SREEKANTH PANNALA

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COMPUTATIONAL SCIENTIST WHO WORKS AT THE CONVERGENCE OF HIGH PERFORMANCE COMPUTING, APPLIED MATHEMATICS, AND DOMAIN SPECIALTIES TO CONSTANTLY PUSH THE ROLE OF COMPUTATIONAL SCIENCE IN ACCELERATING CLEAN ENERGY INNOVATIONS.

EDUCATION:

- Ph.D. in Aerospace Engineering, Georgia Institute of Technology, Atlanta, Georgia (May 2000), [On Large-eddy Simulations of Reacting Two-phase Flows]

- M.S. in Aerospace Engineering, Georgia Institute of Technology, Atlanta, Georgia (Dec. 1994), [Emphasis on CFD and Turbulence]

- B.Tech (Hons.) in Aerospace Engineering, Indian Institute of Technology, Kharagpur, India (Aug. 1993)

NOTABLE HONORS:

- **Secretary of Energy's Achievement Award** - highest non-monetary award from Department of Energy, **2011**
  - For contribution to the multi-agency's effort that was deemed critical to estimating the rate of oil flowing into the Gulf of Mexico and, in turn, developing options to cap the well

- Outstanding Mentor Award, Siemens, **2013**
  - For mentoring high school students who went to the regional finals of Siemens' prize (project was placed in the top 30 in the country)

- Outstanding Mentor Award, US DOE, Office of Science, **2009**
  - For mentoring undergraduate students in science

- Exceptional Mentoring, Research Alliance in Math and Science, ORNL, **2009**
  - For mentoring undergraduate students from HBCU universities

- Oak Ridge National Laboratory **Significant Event Award 2008**
  - For conducting first of the kind HPC simulations of clean coal gasification plants

- Oak Ridge National Laboratory **Significant Event Award 2010**
  - For contributing to the AMP advanced multiphysics software

- Oak Ridge National Laboratory **Significant Event Award 2011**
  - For contributing to the analysis of Fukushima Daiichi accident

- **2007 R&D 100 award**

- o For contributing to the development of MFIX multiphase flow software
- Listed in the **2007** - **2013** Editions of Who's Who in America for scientific contributions
- **2006** Mid Atlantic Regional award of Federal Laboratories Consortium's Technology Transfer Award
  - o For contributing to the development of MFIX multiphase flow software
- Awarded "*Person of the Year*" by India Club of Georgia Tech in **1998** for outstanding service
  - o For providing outstanding leadership and community service

PROJECT PORTFOLIO:

- PI/co-PI on project(s) for modeling batteries from EERE/ARPA-E
- PI on a project for development of multiphase simulation software over the last decade from FE/EERE
- PI on a project from NE for simulations of coating process for nuclear fuel particles
- Co-PI on a project from EERE on HPC for automotive engines
- Co-PI on a project from EERE Biomass program for modeling of catalytic pyrolysis
- Co-PI on a project from OE for dynamic simulations of the electrical grid
- Lead for CASL's ORNL Thermal Hydraulics team
- Co-PI on DOE BRIDGE project on "Using Solid Particles as Heat Transfer Fluid in CSP Plants"
- PI on a DOE multiscale and mathematics research project awarded in **2005** on "Micro-Mesoscopic Modeling of Heterogeneous Chemically Reacting Flows (MMM-HCRF) Over Catalytic/Solid Surfaces"

COMMUNITY SERVICE:

- Editorial Board, Journal of Engineering, **2012** –
- Editorial Board, Journal of Powder Technology, **2012** –
- Founding trustee, Vibha India (Child Relief), **2008** –
- Lead editor of a book titled "Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice," IGI Global, **2011**
- Organizer of Energy Storage session, ASME International Mechanical Engineering Congress and Exposition (IMECE), Vancouver, Canada, **2010**
- Invited participant in the Energy Storage session at DOE Council on Chemical Research Workshop on Hi-Performance Computing, **2011**
- Organizer for a minisymposium titled "Multiscale/Multiphysics Methods for Gas-Solid Reacting Flows" at the **2007** SIAM CSE meeting
- Session Chair, Session III, Track on Computational Sciences, ACM Symposium on Applied Computing, Melbourne, Florida, March 9-12, **2003**
- Reviewer for DOE MICS, DOE FE, DOE NE, ACS PRF, AIAA Journal, ASME conferences, AIChE Journal, I&ECR Journal, SAE conferences, ASME conferences, JES, CEC, CES, IJMF, ChERD, Phy. of Fluids, and CHAOS.
- Co-organizer for several CLEERS workshops (http://www.cleers.org)

RESEARCH EXPERIENCE:

<u>DISTINGUISHED RESEARCH STAFF MEMBER,</u> COMPUTER SCIENCE AND MATHEMATICS DIVISION, OAK RIDGE NATIONAL LABORATORY (2013 – PRESENT)
<u>SENIOR RESEARCH STAFF MEMBER,</u> COMPUTER SCIENCE AND MATHEMATICS DIVISION, OAK RIDGE NATIONAL LABORATORY (2008 – 2013)
<u>RESEARCH STAFF MEMBER,</u> COMPUTER SCIENCE AND MATHEMATICS DIVISION, OAK RIDGE NATIONAL LABORATORY (2001 – 2008)
<u>JICS RESEARCH AFFILIATE,</u> JOINT INSTITUTE FOR COMPUTATIONAL SCIENCES, UNIVERSITY OF TENNESSEE (2003 – PRESENT)
<u>POST GRADUATE/DOCTORAL RESEARCH FELLOW,</u> COMPUTER SCIENCE AND MATHEMATICS DIVISION, OAK RIDGE NATIONAL LABORATORY (1999 –2001)

