Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security

Town Hall Meeting: Energy Breakout

May 17, 2007

Oak Ridge National Laboratory

Joint Institute for Computational Sciences
Room 128 (Auditorium)

http://computing.ornl.gov/workshops/town_hall/index.shtml

Energy Breakout

A Simulation Renaissance for Nuclear Energy

- Assumptions and vision for 2015 (30 min)
- A deeper dive from different perspectives
  - Program integration perspective (45 min)
  - Fuel performance perspective (45 min)
  - Reprocessing perspective (45 min)
  - Fast reactor perspective (45 min)
- Putting it all together (30 min)

2015 Assumptions

- An exaflops platform is successfully designed and deployed
- Next-generation nuclear energy simulation tools have had 8 full years of DOE program support for sustained research, development, deployment, V&V, and application
- Nuclear energy simulation capability requirements, roadmaps, and milestones are established and integrated with a validation experimental plan

2015 Vision

- Nuclear energy simulation is “on par with experiment”
  - First-generation applications are deployed and being used to make mission-critical decisions that previously only experiments could make
- A closed fuel cycle solution is designed and being deployed (perhaps on a regional level)
- Regulatory agency role has changed to accommodate new simulation capabilities

Is This The Right Vision? If Not, What Is? How Do We Get There?

- Is the vision correct and attainable? If not, what should it be?
- What are the payoffs?
- Who are the stakeholders?
- What are the critical timelines?
- What are the enabling technologies and facilities?
- What are the technology barriers?
- What is the technology roadmap?
- What are the major annual program gates?
- What are the management and technological risks?
- What are the budget estimates?

E3SGS Questions to Answer

- What (in broad brush) is feasible or plausible to accomplish in 5-10 years?
- What are the major challenges in the area?
- What is today's state of the art in the area?
- How would we accelerate development with this program?
- What are expected outcomes and impact of acceleration or increased investment (i.e., what problems would we aim to solve or events we would cause to occur)?
- What scale of investment would be needed to accomplish the outcome?
- What are the major risks?

Discussion Leads

- Program integration
  - Sherrell Greene (ORNL)
- Fuel performance
  - Phani Nukala (ORNL)
- Reactor design, analysis, and safety
  - Jess Gehin (ORNL)
- Separations reprocessing
  - Dave DePaoli (ORNL)

Program Integration - Introduction

- Lead - Sherrell Greene
- Opportunities
  - Affordable, safe electrical energy that does not proliferate
- Issues
  - “All models are wrong, some models are useful, the only way to tell between the two is to get some data.”
  - Better become the enemy of good enough
  - Does not have the drivers of
    - Nuclear weapons
    - Climate change
    - Aircraft industry
- Stakeholders
  - Nuclear power industry
    - Hyper-regulated
    - Capital intensive
    - Lots of public security
    - Hyper-risk adverse
    - Only uses COTS
  - Nuclear technology vendors
    - Exist providing services
    - Dominated by proprietary data and tools
    - Have not bought into HCP
  - NRC
    - Hyper-conservative
    - Slow (6 years to license)
  - DOE
    - All but abandoned nuclear energy
    - NE very milestone oriented
    - Nobody owns applied research in nuclear energy
  - Professional societies

Program Integration - Challenges

- Grand challenges
  - Higher temperature
  - Greater burnup
  - Increase efficiency
  - Diversity of plant sizes
  - Affordable high temperature process heat
  - Reduced product development time
- Computational Thrusts
  - Fuel cycle design and optimization (“follow the atom”)
  - Reactor performance (macroscopic, microscopic fuel performance)
  - Radiochemical separation
  - Waste form behavior
- Final Thoughts
  - An epiphany of realization that all stakeholders have to partner together to make this happen
  - Cannot hand everything on GNEP
    - Pick a problem and show results
  - Avoid trite generalizations
    - Keep balance between stretch goals and overselling
  - We need to “go for it”

