AGENDA
Advanced Simulations: A Critical Tool for Future Nuclear Fuel Cycles

December 14-16, 2005

Wednesday, December 14, 2005

7:30 – 8:00	Continental Breakfast	B543 Lobby
8:00 – 9:00	Opening Plenary Session	B543 Auditorium
	Welcome to LLNL	Jane Long
	Starting ASCI: Possible Lessons for Nuclear Power	Vic Reis
	7-Lab Global Nuclear Futures Initiative	Dana Christensen
	Introductory Remarks; Overview of Workshop Objectives	Robert Rosner, William Martin

Concurrent Working Groups

Session 1A. Full System, Enrichment, Fuel Fabrication and Flow, Separation and Recycling Plants, B543 R1258

9:30 — 10:30	Mike Corradini, University of Wisconsin
10:30 — 10:45	Break
10:45 — 11:45	Kemal Pasamehmetaglu, INL

Session 1B. Thermal and Fast Reactors, B543 Auditorium

9:30 — 10:30	Per Peterson, UC Berkeley
10:30 — 10:45	Break
10:45 — 11:45	Philip Finck, ANL

Session 1C. Repository Performance and Design, B543 R1244

9:30 — 10:30	Bob Budnitz, LLNL
10:30 — 10:45	Break
10:45 — 11:45	John Anderson, UNR

12:00 – 12:45	*Lunch*	*B543 Lobby*
1:00 – 1:45	Plenary Speakers	B453 R1001
	NNSA's ASCI Program	Dmitri Kusnezov
1:45 – 1:55	The Grand Challenges of Visualizing and Analyzing ASC Data	Hank Childs, LLNL
1:55 – 2:30	PowerWall and Visualization Demo	
	100+ TFlop/s Solidification Simulations on BlueGene/L	Fred Streitz, LLNL
	Origins of Strength from Dislocation Dynamics	Vasily Bulatov, LLNL

Concurrent Working Groups Reconvene

Session 1A. Full System, Enrichment, Fuel Fabrication and Flow, Separation and Recycling Plants

2:30 — 4:30	Open Discussion Led by Mike Corradini and Kemal Pasamehmetaglu	

Session 1B. Thermal and Fast Reactors

2:30 — 4:30	Open Discussion Led by Per Peterson, Philip Finck, Bill Martin, and Dave Hill	

Session 1C. Repository Performance and Design

2:30 — 4:30	Open Discussion Led by Bob Budnitz and John Anderson	
4:30 — 5:00	Summary Discussion Led by Robert Rosner and William Martin	B543 Auditorium
5:30 — 8:00	Group Dinner	Central Cafeteria
7:00	BlueGene/L – A Case Study from Idea to Reality	Alan Gara, IBM and David Nowak, LLNL
8:00	Adjourn	

Thursday, December 15, 2005

8:00 – 8:30	Continental Breakfast	B543 Lobby
8:30 – 9:00	Plenary Session Objectives for Day 2	B543 Auditorium Robert Rosner, William Martin

Concurrent Working Groups

Session 2A. Computational Sciences/Framework (Chaired by: David Keyes), B543 R1244

9:00 — 9:20	Introductions/Instructions	David Keyes, Columbia
9:20 — 9:35	Models & Simulations for an Advanced, Theory-Based, Fuel Performance Code	Marius Stan, LANL
9:35 — 9:50	Current Status of Simulation on Supercomputers for Engineering Analysis	Jim Tomkins, SNL
9:50 — 10:05	Leadership Computing	Robert Harrison, ORNL
10:05 — 10:20	Software Frameworks to Assist Physics Simulation	Andy Wissink, LLNL
10:20 — 10:35	Supercomputing is Easier Than it Used to Be	Rusty Lusk, ANL
10:35 — 11:45	Discussion	