- Multiscale/Multiphysics models for energy storage devices (Batteries and Supercapacitors), energy conversion and production devices (gasification, pyrolysis, nuclear reactors, etc.), and additive manufacturing (3D printing)

- Thermal hydraulics models for nuclear reactors

- Multiscale models for heterogeneous reacting flows

- Parallel multi-phase DNS and LES models for dense fluidized beds for applications in chemical and fossil industries

- Models for spouted bed CVD coaters for fuel particles for advanced nuclear reactors

- Reduced order models for simulating fluidized beds

- Models for emission reduction components in diesel engines

- Multiscale models for simulating carbon nanotubes

<u>GRADUATE RESEARCH ASSISTANT,</u> GEORGIA INSTITUTE OF TECHNOLOGY (1993 –1999)

- Research was part of MURI (Army's Multi-Disciplinary University Research Initiative) for Intelligent Turbine Engines in developing parallel two-phase LES solvers with Lagrangian droplet tracking using MPI and was a DoD HPCMO grand challenge project.

BOOKS:

1. "Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice," with M. Syamlal and T. J. O'Brien as co-editors, IGI Global, **2011.**

BOOK CHAPTERS:

1. "Multiphase continuum formulation for gas-solids reacting flows," with M. Syamlal, chapter in book titled "Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice," Editors: S. Pannala, M. Syamlal and T. J. O'Brien, IGI Global, **2011**.
2. "Modeling and Simulation of Battery Systems," with Mukherjee, P. P. and J. Turner, chapter in Handbook of Battery Materials: Editor C. Daniel. Weinheim, Wiley-VCH Verlag GmbH & Co. KGaA, **2011**.
3. "Multiscale/Multiphysics Modeling of Biomass Thermochemical Processes," with G. Frantziskonis and S. Simunovic, *ACS book on Computational Modeling of Lignocellulosic Biofuel Production,* **2010.**
4. "Segregated Methods for Two-Fluid Models," with A. Prosperetti, S. Sundaresan, and D. Z. Zhang, Book chapter in *Computational Methods for Multiphase Flows*; Editors: A. Prosperetti and G. Tryggvason, Cambridge University Press, **2007**.

JOURNAL ARTICLES:

1. "A new open computational framework for highly-resolved coupled 3D multiphysics simulations of Li-Ion Cells," with S. Allu, S. Kalnaus, W. Elwasif, S. Simunovic, and J. Turner, *Journal of Power Sources*, **2014**.

2. "Real-time optical diagnostics of isothermal graphene growth induced by pulsed chemical vapor deposition," with A. Puretzky, D. Geohegan, M. Regmi, C. Rouleau, N. Thonnard, J. Readle, and G. Eres, *Nanoscale*, **2013**.

3. "CFD Simulations of Circulating Fluidized Bed Risers, Part I: Grid Study," with T. Li, A. Gel, M. Syamlal and M. Shahnam, Powder Technology, **2013**. (accepted for publication)

4. "CFD Simulations of Circulating Fluidized Bed Risers, Part II: Evaluation of Differences between 2D and 3D Simulations," with T. Li and M. Shahnam, Powder Technology, **2013**. (accepted for publication)

5. "Neutron Imaging at the Oak Ridge National Laboratory: Present and Future Capabilities," *Physics Procedia*, **2013**.

6. "A generalized multi-dimensional mathematical model for charging and discharging processes in a Supercapacitor", with S. Allu, B. Velamur Asokan, B. Philip, and W. A. Shelton, *submitted to Electrochimica Acta*, July **2013**.

7. "Solid Electrolyte Coated High Voltage Layered-Layered Lithium-rich Composite Cathode: $Li_{1.2}Mn_{0.525}Ni_{0.175}Co_{0.1}O_2$," with M. S. Kumar, J. Nanda, Y. Kim, R. Unocic, and N. Dudney, *J. Mater. Chem. A*, **2013**

8. "The AMP (Advanced MultiPhysics) Nuclear Fuel Performance Code," with Clarno, K. T.; Philip, B.; Cochran, W. K.; Sampath, R. S.; Allu, S.; Barai, P.; Simunovic, S.; Berrill, M. A.; Ott, L. J.; Dilts, G. A.; Mihaila, B.; Yesilyurt, G.; Lee, J. H.; Banfield, J. E., *Nuclear Engineering and Design*, **2012**.

9. "Anomalous Discharge Product Distribution in Lithium-Air Cathodes," with Nanda J., H. Bilheux, S. Voisin, G. Veith, R. Archibald, L. Walker, S. Allu, K. Willis, and N. Dudney, *Journal of Physical Chemistry C*, **2012**.

10. "Incremental Growth of Short SWNT Arrays by Pulsed Chemical Vapor Deposition," with A. A. Puretzky, D. B. Geohegan, J. J. Jackson, G. Eres, C. M. Rouleau, K. L. More, N. Thonnard, and J. D. Readle, *Small*, **2012**.

11. "Open-source MFIX-DEM software for gas-solids flows: Part I — Verification," with R. Garg, J. E. Galvin, and T. Li, *Powder Technology*, **2012**.

12. "Open-source MFIX-DEM software for gas-solids flows: Part II — Validation," with T. Li, J. E. Galvin, and R. Garg, *Powder Technology*, **2012**.

