
U.S. DEPARTMENT OF ENERGY | Office of Science

# Future Directions for the Department of Energy's Advanced Computing Tech Team

## ASCR Advisory Committee Meetings

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# Presentation Overview

- **Tech Team vs. Crosscut Explanation**
- **Past History for ACTT**
- **Overview of shared needs**
- **Go-ahead plan**

# Tech Teams vs. Crosscuts

**Tech Teams and Crosscuts exist to address the same challenge: How do we get different parts of the Department of Energy that face similar challenges to work well together?**

- **Example 1: Subsurface flows**
  - Environmental management: Pollutants in ground water.
  - Fossil Energy: Carbon sequestration, petroleum reservoirs.
  - Geothermal: Modeling flow through system.
- **Example 2: High Performance Computing**
  - Office of Science and National Nuclear Security Administration make major investments.
  - Nuclear Engineering, Fossil Energy, Energy Efficiency and Renewable Energy, Environmental Management also investing.

# Tech Teams vs. Crosscuts

| Tech Teams are unfunded vehicles for coordination. | Crosscuts pool together funding and have congressional reporting requirements. |
|---|---|
| - Advanced Computing.<br>- Grid.<br>- Water Energy.<br>- Subsurface.<br>- Supercritical $CO_2$.<br>- Manufacturing.<br>- Energy Storage (New). | - Exascale Computing<br>- Energy-Water Nexus<br>- Grid Modernization<br>- Subsurface Science, Technology, and Engineering<br>- Supercritical $CO_2$. |

Tech teams may or may not grow into cross-cuts.

# Tech Team Purpose

- **Tech team made efforts to move to cross-cut status.**
  - Idea generation across multiple programs in 2014 and 2015.
  - Needs were very heterogenous- programs range from not using HPC at all to making it a key part of their strategies.
  - In many cases, this reflects the industries as a whole.

- **If there isn't a cross-cut, do we need a tech team?**
  - QTR pointed out existing partnerships, need for more.
  - FITARA required a mechanism for all programs to talk to each to other.
  - S4 meeting with team showed interest was there.

**So what should the tech team look like?**

# Common Challenges and Needs

- **Is there a technical basis for keeping the team going ? 2014 survey of needs showed there was.**
  - In some cases, applied groups face exactly the same challenges: Several applied groups want simulation as a tool for finding materials for extreme environments.
  - In other cases, problems are analogous, with the potential to learn from shared approaches.
- **While the physical nature of the problems varied, applied groups pointed to 4 basic sets of needs:**
  1) HPC for discovery/fundamental physics
  2) Using HPC for model reduction
  3) System/Plant Level Simulation
  4) Post-design Simulation

# HPC for Discovery/Fundamental Physics

- **Interest in using HPC at the innovation/discovery stage on a range of topics:**
  - Materials discovery/design.
  - Fluid mechanics and heat transfer at small length scales: carbon sequestration, fuel cells, geothermal, concentrated solar, additive manufacturing.
  - Combustion physics.
- **Discovery/innovation stage definition often varies between the Office of Science and Applied Programs (and between individual applied programs).**
  - Can lead to gaps in both the physical understanding of the problem, and in the computational tools available to attack the problem.

# Using HPC for Model Reduction

- **Moving from discovery to design requires a different approach:**

***The goal is the highest fidelity simulation that allows the engineer to explore the parameter or design space.***

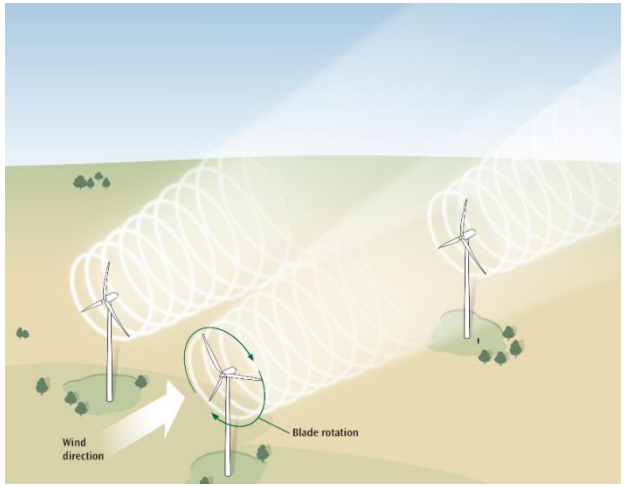
***Often the length and time scales of the problem require us to move from first-principles simulations to models, knowing that "All models are wrong, but some models are useful."***

- **Can be seen most clearly in turbulent flows (Key process in wind energy and combustion, relevant in other areas).**

