U.S. DEPARTMENT OF ENERGY | Office of Science

A New Paradigm for DOE Applied Mathematics

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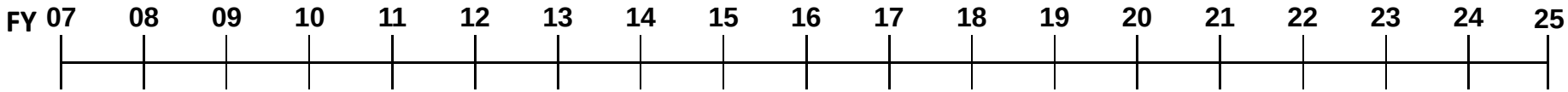
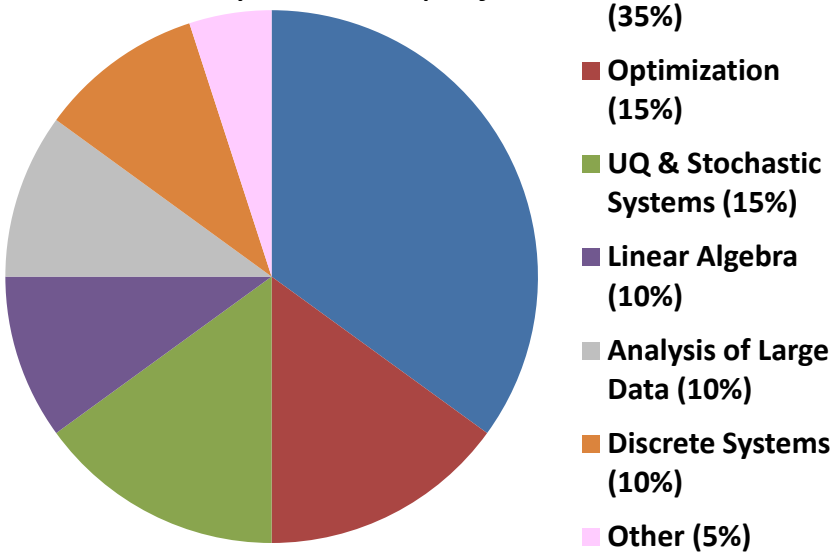
DOE Applied Mathematics paradigm now

The DOE Applied Mathematics program supports basic research leading to fundamental mathematical advances and computational breakthroughs across DOE and Office of Science missions; analysis and development of robust mathematical models, algorithms and software for enabling predictive scientific simulations of DOE-relevant complex systems.

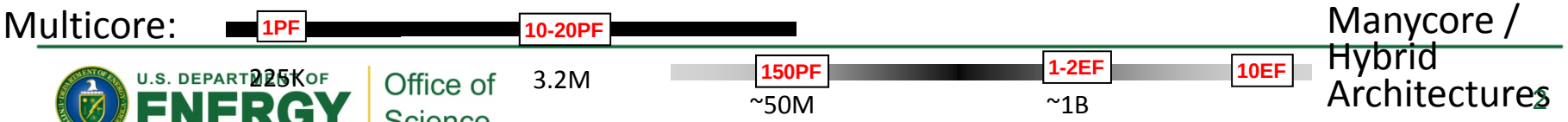


FY12: $40M/year, ~110 projects



Future: Modeling, analysis, and algorithms for simulation of DOE complex systems:

- Increase fidelity: develop new multi-scale, multi-physics models, analysis of coupled systems
- Uncertainty Quantification and V&V
- Approaches for systems that are inherently stochastic
- Methods that integrate data and simulation
- Novel analysis of algorithms for large data / streaming data
- Solvers and optimization methods with reduced global communication
- Higher-order methods; accuracy, stability of methods that move away from bulk synchronous programming models
- Algorithms resilient to machine errors
- Analysis of algorithms for emerging architectures



DOE Applied Mathematics paradigm now

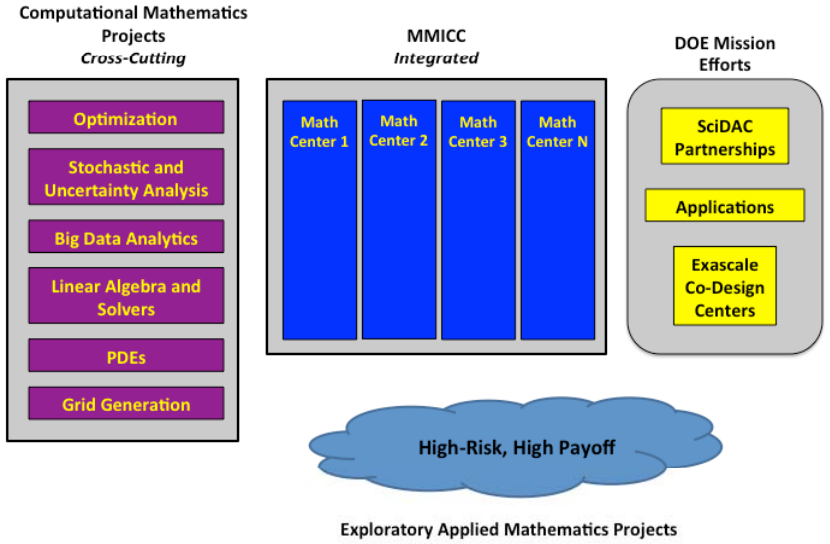
- **Targeted solicitations & unsolicited proposals addressing mathematical topic areas with DOE-relevance**
- **Size of research projects:**
  - Single PI / Two-person team (<$250K) : ~20% of all projects
  - Medium-size teams, 3-5 researchers ($250K-$1M): ~75% of all projects
  - Large- size teams, 5+ researchers (>$1M): ~5% of all projects