13. "High-Resolution Simulations of Coal Injection in a Gasifier," with Li, T., Gel, A., Syamlal, M., and Guenther, C. *Industrial & Engineering Chemistry Research*, doi:10.1021/ie100519s, **2010**.

14. "Modeling the coupling of reaction kinetics and hydrodynamics in a collapsing cavity," with S. K. Mishra, K. Muralidharan, P. A. Deymier, G. Frantziskonis, and S. Simunovic, *Ultrasonics Sonochemistry*, **2010.**

15. "Time-parallel multiscale/multiphysics framework," with G. Frantziskonis, K. Muralidharan, P. Deymier, S. Simunovic, and P. Nukala, *Journal of Computational Physics,* 228, 8085–8092, **2009.**

16. "Advanced Coal Gasifier Designs Using Large-Scale Simulations," Proceedings of the Scientific Discovery Through Advanced Computing Conference, *Journal of Physics*, **2009**.

17. "Modeling the Collisional-Plastic Stress Transition for Bin Discharge of Granular Material," with Sofiane Benyahia, Charles E. A. Finney, Madhava Syamlal, Stuart C. Daw, and Thomas O'Brien, *Powders and Grains, AIP*, **2009**.

18. "Silicon Chemical Vapor Deposition On Macro and Submicron Powders in a Fluidized Bed," with L. Cadoret, N. Reuge, M. Syamlal, C. Rossignol, J. Dexpert-Ghys, C. Coufort, and B. Caussat, *Powder Technology*, 190, pp. 185-191, **2009.**

19. "Wavelet-Based Spatial Scaling of Coupled Reaction-Diffusion Fields" with S. K. Mishra, K. Muralidharan, P. A. Deymier, G. Frantziskonis, and S. Simunovic, *International Journal for Multiscale Computational Engineering*, Issue 6(4), p. 281-297, **2008**.

20. "Multifluid Eulerian Modelling of Dense Gas-Solid Fluidized Bed Hydrodynamics: Influence of the Dissipation Parameters," with N. Reuge, L. Cadoret, C. Coufort, M. Syamlal and B. Caussat, *Chemical Engineering Science*, 63 (22), pp. 5540-5551, **2008**.

21. "Filtered two-fluid models for fluidized gas-particle suspensions," with Yesim Igci, Arthur Andrews, Sankaran Sundaresan, and Thomas O'Brien, *AIChE Journal,* 54(6), 1431-1448, **2008**.

22. "Open-Source Software in Computational Research: A Case Study," with M. Syamlal, T. J. O'Brien, S. Benyahia, and A. Gel, *Modelling and Simulation in Engineering*, Vol. 2008, 937542, **2008**. doi:10.1155/2008/937542.

23. "Spatiotemporal Compound Wavelet Matrix Framework for Multiscale/Multiphysics Reactor Simulation: Case Study of a Heterogeneous Reaction/Diffusion System," with S. K. Mishra, K. Muralidharan, S. Simunovic, C. S. Daw, P. Nukala, R. O. Fox, P. A. Deymier, and G. Frantziskonis, *International Journal of Chemical Reactor Engineering*, Vol. 6: A28, **2008**. http://www.bepress.com/ijcre/vol6/A28.

24. "Dynamic compound wavelet matrix method for multiphysics and multiscale problems", with K. Muralidharan, S. K. Mishra, G. Frantziskonis, P. A. Deymier, P. Nukala, and S. Simunovic, *Phy. Rev. E,* E 77, 026714, **2008**.

25. "Effects of using two- versus three-dimensional computational modeling of fluidized beds: Part II, analysis," with Nan Xie and Francine Battaglia, *Powder Technology,* 182, 14–24, **2008**.

26. "Effects of using two- versus three-dimensional computational modeling of fluidized beds: Part I, hydrodynamics," with Nan Xie and Francine Battaglia, *Powder Technology,* 182, 1–13, **2008**.

27. "In situ time-resolved measurements of carbon nanotube and nanohorn growth," with D. B. Geohegan, A. A. Puretzky, D. Styers-Barnett, H. Hu, B. Zhao, H. Cui, C. M. Rouleau, G. Eres, J. J. Jackson, R. F. Wood, and J. C. Wells, *phys. stat. sol. (b),* 244, No. 11, 3944–3949 / DOI 10.1002/pssb.200776204, **2007**.

28. "Silicon CVD on powders in fluidized bed: Experimental and multifluid Eulerian modelling study," with Loïc Cadoret, Nicolas Reuge, Madhava Syamlal, Carole Coufort and Brigitte Caussat, *Surface and Coatings Technology*, 201, 8919, **2007**.

29. "Simulating the Dynamics of Spouted Bed Nuclear Fuel Coaters," with C. S. Daw, C. E. A. Finney, D. Boyalakuntla, T. J. O'Brien and M. Syamlal. *Chem. Vap. Deposition,* 13, 481-490, **2007**.

30. "Simple model of the interrelation between single- and multi-wall carbon nanotube growth rates for CVD process," with R.F. Wood, J.C. Wells, A. A. Puretzky and D. B. Geohegan, *Physical Review B*, B 75, 235446, **2007**. Also appears in Virtual Journal of Nanoscale Science & Technology, 16, 2, **2007**.

31. "Comparison of Frameworks for Next Generation Multiphase Flow Solver, MFIX. A Group Decision-Making Multiphase Flow Solver," with A. Gel, M. Syamlal, T. J. O'Brien and E. S. Gel, *Concurrency and Computation: Practice and Experience,* Issue 19 (5), p. 609-624 Sp. Iss. SI, **2007**.

