U.S. DEPARTMENT OF ENERGY

Workshop on the Grand Challenges of Advanced Computing for Energy Innovation

Breakout Session #2

Current Users – Grand Challenges

August 1-2, 2012

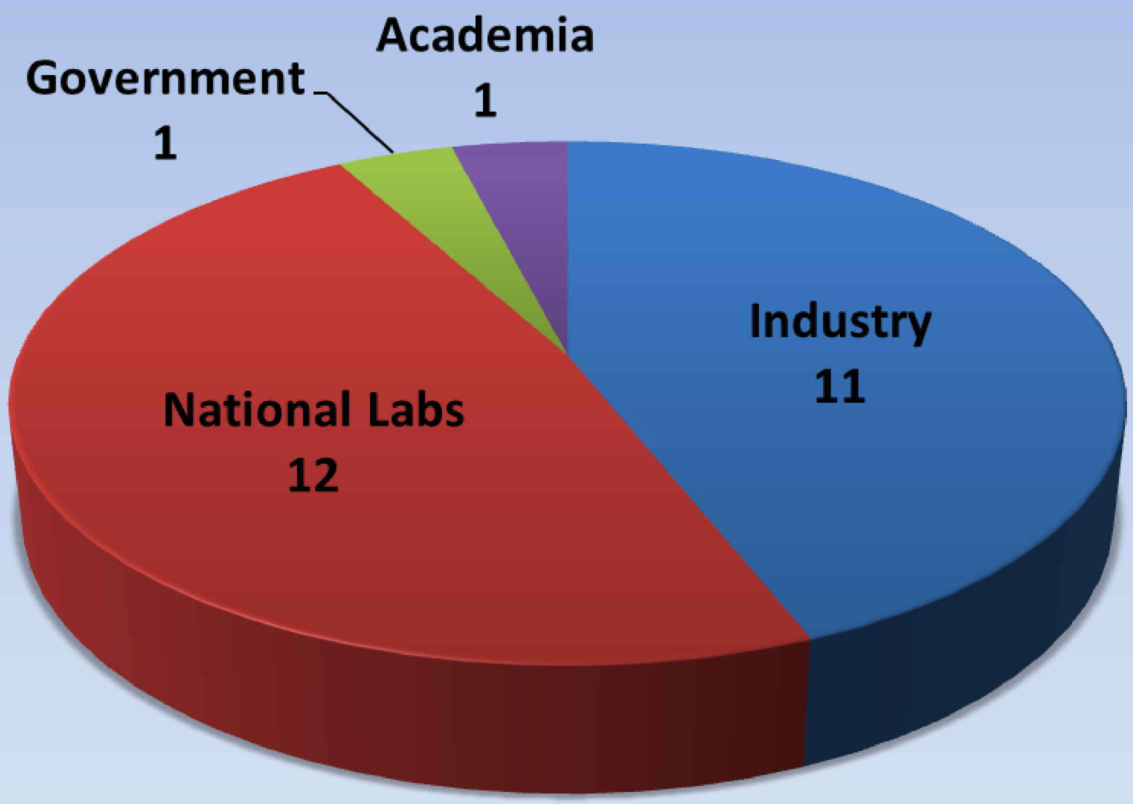
Conference Co-Chair: Steve Ashby

Breakout Session Leads: Moe Khaleel and Steven Lee

Breakout Session Charge:
Energy Innovation via Computing Success Stories

- Where and why advanced computing
  - What role does advanced computing play in your company?
  - What advantages have you realized from advanced computing?
- Challenges faced and overcome
  - What challenges did you face and how did you overcome them?
  - What was the nature of the challenges?
  - Comment with respect to “build, deploy, use” computing lifecycle
- Advice to others
  - How would you advise others considering use of advanced computing?
  - What could DOE do to facilitate wider adoption of advanced computing for energy problems?
- Other observations and recommendations

Breakout Session Participants



25 participants (16 institutions)

