

## 7. Publications

### Structures and Materials

Acharya, A. and A. J. Beaudoin, "Grain-Size Effect in Viscoplastic Mpolycrystals at Moderate Strains," *Journal of the Mechanics and Physics of Solids*, 48, 2213-2230, 2000.

Acharya, A. and Bassani, J. L., "Lattice Incompatibility and a Gradient Theory of Crystal Plasticity," *Journal of the Mechanics and Physics of Solids*, 48, 1565-1595, 2000.

Acharya, A. and Beaudoin, A. J., "Consideration of Lattice Incompatibility in the Evolution of Hardening," to appear in *Proceedings of the Twelfth International conference on textures of materials*, Montreal, Canada, August 9-13, 1999, National Research Council of Canada Press.

Acharya, A., "A Distinct Element Approach to Ball Mill Mechanics," *Communications in Numerical Methods in Engineering* in press, 1999.

Acharya, A., "A Model of Crystal Plasticity Based on the Theory of Continuously Distributed Dislocations," Accepted for publication in *Journal of the Mechanics and Physics of Solids*, 2000.

Acharya, A., "A Nonlinear Generalization of the Koiter-Sanders-Budiansky Bending Strain Measure," *International Journal of Solids and Structures*, 37, 5517-5528, 2000.

Acharya, A., "On Compatibility Conditions for a Left Cauchy-Green Strain Field in 3-Dimensions," *Journal of Elasticity*, 56, 95-105, 1999.

Acharya, A., Cherukuri, H. P. and Govindarajan, R. M., "A New Proposal in Gradient Plasticity: Theory and Application in 1-D Quasi-Statics and Dynamics," *Mechanics of Cohesive-Frictional Materials*, 4, 153-170, 1999

Albe, K., K. Nordlund, J. Nord. And A. Kuronen, "Modeling of Compound Semiconductors: Analytical Bond-Order Potential for GaAs," submitted to *Phys. Rev. B*

Albe, K., K. Nordlund, X. Hu, and R.S. Averback, "Analytical Bond-Order Potential for Platinum-Carbon," submitted to *Phys. Rev. B*

Beaudoin, A. J. and A. Acharya, "A Model for Rate-Dependent Flow of Metal Polycrystals Based on the Slip Plane Lattice Incompatibility," *Materials Science and Engineering A*. in press.

Beaudoin, A. J., A. Acharya, S. R. Chen, D. A. Korzekwa and M. G. Stout, "Consideration of Grain-Size Effect and Kinetics in the Plastic Deformation of Metal Polycrystals," *Acta Materialia* 48, 3409-3423, 2000.

Birnbaum, H. K., Robertson, I. M., and Sofronis, P., "Hydrogen Effects on Plasticity," in *Multiscale Phenomena in Plasticity: From Experiments to Phenomenology, Modelling and Materials Engineering*, pp. 367-381, Ed. Kluwer Academic Publishers, 2000.

Hjelmstad, K. D. and E. Taciroglu, "Analysis and Implementation of Resilient Models for Granular Solids," *Journal of Engineering Mechanics*, v. 126, pp. 821-830, 2000.

Hjelmstad, K. D. and E. Taciroglu, "Mixed Methods and Flexibility Approaches to Bernoulli-Euler Beam Finite Elements: Algorithms and Applications," *Int. Journal for Numerical Methods in Engineering*, (submitted).

Hu, X., K. Albe, R.S. Averback, "Molecular-Dynamics Simulations of Energetic C<sub>60</sub> Impacts on Silicon," *J. Appl. Phys.* 49, 88, 2000.

Jäger, H.-U., K. Albe, "Molecular-Dynamics Simulations Of Steady-State Growth of Ion-Deposited Tetrahedral Amorphous Carbon Films," *J. Appl. Phys.* 1129, 88, 2000.

Kok, S., A. J. Beaudoin, and D. A. Tortorelli, "A Polycrystal Plasticity Model Based on the Mechanical Threshold," accepted for publication in *International Journal of Plasticity*, 2000.

Lufrano, J. and Sofronis, P., "Micromechanics of Hydride Formation and Cracking in Zirconium Alloys" *Computer Modeling in Engineering Science*, 1, 119-131, 2000.

Mishin, Y., McMahon, C. J., Bassani, J. L. and Sofronis, P., "Thermodynamics and Kinetics of Interfacial Decohesion," *Interface Engineering for Optimized Properties II*, Vol. 586, Materials Research Society Symposium Proceedings, accepted for publication.

