4 Outreach and Interaction

4.1 Technical Outreach

Meetings with the Rocket Industry

Critical interactions have continued during the fourth year of the CSAR program. Most significant among industrial/government laboratory meetings in the past year was our participation in the AIAA/ASME/SAE/ASEE Joint Propulsion Conference in Salt Lake City (see below). This followed an equally successful program in 2000 in Huntsville, Alabama.

Our relationship with NASA grew significantly in 2001. A long-awaited Space Act Agreement (the NASA equivalent of a DOE CRADA) was signed in May 2001. The SAA enables CSAR to receive sensitive, unclassified data from NASA that can be used for validation of our simulations, while NASA will receive a copy of the GEN1 and GEN2 codes to use in their research programs. The Validation, Accident, and Specification Team will be working with NASA to get more detailed data to validate the CSAR integrated code in Y5.

NASA and Thiokol teamed to provide the Center with the *Design Data Book for Space Shuttle Reusable Solid Rocket Motor* in 1998. The document contains a detailed description and discussion of the components that comprise the reusable solid rocket motor.

External Advisory Board

The third annual meeting of the CSAR External Advisory Board (EAB) was held 15-16 October 2001. The EAB membership is drawn from the DOE DP laboratories and academia, as well as from the commercial rocket industry, the high-performance computer industry, and other relevant companies. The Board reviewed research studies, was invited to make research recommendations, and continues to provide expertise for translating research findings into practice. The purpose of the EAB is several-fold: assure that the CSAR research program remains aggressive and forward-thinking; gain commercial rocket industry perspective; accelerate high-level technical exchange; catalyze long-term visits; and explore other funding opportunities. Current members of the Board include:

EAB Member	Organization	Title
David H. Bailey	Lawrence Berkeley National Laboratory	Chief Technologist, NERSC Division
Andy Baldi	Lockheed-Martin Missiles & Space	Director, FBM Propulsion and Controls
Felix F. Chen	Aerojet	Technical Principal, Engineering
Fred Culick	Caltech	Professor of Mechanical Engineering and Jet Propulsion
Gary Flandro	University of Tennessee Space Institute	Boling Chair Professor of Advanced Propulsion
Robert L. Glick		Consultant
Robert Keenan	Aerojet	Program Manager, Advanced Programs
Mitchell D.	Yale University	Chair, Mechanical Engineering and Applied

Smooke		Science
Fred S. Blom-shield	Naval Air Warfare Center, China Lake	Head, Propulsion Research Branch
I. Lee Davis	Thiokol Corporation	Senior Research Scientist
Robert Garcia	NASA Marshall Space Center	Group Lead, Applied Fluid Dynamics Analysis
Robert L. Geisler	Geisler Enterprises	Senior Rocket Scientist Consultant
Kent Hennessey	Atlantic Research Corporation	Manager, Thermal Design
Grant Henson	United Technologies/CSD	
Grant B. Hodson	Alliant Techsystems	Technical Manager, Air Force Projects
Taras Jarymowycz	Lockheed-Martin Missiles & Space	
David Kassoy	University of Colorado	Associate Vice President for Technology
Suresh Kulkarni	Thiokol Corporation	Vice President, Systems Engineering
David Mann	Army Research Office	Associate Director, Mechanics and Environmental Sciences Division
Allan J. McDonald	Thiokol Propulsion	Deputy and Technical Director, Science and Engineering
Paul Nielan	Sandia National Laboratory	Manager, Distributed Systems Research Department
Gregory A. Ruderman	Air Force Research Laboratory	Mechanical Engineer
John F. Sparks	Atlantic Research Corpora-tion	Director of Engineering Research

Technical Conferences

The Center provides travel funds to investigators to participate in conferences in core areas to enhance their technical expertise and to build global awareness of the ASCI/ASAP simulation program. Especially important to the technical community has been CSAR's annual participation in the AIAA/ASME/SAE/ASEE Joint Propulsion Conferences (JPC) in 2000 and 2001. A nine-paper session was organized in July 2001 for the JPC in Salt Lake City:

AIAA-2001-3040 —Dick, W. A., M. T. Heath, and R. A. Fiedler, "Integrated 3-D Simulation of Solid Propellant Rockets"

