Multiscale Mathematics Initiative

Gary M. Johnson
OASCR/MICS

Advanced Scientific Computing Advisory Committee Meeting
April 5 and 6, 2004
Hilton Washington Embassy Row Hotel
Washington, DC

President's FY2005 Budget Request:

Atomic to Macroscopic Mathematics

The FY 2005 budget also includes $8,500,000, for the new "Atomic to Macroscopic Mathematics" (AMM) research effort to provide the research support in applied mathematics needed to break through the current barriers in our understanding of complex physical processes that occur on a wide range of interacting length- and time-scales. The current state-of-the-art in the theory and modeling of complex physical systems generally requires that the physical phenomena being modeled either occur at a single scale, or widely separated scales with little or no interaction. Complex physical systems frequently involve highly nonlinear interactions among many phenomena at many different scales. Increases in computational power over the last decade have enabled scientists to begin the process of creating sophisticated models with fewer simplifying assumptions. These new models cannot succeed without a deeper understanding of the mathematics of phenomena at multiple scales and how they interact, from the atomic scale through the mesoscopic to the macroscopic. Achieving this basic mathematical understanding will provide enabling technology to virtually every challenging computational problem faced by the Office of Science.

Progress in AMM will best be achieved through a combination of investments, including (1) funds for innovative approaches to multiscale mathematics at universities throughout the country, (2) investments in partnerships between university researchers and investigators at the national laboratories, and (3) additional investments in multidisciplinary teams at the national laboratories. Category (1) represents investment in relatively high-risk / high-payoff approaches. Categories (2) and (3) follow the SciDAC model of building teams that involve national laboratory researchers in various critical applications. AMM research will support the development of new high-fidelity simulations that are crucial to our improved understanding of important problems across the Office of Science, including fuel cell design, understanding of microbial cells and communities, accelerator design and optimization, combustion processes including clean and efficient engine design, fusion reactor design and optimization, design of materials atom-by-atom, and many more.

DOE Multiscale Mathematics Workshop

The Sheraton Pentagon South Hotel
Alexandria, VA

May 3-5, 2004

http://www-fp.mcs.anl.gov/multiscale-workshop/

Workshop Co-Chairs

Linda Petzold
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Workshop Program

Monday, 3 May 2004

7:30 – 8:00	Continental breakfast provided
8:00 – 9:00	Welcome and Overview Includes description of process, including discussion of goals, concrete questions to be answered, logistics, etc.
9:00 – 10:00	Plenary Talk on fundamental issues of multiscale mathematics.
10:00 – 10:30	BREAK
10:30 – 11:30	Plenary Talk from illustrative application (illustrate challenge of multiscale with reference to *specific* roadblocks)
11:30 – 12:00	Assignment of breakout sessions and rooms
12:00 – 1:00	LUNCH
1:00 – 4:00	Breakout sessions led by applications
4:00 – 5:30	Brief presentation of findings from breakout sessions

Workshop Program

Tuesday, 4 May 2004

8:00 – 8:30	Continental breakfast provided
8:30 – 9:00	Clarification of charge, if necessary
9:00 – 12:00	Breakout sessions led by mathematicians
12:00 – 1:00	LUNCH
1:00 – 2:30	Brief presentations of findings from breakout sessions
2:30 – 3:00	BREAK
3:00 – 4:15	Panel discussion, applications panelists Includes search for unifying principles, common threads, etc.
4:15 – 5:30	Panel discussion, mathematician panelists. (This is where the fundamental mathematical underpinnings of multiscale issues will be discussed).

Workshop Program

Wednesday, 5 May 2004

8:00 – 8:30	Continental breakfast provided
8:30 – 9:00	Revisit charge for roadmap
9:00 – 12:00	Breakout sessions devoted to creating outlines for roadmap
12:00 – 1:00	LUNCH (General participants free to leave).
1:00 – 5:30	Session leaders meet to create first rough draft of roadmap document

Breakout session titles and co-leaders

Materials Science	Russ Caflisch (UCLA) Giulia Galli (LLNL)
Environmental and Geosciences	Mary Wheeler (UT-Austin) Casey Miller (UNC)
Biosciences	John Doyle (CalTech) TBA
Fusion	Phil Colella (LBNL) Steve Jardin (PPPL)
Combustion	John Bell (LBNL) Ahmed Ghoniem (MIT)
High Energy Density Physics	David Livermore (Maryland) Bob Rosner (ANL/Uchicago)
Uncertainty Quantification	George Ostrouchov (ORNL) Roger Ghanem (JHU)
Information Sciences	Ewing Lusk (ANL) Jim Thomas (PNNL)