32. "Bifurcation Analysis of Bubble Dynamics in Fluidized Beds," with Peter Blomgren, Antonio Palacios, Bing Zhu, Stuart Daw, Charles Finney and John Halow, *CHAOS*, 17 (1), 013120, **2007**.

33. "Wavelet-based Spatiotemporal Multi-scaling in Diffusion Problems with Chemically Reactive Boundary," with George Frantziskonis, Sudib K. Mishra, Srdjan Simunovic, C. Stuart Daw, Phani Nukala, Rodney O. Fox, and Pierre A. Deymier, *International Journal for Multiscale Computational Engineering*, Issue 5-6, p. 755-770, **2006**.

34. "Dynamic Interacting Bubble Simulation (DIBS): An Agent-Based Bubble Model for Reacting Fluidized Beds," with C. S. Daw and J. S. Halow, S*pecial issue of CHAOS on "Nonlinear dynamics in spatially extended mechanical systems,"* CHAOS, Vol. 14(2), **2004**.

35. "Multiscale Simulations of Carbon Nanotube Nucleation and Growth: Mesoscopic Continuum Calculations," with R. F. Wood, *Special issue on SWNT Growth Mechanisms*, J. Nanosci. Nanotech., Vol. 4(4), **2004**.

36. "Simulations of Reacting Fluidized Beds Using an Agent-Based Bubble Model," with C. S. Daw and J. Halow, *International Journal of Chemical Reactor Engineering*, Vol. 1: A20, **2003**. http://www.bepress.com/ijcre/vol1/A20

TECHNICAL PUBLICATIONS:

1. "Demonstration & Assessment of Advanced Modeling Capabilities for Multiphase Flow with Sub-cooled Boiling L2.THM.P7.01," CASL Milestone Report, July, 2013.

2. "Lift Forces in Bubbly Flows THM.CLS.P7.06," CASL Milestone Report, June, 2013.

3. "Parameter Sweep and Optimization of Loosely Coupled Simulations Using the DAKOTA Toolkit," with W. Elwasif, D. Bernholdt, S. Allu, and S. Foley, *IEEE CSE 2012*, Cyprus.

4. "Computer Aided Engineering of Batteries Effort (ORNL)," *2012 DOE VT Annual Report*

5. "Engine Efficiency Fundamentals – Accelerating Predictive Simulation of Internal Combustion Engines with High Performance Computing," *2012 DOE VT Annual Report*

6. "CAEBAT OAS BETA RELEASE V1," S. Pannala, S. Allu, W. Elwasif, S. Simunovic, D. Bernholdt, and J. Turner, Internal report to CAEBAT partners, **2012**.

7. "Application of high performance computing for simulating the unstable dynamics of dilute spark-ignited combustion,"   CEA Finney, MK Stoyanov, S Pannala, CS Daw, RM Wagner, KD Edwards, CG Webster, and JB Green Jr, *2012 International Conference on Theory and Applications of Nonlinear Dynamics (ICAND)*, Seattle, WA, USA; 26-30 August **2012**.

8. "High performance computing: clean coal gasifier designs using hybrid parallelization," with M. Syamlal, C. Guenther, and A. Gel, *Proceedings of Fluidization XIII*, Gyeong-ju, Korea, **2010**. (http://www.osti.gov/energycitations/product.biblio.jsp?osti_id=983571; http://services.bepress.com/eci/fluidization_xiii/108/)

9. "Test Problem 4: 2009 Three-Dimensional Assembly Simulations Report," with E. Popov, R. Deiterding, and B.   Neykov, *ORNL/TM-2009/246*, November, **2009**.

10. "Accelerating Clean Coal Gasifier Designs with Hybrid MPI/OpenMP High Performance Computing," with A. Gel, S. Pannala, R. Sankaran, C. Guenther, M. Syamlal, and T. O'Brien, *Proceedings of the Parallel Computational Fluid Dynamics (ParCFD)*, May 18-22, Moffett Field, CA, USA, **2009**.

11. "Wavelet Based Spatial Scaling of Coupled Reaction Diffusion Fields," with S. K. Mishra, K. Muralidharan, P. Deymier, G. Frantziskonis, and S. Simunovic, *Proceedings of the **2008** ICCS conference*, Lecture Notes in Computer Science, Springer.

12. "Parallel-in-Time Multiscale/Multiphysics Framework," with G. Frantziskonis, K. Muralidharan, P. Deymier, and S. Simunovic, Proc. 3rd International Conference "From Scientific Computing to Computational Engineering," *3rd IC-SCCE*, Athens, 9-12 July, **2008**, D. Tsahalis, Ed., pp. 1-6.

13. "Micro-Mesoscopic Modeling of Heterogeneous Chemically Reacting Flows (MMM-HCRF) Over Catalytic/Solid Surfaces: 2007 Annual Progress Report," with S. Simunovic, C. S. Daw, P. K. Nukala, G. Frantziskonis, S. Mishra, P. Deymier, R. Fox, T. J. O'Brien and M. Syamlal, **2007**.

14. "Process Modeling Phase II Summary Report for the Advanced Gas Reactor Fuel Development and Qualification Program," with Charles E. A. Finney and C. Stuart Daw, *ORNL Technical Report for INL MPO 00056009*, **2006**.

15. "Micro-Mesoscopic Modeling of Heterogeneous Chemically Reacting Flows (MMM-HCRF) Over Catalytic/Solid Surfaces: 2006 Annual Progress Report," with S. Simunovic, C. S. Daw, P. K. Nukala, G. Frantziskonis, S. Mishra, P. Deymier, R. Fox, T. J. O'Brien and M. Syamlal, **2006**.