Program Integration - Discussion

- Is the 10 years realistic?
  - Yes - focused on achieving success on a single project (maybe 2 or 3)
- Are there other international efforts that can be leveraged?
  - The French have a similar program, but overall very few. Most players are just porting legacy codes to new platforms
- Problem of lack of leadership.
  - Yes, and this needs to change. We need someone to own the problem
- What could be the “near death” experience that will drive the changes in the nuclear design process
  - The Federal Requirement for safe, reliable and affordable nuclear power
- How can we close the gap between industry and the modeling and simulation worlds
  - New orders for plants will motivate (and finance) the shift to new technologies

Reprocessing Issues

- Lead - Dave DePaoli
- Issues
  - Process very complicated (more than just solvent extraction) with a large number of different materials
  - Multiple pathways being considered
  - Treatment of waste streams
  - Improving coupling between computations and experiments
    - High temperature & radiation
  - Need for multi-scale modeling

Reprocessing - Opportunities

- Opportunities
  - Research on developing of separation agents
    - Can they be “engineered” to get desired results
  - Full scale plant simulations using first principles
  - Some codes are adequate, others need work
  - Integrating multiple codes
  - Separations simulations
    - Empirical understanding does not lead to appropriate scale-up
    - Requires exascale computing
- Payoffs
  - Reduced R&D cost and time
  - Improved/accelerated design
    - Process scale-up
    - Reduced facility cost
  - Opportunity for major change
    - Shorten path to X by Y years
  - Waste form design

Reprocessing - Discussion

- How accurate do the chemical models have to be?
- Can it be done?
- Why not put the waste in space?
  - The waste is so dangerous it would be too dangerous go through the launch process
- European are currently reprocessing - how are they using modeling and simulation to support that?
  - They are not as far along, are using empirical data and they are using well understood reprocessing processing.
- What are the computational science gap that prevent the modeling of waste forms?
  - A lot can be done now, but some improvements are needed
  - Other models are quite limited (zero dimensional)
- Another driver might be safety.
- Biggest payoff?
  - Waste forms - can not do satisfactory experimentation of long life waste forms

Modeling of Fuel Rod - Opportunities

- Lead - Phani K. Nukala
- Predictive capability
  - Reduce fuel development & qualification
  - Life cycle performance assessment
  - Address safety concerns
  - Predict fuel rod behavior in DBA
- TRU fuels
  - Extreme temperatures

Modeling of Fuel Rod - Issues

- Material properties
  - Swelling
  - Phase change in mirostructure
  - Thermal properties
  - Crack formation and mechanical property changes
- Inherently multiscale
  - Point defects
  - Defect and fission product
- Current state of the arit
  - Axi-symmetric models (2D)
- Cladding behavior governed by
  - Multi-physics
  - Feedback from multiscale
- Need for capacity and capability computing
- Need for higher resolution and larger model size
- Coupling time scales requires algorithmic advances

Modeling of Fuel Rod - Discussion

- What are the justification for exascale?
  - Calculations based only on thermodynamics. When adding additional physics, this will scale even higher
  - Also, incorporation of uncertainties and optimization

Recycling Reactors - Opportunities

- Lead - Jess Gehin
- Opportunities
  - Eliminate unrealistic assumptions that drive to more conservative designs and thus higher installation costs
  - Higer power efficiencies
  - Reduction of learning curves to get efficiencies
  - Reduction in the required number of repositories
  - Increase in safety
  - Optimize design of
    - Power Grid
    - Fuel cycle
    - Operations
    - On-line monitoring
    - Operator training