Session 2B. Neutronics (Chaired by: Forrest Brown), B543 R1258

9:00 — 9:15	Introductions/Instructions	Forrest Brown, LANL
9:15 — 9:30	Hybrid & Parallel Computing Particle Transport Methods in Shielding Core Physics	Ali Haghighat, Univ. of Florida
9:30 — 9:45	Recent Reactor Core Modeling R&D at the INL: Advanced Test Reactor & Pebble-bed Reactor	Hans Gougar, INL
9:45 — 10:00	Modern Transport Codes at LLNL for use on High Performance Computers	Spike Procassini, LLNL

10:00 — 10:15	Nodal Neutron Transport Methods	Elmer Lewis, Northwestern
10:15 — 10:30	The Numerical Nuclear Reactor: Full Core, 3-D Reactor Simulation with Coupled Integral Neutron Transport & CFD	Tom Downar, Purdue
10:30 — 10:45	Advanced Deterministic Transport Methods	Jim Morel, Texas A&M
10:45 — 11:00	Advanced Neutronics Simulation Development and Directions	Jess Gehin, ORNL
11:00 — 11:15	Nuclear Modeling for Cross Sections	Paul Dotson, LANL
11:15 — 11:30	Neutronic Analysis Needs for Future Nuclear Energy Systems	Hussein Khalil, ANL
11:30 — 11:45	Neutronics for Multiphysics Frameworks	Cassiano Oliveira, Georgia Tech.

Session 2C. Thermal Hydraulics and Computational Fluid Dynamcs (Chaired by: Tom Downar), B543 Aud.

9:00 — 9:20	Introductions/Instructions	Tom Downar, Purdue
9:20 — 9:35	Complete CFD for a Research Reactor–A Step Toward Power Reactors	Rizwan Uddin, Univ. of Illinois
9:35 — 9:50	Applying Multi-Scale Multi-Physics Modeling Methods to the Nuclear Reactor Design	Vlad Georgevich, LLNL
9:50 — 10:05	Modern Computational Tools for Reactor Safety	Paul Dotson, LANL
10:05 — 10:20	Simulations of Granular Flow in Pebble-bed Nuclear Reactors	Martin Bazant, MIT
10:20 — 10:35	Status & Future Needs of Reactor Safety Codes for Future Reactors	Karen Vierow, Purdue
10:35 — 10:50	Advanced Modeling & Simulation for Fluid Flow & Heat & Mass Transfer Applications	Randy Summers, SNL
10:50 — 11:05	Advanced Computational Techniques and Platforms for Solution of Thermal Hydraulic Problems	Graydon Yoder, ORNL
11:05 — 11:20	Particle & Grid-based Methods for Multiphase Fluid Flow	Paul Meakin, INL
11:20 — 11:35	Multi-physics Simulation Capability at the INL for High-resolution Analysis of Reactor Systems	Richard Martineau, INL
11:35 — 11:50	Challenges for CFD in Nuclear Applications	Yassin Hassan, Texas A&M

Session 2D. Structural Mechanics (Chaired by: Tinsley Oden), B543 R2234

9:00 — 9:20	Introductions/Instructions	Tinsley Oden, Univ. of Texas
9:20 — 9:35	Estimation and Control of Modeling and Discretization Error in Structural and Solid Mechanics	Tinsley Oden, Univ. of Texas
9:35 — 9:50	Advanced Modeling & Simulation for Structural Analyses	Hal Morgan, SNL
9:50 — 10:05	The Analysis Enterprise	Robert Ferencz, LLNL
10:05 — 10:20	Radiation Effects on Material Performance	Brian Wirth, UC Berkeley
10:20 — 11:45	Discussion	

Session 2E. Material Science (Chaired by: Steve Zinkle), B543 R1297

9:00 — 9:20	Introductions/Instructions	Steve Zinkle, ORNL
9:20 — 9:35	A Fundamental Science Approach to Optimizing Nuclear Fuel & Waste Form Design	Kurt Sickafus, LANL
9:35 — 9:50	Application of Computational Materials Science Multiscale Modeling to Fission Reactors	Steve Zinkle, ORNL
9:50 — 10:05	Simulations of Radiation Damage Processes in Silicon Carbide	Bill Weber, PNL
10:05 — 10:20	Advanced Modeling & Simulation for Material Science Applications	John Aidun, SNL
10:20 — 10:35	Modeling Materials in Reactor Environments	Tom Arsenlis, LLNL
10:35 — 10:50	Void Swelling and Radiation-induced Segregation: An Example of the Need for Advances in Computational Modeling	Todd Allen, Univ. of Wisconsin
10:50 — 11:05	Material Simulation Needs for Advanced Reactors	Bill Halsey, LLNL
11:05 — 11:45	Discussion	