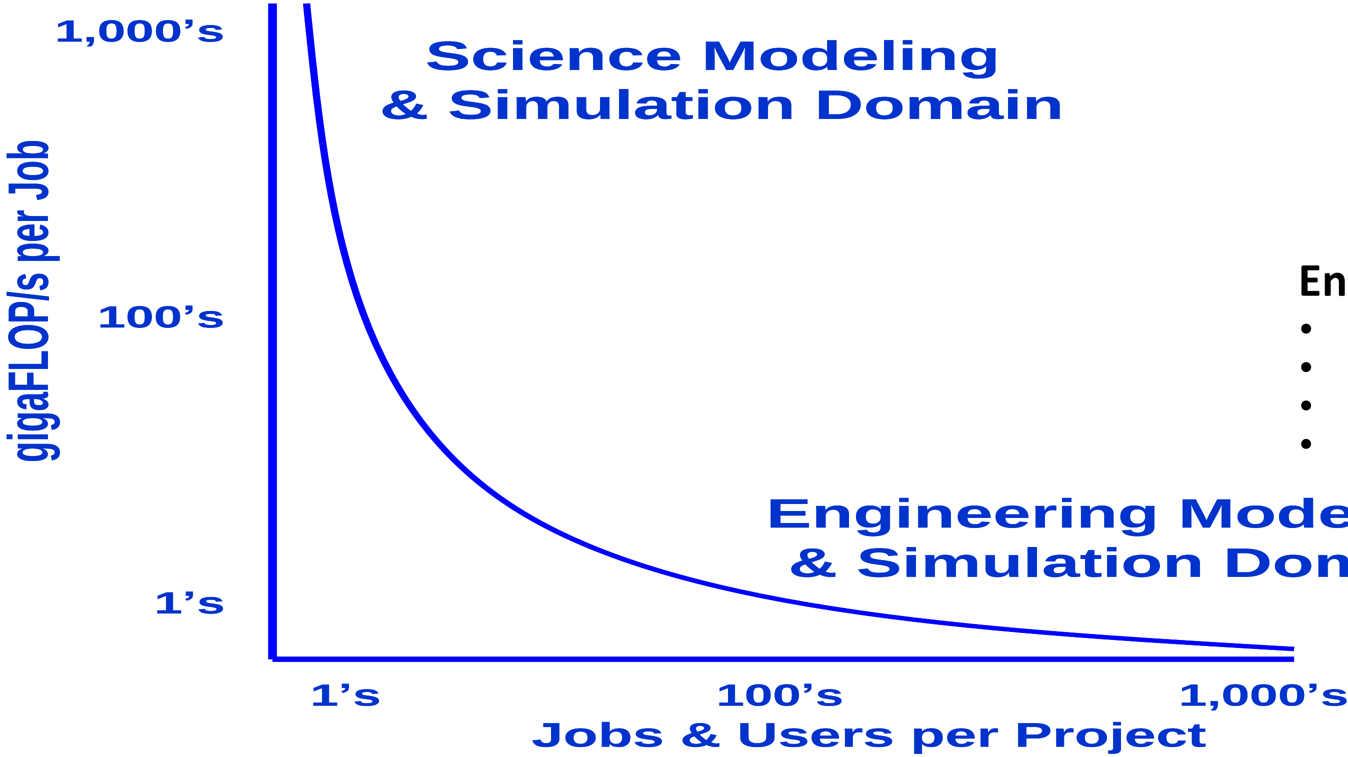
What does Advanced Computing Mean to you?

- Better answers/decisions faster
- Higher fidelity/improved coupling/etc. are means to that end
- Reduced uncertainties in the result
- Lowers risk to making consequential decisions based on the result “predictive”
- Wide range of computers (anything beyond single core, and includes Linux, Unix, Windows)
- Modeling and simulation and data analytics are all important for power grids
- Modeling and simulation, analytics, …
- Substantial scale >=10K cores
- The ability to solve complex analytical business/scientific challenges that are beyond the means of historic data and established knowledge
- Gain near physical insights → scientific discovery
- Virtual microscope
- Assure safety of existing systems
- Design new systems from first principl
- 100TF-class clusters in house
- Access to larger resources
- Focus on the applications and the science they can enable
- Analytics and the insights and decisions it enables
- Everything on Alex’s slide (3)
- Large HPC system
- The development, implementation, and validation of high fidelity modeling and simulation tools that can be deployed on a variety of computing platforms
- A simulation strategy that puts the increased performance, reduced price of computing to use
- Solutions
- Reduced risk
- Accelerated time to market
- New insights
- Higher fidelity (when necessary)
- Computation → knowledge → decision