16. "ORNL FY06 Progress Report on FBCVD Process Modeling for the Advanced Gas Reactor Fuel Development and Qualification Program," with Charles E. A. Finney, Dhanunjay Boyalakuntla and C. Stuart Daw, Oak Ridge National Laboratory Technical Report, *ORNL/CF-06/06*, **2006**.

17. "Process Modeling Phase I Summary Report for the Advanced Gas Reactor Fuel Development and Qualification Program," with C. S. Daw, D. Boyalakuntla and C. E. A. Finney, *ORNL/TM-2006/520*, March, **2006**.

18. "ORNL FY05 Process Modeling Summary Report for the Advanced Gas Reactor Fuel Development and Qualification Program: Hydrodynamics, Heat and Mass Transfer for NU UCO particles," with D. Boyalakuntla, C. E. A. Finney and C. S. Daw, Oak Ridge National Laboratory Technical Report, *ORNL/CF-05/14*, September, **2005**.

19. "ORNL FY05 Process Modeling Summary Report for the Advanced Gas Reactor Fuel Development and Qualification Program: Hydrodynamics, Heat and Mass Transfer," with D. Boyalakuntla, C. E. A. Finney, and C. S. Daw, Oak Ridge National Laboratory Technical Report, *ORNL/CF-05/13*, August, **2005**.

20. "Hybrid (mixed SMP/DMP) parallelization of MFIX: A Multiphase CFD code for modeling fluidized beds," with E. D'Azevedo, T. O'Brien and M. Syamlal, *Proceedings of ACM Symposium on Applied Computing*, Melbourne, Florida, 9-12 March, **2003**.

21. "Automotive Underhood Thermal Management Analysis Using 3-D Coupled Thermal-Hydrodynamic Computer Models: Thermal Radiation Modeling," with E. D'Azevedo and T. Zacharia, *ORNL CRADA Report C9800401*, **2002**.

22. "On Large Eddy Simulations of Reacting Two-phase Flows," *Ph. D Dissertation – Georgia Institute of Technology*, May **2000**.

23. "Large Eddy Simulations of Reacting Two-phase Flows," with S. Menon, *Georgia Tech Report CCL-00-005*, Prepared with the support of the Army Research Office – Contract DAAH04-96-1-0008, **2000**.

24. "Subgrid Two-Phase Mixing and Combustion Modeling for Large-Eddy Simulations," with S. Menon, *ASME Turbo Expo'98,* Stockholm International Fairs, Stockholm, Sweden*,* June, **1998**.

25. "Simulations of Underwater Explosion Bubble Dynamics Using an Arbitrary Lagrangian-Eulerian Formulation," with S. Menon, FEDSM97-3492, *ASME Fluids Engineering Division Summer Meeting, FEDSM'97 (Symposium)*, Vancouver, June, **1997**.

26. "Numerical Study of Bubble Collapse and Rebound Near a Wall," with S. Menon, FEDSM97-3244, *1997 ASME Fluids Engineering Division Summer Meeting*, FEDSM'97 (Forum), Vancouver, June, **1997**.

INVITED PRESENTATIONS:

1. "Delivering Breakthrough Science through High-Performance Computing: Relevance to Additive Manufacturing Computational End Station (ACE)," S. Pannala, Z. Feng, R. DeHoff, C. Duty, L. Love, C. Blue, T. R. Watkins and S. S. Babu, *Invited presentation* at Smoky Mountain HPC conference, Gatlinburg, **2013**.

2. "Multiscale/Multiphysics simulation strategy for reacting multiphase flows," *Invited presentation* at North Carolina State University, Raleigh, NC, March 14, **2013**.

3. "Bridging atomistic to continuum scales for designing energy materials: challenges and opportunities," *Invited presentation* at IIT Jodhpur, Jodhpur, India, February 8, **2013**.

4. "Multiscale/Multiphysics simulation strategy for heterogeneous chemically reacting flows," *Invited presentation* at Florida International University, Miami, FL, March 30, **2012**.

5. "Hierarchical Models for Batteries: Overview with Some Case Studies," *Invited presentation* at AABC (Advanced Automotive Battery Conference), Orlando, February 6-10, **2012**.