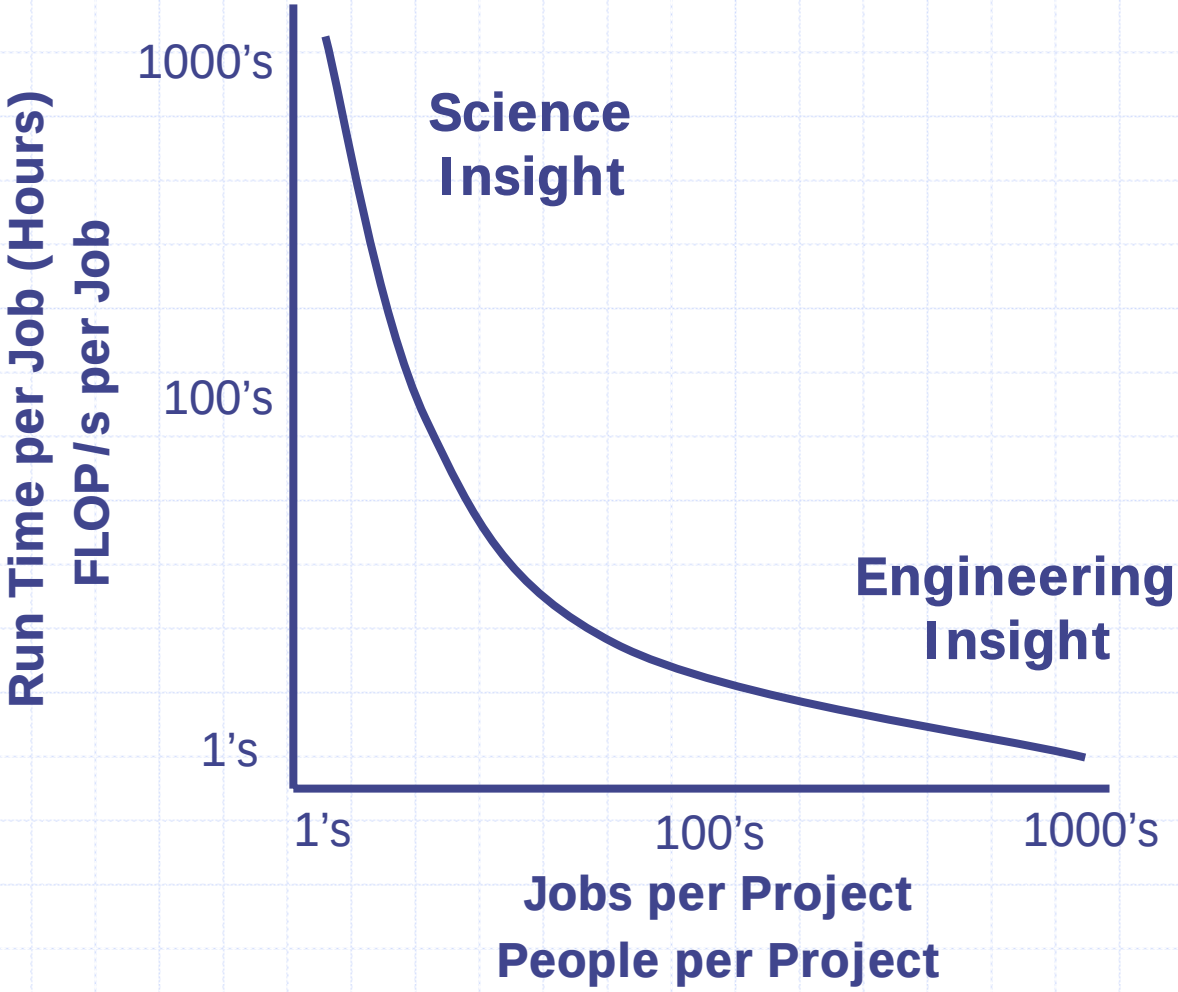
Recycling Reactors - Issues

- Core a coupled physics problem (not currently being done very well today)
- Need to look at full system
- Designs excessively conservative
- On par with experiment
  - Possible in areas that physics are well known and data exisit
  - Difficult when it does not
- Regulatory need to accommodate new simulation capabilities
  - Experimental needs
  - QA

