



*U.S. Department of Energy's*  
**Office of Science**

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# **A Science-based Case for Large-Scale Simulation (SCaLeS)**

*Advanced Scientific Computing Research*  
*Strategic Planning workshop*

**Dan Hitchcock**

*22 July 2003*



# Original Charge (April 2003, Polansky)

- “Identify rich and fruitful directions for the computational sciences from the perspective of scientific and engineering applications”
- Build a “strong science case for an ultra-scale computing capability for the Office of Science”
- “Address major opportunities and challenges facing computational sciences in areas of strategic importance to the Office of Science”
- “Report by July 30, 2003”
- “Foster additional workshops, meetings and discussions on specific topics that can be identified and analyzed over the course of the next year”
- Though our formal charge is Office of Science-centric, the report may ultimately be combined with others in a multiagency thrust, and should be prepared with a broader science case and need not be confined scientifically to Office of Science interests alone



# Envisioning the report

- Dozens of authors from labs and universities
- Editorial oversight by small board, including expertise from each Office
- Written hierarchically, with easy-to-read summaries for Congressional staffers and in-depth sections to impress non-computational experts from scientific community
- Broad and as comprehensive as possible, as to areas touched
- Deep in a number of illustrative places, through case studies
- Written with strong awareness of antecedents and distinct mission
- Laden with good charts and good (but not gimmicky) scientific eye-candy



# Workshop planning

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- Selected plenaries on context and structure
- Selected plenaries on scientific content and scaling analyses
- Parallel sessions of breakout groups organized by:
  - Disciplinary areas (one session, w/approx. 10 breakouts)
  - Cross-cutting discussions (two sessions)
- Parallel sessions scribed by invited and prepared graduate students; overall meeting and written products professionally scribed with DOE HQ support
- Web supported (with *a priori* and *a posteriori* postings of position papers and presentations)



# Antecedent reports

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- 1982: “Large Scale Computing in Science and Engineering” (convened by NSB)
- 1992: “Grand Challenges: High Performance Computing and Communications” (OSTP)
- 1993: “From Desktop to Teraflop: Exploiting the U.S. Lead in High Performance Computing” (NSF)
- 1995: “Report of the Task Force on the Future of the NSF Supercomputer Centers Program” (NSF)
- 1999: “Information Technology Research: Investing in Our Future” (PITAC)
- 2000: “Scientific Discovery through Advanced Computing” (DOE SC)
- 2003: “Revolutionizing Science and Engineering through Cyberinfrastructure” (NSF)



# SCaLeS Workshop

- Held on 24—25 June, to provide input for a report required by 30 July(!)
- Approximately 325 participants from 11 applications areas, 8 applied mathematics areas and 8 computer science areas
- Patterned on the SciDAC approach (interdisciplinary, balance among hardware resources, applications and “enabling technologies”)
- Three main chapters for the report: *Applications*, *Mathematics*, *Computer Science*
- Chapter editors are (resp.) Thom Dunning, Phil Colella and Bill Gropp, with David Keyes the report editor
- Two reports envisioned: Short digestible overview report (30 July), and a longer detailed report, to be published by SIAM



# Chapter Authors / Workshop Leaders

- Applications
  - Accelerator Modeling – Kwok Ko, Rob Ryne
  - Astrophysics – Tony Mezzacappa, Bob Rosner
  - Biology – Mike Colvin, George Michaels
  - Chemistry – Robert Harrison, Theresa Windus
  - **Climate – John Drake, Bob Malone, Phil Jones\***
  - Combustion – John Bell, Larry Rahn
  - Environmental – Mary Wheeler, Steve Yabusaki
  - Materials – Francois Gygi, Malcolm Stocks
  - Nanoscience – Peter Cummings, Lin-Wang Wang
  - Plasma Science – Steve Jardin, Bill Nevins
  - QCD – Bob Sugar

\* Offsite



# Chapter Authors / Workshop Leaders

- Mathematics
  - CFD/MHD – Phil Colella, Paul Fischer
  - Discrete Math – Bruce Hendrickson, Alex Pothen
  - Solvers and “Fast” Algorithms – Van Henson, Juan Meza
  - Meshing Methods – Lori Freitag, David Serafini, David L. Brown
  - Multiphysics – Dana Knoll, John Shadid
  - Multiscale – Tom Hughes, Mark Shephard
  - Radiation Transport / Kinetic Methods – Frank Graziani, Jim Morel
  - Uncertainty – Jim Glimm, Sallie Keller-McNulty



# Chapter Authors / Workshop Leaders

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- Computer Science
  - Architecture – Bill Gropp, Jim Tomkins
  - Access / Resource Sharing – Ian Foster\*
  - Data – Arie Shoshani, Dorom Rotem
  - Frameworks / Environments – Rob Armstrong, Kathy Yelick
  - Performance Tools / Evaluation – David Bailey
  - Software Management – Steve Hammond, Rusty Lusk
  - System Software – Al Geist
  - Visualization – Wes Bethel, Chuck Hansen

\* Offsite



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