6. "Using Uncertainty Quantification to Bridge Atomistic to Continuum Scales for Designing Energy Storage Devices: Challenges and Opportunities," *Invited presentation* at 9th Annual NanoTechnology for Defense Conference (NT4D), Bellevue, Washington, October 24 – 27, **2011**.
7. "Bridging atomistic to continuum scales for designing battery chemistry and materials: Challenges and opportunities," *Invited presentation* at 242nd ACS National Meeting & Exposition, Denver, Colorado, August 28-September 1, **2011**.
8. "A Multi-scale Modeling Framework for Li-Ion Batteries," with P. P. Mukherjee, S. Allu, and J. Turner, *Invited presentation* at the 7th Annual International Conference on Lithium Battery Power, Las Vegas, NV, **2011**.
9. "Bridging atomistic to continuum scales for designing energy materials: challenges and opportunities," *Invited presentation* at ASME International Mechanical Engineering Congress and Exposition (IMECE), Vancouver, Canada, Nov. 12-18, **2010**.
10. "Multiscale/Multiphysics simulation strategy for gas-solids flow reactors," *Invited presentation* at Vanderbilt University, September 27, **2010**.
11. "Multiscale and Multiphysics Models for Interfacial and Bulk Processes in Electrochemical Systems", *Invited presentation* at *Electrochemical Energy Storage beyond Lithium Ion: Computational Perspectives Symposium*, ANL, Chicago, Illinois, USA, May 03, **2010**.
12. "Bridging atomistic to continuum scales for designing energy materials: challenges and opportunities," *Invited presentation* at Georgia Tech, January 27, **2010**.
13. "Multiphase flow modeling using MFIX," Weeklong short-course at SATC in Criciuma, Brazil as part of the NETL-Brazilian coal association MOU, May **2010**.
14. "Bridging atomistic to continuum scales for designing energy materials: challenges and opportunities," *Invited presentation* at UTK Math Colloquium, Oct. 26, **2009**.
15. "Multiscale/Multiphysics simulation strategy for gas-solids flow reactors," *Invited presentation* at Duke University, September 22, **2009**.
16. "Multiscale/Multiphysics simulations for multiphase gas-solids flow reactors," *Invited presentation* at University of Kentucky, July 23, **2009**.
17. "Multiscale/Multiphysics simulations for clean energy solutions: HPC challenges and opportunities," *Invited presentation* at Workshop on Trends, Technologies and Collaborative Opportunities in High Performance Computing WTTC09, Theme: "High Performance Computing: Enabling Technologies for Knowledge Economy," May 25-26, **2009**, Software Park Building, Chaengwattana Road, Nonthaburi (Greater Bangkok), Thailand.
18. "Multiscale/Multiphysics simulations for clean energy solutions: HPC challenges and opportunities," *Invited presentation* at Workshop on Trends, Technologies and Collaborative Opportunities in High Performance Computing WTTC09, Theme: "High Performance Computing: Enabling Technologies for Knowledge Economy," May 28, **2009**, Mae Fah Luang University, Chiang Rai, Thailand.
19. "Reduced Models for Gas-Solids Flows: Coarse Discrete Element Method and Phase-Space Proper Orthogonal Decomposition," *Invited presentation* at NETL 2009 Workshop on Multiphase Flow Science, Morgantown, WV, April 22-23, **2009**.
20. "Bridging atomistic to continuum scales for designing energy materials: challenges and opportunities," *Invited Presentation at Young Investigators Symposium* (EU, US and Japan), **2008**. (http://computing.ornl.gov/workshops/symposium08/)
21. "Multiscale/Multiphysics (MSMP) Simulations of Heterogeneous Chemically Reacting Flows (HCRF): Role in Energy Security and Sustainability," *Invited presentation at DOE ASCR workshop on Scientific Impacts and Opportunities for Computing*, January 9 -12, 2008, http://computing.ornl.gov/workshops/peta08/.

22. "In Situ Time-resolved Measurements of Carbon Nanotube and Nanohorn Growth," with D. B. Geohegan, A. A. Puretzky, G. Eres, D. Styers-Barnett, C. M. Rouleau, Z. Liu, I. N. Ivanov, J. Jackson, R. F. Wood, J. Wells, M.-D. Cheng, H. Cui, H. Hu, B. Zhao, M. Yoon, K. Xiao and M. Garrett, *Invited presentation at IWEPNM 2007 International Winterschool on Electronic Properties of Novel Materials: Molecular Nanostructure*, March 10-17, Kirchberg, Austria, **2007**.

23. "Multiphysics/MultiscaleModeling of Heterogeneous Chemically Reacting Flows (HCRF)," Invited presentation at US France Young Engineering Scientists Symposium, **2007**. (http://france-science.org/symposium2007/)

24. "Simulations in Chemical Processing," ***Invited presentation*** *at the Town Hall Meeting on Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security an Initiative* (Breakout: Industrial Processes and Manufacturing), ORNL, May 17-18, **2007**.

25. "Multiscale/Multiphysics Modeling of a Chemical Reactor," ***Invited presentation*** *at the Simulation and Modeling for Advanced Nuclear Energy Systems Workshop organized by DOE*, Washington DC, August, **2006**.

PRESENTATIONS:

1. "The effects of soft-sphere contact models on heat transfer to particles flowing over a heated surface," A Morris, C Hrenya, Z Ma, S Pannala, T O'Brien, *Bulletin of the American Physical Society*, November **2013**

2. "Optimization of Tab Placement in Li-Ion Battery Using Multi-Physics Simulations," S Allu, W Elwasif, S Pannala, S Kalnaus, S Simunovic, and JA Turner, *ECS Meeting Abstracts*, Oct. **2013**

3. "Understanding the Effect of Temperature Gradients in Modules On Cell Balance Using Coupled Multi-Physics Modeling approach," S Pannala, S Allu, W Elwasif, S Kalnaus, S Simunovic, JA Turner, *ECS Meeting Abstracts*, 1229-1229, Oct. **2013**

4. "Three dimensional thermal, electrical and electrochemical modeling of Li-ion batteries," S Kalnaus, S Allu, W Elwasif, S Simunovic, S Pannala, JA Turner, *ECS Meeting Abstracts*, 1210-1210, Oct. **2013**

5. "Direct Fluorination of Iron (II, III) Oxide Conversion Electrodes," Hui Zhou, Jagjit Nanda, Surendra K. Martha, Juan Carlos Idrobo, Loïc Baggetto, Gabriel M. Veith, Sheng Dai, S Pannala, NJ Dudney, J Adcock, *ECS Meeting Abstracts*, Oct. **2013**

6. "Design of scalable three-dimensional electrode and device architectures with good rate capabilities," S. Pannala, J. Nanda, and B. Dunn, *ECS Spring Meeting*, **2013**

7. "Open Architecture Software (OAS) for modeling multi-physics phenomenon of Li-Ion Batteries," S. Pannala, S. Allu, WR Elwasif, S. Simunovic, and JA Turner, *ECS Spring Meeting*, **2013**

8. "DEM Simulations of Falling Particles Flowing in Crossflow Around a Heated Cylinder," with A. Morris, C. Hrenya, and Z. Ma, *NETL 2013 Conference on Multiphase Flow Science*, Morgantown, West Virginia, USA, August, **2013**.