Namazifard, A. and I. D. Parsons, "A Distributed Memory Parallel Implementation of the Multigrid Method," Submitted to the *International Journal for Numerical Methods in Engineering*.

Namazifard, A. and I. D. Parsons, "An MPI Implementation of Newmark's Method. *Computer-Aided Civil and Infrastructure Engineering*," 15, 189-195, 2000.

Namazifard, A., I. D. Parsons, A. Acharya, E. Taciroglu and J. H. Hales, "Parallel Structural Analysis of Solid Rocket Motors," *AIAA/ASME/SAE/ASEE Joint Propulsion Conference*, Huntsville, Alabama, July 16-19, 2000.

Parsons, I. D. P., Acharya, A., Alavilli, P., Fiedler, R., Jiao, X., and Namazifard, A., "Coupled Simulation of Solid Rocket Motors," *AIAA paper 2000-3456*, 36<sup>th</sup>. *AIAA/ASME/SAE/ASEE Joint propulsion conference and exhibit*, Huntsville, Al, July 16-19, 2000.

Parsons, I. D. P., Alavilli, P. V. S., Namazifard, A., Acharya, F. Najjar, D. Tafti, and X. Jiao, "Loosely Coupled Simulations of Solid Rocket Motors," 5<sup>th</sup>. *National Congress on Computational Mechanics (USACM)*, Boulder, Colorado, August 2000.

Parsons, I. D. P., Alavilli, P., Namazifard, A., Jiao, X., and Acharya, A., "Fluid-Structure Interaction Through A Non-Material Interface: Simulations Of Solid Rocket Motors," Invited paper in *ASCE Fourteenth Engineering Mechanics Conference (EM 2000)*, May, Austin, TX, 2000.

Parsons, I. D., P. Alavilli, A. Namazifard, X. Jiao, A. Acharya, "Simulations Of Solid Rocket Motors Using A Partitioned Fluid-Structure Interaction Algorithm," *Proceedings of the Fifth International Conference on Computational Structures Technology*, Leuven, Belgium, 6-8 September 2000.

Parsons, I. D., P. V. S. Alavilli, A. Namazifard, J. Hales, D. Tafti, "Coupled Multi-Physics Simulations of Solid Rocket Motors," *Proceedings of the PDPTA '99 International Conference*, 3101-3107, 1999.

Sheffer, A. and E. Taciroglu, "Hexahedral Mesh Adjustment for the Simulation of Solid Propellant Rockets," ICES'2K, Los Angeles, CA, 2000.

Sofronis, P. and Lufrano, J., "Interaction of Local Elastoplasticity with Hydrogen: Embrittlement Effects," *Materials Science and Engineering A*, 260, 41-47, 1999.

Sofronis, P. and Aravas, N., "Hydrogen Enhanced Localized Plasticity," *Proceedings of 3<sup>rd</sup> National Congress on Computational Mechanics*, Eds. N. Aravas and J. T. Katsikadelis, pp. 129-135, University of Thessaly, Volos, Greece, June 24-26, 1999.

Sofronis, P. and Birnbaum, H. K., "The Mechanics of Hydrogen-Induced Fracture by Hydride Formation," *Proceedings of 3<sup>rd</sup> National Congress on Computational Mechanics*, Eds. N. Aravas and J. T. Katsikadelis, pp. 369-376, University of Thessaly, Volos, Greece, June 24-26, 1999.

Sofronis, P. and Taha, A., "Micromechanical modeling of hydrogen transport-A review," *Environmentally assisted cracking: Predictive Methods for Risk Assessment and Evaluation of Materials Equipment, and Structures*, ASTM STP 1401, R. D. Kane, Ed., American Society for Testing of Materials, West Conshohocken, PA, 2000.

Taciroglu, E. and K. D. Hjelmstad, "Isotropic Limit Tension of Compression Elasticity," *ASCE 13th Engineering Mechanics Conference*, Baltimore, MD, 1999.

Taha, A. and Sofronis, P., "A Micromechanics Approach to the Study of Hydrogen Transport and Embrittlement," *Engineering Fracture Mechanics*, To appear.

Yin, L., Acharya, A., Sobh, N., Haber, R. B. and Tortorelli, D. A., "A Space-Time Discontinuous Galerkin Method For Elastodynamic Analysis, In *Discontinuous Galerkin Methods: Theory, Computation And Applications*," Ed. B. Cockburn, G. Karriadakis and C. W. Shu, *Lecture Notes in Computational Science and Engineering*, 11, 459-464, Springer Verlag. 1999.

