4. Outreach and Interaction

Industrial Outreach

Meetings with the Rocket Industry

Critical interactions have continued during the third year of the CSAR program. Most significant among industrial/government laboratory meetings in 1999-2000 was our participation in the AIAA/ASME/SAE/ASEE Joint Propulsion Conference in Huntsville, Alabama, 18 July (see below). Another key meeting was the AIAA Aerospace Sciences Meeting and Exhibit in Reno, Nevada in January 2000. The latter meeting led to renewed interaction between CSAR and NASA. A Space Act Agreement (the NASA equivalent of a DOE CRADA) is likely to develop from this interaction defining the data and research relationship between NASA and CSAR.

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. The Validation, Accident, and Specification Team will be working with NASA to get more detailed data to validate the CSAR integrated code in Y4.

External Advisory Board

The second annual meeting of the CSAR External Advisory Board (EAB) was held 21-22 August 2000. 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:

Felix F. Chen	Aerojet	Technical Principal, Engineering
Robert Keenan	Aerojet	Program Manager, Advanced Programs
Gregory A. Ruderman	Air Force Research Laboratory	Mechanical Engineer
Grant B. Hodson	Alliant Techsystems	Technical Manager, Air Force Projects
David Mann	Army Research Office	Associate Director, Mechanics and Environmental Sciences Division
Kent Hennessey	Atlantic Research Corporation	Manager, Thermal Design
Fred Culick	Caltech	Professor of Mechanical Engineering and Jet Propulsion
Robert L. Glick	Consultant	Consultant
Robert L. Geisler	Geisler Enterprises	Senior Rocket Scientist Consultant
Greg Astfalk	Hewlett-Packard Company	Chief Scientist
Marc Snir	International Business Ma-	Senior Manager, Parallel Systems Organi-

	chines Corporation	zation
David H. Bailey	Lawrence Berkeley National Laboratory	Chief Technologist, NERSC Division
Andy Baldi	Lockheed-Martin Missiles & Space	Director, FBM Propulsion and Controls
Taras Jarymowycz	Lockheed-Martin Missiles & Space	
Robert Garcia	NASA Marshall Space Center	Group Lead, Applied Fluid Dynamics Analysis
Fred S. Blomshield	Naval Air Warfare Center, China Lake	Head, Propulsion Research Branch
Paul Nielan	Sandia National Laboratory	Manager, Distributed Systems Research Department
I. Lee Davis	Thiokol Corporation	Senior Research Scientist
Suresh Kulkarni	Thiokol Corporation	Vice President, Systems Engineering
Allan J. McDonald	Thiokol Propulsion	Deputy and Technical Director, Science and Engineering
Grant Henson	United Technologies/CSD	
David Kassoy	University of Colorado	Associate Vice President for Technology
Gary Flandro	University of Tennessee Space Institute	Boling Chair Professor of Advanced Propulsion
Mitchell D. Smooke	Yale University	Chair, Mechanical Engineering and Applied Science

Travel and ASCI Technical Interaction

Center personnel traveled extensively in the third 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 Recent Collaboration	**DP Lab**	**Lab Contact**	**CSAR Contact**
CSAR Seminars and Visits to ASCI			
Seminar on computational environments; February 2000	LLNL	J. May	D. Padua
Seminar on hydrogen degradation of steels; September 1999	SNL	D. Bammann	P. Sofronis
I/O characterization and performance tools; December 1999	LANL	J. Reynders	D. Reed

Invited speaker at CNLS Meeting; June 2000	LANL		D. Ceperley
Path integral calculations presentation; March 2000	LLNL	E. Pollock	B. Militzer
Asymptotic theories for detonation front evolution and methods for propagating interfaces; June 2000	LANL	J. Bdzil	M. Short
Seminar on modeling solid propellant combustion; April 2000	LANL		J. Murphy
Seminar on Krylov subspace methods; December 1999	LANL	Tri-lab	E. de Sturler
Visit to discuss linear solvers and preconditioners	LLNL	A. Cleary, E. Chow, et al.	E. de Sturler
Discussion of ASCI/CSAR development; June 1999, November 1999, February 2000	LLNL	K. Mish	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
Seminar at Stanford ASAP Center; May 2000	Tri-lab	W. Reynolds and G. Golub	M. Heath
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
ASCI/Tri-lab Seminars and Visits to CSAR			
Long-term collaborative visit for code coupling research; March-June 2000	LLNL	J. Grandy	M. Heath
CSAR External Advisory Board Meeting; August 1999	SNL	P. Hommert	M. Heath
CSAR seminar; September 1999	SNL	R. Lehoucq	M. Heath
CSAR seminar; November 1999	LLNL	S. Ashby	M. Heath
CSAR seminar; November 1999	LLNL	K. Mish	M. Heath
CSAR seminar; April 2000	SNL	S. Wunsch	R. Moser
CSAR/AAE seminar; April 2000	LLNL	B. Goodwin	M. Bragg
ASCI Workshops			
Software Frameworks — February 2000	Tri-Lab		
Scalability Workshop (CSAR hosted) — May 2000	LLNL, SNL	40 attendees	J. Hoeflinger and F. Najjar
Code sharing			
CUBIT	SNL	J. Zepper	A. Sheffer
ZOLTAN	SNL	K. Devine	D. Parsons
Pronto2-D and 3-D	SNL		