AIAA-2001-3579 — Buckmaster, J., T. L. Jackson, and M. Ulrich, "Numerical Modeling of Heterogeneous Propellant Combustion"

AIAA-2001-3947 — Melcher, J. C., H. Krier, and R. L. Burton, "Burning Aluminum Particles Inside a Laboratory-Scale Solid Rocket Motor"

AIAA-2001-3950 — Venugopal, P., F. M. Najjar, and R. D. Moser, "Numerical Simulations of Model Solid Rocket Motor Flows"

AIAA-2001-3951 — Ferry, J. and S. Balachandar, "Multiphase Flow Research and Implementation at CSAR"

AIAA-2001-3952 — Jackson, T. L., J. Buckmaster, M. Campbell, S. Kochevets, and L. Massa, "The Burning of 3D Random-pack Heterogeneous Propellants"

AIAA-2001-3953 — Geubelle, P. H., C. Hwang, R. A. Fiedler, S. Breitenfeld, and A. Haselbacher, "Simulation of Dynamic Fracture Events in Solid Propellant Rockets"

AIAA-2001-3954 — Fiedler, R. A., X. Jiao, A. Namazifard, A. Haselbacher, F. M. Najjar, and I. D. Parsons, "Coupled Fluid-Structure 3-D Solid Rocket Motor Simulations"

AIAA-2001-4502 — Tang, K. C. and M. Q. Brewster, "Dynamic Combustion of AP Composite Propellants: Ignition Pressure Spike"

In Y3 CSAR supported a full-day technical paper session presented by Center researchers at the JPC in Huntsville, Alabama, 18 July 2000. Thirteen papers were presented to the conference attendees that fully overviewed the research program and invited industrial and government researchers in the field to collaborate with CSAR.

AIAA-2000-3455 — Heath, M., R. Fiedler, and W. Dick, "Simulating Solid Propellant Rockets at CSAR"

AIAA-2000-3456 — Parsons, I. D., P. Alavilli, A. Namazifard, A. Acharya, X. Jiao, and R. Fiedler, "Coupled Simulations of Solid Rocket Motors"

AIAA-2000-3457 — Namazifard, A., I. Parsons, A. Acharya, E. Taciroglu, and J. Hales, "Parallel Structural Analysis of Solid Rocket Motors"

AIAA-2000-3459 — Hegab, A., T. Jackson, J. Buckmaster, and S. Stewart, "The Burning of Periodic Sandwich Propellants"

AIAA-2000-3460 — Knott, G. and M. Brewster, "A Two-dimensional Model of Composite Propellant Flame Structure and Burning Rate"

AIAA-2000-3461 — Kochevets, S., J. Buckmaster, and T. Jackson, "Random Propellant Packs and the Flames They Support"

AIAA-2000-3567 — Alavilli, P., J. Buckmaster, T. Jackson, and M. Short, "Ignition-Transient Modeling for Solid Propellant Rocket Motors"

AIAA-2000-3568 — Najjar, F., S. Balachandar, P. Alavilli, and J. Ferry, "Computations of Two-Phase Flow in Aluminized Solid Propellant Rockets"

AIAA-2000-3569 — Balachandar, S., J. Ferry, and P. Bagchi, "Fundamental Two-Phase Flow Modeling Efforts at CSAR"

AIAA-2000-3570 — Rani, S. and S. Vanka, "Direct Numerical Simulation of Two-Way Coupling Effects in a Particle-Laden Turbulent Pipe Flow"

AIAA-2000-3571 — Venugopal, P., F. Najjar, and R. Moser, "DNS and LES Computations of Model Solid Rocket Motors"

AIAA-2000-3572 — Tang, K. and M. Brewster, "Nonlinear Dynamic Combustion in Solid Rockets: L* Effects"

AIAA-2000-3573 — Surzhikov, S., J. Murphy, and H. Krier, "2D Model for Unsteady Burning Heterogeneous AP/Binder Solid Propellants"

4.2 NNSA/ASCI Interaction

Center personnel traveled extensively in the fourth year of the ASAP program and were involved in a large number of technical and informational meetings. These included meetings intended to explore rocket science and technology, identify technical collaborators, describe the ASCI/ASAP program, and establish relationships among Center investigators, DOE lab scientists, and industry leaders. Individual CSAR senior investigators and technical staff have traveled to DOE DP labs to serve on ASCI/ASAP panels, to participate in ASAP-wide workshops (materials and computational environment), to offer research seminars and technical interaction, to receive training on the ACSI computational resources, and to discuss ASCI resource issues with the CRT.