## **Combustion and Energetic Materials**

Artacho, E., D. Sanchez-Portal, P. Ordejon, A. Garcia, J. M. Soler, "Linear-scaling ab-initio calculations for large and complex systems," *Phys. Stat. Sol. (b)* 215, 809 (1999).

Ben-Nun, M. and T. J. Martínez, "A Multiple Spawning Approach to Tunneling Dynamics," *J. Chem. Phys.*, 112, 6113, 2000.

Ben-Nun, M. and T. J. Martínez, "Exploiting Temporal Non-Locality to Remove Scaling Bottlenecks in Non-Adiabatic Quantum Dynamics," *J. Chem. Phys.*, 110, 4134, 1999.

Ben-Nun, M. and T. J. Martínez, "Photodynamics of Ethylene: Ab Initio Studies of Conical Intersections, *Chemical Physics*," 259, 237, 2000.

Ben-Nun, M. and T. J. Martínez, "Semiclassical Tunneling Rates from Ab Initio Molecular Dynamics," *J. Phys. Chem.*, 103, 6055. 1999.

Ben-Nun, M. and T. J. Martínez, "Electronic Absorption and Resonance Raman Spectroscopy from Ab Initio Quantum Molecular Dynamics," invited article for K. R. Wilson *Festschrift*, *J. Phys. Chem.*, 103, 10517, 1999.

- Ben-Nun, M., J. Quenneville, and T. J. Martínez, “Ab Initio Multiple Spawning: Photochemistry from First Principles Quantum Molecular Dynamics,” *J. Phys. Chem. Invited Feature Article*, 104, 5161, 2000.
- Buckmaster, J. and M Short, “Cellular Instabilities, Sublimit Structures and Edge-flames in Premixed Counterflows,” *Combustion Theory and Modeling*, vol. 3, 199-214, 1999.
- Buckmaster, J. and T.L. Jackson, “Response of Propellant Flames to Unsteady Flows, and Related Questions,” *AIAA Paper No. 99-0323*, 1999.
- Buckmaster, J., Hegab, A., and Jackson, T., “Further Results on Oscillating Edge-Flames,” *Proceeding of the 17th. International Colloquium on the Dynamics of Explosives and Reactive System, Heidelberg, Germany, 1999.*
- Buckmaster, J., Hegab, A., and Jackson, T., “More Results on Oscillating Edge-Flames,” *Journal Physics of Fluid, Vol. 12, No. 6, 2000.* <http://ojps.aip.org/phf/>, 2000.
- Buckmaster, J., Hegab, A., and Jackson, T., “The Effect of Convection and Cold Probes Oscillating Edge-Flames,” *AIAA 2000-0847*, 38th. Aerospace Science Meeting, Reno, NV, 2000.
- Buckmaster, J., T.L. Jackson & J. Yao, “An Elementary Discussion of Propellant Flame Geometry,” *Comb. & Flame*, 117, pp. 541-552, 2000.
- Buckmaster, J., Yi Zhang, “Oscillating Edge Flames,” *Combustion Theory and Modelling*, vol.3, 547-565, 1999.
- Ceperley, D. M. “Microscopic Simulations in Physics ,” *Rev. Mod. Phys.* 71, S438, 1999.
- Ceperley, D. M. “Understanding Electronic WaveFunctions,” in *Electron Correlations and Materials Properties*, eds. A. Gonis and N. Kioussis, Plenum, 1999.
- Ceperley, D. M. and M. Dewing, “The Penalty Method for Random Walks with Uncertain Energies,” *J. Chem. Phys.*, 110, 9812, 1999.
- Chorpening, B. T., G. M. Knott, and M. Q. Brewster, “Flame Structure and Burning Rate of AP/HTPB Propellant Sandwiches,” *Proceedings of the 28<sup>th</sup> International Symposium on Combustion*, The Combustion Institute, Pittsburgh, PA, August 2000.
- Fried, E. and A. Q. Shen, “Supplemental Relations at a Phase Interface Across Which the Velocity and Temperature Jump,” *Continuum Mechanics and Thermodynamics*, 11: 277-296, 1999.
- Hegab A., Buckmaster J., Jackson T., and Stewart, S. “The Burning of Periodic Sandwich Propellants,” *AIAA Paper #2000-3459*, 36th. AIAA/ASME/SAE/ASEE Joint Propulsion, Huntsville, Al., 2000.
- Hegab, A. and Kassoy, D., “Internal Flow Temperature Dynamics in a Channel with Time-dependent Mass Injection,” submitted to *Journal of Power and Propulsion*.
- Hegab, A. and Kassoy, D., “The Thermal Response of an Internal Flow in a Solid Rocket Motor Chamber/Nozzle Model,” *AIAA paper 2001-0338*, 39th. Aerospace Science Meeting, Reno, NV, 2000.