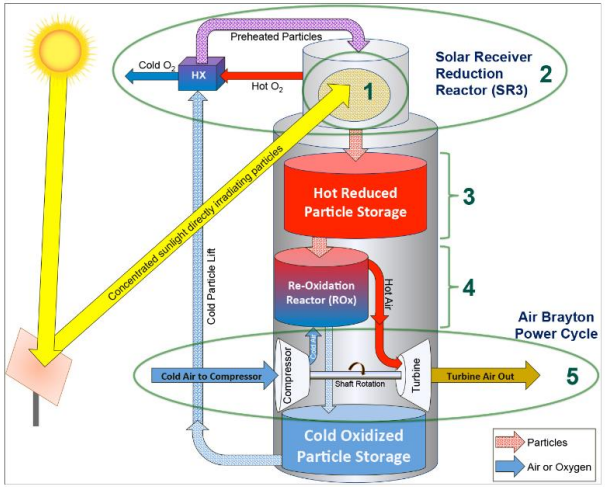

- **How do we use approaches that require leadership-class simulation in an integrated manner with modeling?**

# Using HPC for System/Plant Level Simulation

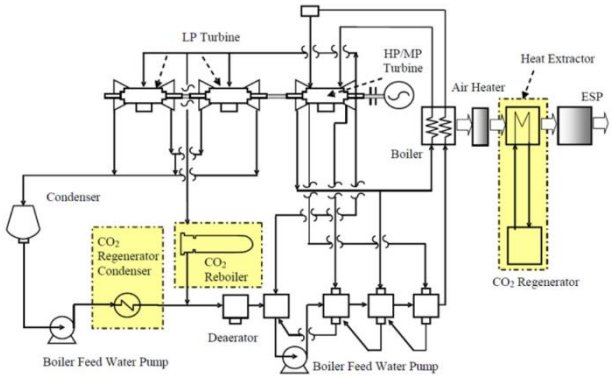
- **Many technologies have problems that require multiple sub-systems to be simulated to capture interactions.**
  - High physical fidelity required in each sub-system (or physical model.)
  - Need an integrated framework for integrating these.
  - Approach taken by CASL- does it translate elsewhere?




Wind Farm with wake interactions (Sandia)




Concentrated Solar Schematic (Sandia)

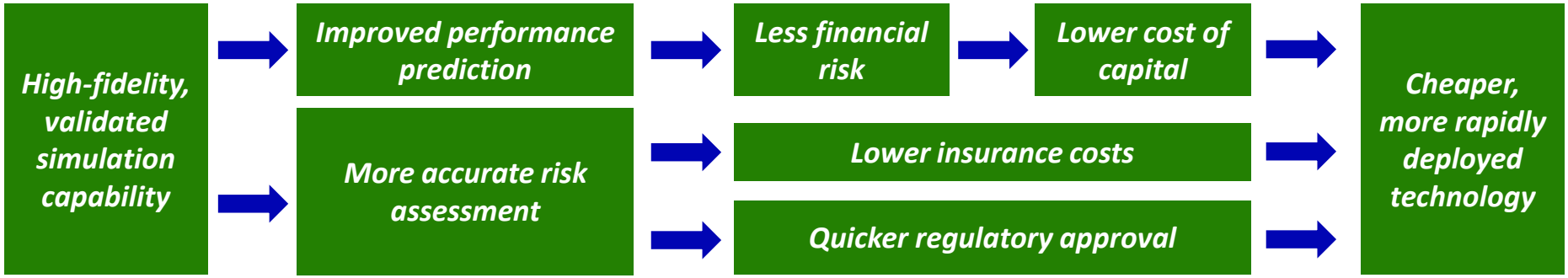



Integrated Coal-Fired Plant with Carbon Capture (NETL)

# Post-Design Simulation (1)

- **Traditionally, engineering simulation used to *compare options and pick the most effective.* This is only one of the potential uses.**

**Accurate simulations may contribute to deployment of new technologies by improving assessment of risk in three areas: performance, insurance, and regulation.**




- **Analogous to mission assurance approach taken in aerospace.**
  - Requires simulations that *financers, insurers, and regulators* trust.
  - CFD used in this manner in the post-2010 offshore drilling industry.
  - Model comes from solar, wind, and carbon sequestration, but similar issues likely to be seen in geothermal, wave, tidal, etc.

# Post-Design Simulation (2)

**Other deployment and post-deployment related problems may be HPC driven**

- **Prediction of wind and solar performance on daily basis for grid integration is a potential HPC application.**
  - Using weather data (NOAA?) to understand expected weather, and then using plant-level models to turn this into an expected performance.
  - Requires a level of data handling similar to that of integrated experiment/HPC done by DOE, or NOAA in hurricane prediction.
- **Using plant-level simulations to determine operational responses (manufacturing, wind energy de-tuning, etc.)**

# So where does ACTT go?

- **“If we can’t communicate, we can’t collaborate.”**
  - Tech team’s primary goal is to allow communication across the department.
  - Deputy Undersecretary’s discussion with the team got labs interested in presenting.
- **Strike a balance between technical and program presentations.**
  - ACTT will highlight approaches that have the potential to jump between programs- both technologies and partnership approaches.
  - Peter Nugent of LBNL talking about combining HPC and large-scale experiments.
  - Sibendu Som of Argonne highlighting collaboration with industry.
  - Move towards steady monthly meetings, with 10-15 minute “updates” and 30-40 minute “deep dives”
  - Add more Lab members, broaden participation.
- **Goal is now to enable collaboration and partnership across programs and labs rather than be the partnership.**

# Thank You!  Questions?