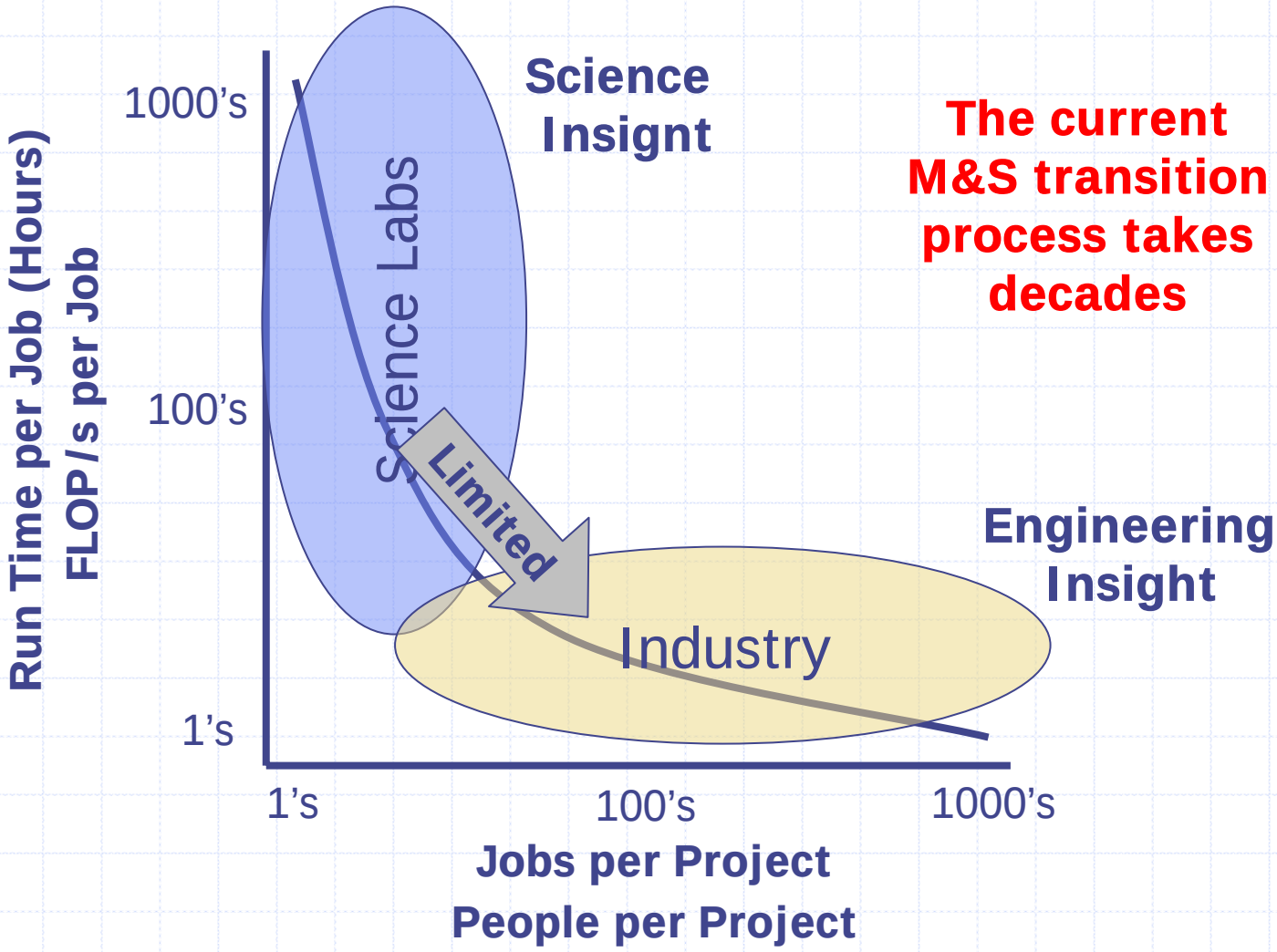
Modeling and Simulation Characteristics

- **Scientific**
  - As much “first principles” as possible required for modeling and simulations
  - Codes usually developed and validated as part of the discover process
  - Models then to be relatively static (i.e. not part of a design process)
  - Capability jobs are critical to advancing this type of insight
  - Limited number of users (1’s or 10’s of scientists) per project
  - Deliberate (slow) turn around on “projects”
- **Engineering**
  - Models are dynamic to support a design process
  - Turn around on “jobs” required to be hours and days
  - Use of existing, validated codes
  - Users that number in the 10’s to 100’s per project
  - Codes use of “abstractions” of physical properties
  - Capacity computing critical to success