Nature of Collaboration	DOE Lab	Lab Contact	CSAR Contact
CSAR Visits to DOE Labs			
Two lectures at Materials Institute Summer School; July 2001	LLNL	M. Kalos, L. Fried, V. Bulatov	D. Ceperley
Seminar on mechanics modeling; May 2001	LLNL	J. Belak, R. Minich	P. Sofronis
Lecture at "Limits of Simulation" workshop; Oct 2000	LLNL	G. Galli	D. Ceperley
Invited speaker at CNLS Meeting; June 2000	LANL		D. Ceperley
Asymptotic theories for detonation front evolution and methods for propagating interfaces; June 2000	LANL	J. Bdzil	M. Short
Seminar at Stanford ASAP Center; May 2000	Tri-lab	W. Reynolds and G. Golub	M. Heath
Seminar on modeling solid propellant combustion; April 2000	LANL		J. Murphy
Path integral calculations presentation; March 2000	LLNL	E. Pollock	B. Militzer
Seminar on computational environments; February 2000	LLNL	J. May	D. Padua
Seminar on Krylov subspace methods; December 1999	LANL	Tri-lab	E. de Sturler
Visit to discuss linear solvers and preconditioners; 2000	LLNL	A, Cleary, E. Chow, et al.	E. de Sturler
Discussion of ASCI/CSAR development	LLNL	K. Mish	M. Heath
I/O characterization and performance tools; December 1999	LANL	J. Reynders	D. Reed
Seminar on hydrogen degradation of steels; September 1999	SNL	D. Bammann	P. Sofronis
Lectures on (new) iterative solvers for linear systems of equations; March 1999	SNL	R. Lehoucq	E. de Sturler

Seminar on analysis of iterative methods; March 1999	LANL	M. Benzi	E. de Sturler
Seminar on non-linear studies; November 1998	LANL		R. Adrian
Summer Student Interns at DOE Labs			
Graduate student K. Esler spent summer 2001 as a participant in the Materials Summer School Program.	LLNL	M. Kalos	D. Ceperley
Graduate student S. Hwang interned with Scientific Data Mgmt R&D, Summer 2001	LBL	A. Shoshani	M. Winslett
Graduate student A. Pinar spent Summer 1999 and 2000 at SNL.	SNL	B. Hendrickson	M. Heath
Graduate student D. Pattillo spent summer 1999 as a participant in the Engineering Science Summer Institute Program	SNL Livermore	M. Horstemeyer	P. Sofronis
Interaction on mesh generation. Graduate student Alper Ungor spent summer 1999 at SNL	SNL	S. Mitchell	S. Teng
Graduate student B. Militzer spent the summer 1998 and 1999 at LLNL. New method for simulations of high-pressure hydrogen.	LLNL	E. L. Pollock, Nellis, Cauble, Alder	D. Ceperley
Graduate student M. E. Bange, spent summers (1999 and 1998) doing mechanical testing	LANL	M. Stout	A. Beaudoin
DOE ASCI/ASAP/PI Meetings			
Participated in ASCI PI Meeting at LANL; February 2001	Tri-lab	W. Reed	M. Heath
Participated in ASCI PI Meeting; February 2000	Tri-lab	P. Messina	M. Heath
Participated in ASCI/ASAP Directors' Meeting; February 2000	Tri-lab	P. Messina	M. Heath
DOE Panel Reviews			
LDRD proposal review panel; two visits, 2001	LLNL-H		R. Martin
ASCI/Tri-lab Visits and Seminars at CSAR			
CSAR seminar; June 2001	SNL	B. Hendrickson	M. Heath
CSAR seminar; May 2001	LBNL	P. Concus	M. Heath
CSAR/Physics Dept seminar; April 2001	LANL	G. Ortiz	D. Ceperley
CSAR seminar; Feb 2001	SNL	S. Owen	M. Heath
CSAR seminar; Nov 2000	SNL	J. Stewart	M. Heath
CSAR seminar; Oct 2000	LLNL	D. Quinlan	M. Heath
CSAR seminar; Oct 2000	UC/Flash	B. Frixell	M. Heath
CSAR seminar; Oct 2000	LANL	C. Liu	M. Heath
CSAR seminar; Oct 2000	SNL	B. Hendrickson	M. Heath