Jackson T., J. Buckmaster, and A. Hegab, "Periodic Propellant Flames and Fluid-Mechanical Effects," *Journal of Power and Propulsion*, in press.

Jackson, T., Buckmaster, J., Hegab, A., and Knott, "Random Packing of Heterogeneous Propellants and the Flame They Support," ICTAM, 2000-1498, 20th International Congress of Theoretical and Applied Mechanics, Chicago, 2000.

Jackson, Tom, John Buckmaster, and Jay Hoeflinger, "Three-dimensional Flames Supported by Heterogeneous Propellants," JANNAF Combustion Subcommittee, Airbreathing Propulsion Subcommittee and Propulsion Systems Hazards Subcommittee Joint Meeting, Cocoa Beach, Florida, 1999.

Knott, G. M. and M. Q. Brewster, "A Two-Dimensional Model of Composite Propellant Flame Structure and Burning Rate," 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Huntsville, AL, AIAA Paper No. 2000-3460, July 16-19, 2000.

Knott, G. M. and M. Q. Brewster, "Numerical Analysis of Solid Propellant Sandwich Combustion," 36<sup>th</sup> JANNAF Combustion Subcommittee Meeting, Cocoa Beach, FL, CPIA Publ. No. 691, I, 311-324, 1999.

Knott, G. M. and M. Q. Brewster, "Two-Dimensional Combustion Modeling of Heterogeneous Solid Propellants with Finite Peclet Number," *Combustion and Flame*, 121, 91-106, 2000.

Knott, G.M., M.Q. Brewster & T.L. Jackson, "A Simplified Model for Composite Propellant Burning Rate," AIAA Paper No. 99-0591, 1999.

Lasseigne, D.G., R.D. Joslin, T.L. Jackson & W.O. Criminale, "The Transient Period for Boundary Layer Disturbances," *J. Fluid Mech.*, 381, pp. 89-119, 1999.

Martin, Richard M., "Condensed-matter Physics - Simple Metals Under Pressure," *Nature* 400, 117, 1999.

Militzer, B., W. Magro and D. Ceperley, "Characterization of the State of Hydrogen at High Temperature and Density," *Contr. Plasma Physics* 39, 151, 1999.

Murphy, J.J. and H. Krier, "Heterogeneous Effects on the Dynamic Burning in Composite Solid Propellants," 28th Int'l Combustion Symposium; Edinburgh, Scotland, August 1-4, 2000.(Proceedings book to appear in March 2001.)

Sanchez-Portal, D., I. Souza, R. M. Martin, "LCAO calculation of dynamical charges and ferroelectricity," Proceedings of the workshop on "Fundamental Physics of Ferroelectrics," Aspen Center for Physics, February 13-20, 2000 (in press).

Short, M., J Buckmaster, S.Kochevets, "Edge-flames and sublimit hydrogen combustion," *Combustion and Flame*, 2000, to appear.

Srinivasan, A., D. M. Ceperley and M. Mascagni, "Random Number Generators for Parallel Applications in Monte Carlo Methods in Chemical Physics," Vol. 105, *Advances in Chemical Physics*, eds. D. M. Ferguson, J. I. Siepmann and D. G. Truhlar, Wiley, 1999.

Stephan, Uwe, "A Comparison of the Convergence Properties of First-Principles Linear-Scaling Electronic-Structure Schemes," submitted to *Phys. Rev. B*, 2000.

Stephan, Uwe, Richard M. Martin and David A. Drabold, "Extended-range computation of Wannier-like Functions in Amorphous Semiconductors," accepted in Phys. Rev. B, 2000.

Surzhikov, S.T., J.J. Murphy, and H. Krier, "2D Model for Unsteady Burning of Heterogeneous AP/Binder Solid Propellants," AIAA paper 2000-3573 at the AIAA Joint Propulsion Conference, Huntsville, AL; July 16-19, 2000, submitted to the Journal of Propulsion and Power.

Surzhikov, S.T. and H. Krier, "A Quasi One Dimensional Model for the Burning of Layered Heterogeneous Solid Propellants," submitted to Combustion & Flame.

Surzhikov, S.T. and H. Krier, "Unsteady Dynamic Variables Method for modeling Heterogeneous Propellant Burning," submitted to AIAA Journal.

Tang, K. C. and M. Q. Brewster, "Analysis of Molecular Gas Radiation: Real Gas Property Effects," Journal of Thermophysics and Heat Transfer, Vol. 13, No. 4, pp. 460-466, 1999.

