge - 10 years
  4. 44. The system can identify a gap in experimental methods that would be needed to complete my experiment - 10 years
  5. 43. Hypothesis to physical exploration - mathematical mapping - 15 years.
     + Comments
     + Relates to the mental model mapping. (#61)
  6. 103. Optimal experimental design a priori and during the experiment building on real time data - connected to monitoring, data logging trail, digital twins
  7. 30. The system suggests a physically valid experiment to me that is better than or a valuable addition to my own ideas - 30 years
     + Comments
     + +1 (#50)
  8. 39. I can discuss different possible hypothesis (interpretation of full or partial results, or which approaches to take) with the system - 40 years
* Experimental verification, Explainability, Reproducibility - 0-15 years; Medium but necessary! (4)
  1. 102. Uncertainty quantification, etc.
  2. 100. Trustworthiness of autonomous system, decisions.
  3. 20. Interpretability of AI results (10 years)
  4. 73. Full experimental reproducibility is available - 5 years (sufficient information available), 15 years (digital information and resources available to automatically rerun an experiment)

2.2 Breakout 4 - Signpost Plausibility

Participants: 2

**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)

* 10. SIGNPOSTS WERE COLLECTED AND ARE BEING ORGANIZED IN THE BREAKOUT 3 AREA.
* 2. V1: The future of self-driving facilities closes the loop on scientific experiments with end-to-end design-to-execution, in silico-to-in vivo, enabling accelerated scientific discovery.
  + Comments
  + This system will prioritize, optimize, and control its trajectory. Offer new hypotheses and explore them - potentially informing the human to change goals. (#3)
    - [Coordination, logs, multiple facilities - coscheduling] (#4)
    - Will science be automated itself? (#5)
  + Near term (5-10 years) should be able to automate a individual tasks (#6)
  + Self-driving facilities will include both large laboratory facilities as well as automated field sites operating in coordination (10 years) (#7)
  + Simulations will need to be advanced enough to produce high fidelity data indistinguishable from real experimental measurements (15 years). (#8)
  + Continuous interaction of computational and experimental facilities throughout the experimental design, execution and optimization (#9)