9. "Accelerating predictive simulation of IC engines with high performance computing (ACE017)," *DOE VT Annual Merit Review*, **2013**.

10. "Real-time Optical Diagnostics of Graphene Growth Induced by Chemical Vapor and Pulsed Laser Deposition," *12th International Conference on Laser Ablation (COLA 2013)*, Italy, Oct. **2013**.

11. "Computational Framework for Modeling Multi-Physics Phenomenon of Li-Ion Batteries across Various Hierarchies," S Allu, S Pannala, P Mukherjee, W Elwasif, J Turner, *ECS Fall Meeting Abstracts*, 1067-1067, Oct. **2012**.

12. "Electrode Architectures for Conversion-Based Cathodes: Case of Iron Fluorides and Oxyfluorides," SK Martha, J Nanda, JC Idrobo, S Pannala, S Dai, NJ Dudney, J Wang, PV Braun, *ECS Fall Meeting Abstracts*, 734-734, Oct. **2012**.

13. "Accelerating the Development of High Efficiency Engines," *The 5th International Symposium on Clean and High Efficiency Combustion in Engines*, Tianjin, China, July **2013**.
14. "A Duality Framework for Optimal Control of Battery Management Systems in Hybrid Electric Vehicles," *2014 American Control Conference*, June, **2014**.
15. "Coupled Multi-Physics Model for Li-ion Battery Cells during Impact," *EUROMAT 2013, European Congress and Exhibition on Advanced Materials and Processes*, Spain, Sept. **2013**.
16. "Computational framework for modeling thermal response of Lithium-Ion batteries under abusive conditions," *EUROMAT 2013, European Congress and Exhibition on Advanced Materials and Processes*, Spain, Sept. **2013**.
17. "High Dimensional Multiphysics Metamodeling for Combustion Engine Stability," *SIAM Annual Meeting*, July **2013**.
18. "Computational Pyrolysis Consortium," *Biomass Energy Technology Review Meeting*, May 2013.
19. "State-of-the-Art Neutron Techniques for Studying Electrochemical Storage Materials and Interfaces," *Beyond Lithium IV*, June **2013**.
20. "High Dimensional Multiphysics Metamodeling for Combustion Engine Stability," *SIAM CSE*, Feb. **2013**.
21. Electrochemical and Transport Behavior of Lithium Ion Battery 3-D Electrode Architectures," Michael Martin, Partha P Mukherjee, Sreekanth Pannala, Srikanth Allu, Devesh Ranjan, John Turner, Electrochemical Society Meeting, Seattle, May 6-10, **2012**.
22. "A micro-macroscopic volume-averaged model for batteries," with S. Allu, P. Mukherjee, J. Nanda, N. Dudney, S. Martha, and J. Turner, Electronic Materials and Applications 2012, American Ceramic Society, Orlando, January 18-20, **2012.**
23. "Particle Morphology and Interactions in the Lithium Ion Battery Electrode," with P. P. Mukherjee, S. Allu, J. Nanda, N. Dudney, and J. A. Turner, ECS Meeting, Boston, MA, October 9 – 14, **2011**.
24. "A Micro-mesoscopic Model for Li-Ion Intercalation Batteries," with P. P. Mukherjee, S. Allu, J. Nanda, S. Martha, N. Dudney, and J. A. Turner, Electrochemical Society Meeting, Montreal, Canada, May 1-6, **2011**.
25. "Electrochemical and Thermal Modeling of Reactions for Lithium-ion Batteries along with Multidimensional Transport," with C. E. Shaffer, A. Sabau, S. Allu, and P. P. Mukherjee, Electrochemical Society Meeting, Montreal, Canada, May 1-6, **2011**.
26. "2D and 3D Imaging of Lithium in Porous Electrodes: Neutron Tomography Studies," with J. Nanda, H. Bilheux, K. Willis, S. Voisin, S. Allu, P. P. Mukherjee, G. Veith, and N. Dudney, MRS Spring Meeting, San Francisco, CA, USA, April 25-29, **2011**.
27. "Validation studies of open-source MFIX-DEM software for gas-solids flows," T. Li, R. Garg, J. Galvin, and S., Pannala, presented at AIChE annual meeting, November, **2010**.
28. "Validation Studies on Filtered Model Equations for Gas-Particle Flows in Risers," with Y. Igci, S. Benyahia, S. Sundaresan, presented at AIChE annual meeting, November, **2010**.
29. "Initial Validation of the AMP Nuclear Fuel Performance Code," with S. Allu, J. Banfield, P. Barai; J. Billings, K. T. Clarno, W. K. Cochran, G. A. Dilts, S. Kadioglu, J. Lee, G. I. Maldonado, R. Martineau, B. Mihaila, L. Ott, B. Philip, R. Sampath, S. Simunovic, J. A. Turner, C. Unal, G. Yesilyurt, to be presented at ANS winter meeting, **2010**.
30. "Multiscale and Multiphysics Models for Interfacial and Bulk Processes in Electrochemical Systems" ORNL User Week, Scientific Basis for Solar Energy and Energy Storage, ORNL, September 13, **2010**.
31. "Computational Approaches for Investigating Electrochemical Energy Storage Materials and Devices," with B. Sumpter, Poster presentation at SciDAC conference, July, **2010**.