Tang, K. C. and M. Q. Brewster, "Computational Simulation of Nonlinear  $L^*$  Combustion Instability in Solid Rockets," AIAA 99-0859, the 37th AIAA Aerospace Sciences Meeting, Reno, NV, January 11-14, 1999.

Tang, K. C. and M. Q. Brewster, "Nonlinear Bulk-mode ( $L^*$ ) Combustion Simulations," the JANNAF 37th Combustion Meeting, Monterey, CA, November 13-17, 2000.

Tang, K. C. and M. Q. Brewster, "Nonlinear Dynamic Combustion in Solid Rockets:  $L^*$  Effects," submitted to the Journal of Propulsion and Power.

Tang, K. C. and M. Q. Brewster, "Nonlinear Dynamic Combustion in Solid Rockets:  $L^*$  Effects," AIAA 2000-3572, the 37th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, Alabama, July 16-19, 2000.

Thompson, K. and T. J. Martínez, "Ab Initio/Interpolated Quantum Dynamics on Coupled Electronic States with Full Configuration Interaction Wavefunctions," J. Chem. Phys., 110, 1376, 1999.

## Fluid Dynamics

Alavilli, P., Buckmaster, J., Jackson, T., and Short, M., "Ignition-transient Modeling for Solid-propellant Rocket Motors," AIAA-Paper 2000-3567, AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, AL, July 16-19, 2000.

Allavilli, P.V.S., Tafti D. K. and Najjar, F., "The Development of an Advanced Solid-Rocket Flow Simulation Program ROCFLO," 38<sup>th</sup> AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 2000.

Allen J. Toreja and Rizwan-uddin, "A Hybrid Numerical Method For Time-Dependent Convection-Diffusion Problems In Arbitrary Geometries," to appear in the Trans. Am. Nucl. Soc., Washington, D.C., 2000.

Allen J. Toreja and Rizwan-uddin, "Hybrid Numerical Methods for the Convection-Diffusion Equation in Arbitrary Geometries," in the Proc. M&C'99—International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications, Madrid, Spain, September, 27-30, 1999.

Bagchi, P. and Balachandar, S., "Linearly Varying Ambient Flow Past a Sphere at Finite Reynolds Number. Part 2: Equation of Motion" to be submitted to J. Fluid Mech.

Bagchi, P. and Balachandar, S., "Linearly Varying Ambient Flow Past a Sphere at Finite Reynolds Number - Part 1: Wake Structure and Forces In Steady Straining Flow" TAM Report # 938. Dept. of Theoretical & Applied Mech., UIUC.

Bagchi, P. and Balachandar, S., "Unsteady Motion and Forces On a Spherical Particle In Nonuniform Flows," Proceedings of 2000 ASME Fluids Engg. Summer Conf., Boston, MA.

Bagchi, P., Ha, M. Y. and Balachandar, S., "Direct Numerical Simulation of Flow and Heat Transfer From a Sphere in a Uniform Cross Flow," to appear in ASME J. Fluids Engg.

Balachandar, S. and Ha, M. Y., "Unsteady heat transfer from a sphere in a uniform cross-flow, submitted to Intl. J. Heat & Mass Transfer.

Balachandar, S., J.P. Ferry, and P. Bagchi, "Fundamental Two-Phase Flow Modeling Efforts at CSAR," AIAA 2000-3569, AIAA, July 16-19, 2000.

Deng, Z., Adrian, R.J., and Tomkins, C.D., "Structure of Turbulence in Channel Flow with a Fully Transpired Wall," AIAA 2001-1019, 39th AIAA Aerospace Sciences Meeting & Exhibit, Nevada, Jan. 2001.

Ferry, J. and S. Balachandar, "A Fast Eulerian Method for Two-phase Flow," IJMF (accepted).

Ferry, J. and S. Balachandar, "Behavior of Particles in a Turbulent Channel Flow," FEDSM2000-11136, ASME, June 2000.

Ferry, J. and S. Balachandar, "Estimate of the Effect of Flow Inhomogeneity on Forces on Particles in a Wall-bounded Flow," Phys. Fluids (submitted).

Huang, W. and Tafti D. K., "A Parallel AMR Algorithm for Solving Nonlinear Dynamical Systems," Int. J. of Supercomputing Applications and High Performance Computing, submitted May 2000.

Huang, W. and Tafti D. K., "A Parallel Computing Framework for Dynamic Power Balancing in Adaptive Mesh Refinement Applications," Parallel CFD '99, Summer 2000.

