Group #12: Community of Interest on the Future of Scientific Methodologies

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| Date | November 2, 2020 |

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Contents

[1 Day One - November 2, 2020 3](#_Toc55483962)

[1.1 Discussion: Breakout 1 - Define the Scope of the Problem. 3](#_Toc55483963)

[1.2 Discussion: Breakout 2 - Implications of this Problem. 6](#_Toc55483964)

[1.3 Brainstorm: Day 1 Reflections 8](#_Toc55483965)

[2 Day Two - November 5, 2020 8](#_Toc55483966)

[2.1 Brainstorm: Breakout 3 - Signposts 8](#_Toc55483967)

[2.2 Brainstorm: Breakout 4 - Signpost Plausibility 9](#_Toc55483968)

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 Ishihara, Dantong Yu

**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?
	+ Notes from round-robin at the beginning (#1)
		- Digital twins have been used in manufacturing for a while. (#2)
			* in 30 years, can we have digital twins of individuals and their health, physiology and interaction with devices? (#8)
		- Digital twin has the ability to incorporate history of past experiments/diagnoses/data into currently-running context (#3)
	+ Adapt measurements real-time (#4)
		- Current methods have static measurement locations (#5)
		- For example, send a drone into a hurricane when data or models indicate that the time/location is beneficial (#6)
		- Similar to Adaptive Mesh Refinement for sensor deployment, but more sophisticated (#7)
			* This goes beyond zooming in and out to capture hot spots of interest. This can lead to an expansion of the model domain itself, or also more adaptive high-temporal resolution at moments of interest. (#12)
		- And also integrate models and measurements in near-real time. For e.g. can we test out scenarios in the models so we can be better prepared - in terms of planning measurements, deploying emergency response etc. (#16)
	+ Chemical process/manufacturing - ability to inform later stages of a process pipeline based on observations in previous stages (#9)
	+ How to make digital twin become actuator, the portal that allows operators to remotely monitor, control and manage the real-twin (#10)
	+ Ability to instrument EM stewardship locations and couple that information with simulations - reconfigure sensors as necessary, inform future discussions (#11)
	+ AI and Machine learning will be indispensable components in the digital twin? What particular roles can AI play in digital twins? (#13)
	+ Intent-based networking - as digital twins and experimental capabilities interact, the network can reconfigure itself according to their needs (#14)
	+ Interfaces between digital twins and other technology components (this points toward needed capabilities) (#15)
		- Need a language or other communication mechanism to accomplish this - real-time communication is key, but limited by physical distance (longer control loops over longer distances.....extreme case is NASA control of Mars Rovers) (#17)
		- AI is likely to play an important role here (#18)
	+ Fault tolerance in digital twins - integrity of operation, trust, reliability, protection from hacking/malice (#19)
		- ethical digital twins - how would you teach digital twins ethics? (#23)
		- can digital twins learn from each other? (#25)
	+ Data capture and storage (#20)
	+ Data QA/QC in real-time applications is challenging - need to have confidence in individual components as well as the entire pipeline (#21)
	+ Computing near/at the edge (#22)
	+ Need enough benchmarking/background/training data to gain confidence that the models are correct and are operating correctly (#24)
	+ 30 years from now, we'll be doing measurements differently (#26)
		- VR-based - can we drive remote sensors from our desks or from control centers? (#27)
		- Can we operate remote sensors using digital twins to reconfigure them as appropriate? (#28)
	+ Multi-physics models are key - integrate multiple scientific processes from different domains in the digital twin (#29)
	+ Sensors change/degrade/drift over time - models will need to adapt. Can we use the digital twin to keep calibration information fresh? (#30)
	+ Different entities will own/operate/contribute different parts of the overall ecosystem, especially in large projects. If digital twin elements or models confer competitive advantage, how does this affect the landscape? (#31)
	+ Uncertainty quantification - how do you manage uncertainty, esp. when coupling models with sensors/observations? (#32)
		- Need a process to make decisions based on confidence, behavior of pipeline elements, etc (#33)
		- In decision support, some uncertainties are more important than others (#34)
		- Understand the sensitivity of certain models to certain parameters - can we manage this better? (#35)
		- Can we solve this by just collecting massive amounts of data in order to reduce uncertainty? (#36)
		- Use physics model to bound/constrain/sanity-check AI models (#38)
	+ Combine a physics model with sensor data and AI/ML - physics model might reduce uncertainty (#37)
	+ Tension between mechanistic physics models that we understand and trust, and emergent/AI/ML models that may give us new insights. (#39)
		- In some cases we don't have the instrumentation or measurements to inform a mechanistic model or evaluate an AI model (#40)
			* We want the new insights - need for explainable AI/ML (#41)
		- There are gaps in the data needed to develop/validate mechanistic model (#42)
		- AI/ML models can do things that mechanistic models cannot, but then we hit the explainability issue (#43)
		- Lots to do there - effort for roadmap/path between now and 30 years from now (#44)
		- Different domains/time-scales have different tolerance for errors (#45)
			* For example, a Roomba vacuum and a self-driving car may use the same sensors, models, and algorithms - one requires much more assurance than the other for useful/safe operation (#46)
	+ Models are likely to be very different in 30 years. For example, AI has changed the modeling community in a few short years. (#47)
		- Modeling will change - we need our environment/ecosystem to be resilient/adaptable to changes in technologies (this is also true of sensor technology) (#48)
		- Quantum computing will change the computing environment significantly - need to be able to adapt/incorporate (#49)
		- Heterogeneous computing will almost certainly provide some significant wins here - different model components running on different processors, multiple machines/resources integrated into a functioning whole, edge computing at the sensor, etc. (#50)
			* Many science domains have significant scale issues - fractal aspects of the domain (e.g. earth sciences) (#52)
	+ Rate of data collection is dramatically increasing. Also detail level will increase significantly. Also time scale will increase. (#51)
* Who would develop it (basic research to advanced deployment)?
	+ Need significant infrastructure investments in order to bring this about (#54)
		- There are several different parts of this - computing, sensors, data, networking, domain scientists, etc. (#53)
	+ End to end issues - sensor to facility to human (#55)
	+ (1) Previous points all argue for a large-scale interdisciplinary approach - there isn't one "who" that will develop this (#56)
	+ Industry will do some parts of this (e.g. cloud computing, semiconductor technologies for sensors) (#57)
		- Industry will not do everything (we've seen this from history - no reason to expect this to change) (#58)
		- Need to track gaps between industry technologies and science needs, ideally there is interplay/synergy/iteration (#59)
		- Focus on filling the gaps (#60)
	+ Data needs to be easily accessible to the scientific community, within the full scope of the science collaboraiton (#61)
		- e.g. cloud providers often come with data lock-in or with costs to retrieve/use data (#62)
	+ Need a widely-deployed machine-readable data storage/annotation/publication/access standard (or standards) to facilitate data use and re-use at scale. (#63)
	+ Need to compare with the self-driving facilities people. (#75)
* Who would use it and what skills would they need to use it effectively?
	+ Senior leadership is a user of digital twin technology - strategic forecasting, proposal bids, etc. (#64)
	+ Scientific community - data taking, data analysis, experiment design, etc. (#65)
	+ Data analysts (not just domain scientists) (#66)
	+ User-centered design, UI/UX, etc - key not just for scientists, but also for citizen science (#67)
		- Allow the public to gain familiarity with science and data - e.g. Fukushima, wildfires, air pollution, etc. (#68)
			* WiFire is a perfect example of this (UCSD/SDSC) (#69)
	+ UI/UX for human-in-the-loop operation (augmented reality, etc) (#70)
		- specialized skill requirements are significant barriers (#71)
		- need to democratize access to these assets - significant increase in utility/productivity (#72)
		- allows senior leadership use case also (#73)
			* adjust parameter inputs, see how behavior changes - scenario planning, strategy, etc. (#74)
* When would it be expected to be in production use (N years in the future)?
* Where, and how widely, would it be deployed?
* What is the setup time and/or process for using it?