CSAR External Advisory Board Meeting; August 2000	SNL	P. Nielan	M. Heath
Long-term collaborative visit for code coupling research; March-June 2000	LLNL	J. Grandy	M. Heath
CSAR seminar; April 2000	SNL	S. Wunsch	R. Moser
CSAR/AAE seminar; April 2000	LLNL	B. Goodwin	M. Bragg
CSAR seminar; November 1999	LLNL	S. Ashby	M. Heath
CSAR seminar; November 1999	LLNL	K. Mish	M. Heath
CSAR seminar; September 1999	SNL	R. Lehoucq	M. Heath
CSAR External Advisory Board Meeting; August 1999	SNL	P. Hommert	M. Heath
ASCI Workshops			
Scalability Workshop (CSAR hosted) — May 2000	LLNL, SNL	40 attendees	J. Hoeflinger
Software Frameworks — February 2000	Tri-Lab		
Code Sharing			
CUBIT	SNL	J. Zepper	A. Sheffer
ZOLTAN	SNL	K. Devine	D. Parsons
Pronto2D and 3D	SNL		
3D mesh generation tools: LAGriT and GEOMESH	LANL		
Software/Hardware Visits from Labs			
SIERRA software — Feb 1999	SNL	L. Taylor	
OVERTURE software — Feb 1999	LLNL	B. Henshaw and D. Quinlan	
Computational resources needed by CSAR — Feb 1999	LANL	A. White	
Blue Pacific — Dec 1998	LLNL	M. Seagar and J. Shuler	

Faculty Sabbaticals at DOE Labs			
R. Martin (Physics) at H Division, 2001-2.	LLNL	G. Galli , A. K. McMahan	R. Martin
Joint Research			
Dislocation mechanisms and void growth modeling; 2001-3	LLNL	J. Belak, R. Minich	P. Sofronis
Simulations of high-pressure hydrogen; 2000-1	LLNL	B. Militzer	D. Ceperley
Iterative solvers for linear systems of equations	SNL	R. Lehoucq	E. de Sturler
Linear solvers and preconditioners	LLNL	E. Chow	E. de Sturler
Meshing discussions	SNL		A. Sheffer
Many-body calculations	LLNL	J. Grossman, M. Rohlfing, S. Louis, M. Cohen	L. Mitas

Dislocation based analysis of void growth in metals	LLNL	R. Minich	P. Sofronis
Hydrogen degradation of 304L steels	SNL	D. Bammann	P. Sofronis
Laser ignition of high explosives	LANL	S. Son	M. Q. Brewster
Curing of viscoelastic composites, residual stresses	SNL	D. Adolf	H. Hilton
Fracture behavior of the nickel base super-alloy 690	Atomic Power Lab	D. Symons, Bettis	P. Sofronis
Dislocation-based analysis of micromechanical phenomena in materials	LLNL	D. Lassila	P. Sofronis
Potential joint efforts among CSAR, LANL, and NCSA	LANL	A. White and J. Reynders	M. Heath
Discuss potential speakers and topics for a major SIAM conference in 2000 focusing on CSE, and especially on ASCI-scale interdisciplinary simulation	LLNL	S. Ashby	M. Heath
Iterative methods for sparse linear systems	LLNL	S. Ashby and S. Lee	P. Saylor
Pycnonuclear fusion calculations	LLNL	B. J. Alder	D. Ceperley
Simulation of systems at high magnetic fields and correlated electron gas	LLNL	M. Jones and G. Ortiz	D. Ceperley
Implementation of mechanical threshold stress model in polycrystalline plasticity	LANL	C. Tome ad P. Maudlin	A. Beaudoin
Development of a polycrystal finite element model	LANL	U. F. Kocks	A. Beaudoin
Experimental testing and the fitting of data to constitutive models	LANL	M. Stout, S. R. Chen, M. Lovato	A. Beaudoin
Applications of polycrystal plasticity models	LANL	C. Tome	A. Beaudoin
Modeling of plastic inhomogeneity using finite element codes	LANL	P. Maudlin	A. Beaudoin
Selected Technical Discussions			
Discussion on combinatorial problems in scientific computing; June 2001	SNL	B. Hendrickson	M. Heath
Technical talks, May, June 2001	ANL	D. Weber, D. Bartels, T. Wei	Rizwan-uddin
Discussions on environmental degradation of materials; May 2001	LLNL	D. Bammann	P. Sofronis
Discussion on mesh generation; Feb 2001	SNL	S. Owen	M. Heath
Dislocation mechanisms and void growth modeling; 2001-3	LLNL	J. Belak, R. Minich	P. Sofronis
Discussion of unstructured fluids code development, V&V, and source-code mgmt; Feb 2001	SNL	J. Stewart, C. Ober, T. Smith	A. Haselbacher
Discussion on frameworks for multiphysics integration; Nov 2000	SNL	J. Stewart, A. Gullerud	M. Heath
Discussion of ASCI/CSAR development at	LLNL	K. Mish	M. Heath