Landscape

Science Domain

- Few users
- Few jobs
- Very big computers/job
- Long runtime



Engineering Domain

- Short, high pressure timelines
- Requirement for many, short jobs
- Many users
- User environment straightforward

Where and Why Advanced Computing

- **Role of advanced computing**
- Enabler
- Solve problems on larger scale and/or with greater details
- Develop by simulations rather than expensive testing
- High throughput computations

- **Advantages realized from advanced computing**
- Quick design time, reduction of cost
- Time speedup to build prototypes
- Only choice to solve a problem (big data)

Challenges Faced and Overcome

- **Characterize the Challenges you Faced**
- Knowing level of fidelity needed to deal with specific problem
- V& V of models
- How to engage with the National Labs
- IP issues

- **Overcome Challenges**
- Industry should be vocal about need for software and support from labs
- Rigorous process for "business pull" to understand business dirivers
- Embark on "umberall" agreements or CRADAs

Computing Life Cycle - “Build, Deploy, Use”

- Own in-house developed codes as well as commercial codes.
- For the in-house codes we have user development and support teams with “help desks”. Those teams keep the software up to date with new releases as needed.
- For the commercial codes we rely on the vendor support help lines
- Commercial applications supported by vendors. R&D applications supported internally
- Come to national labs to scale, refresh, test and/or benchmark their codes; determine if can do before make internal investment

Advice to Others

- **Valuable lessons learned**
- Must be clear about business value and the problem you are trying to solve
- Must be sure the tool can provide an answer

- **Justify HPC investments**
- Must make sure all the HPC hardware, software and support costs are included in the ROI calculation.
- Establish a clear business case for advanced computing in a specific domain
- Try with labs or others to test out the HPC system to justify the need

What could DOE Do?

- DOE could help accelerate the use of simulation by demonstrating the ability to get "right answers" to tough problems – model validation, best practice
- Send lab experts on sabbaticals to companies. Reciprocal sabbaticals too.
- Make national lab codes easier to use
- Algorithms and software development tools are a long-time national labs strength
- Computing environments available for trial use

Observations -- DOE Applied Programs

- DOE Applied Programs have lesser HPC resources/infrastructure than NNSA or SC
- DOE Applied Programs lack a SciDAC-like mechanism to fund advances in applications and middleware
  - INDUSTRY is the end user for what the Applied Programs deliver, not DOE!
  - Piecemeal approach: e.g.
    - Advanced Modeling & Simulation, NEAMS
    - Power grid funding, OE
    - NETL APECS, CCSI
    - Hubs

▶ There is a perception that the "missing middle"* issue impacts the pace of innovation in companies addressing the nation's critical energy problems

* June 15, 2011, **The Invisible Innovators: What Is the Missing Middle? And Why Do We Need Them,** Jon Riley; http://www.digitalmanufacturingreport.com/

The Missing Middle*

- The missing middle – companies that employ < 500 people.

- In the past 30 years, R&D investment in the larger companies has plummeted — from 72 percent of total in 1981 to 40 percent in 2007. (Source: National Science Foundation, Science Resource Studies, Survey of Industrial Research Development) .

- The Bell Labs, Xerox PARCs, Eastman Kodaks are history; The smallest enterprises now shoulder the burden of innovation.

- The missing middle has taken over innovation. It's R&D investment share has risen from 23% in 1983 to 64% in 2008.

- Industry as a whole is moving toward a 21st century digital paradigm, and the missing middle, the new torchbearers of innovation, need those 21st century tools to compete.

* June 15, 2011, **The Invisible Innovators: What Is the Missing Middle? And Why Do We Need Them,** Jon Riley; http://www.digitalmanufacturingreport.com/

Recommendations - Summary

- Make national lab technologies more accessible to the whole (open sources software is not necessarily an effective way)
- Lead in creating an ecosystem for computational innovation, supply vision, leadership and tools
- Incentivize greater adoption/use
- Be pro-active in outreach to industry, and key stakeholders including education
- Establish staff exchange mechanism between national labs and industry (see sabbatical comments from previous question discussion)

Example of What Does Success Look Like?

- Like an experimental beam line with end station