Joint research			
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	S. Mitchell	A. Sheffer
Many-body calculations	LLNL	J. Grossman, M. Rohlfing, S. Louis, and 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
Fracture behavior of the nickel base superalloy 690	Atomic Power Lab	D. Symons, Bettis	P. Sofronis
Dislocation-based analysis of micromechanical phenomena in materials	LLNL	D. Lassila	P. Sofronis
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 and 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
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	
Summer Student Interns			
Graduate student S. Hwang interning in Scientific Data Mgmt R&D Group	LBL	A. Shoshani	M. Winslett
Graduate student A. Pinar spent Summers 1999 and 2000 at SNL.	SNL	B. Hendrickson	M. Heath
Graduate student T. Berger-Wolf spent Summer 2000 at SNL.	SNL	B. Hendrickson	M. Heath

Graduate student D. Bunde spent Summer 2000 at SNL.	SNL	C. Phillips	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
New method for simulations of high-pressure hydrogen. Graduate student B. Militzer spent the summer 1998 and 1999 at LLNL.	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
Selected Technical Discussions			
Discussion of ASCI/CSAR development at NSF Model-based Simulation Workshop	LLNL	K. Mish	M. Heath
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	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
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
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.	D. S. Stewart

		Hull	
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

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 in Y3 was a full-day technical paper session presented by Center researchers at the AIAA/ASME/SAE/ASEE Joint Propulsion Conference 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 — Simulating Solid Propellant Rockets at CSAR — M. Heath, R. Fiedler, and W. Dick
AIAA-2000-3456 — Coupled Simulations of Solid Rocket Motors — I. D. Parsons, P. Alavilli, A. Namazifard, A. Acharya, X. Jiao, and R. Fiedler
AIAA-2000-3457 — Parallel Structural Analysis of Solid Rocket Motors — A. Namazifard, I. Parsons, A. Acharya, E. Taciroglu, and J. Hales
AIAA-2000-3459 — The Burning of Periodic Sandwich Propellants — A. Hegab, T. Jackson, J. Buckmaster, and S. Stewart
AIAA-2000-3460 — A Two-dimensional Model of Composite Propellant Flame Structure and Burning Rate — G. Knott and M. Brewster
AIAA-2000-3461 — Random Propellant Packs and the Flames They Support — S. Kochevets, J. Buckmaster, and T. Jackson
AIAA-2000-3567 — Ignition-Transient Modeling for Solid Propellant Rocket Motors — P. Alavilli, J. Buckmaster, T. Jackson, and M. Short
AIAA-2000-3568 — Computations of Two-Phase Flow in Aluminized Solid Propellant Rockets — F. Najjar, S. Balachandar, P. Alavilli, and J. Ferry
AIAA-2000-3569 — Fundamental Two-Phase Flow Modeling Efforts at CSAR — S. Balachandar, J. Ferry, and P. Bagchi
AIAA-2000-3570 — Direct Numerical Simulation of Two-Way Coupling Effects in a Particle-Laden Turbulent Pipe Flow — S. Rani and S. Vanka
AIAA-2000-3571 — DNS and LES Computations of Model Solid Rocket Motors — P. Venugopal, F. Najjar, and R. Moser
AIAA-2000-3572 — Nonlinear Dynamic Combustion in Solid Rockets: L* Effects — K. Tang and M. Brewster
AIAA-2000-3573 — 2D Model for Unsteady Burning Heterogeneous AP/Binder Solid Propellants — S. Surzhikov, J. Murphy, and H. Krier

Student Interns at DOE Labs

Five graduate students served as research interns in 1999-2000. Students were placed at Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Sandia National Laboratory (2), and Sandia-Livermore National Laboratory.