New DOE Applied Mathematics paradigm

Support the research and development of applied mathematical models, methods and algorithms for understanding natural and engineered systems related to DOE's mission … Support ASCR Challenge: Discover new applied mathematics, computer science, and networking tools for the ultra-low power, multicore-computing future and data-intensive science

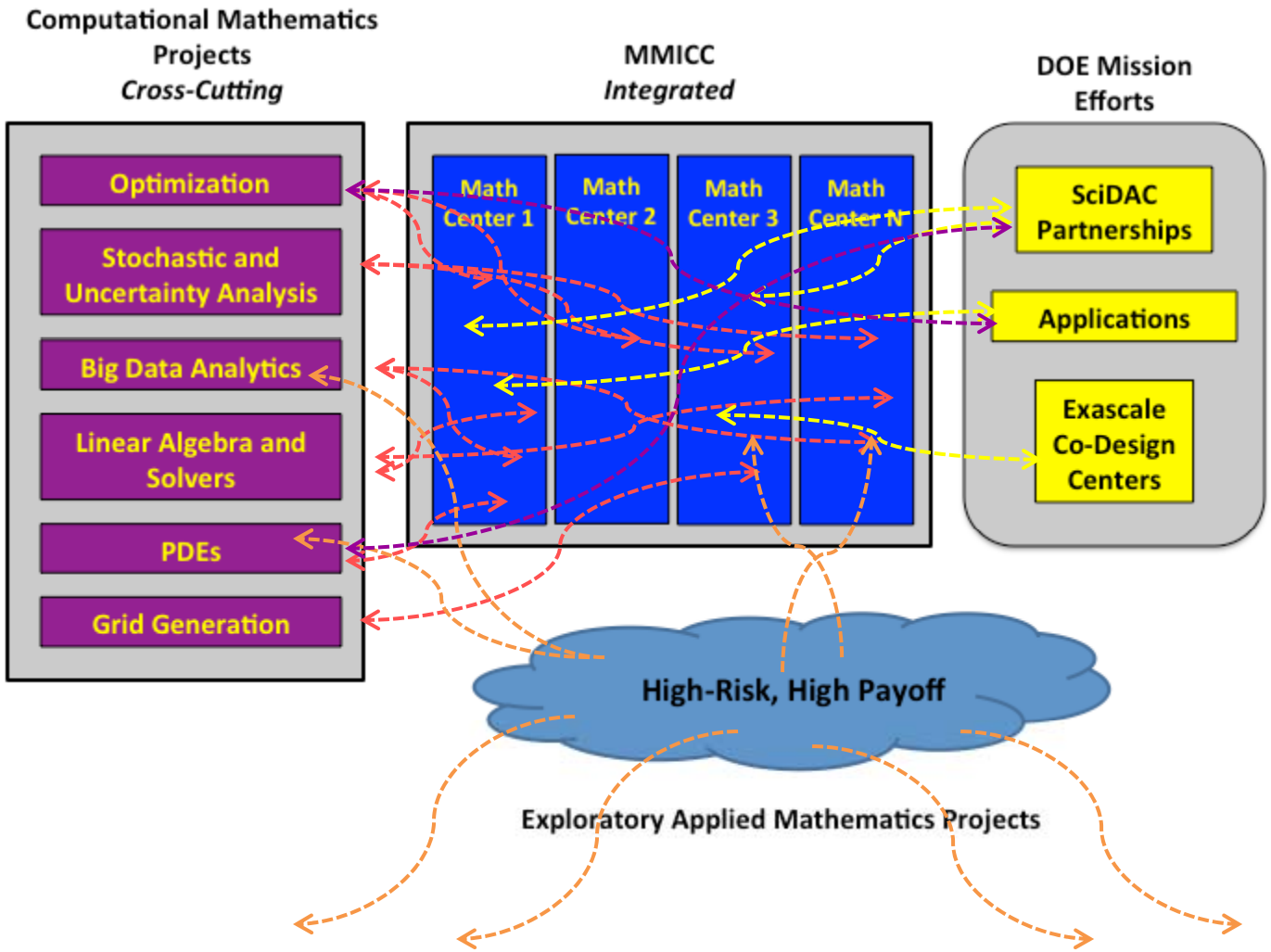
Long-term goals:

- Mathematics research that 5-10+ years out will impact DOE mission efforts: DOE Applications, SciDAC Partnerships, and Exascale Co-Design
- New Mathematical Multifaceted Integrated Capability Centers (MMICCs) directly enhances impact of applied math on DOE mission