Jimenez, J. and Moser, R. D., "LES: Where Are We and What Can We Expect," AIAA J. 38, 605-612, 1999.

Langford, J. A. and Moser, R. D., "Optimal LES Formulations for Isotropic Turbulence," J. Fluid Mechanics, 398, 321-346, 1999.

Michael, E.P.E., J.J. Dorning and Rizwan-uddin, "Studies on Nodal Integral Methods for the Convection-Diffusion Heat Equation," accepted for publication in Nuclear Science & Engineering.

Moser R. D., Norman M. L., Balachandar S. and Tafti D., "Simulating Flows in Solid Rocket Motors," AIAA 99-3648, by invitation at the 30<sup>th</sup> AIAA Fluid Dynamics Conference, Norfolk VA, June 28-31, 1999.

Moser, R. D., Langford, J. A. and Volker, S., "Optimal LES: How Good Can an LES Be?" Proceedings of the Second AFOSR International Conference on DNS and LES, June 7-9, Rutgers University, 1999.

Najjar, F.M., S. Balachandar, P.V.S. Alavilli, and J. Ferry, "Computations of Two-Phase Flow in Aluminized Solid Propellant Rockets," AIAA 2000-3568, 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Huntsville, AL, July 16-19, 2000.

P. Venugopal, F.M. Najjar, and R.D. Moser, "DNS and LES Computations of Model Solid Rocket Motors," AIAA 2000-3571, 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, AL, July 16-19, 2000.

Parsons, I., Alavilli, P., Namazifard, A., Acharya, A., Xiao, J., and Fiedler, R. "Coupled Simulations of Solid-rocket Motors," AIAA-Paper 2000-3456, 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, AL, July 16-19, 2000.

Parsons, I., Alavilli, P., Namazifard, A., Jiao, X., and Acharya, A. "Fluid-Structure Interaction Through a Non-material Interface: Simulations of Solid Rocket Motors," May 2000, Invited paper, ASCE 14<sup>th</sup> Engineering Mechanics Conference(EM2000), Austin, TX, 21-24 May, 2000.

Rani, Sarma L. and S. P. Vanka, "Direct Numerical Simulation of Two-Way Coupling Effects In a Particle-Laden Turbulent Pipe Flow," Paper No. AIAA2000-3570, 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, AL, July 16-19, 2000.

Rani, Sarma L. and S. P. Vanka, "Large Eddy Simulation of Turbulence Modification and Particle Dispersion In a Fully-Developed Pipe Flow," 52<sup>nd</sup> annual meeting of Division of Fluid Dynamics, American Physical Society, New Orleans, 1999

Rani, Sarma L. and S. P. Vanka, "Numerical Simulation of Two-Way Coupling Effects In a Particle-Laden Turbulent Pipe Flow," Proceedings of FEDSM'00, ASME Fluids Engineering Summer Conference 2000, Paper No. FESM2000/11147, Boston.

Rizwan-uddin, "A Nodal Method for Phase Change Moving Boundary Problems," Int. J. Computational Fluid Dynamics, 11, 211-221, 1999.

Rizwan-uddin, "Alternative Treatments of the Time and Spatial Directions in the Nodal Integral Method," in Proc. M&C'99—International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications, Madrid, Spain, September, 27-30, 1999.

Rizwan-uddin, "Comparison of the Nodal Integral Method and Non-Standard Finite-Difference Schemes for the Fisher Equation," accepted for publication in SIAM J. Scientific Computing.

Rizwan-uddin, "One-Dimensional Phase Change with Periodic Boundary Conditions," Numerical Heat Transfer, Part A: Applications, 35, 361-372, 1999.

Rock, D. T. and Rizwan-uddin, "Subchannel Analysis of Nuclear Reactor Thermalhydraulics Using CFD," Proc. High Performance Computing Symposium—Grand Challenges in Com-



puter Simulation, 1999 Advanced Simulation Technologies Conference, San Diego, CA, pp. 110-115, April 11-15, 1999.

Wang, Fei and Rizwan-uddin, "A Nodal Scheme for the Time-Dependent, Incompressible Navier-Stokes Equations," to appear in the Trans. Am. Nucl. Soc., Washington, D.C., 2000.

Wang, G. and Tafti D.K., "Performance Enhancement on Microprocessors with Hierarchical Memory Systems for Solving Large Sparse Linear Systems," Int. J. of Supercomputing Applications and High Performance Computing, Vol. 13, No. 1, pp. 63-79, Spring 1999.