Session 2F. Fuel Development (Chaired by: Kemal Pasamehmetaglu), B543 R2074

9:00 — 9:20	Introductions/Instructions	Kemal Pasamehmetaglu, INL
9:20 — 9:35	Modeling & Simulation of Fuel Material Performance Under Reactor Conditions	Jim Tulenko, Univ. of Florida
9:35 — 9:50	Modeling to Support Fuel Development for an Advanced Fuel Cycle	Dave Williams, ORNL
9:50 — 10:05	Advance Fuel Matrix for Next Generation Reactors	John Abrefah, PNL
10:05 — 10:20	Molecular Scale Heavy Element Science	Theresa Windus, PNL
10:20 — 10:35	Advanced Methodology for Fuel Cycle Analysis	John Lee, Univ. of Michigan
10:35 — 10:50	Advanced Modeling & Simulation for Nuclear Fuel Development	Paul Pickard, SNL
10:50 — 11:05	Chemical Reprocessing Plant Simulation	Monica Regalbuto, ANL
11:05 — 11:45	Discussion	

Session 2G. Probabilistic Risk Assessment (Chaired by: Paul Turinsky), B543 R1038

9:00 — 9:20	Introductions/Instructions Evaluation of Uncertainties of Predicted System Attributes	Paul Turinsky, NC State Univ.
9:20 — 9:35	Dynamic PRA Methods	Tunc Aldemir, OSU
9:35 — 9:50	Advanced Modeling & Simulation in PRA	John Kelly, SNL
9:50 — 10:05	The Use of Simulation for Sensitivity Analyses in PRA	Bob Budnitz, LLNL
10:05 — 10:20	Probabilistic Seismic Design and Evaluation of Nuclear Facility Structures	Bozidar Stojadinovic, UC Berkeley
10:20 — 10:35	Next-generation Simulation Models for Nuclear Waste Repositories	Bruce Robinson, LANL
10:35 — 11:45	Discussion	

12:00 – 12:45	*Lunch*	*B543 Lobby*
1:00 – 1:30	Plenary Speaker Large Scale Simulations in the Office of Science	B543 Auditorium Michael Strayer, DOE

Concurrent Working Groups Reconvene

Session 2A. Computational Sciences/Framework
2:00 — 3:15 Open Discussion Led by David Keyes

Session 2B. Neutronics
2:00 — 3:15 Open Discussion Led by Forrest Brown

Session 2C. Thermal Hydraulics and Computational Fluid Dynamics
2:00 — 3:15 Open Discussion Led by Tom Downar

Session 2D. Structural Mechanics
2:00 — 3:15 Open Discussion Led by Dave McCallen

Session 2E. Material Science
2:00 — 3:15 Open Discussion Led by Steve Zinkle

Session 2F. Fuel Development
2:00 — 3:15 Open Discussion Led by Kemal Pasamehmetaglu

Session 2G. Probabilistic Risk Assessment
2:00 — 3:15 Open Discussion Led by Paul Turinsky

3:15 — 3:30	*Break / Refreshments*	*B543 Lobby*
3:30 – 5:30	Summary/Preparation for Friday Plenary Session Co-Chairs Meet with Working Group Chairs and Keynote Speakers Only	B543 R1258
3:30 – 5:30	Open Time for Participant Discussions	B543 Conference Rooms
5:30	Adjourn	

Friday, December 16, 2005

8:00 – 8:30	Continental Breakfast	B543 Lobby
8:30 – 12:00	Plenary Session – Wrap Up *Session Summaries and Results,* *Concluding Remarks, Path Forward*	B543 Auditorium Session Chairs Robert Rosner, William Martin
12:00	Adjourn	