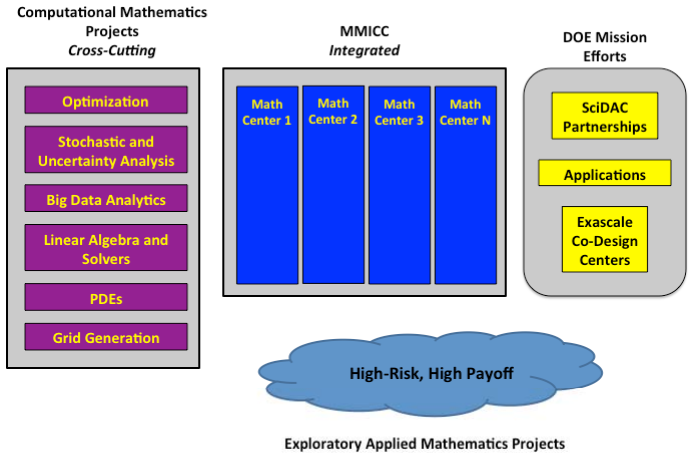
- Cross-cutting mathematics projects: addresses foundational, algorithmic and extreme-scale mathematical challenges
- High-risk, high-payoff: new mechanism to bring in highly innovative research

New Applied Mathematics Paradigm



Applied Mathematics:
Mathematical Multifaceted Integrated Capability Centers (MMICCs)

- Background
  - 2005 Multiscale Mathematics solicitation
  - 15 projects awarded under Multiscale Mathematics and Optimization of Complex Systems (ending 8/2012)
  - 7 projects awarded under Mathematics for Complex Distributed Interconnected Systems (ending 8/2012)
  - 7 projects awarded under ARRA Multiscale Mathematics and Optimization of Complex Systems (ending 8/2012)



  - Workshop: Sept 13-15, 2011; Workshop report, *"A Multifaceted Mathematical Approach for Complex Systems"* March 2012.
  - Applied Math Summit 3/7/2012.
- New Paradigm
  - Holistically address mathematics for increasingly complex DOE-relevant systems for scientific discovery, design, optimization and risk assessment.
  - Broader view of the problem as a whole, and devise solution strategies that attack the problem in "its entirety" by building fundamental, multidisciplinary mathematical capabilities
  - Enable applied mathematics researchers to work together in large, collaborative teams to more effectively address application problems earlier in the problem solving process.

Summit Discussion (3/7/2012)

- What are the pro's and con's of this new paradigm? Are there examples of other centers that we can learn from?
- What should the MMICCs focus on, e.g. themes?
- How close to, or removed from, an application should the center be?
- Can a MMICC focus on foundational and computational mathematics effectively for multiple domain applications?
- How might they change over time?
- How will this be received within the applied mathematics community? How should this be socialized?
- How do you measure success of a center?
- After this meeting what should be the next step in accomplishing this paradigm shift.

Summit Summary – Key Points(3/7/2012)

- MMICCs are a good idea but note that long-term cross-cutting mathematics projects have been mainstay of success of DOE Applied Mathematics program.
- MMICCs structure should have clear relevance and impact to DOE mission areas
- If successful, MMICCs will grow entire Applied Math program
- MMICCs: Let the applicants define a “Grand Challenges”.
  - Grand Challenges for MMICCs include defining one or more DOE-relevant scientific or engineering challenges; these are then abstracted into a set of mathematical research challenges that must be addressed through an multifaceted, integrated, iterative process.

Summit Summary – Key Points(3/7/2012)

- Extended discussion of MMICCs themes:
  - Is it feasible to focus on more than one application?
    - Yes, MMICCs should focus on mathematical abstractions of science problems, but also ensure that results, e.g. models, methods and algorithms, will have long-term science impact.
  - Areas that are ripe for investment:
    - Materials & Chemistry for Energy Applications
    - Complex Engineered Systems e.g. power grid with a focus on real time, predictive capabilities
    - Fluid-structures interactions, but choose illustrative example carefully
    - SC Facilities, e.g. light sources (Note: math challenges not well articulated)
  - Areas that already have a lot of investment:
    - Fusion
    - Accelerator modeling
    - Climate
    - CFD,
    - Nuclear weapons design code

Summit Summary – Key Points(3/7/2012)

- Binding pre-applications are a good idea; won't waste applicants' time and reviewers' time
- Center director is critical for success; identify key senior staff; allow flexibility of junior staff and collaborations
- Socialization with Applied Mathematics community is important; it will be challenging and take time.

- MMICCs will need to:
  - Address the ***long-term mathematical challenges*** one or more DOE grand challenges of increasing complexity and that require new multifaceted, integrated processes across multiple mathematical disciplines.
  - Identify ***a set of mathematics research challenges that represent abstractions*** of the grand challenges. These abstractions would then be optimally addressed through a multifaceted, integrated approach.
  - Have ***potential impact*** to the DOE mission ***in the 5-10+ year timeframe*** by transitioning to SciDAC Partnerships, SciDAC Institutes, Co-Design Centers, and/or directly to DOE application scientists.

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Questions?

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