Weber, D.P., Thomas Y.C. Wei, D.T. Rock, Rizwan-uddin, R.A. Brewster and S. Jonnavithula, "Computational Fluid Dynamics (CFD) and its Potential for Nuclear Applications," Proc. American Power Conference, Chicago, Vol. 61, pp. 338-348, Illinois Institute of Technology, April 6-8, 1999.

Weber, D.P., Thomas Y.C. Wei, R.A. Brewster, D.T. Rock and Rizwan-uddin, "High Fidelity Thermal-Hydraulic Analysis Using CFD and Massively Parallel Computers," submitted for presentation at the Fourth Int. Meeting on Supercomputing Applications in Nuclear Engineering, Japan, September, 2000.

Wescott, Bradley and Rizwan-uddin, "An Efficient Formulation of the Modified Nodal Integral Method and Application to 2-D Burger's Equation," in Proc. Ninth Int. Conference on Nuclear Reactor Thermal Hydraulics (NURETH-9), San Francisco, CA, October 3-8, 1999.

Wescott, Bradley and Rizwan-uddin, "An Efficient Formulation of the Modified Nodal Integral Method and Application to 2-D Burgers' Equation," accepted for publication in Nuclear Science & Engineering.

## **Computer Science**

Bhandarkar, Milind A. and Laxmikant V. Kale, "A Parallel Framework for Explicit FEM," Accepted for International Conference on High Performance Computing (HiPC), Bangalore, India, December 2000.

Bhandarkar, Milind, L. V. Kale, Gengbin Zheng, Eric de Sturler, and Jay Hoeflinger, "Object-Based Adaptive Load Balancing for MPI Programs," in Preparation, May 2000.

de Sturler, E., "Improving the Convergence of the Jacobi-Davidson Algorithm," Technical Report, UIUCDCS-R-2000-2173/UILU-ENG-2000-1730, June 2000 (submitted for publication).

de Sturler, E., "Truncation Strategies for Optimal Krylov Subspace Methods," SIAM Journal on Numerical Analysis Vol. 36, pp. 864-889. Proceedings of the 1999 International Conference on Parallel and Distributed Processing Techniques and Applications (PDPTA'99) Las Vegas, Nevada, USA. Associate Editor, June 28 - July 1, 1999.

de Sturler, E., "Variations on the Jacobi-Davidson Theme. In Iterative Methods in Scientific Computation II," proceedings of the Fourth IMACS International Symposium on Iterative Methods in Scientific Computation, honoring the 75th birthday of David M. Young, Austin Texas, October 18-20, 1998, IMACS series in Computational and Applied Mathematics 1999.

de Sturler, E., Jay Hoeflinger, Laxmikant Kale, Milind Bhandarkar, "A New Approach to Software Integration Frameworks for Multi-physics Simulation Codes," Proceedings of the 8<sup>th</sup> Conference of the IFIP WG 2.5 Working Committee on Software Architecture for Scientific Computing Applications, October 2000 (to appear).

de Sturler, Eric, Jay Hoeflinger, Milind Bhandarkar, and Laxmikant Kale, "A New Approach to Software Integration Frameworks for Multi-physics Simulation Codes," International Conference on Software Architecture for Scientific Computing Applications, Ottawa, Ontario, Canada, October 2-6, 2000.

Heath, M. T., R. A. Fiedler, and W. A. Dick, "Simulating Solid Propellant Rockets at CSAR," AIAA 2000-3455, 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, AL, July 16-19, 2000.

Heath, M. T. and W. A. Dick, "Virtual Prototyping of Solid Propellant Rockets," Comput. Sci. Engr., Vol. 2, No. 2 (March-April 2000), pp. 21-32.

Heath, M. T., A. Ranade, and R. S. Schreiber, editors, "Algorithms for Parallel Processing," Springer-Verlag, New York, 1999.

Heath, M. T., and P. Raghavan, "Performance of Parallel Sparse Triangular Solution," Algorithms for Parallel Processing, ed. by M. T. Heath, A. Ranade, and R. S. Schreiber, Springer-Verlag, New York, pp. 289-305, 1999.

Hoeflinger, Jay and Yunheung Paek, "A Comparative Analysis of Dependence Testing Mechanisms," Workshop on Languages and Compilers for Parallel Computers, August 2000.

Hoeflinger, Jay and Yunheung Paek, "Unified Interprocedural Parallelism Detection," accepted by the International Journal of Parallel Processing, 2000.

Hoeflinger, Jay, Prasad Alavilli, Thomas Jackson, and Robert Kuhn, "Producing Scalable Performance with OpenMP: Experiments with Two CFD Applications," accepted by Journal of Parallel Computing, 2000.

