Computational Subsurface Sciences Workshop

Marriott Bethesda North Conference Center
9-12 January 2007

http://subsurface2007.labworks.org/

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Collaborating Offices

- ## Office of Science (SC)
  http://www.sc.doe.gov/

- ## Office of Environmental Management (EM)
  http://www.em.doe.gov/pages/emhome.aspx

- ## Office of Fossil Energy (FE)
  http://www.fossil.energy.gov/

- ## Office of Civilian Radioactive Waste Management (RW)
  http://www.ocrwm.doe.gov/

Workshop Charge

- Identify computational science research needs and opportunities in the subsurface sciences and related areas, with a focus on developing a next generation of numerical models of subsurface flow and process simulation.

- Highlighted areas will include potential tera-scale (and future peta-scale) computational algorithms to enable high fidelity subsurface simulation models that fully couple key physical, chemical, geological and biological processes, with new capabilities to quantify and reduce model uncertainty.

- Prepare a preliminary letter report within one week of workshop completion and follow with a full report within 60 days of workshop completion.

Organizing Committee

Todd Arbogast	University of Texas at Austin
Ken Eggert	Los Alamos National Laboratory
Mike Heroux	Sandia National Laboratories
Tissa Illangasekare	Colorado School of Mines
Moe Khaleel	Pacific Northwest National Laboratory
Paul Meakin	Idaho National Laboratory
Jack Parker	Oak Ridge National Laboratory
Barry Smith	Argonne National Laboratory
Andy Tompson	Lawrence Livermore National Laboratory
Dave Zachmann	Colorado State University
George Zyvoloski	Los Alamos National Laboratory

Participation

- More than 150 registered for this invitation-only workshop

- Broad representation of discipline and computational scientists working in the subsurface sciences

- Participants from:
  - 11 DOE Laboratories
  - 25 Universities
  - Industry
  - DOE Headquarters (observers)

Workshop Structure

- Welcoming remarks by workshop organizers and representatives of the collaborating DOE offices

- Morning and afternoon plenary talks by leading experts

- Five panels:
  - morning led by discipline scientists
  - afternoon led by computational scientists

- Details at http://subsurface2007.labworks.org/

Disclaimer

This is a preview of *potential* coming attractions…

The workshop final report has not yet been submitted. Thus, all findings reported here should be viewed as preliminary and subject to change.

Crosscutting Findings and Challenges

- Uncertainty Analysis

- New Multi-Scale Computational Tools

- HPC High Fidelity Simulations

- Increased Collaboration

Tentative Panel Findings and Proposed Research Directions

Advanced Scientific Computing Research Program

1. Integrated Site Characterization
2. Protocols for "Soft" Data
3. Optimized Decision Making
4. Cyber Infrastructure
5. New Algorithms for Coupled Phenomena
6. High Performance Computing Data Management
7. Improved Multiphase Flow Simulators
8. New Algorithms for Parallel Computations
9. Risk Analysis
10. Community Building
11. High Fidelity CO_2 Sequestration Model
12. Physically Based Process Representation
13. New Algorithms for Parallel in Time Computations
14. Heterogeneity at Multiple Scales
15. Testbed of Upscaling Benchmarks
16. Pore Scale Particulate Transport
17. Pore Scale Reactive Flow

Conclusions

Advanced Scientific Computing Research Program

- Computational subsurface sciences research agenda challenges the limits of current simulation capabilities
- Many opportunities for significant advances in simulation capabilities and mutually beneficial collaborations exist
- Advanced computational capabilities would be of immediate use to the DOE Applications Offices (EM, FE, RW)
- Computational subsurface sciences research agenda will require new enabling technologies :
  - parallel programming models for MPI and multithreading
  - dynamic load balancing
  - language interoperability
  - high-performance data management
  - performance monitoring metrics
  - debugging tools
  - distributed data archiving
  - visualization
  - data mining
  - model validation and code verification
- Need to address daunting challenges related to the multi-scale, multi-physics nature of subsurface sciences
- Will require collaboration between discipline scientists in the DOE Applications Offices and computational scientists in SC's OASCR

Postscript

SC's Office of Basic Energy Sciences has just held the following workshop:

Basic Research Needs for Geosciences:
Facilitating 21st Century Energy Systems

Marriott Bethesda North Conference Center
21-23 February 2007
http://esd.lbl.gov/BRN-Geosciences2007/index.htm

"This workshop's goal is to identify the research needed to understand geological systems that can accommodate storage of energy byproducts over decadal, century and millennial time scales, and over a range of length scales. DOE initiatives on developing a hydrogen economy, zero emission fossil fuel power plants and advanced nuclear energy systems, among others, all assume large increases in the ability to dispose of energy-related byproducts."