1.2 Breakout 2 - Implications of this Problem.

Participants: 2

**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?
	+ Need much better data - we can see norm and deviation from the norm, but we don't have good data for extremes (#3)
	+ (2) Need two types of digital twins (at least) - one for the sensor itself (to assess sensor operation, calibration, failure modes, etc), and for the environment that the sensor is observing (e.g. to guide sensor placement, change observation spectra/angle/parameters, etc.) (#4)
	+ Sensor management - software, configuration, etc - incorporate/adopt tooling/methodologies from IoT/industry world where there is already work on managing large fleets of small devices (#5)
	+ (2) Interfaces between components (#6)
		- Example: Google project to allow bots to develop their own communication language (#7)
		- Need feedback/iteration mechanism - communication is two-way, not just control or information retrieval (#8)
		- Streaming/real-time interfaces needed also (#9)
		- (1) Clear need for a "data facility" for DOE which can integrate, process, publish, etc. (#10)
			* Some components are common/re-usable across science domains (data publication capabilities, high-speed storage, data transfer/placement, orchestration, etc) (#12)
			* Some components are science-specific (domain, facility, collaboration) and need to be done by the science community (but hopefully using scalable infrastructure) (#13)
		- Provenance capture and other data use/assimilation issues - which data set did you use, which version, if the model or calibration gets updated how is that tracked, etc. (#11)
	+ The same is true for models - different software versions/environments, porting to new systems, advances in algorithms, etc. (#23)
		- Sensors and models are essentially the same in this way (at least in the abstract) - both will change in behavior over time, and those changes need to be quantified and tracked (#24)
	+ Error propagation is another important point - how do we track errors through systems and through data use? (#25)
		- Broad uncertainty (UQ) topic (the intent was to create an umbrella for the above several topics) (#26)
	+ Broad topics/groupings (#31)
		- Additional mathematics (#32)
			* We need a mathematics for optimizing sensor placement, ability to acquire specific types of data, etc. (#27)
				+ Better optimization algorithms, esp. those that can deal with high dimensional datasets, and real-time data assimilation (#28)
				+ Includes modeling environment to understand sources of interference, and therefore accounting for it (adjust sensor placement, filter data, etc) (#29)
			* Need ways to deal with sparse/missing data (COVID pandemic is a good example - we have incomplete/missing data, and yet we need to feed what we have into models and do the best we can - how do we do this better?) (#30)
		- (2) Uncertainty Quantification and related topics (#33)
			* (1) Digital twin behavior needs to be reproducible. How do you get back to a known state? Need tools to manage/characterize digital twin/simulation components. (#14)
				+ Bitwise reproducibility is hard. How important is that? Is semantic reproducibility, or reproducibility within some threshold, sufficient? (#15)
				+ How do you know what cause variance? Sensor calibration/firmware, other stuff? (#16)
				+ There is sufficient variability in the computing environment in modern systems that there will be variance/variability between runs in the general case. (#17)