Jiao, X., H. Edelsbrunner, and M. T. Heath, "Mesh Association: Formulation and Algorithms, Proc. 8th International Meshing Roundtable, Lake Tahoe, CA, October 1999.

Kale, L. V., Milind Bhandarkar and Robert Brunner, "Run-time Support for Adaptive Load Balancing," In: Rolim J. (Ed.), Parallel and Distributed Processing. Springer Verlag, 2000, ISBN 3-540-67442-X, Lecture Notes in Computer Science, Vol. 1800, Proceedings of 4th Workshop on Runtime Systems for Parallel Programming (RTSPP) Cancun - Mexico, March 2000.

Paek, Yunheung, Jay Hoeflinger, and David Padua, "Efficient and Precise Array Access Analysis," submitted to Transactions on Programming Languages and Systems, 1999.

Pinar, A., and M. T. Heath, "Improving Performance of Sparse Matrix-Vector Multiplication," Proc. Supercomputing 99, Portland, OR, November 1999.

Shaffer, Eric, Shannon Whitmore, Benjamin Schaeffer, and Daniel A. Reed "Virtue: Immersive Performance Visualization of Parallel and Distributed Applications," IEEE Computer, pp. 44-51, December 1999.

Sheffer, A., "Model Simplification for Meshing Using Face Clustering," Computer-Aided Design (CAD), to appear.

Sheffer, A., A. Ungor, S.-H. Teng, and R. B. Haber, "Generation of 2D Space-Time Meshes Obeying the Cone Constraint," Advances in Computational Engineering & Sciences, 2000. Eds. Alturi, S.N. and Brust, F.W., Tech Science Press, pp. 1360-1365, 2000.

Sheffer, A., E. de Sturler, "Parameterization of CAD Surfaces for Meshing by Triangulation Flattening," Proc. of 7th International Conference on Numerical Grid Generation in Computational Field Simulations, Whistler, British Columbia, Canada, September 2000. Also Technical Report UIUCDCS-R-2000-2174, University of Illinois at Urbana-Champaign, 2000.

Sheffer, A., E. de Sturler, "Surface Parameterization for Meshing by Triangulation Flattening," Proc. of 9th International Meshing Roundtable, New-Orleans, Louisiana, October 2000. Also Technical Report UIUCDCS-R-2000-2175, University of Illinois at Urbana-Champaign, 2000.

Sheffer, A., E. Taciroglu, "Hexahedral Mesh Adjustment for the Simulation of Solid-Propellant Rockets," Advances in Computational Engineering & Sciences, 2000. Eds. Alturi, S.N. and Brust, F.W., Tech Science Press, pp. 1366-1371, 2000.

Ungor, A., A. Sheffer, "Tent-Pitcher: A Meshing Algorithm for Space-Time Discontinuous Galerkin Methods," Proc. of 9th International Meshing Roundtable, New-Orleans, Louisiana, October 2000.

Ungor, A., A. Sheffer, and R. B. Haber, "Space-Time Meshes for Nonlinear Hyperbolic Problems Satisfying a Nonuniform Angle Constraint," Proc. of 7th International Conference on Numerical Grid Generation in Computational Field Simulations, Whistler, British Columbia, Canada, September 2000.

Ungor, A., C. Heeren, X.-Y. Li, A. Sheffer, R. B. Haber, and S.-H. Teng, "Constrained 2D Space-Time Meshing with All Tetrahedra," Proc. of IMACS World Congress on Scientific Computation, Applied Mathematics and Simulation, Lausanne, Switzerland, August 2000.

## **General and System Integration**

Fiedler, R. A., and Norris, J. C., "Rocketeer v1.1 User's Guide," [http://www.csar.uiuc.edu/F\\_software/rocketeer](http://www.csar.uiuc.edu/F_software/rocketeer), August 2000.

Heath, M. T., R. A. Fiedler, and W. A. Dick, "Simulating Solid Propellant Rockets at CSAR," AIAA 2000-3455, 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, AL, July 16-19, 2000.

Heath, M. T. and W. A. Dick, "Virtual Prototyping of Solid Propellant Rockets," Comput. Sci. Engr., Vol. 2, No. 2, pp. 21-32, March-April 2000.

Parsons, I. D., P. Alavilli, A. Namazifard, A. Acharya, X. Jiao and R. Fiedler, "Coupled Simulations of Solid Rocket Motors," AIAA Paper 3456, 36<sup>th</sup> AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, Huntsville, AL, July 16-19, 2000.