Report from the Subcommittee on the Evaluation of the

# Long Term Goal of Enabling Effective Modeling of Complex Systems

Subcommittee Members:

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# The Charge:

- The subcommittee was asked to evaluate progress toward the long term goal:

***"By 2015, demonstrate progress toward developing mathematics, algorithms, and software that enable effective scientifically critical models of complex systems, including highly nonlinear or uncertain phenomena, or processes that interact on vastly different scales or contain both discrete and continuous elements."***

# Evaluation:

- The subcommittee finds that:

***"The Office of Advanced Scientific Computing Research (OASCR) has made an excellent start toward achieving the goal of enabling effective modeling of complex systems, in particular those systems with processes that interact on vastly different scales."***

Ref: Subcommittee Report

# Background on OASCR Efforts

- OASCR has initiated two key efforts to address the long term goal of enabling effective modeling of complex systems
  - First effort focused on advancing multi-scale mathematics to address processes that interact on vastly different scales
    - Widespread agreement that multi-scale mathematics is a research area ripe for the greatest payoffs
  - Second effort just getting underway will begin to address the broader set of mathematical challenges in the field of Complex Systems
    - Workshop scheduled for Dec 7-8, 2006

# Finding on the Planned Workshop for December 2006

- "Mathematical Research Challenges in Optimization of Complex Systems"
- Shows enormous promise
  - Based on:
    - Credentials and dedication of the organizers
    - Invitation list
- Addresses the broader set of issues beyond multi-scale mathematics
  - Necessary to fully address the long term goal

# Multi-scale Mathematics Research and Education Program: Workshops

- Initiated in 2004 with a series of three workshops and reports
  - May, July, and Sept 2004
  - Broad representation from the mathematics and computational science community
  - Defined the opportunity and a path forward
    - Strategic Plan for addressing the mathematical challenge of multi-scale phenomena
  - Increased awareness of the program and research challenges
  - http://www.sc.doe.gov/ascr/mics/ams/index.html
- Important conclusion
  - Multi-scale challenge will not be advanced solely by increasing capability computing
  - Will necessarily require the development of
    - new mathematics
    - new algorithms
    - Collaborations amongst domain scientists with mathematicians

# Multi-scale Mathematics Research and Education Program: Request for Proposals

- Posting to Awards ~7 months
  - Posted 7-January-2005
  - Closed 28-March-2005 (< 3 months)
  - Awards announced 4-August-2005
- **13 funded from 170 proposals received (<8%)**
  - 25 institutions
    - 17 Universities, 8 DOE Laboratories
  - Some single PI, some large teams from multiple organizations
- $20.6M over three years
  - Minimum $650K to a Maximum $2.6M per proposal, $1.6M Average
- Covers a good cross-section of important problems, including
  - Biological systems
  - Plasma physics
  - Nano-scale materials
  - Climate systems
- Making good progress

# Conclusions

- The multi-scale mathematics program needs to grow
  - First opportunity for any new proposals will be in FY08
  - Expect many excellent proposals from this first round could not be funded
- "Mathematical Research Challenges in Optimization of Complex Systems" will also require new funding
  - If OASCR is to continue to make progress towards the long term goal.
- Portfolio breadth of the core applied and computational mathematics needs to be maintained
- Growth in these mathematics programs should not fall to lower priority than investments in hardware to achieve peta-scale computing
  - Mathematical and algorithmic advances are absolutely necessary to address the modeling challenges in complex systems and therefore to meet the long term goal