Brings up the importance of uncertainty quantification (#18)

Same is true for sensors - explore what "reproduce" means (#19)

* + - * (1) Additional angle on UQ - people shouldn't blindly believe sensors. Need to understand the sensor, how it behaves, comparison to other sensors that measure the same thing in different ways, etc. (#20)
				+ If you're using data from different sources, need to be able to understand which things are comparable and in what ways (#21)
				+ Need a way to track changes in sensors/data over time (#22)
		- Feedback between sensors/hardware/software/models (#34)
		- (1) Better/more reliable sensor hardware/packaging (#35)
			* Hardened sensors that can survive their environment (#1)
				+ Currently sensors fail or are intermittent - need a way to ensure that they will continue to operate (#2)
		- (1) Multiple computing topics (edge computing, ability to incorporate different computing models into the overall architecture over time, impact of quantum computing as it's developed, etc) (#36)
	+ (1) Some things change very slowly (#37)
		- Data formats (#38)
		- Agreements/treaties between people and organizations (#39)
		- Communication protocols (e.g. TCP/IP in the Internet) (#40)
		- Large software code bases (#41)
	+ Some things change quickly (#42)
		- Computing hardware (#43)
			* Networking hardware (#44)
* Who is/will develop this companion technology/service?
	+ Partnership between research and industry will be key (#45)
	+ Industry does what they do for specific applications - good stuff to use if it fits our needs, but we need to be clear that there is some stuff that the science complex will have to develop (#46)
	+ Industry is already doing some good digital twin work (e.g. aircraft engine condition-based maintenance). Leverage their work if we can. (#47)
* 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

**The following participants have not been active:**
Devarshi Ghoshal, Josh Greenberg, Deep Medhi, Dantong Yu, Dantong Yu

**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. Human-computer interfaces - how do we interact with Digital Twins, or with the system of experiment + Digital Twin?
	+ Comments
	+ Technology already exists today (precursor) (#6)
	+ ability to communicate using mechanisms other than speech and text would allow scientists to be much more productive (#14)
	+ virtual reality, holographic, haptics etc. how can that influence our ability to get better understanding of the physical system (#15)
	+ ability to share skills/expertise via human/computer interfaces (#16)
	+ visualization of model results and observational data - new types of 3D viz? (#17)
* 2. Computing will not be separate from the environment, and will be integrated both with the experiment and form the basis for the digital twin
* 3. Uncertainty and managing uncertainty, error detection/correction, etc. will be key
* 4. Data acquisition will be part of the experiment environment and help guide the experiment, as well as collect the data from the subject of the experiment
* 5. Automation of control and decision-making will be key
* 7. Integration of data will be critical for digital twins
	+ Comments
	+ data needs to be easily available (#8)
	+ data needs to be easy to integrate into digital twin model (#9)
	+ integration of heterogenous data from multiple sources, and that are prone to human error and bias (#11)
	+ Policy item: data from DOE-funded experiments must be published and curated at scale (TB to PB) in a way that makes the data easy to ingest by running simulations (#12)
		- over time, this will help bring about an ecosystem within which data sets are easily available using machine-to-machine interfaces (#13)
* 10. What are the components of a digital twin/simulation and what are the data we need to be able to capture that

2.2 Breakout 4 - Signpost Plausibility

Participants: 1

**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. https://docs.google.com/document/d/1ngpIRwApPCz7u5zSpD6\_lxQ6FTDigDRz36TVVWbN4GY/edit#