Modeling and Simulation Requirements Relationship

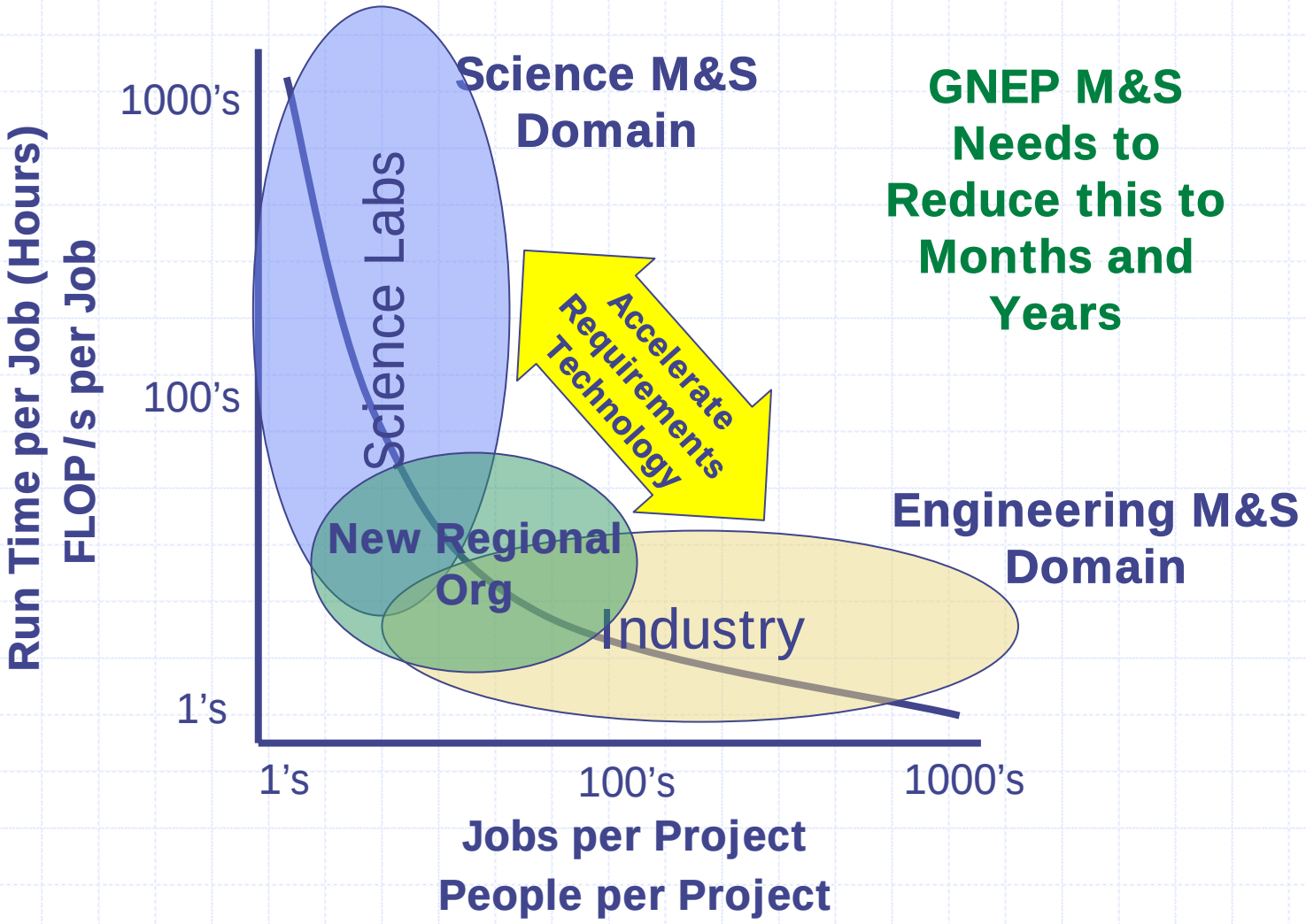
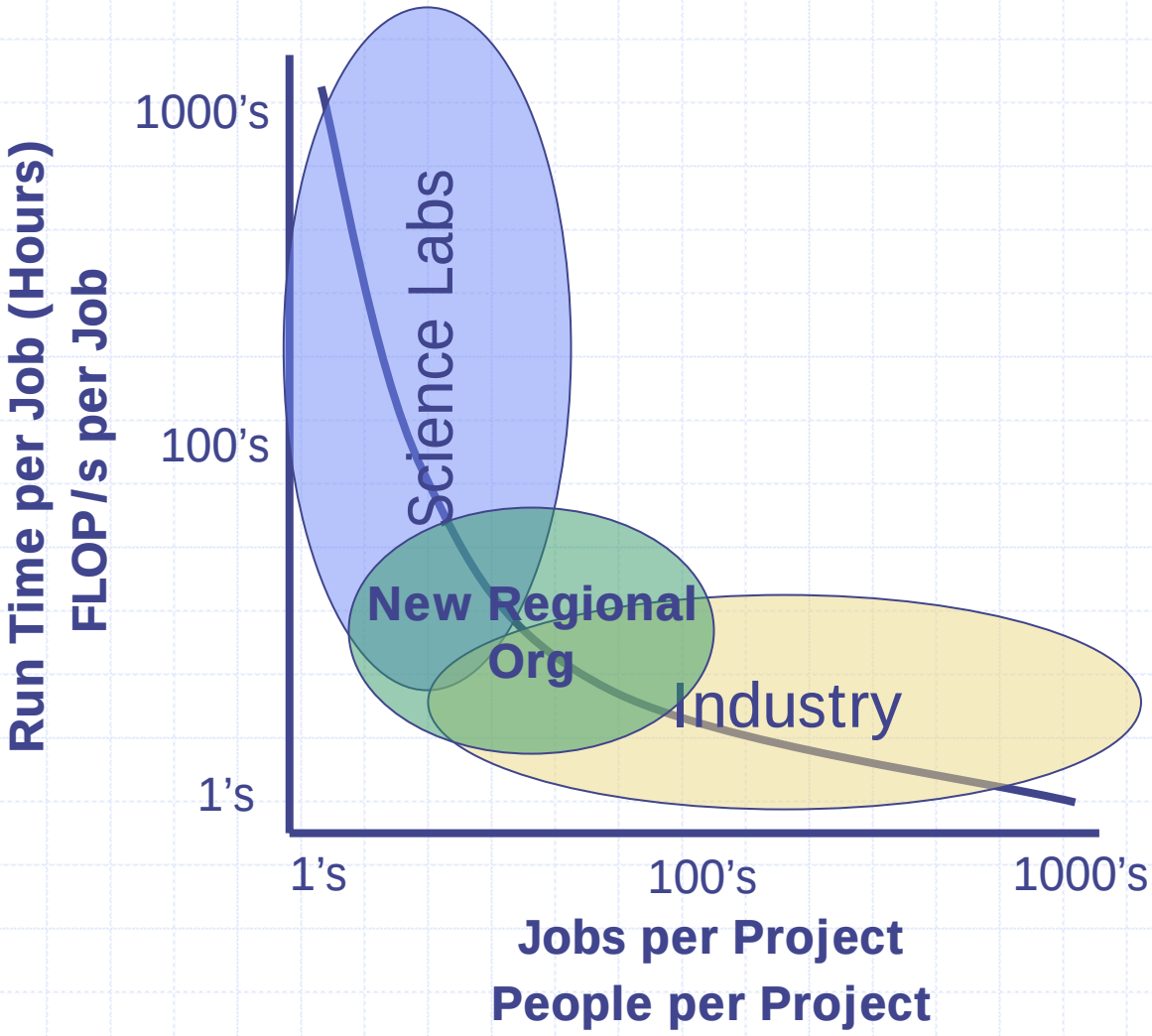


The GNEP Challenge -
Increasing the Pace and Quality of the Transition



The current M&S transition process takes decades

Potential Organization to “Fill the Gap”



Roles Needed for GNEP