NSF Model-based Simulation Workshop			
Discussion of ASCI/CSAR development at DOE Comp Sci Grad Fellowship Conf	Tri-lab		M. Heath
Quantum simulations	LLNL	B. Alder	D. Ceperley
Computational materials science workshop	LLNL	G. Galli and F. Gygi	D. Ceperley
Materials modeling discussions	LLNL	T. Diaz de la Rubia	R. Averback
Guest appointment for facility usage; 2000, 2001	ANL	L. Frietag	J. Norris
Discussion on using Rocketeer for FLASH data; 2001	ANL	L. Frietag	J. Norris
Discontinuous Galerkin Methods	LANL	R. Lowrie	R. Haber
I/O characterization and performance tools	LANL	J. Reynders	D. Reed
Meshing discussions	SNL	R. Leland	A. Sheffer
Conical intersections in TATB and PETN and connections to detonation sensitivity	LLNL	C. Wu	T. Martinez
Modeling of damage in solids	SNL Livermore	D. Bammann and M Horstemeyer	E. Fried
Role of electronic excited states in shock-induced chemistry	LLNL	C. Tarver	T. Martinez
Parallel C++ based frameworks, supporting irregular computations	LLNL	D. Quinlan and B. Henshaw	L. Kale
Detonation physics, multiphase flow, ignition and combustion of energetic materials, advanced numerical algorithms and strategies	LANL	J. Bdzil, T. Aslam, B. Asay, P. Howe, R. Menikoff, L. Hill, S. Son, L. Hull	D. S. Stewart
Detonation physics modeling in thin layers	SNL	A. Ratzel	D. S. Stewart
Combustion Modeling	LLNL	C. Westbrook	D. S. Stewart
Computational Materials Science Summer lectures and the NCSA Alliance program	LLNL	G. Galli and F. Gygi	D. Ceperley

4.3 CSAR Students and Staff Hired by DOE DP Labs

Former CSAR/CSE Students at DP Labs

- Michelle Duesterhaus, SNL (MS, Mechanical and Industrial Engineering, 2001)
- Jason Hales, SNL (PhD, Civil and Environmental Engineering, 2001)
- Benjamin T. Chorpening, SNL-L (PhD, Mechanical Engineering, 2000)
- Burkhard Militzer, LLNL (PhD, Physics, 2000)
- C. D. Tomkins, LANL (PhD, Theoretical and Applied Mechanics, 2000)
- Jeff J. Murphy, SNL-L (PhD, Mechanical Engineering, 1999)
- Donald Siegel, SNL (PhD, Physics, 1999)

- Steven F. Wojtkiewicz, SNL (PhD, Aero and Astro Engineering, 1999)
- Giulia Galli, LLNL (PhD, Physics, 1998)
- Arne Gullerud, SNL (PhD, Civil Engineering, 1998)
- Mike Ham, LANL (MS, Computer Science, 1998)

Former CSAR Employees at DP Labs

- Jeffrey Vetter, LLNL
- James Quirk, LANL
- Dennis Parsons, LLNL