32. "High-Resolution Simulations of Coal Injection in a Gasifier," with Li, T., Gel, A., Syamlal, M., and Guenther, C., ISCRE 21: 21st International Symposium on Chemical Reaction Engineering, Loews Philadelphia Hotel, Philadelphia, PA, USA, June 13th - 16th, **2010**.

33. "Coupled MFIX-DEM: Verification and Validation," with J. Galvin, R. Garg, and T. Li, Multiphase Flow Science Workshop, Pittsburgh, Pennsylvania, May 3-6, **2010**.

34. "High Resolution Numerical Simulations of Coal Gasifiers Using High Performance Computing," with A. Gel, T. Li, C. Guenther, and M. Syamlal, Multiphase Flow Science Workshop, Pittsburgh, Pennsylvania, May 3-6, **2010**.

35. "A generalized multi-dimensional mathematical model for charging and discharging processes in a Supercapacitor", with S. Allu, B. Velamur Asokan and W. A. Shelton, MRS Spring Meeting, San Francisco, California, April 05, **2010.**

36. "A Generalized multi-dimensional mathematical model for Li-Ion intercalation batteries", with S. Allu, J. Nanda, P. Mukherjee, and W. A. Shelton, ECS Spring Meeting, Vancouver, Canada, April 25, **2010**.

37. "How Can Detailed Modeling in Fuel Cells Be Adapted to Li/Air Batteries?", with P. P. Mukherjee and J. A. Turner, Poster presentation, *Beyond Lithium-Ion: Computational Perspectives Symposium*, Argonne National Laboratory, IL, USA, May 3-4, **2010**.

38. "Thermal and electrochemical behavior of high energy density carbon fiber paper (CFP)-LiFePO4 positive electrodes," with S. K. Martha, J. Nanda, J. Kiggans, A. Kercher, H. Wang, W. D. Porter, E. E. Kalu, and N. J. Dudney, *MRS Fall meeting*, 2010.

39. P. P. Mukherjee, S. Pannala, S. Allu, J. Nanda, and J. A. Turner, "Solid-Phase Diffusion Modeling in Lithium Ion Batteries", Oral presentation, Electrochemical Society Meeting, Las Vegas, NV, USA, October 10-15, **2010**.

40. "Large-scale parallel flow simulations for nuclear fuel performance," with S. Allu and E. Popov, SIAM CSE, January **2010**.

41. "Multiscale/Multiphysics Modeling for Gas-granular Reacting Flows," DARPA workshop on Granular Dynamics, February **2010**.

42. "Coarse Discrete Element Simulations for Gas-Solids Flows," with J. E. Galvin, S. Benyahia, R. Garg and C. Guenther, AIChE annual meeting, Nashville, Nov. 7-13, **2009**.

43. "High Resolution Simulations of a Coal Gasifier," with M. Syamlal, C. Guenther, and A. Gel, AIChE annual meeting, Nashville, Nov. 7-13, **2009**.

44. "Advanced Coal Gasifier Designs Using Large-Scale Simulations," with M. Syamlal, A. Gel, and C. Guenther, Scientific Discovery Through Advanced Computing Conference, San Diego, CA, June 14-18, **2009**, JP.

45. "Accelerating Clean Coal Gasifier Designs with Hybrid MPI/OpenMP High Performance Computing," with A. Gel, S. Pannala, R. Sankaran, C. Guenther, M. Syamlal, and T. O'Brien, Parallel Computational Fluid Dynamics (ParCFD), May 18-22, Moffett Field, CA, USA, **2009**.

46. "Modeling the Collisional-Plastic Stress Transition for Bin Discharge of Granular Material," with Sofiane Benyahia, Charles E. A. Finney, Madhava Syamlal, Stuart C. Daw, and Thomas O'Brien, Presented at the Powders and Grains **2009**: 6th International Conference on Micromechanics of Granular Media, Golden (Colorado).

47. "Discriminating characteristics for simulation-based design and scaling of spouted beds," with C. E. A. Finney and C. S. Daw, *Computational Fluid Dynamics in Chemical Reaction Engineering V*, Whistler, BC, Canada, June 15-10, **2008**. {URL: http://www.cfdcre5.org/cfdcre5-Finney.pdf}

48. "Understanding the interactions between hydrodynamics and chemistry in coal gasifier simulations," with C. Guenther, J. Galvin, M. Syamlal and A. Gel, *Computational Fluid Dynamics in Chemical Reaction Engineering V*, Whistler, BC, Canada, June 15-10, **2008**. {URL: http://www.cfdcre5.org/cfdcre5-Pannala.pdf}

49. "Wavelet Based Spatial Scaling of Coupled Reaction Diffusion Fields," with S. K. Mishra, K. Muralidharan, P. Deymier, G. Frantziskonis, and S. Simunovic, *2008 ICCS conference*, Poland, **2008**.

50. "Time-parallel multiscale/multiphysics framework," with G. Frantziskonis, K. Muralidharan, P. Deymier and S. Simunovic, *3rd IC-SCCE conference*, Athens, **2008**.

51. "Wavelet-based Spatiotemporal Multiscaling in Diffusion Problems with Chemically Reactive Boundary," with S. Simunovic, C. S. Daw, P. K. Nukala, G. Frantziskonis, S. Mishra, A. Mallik, K. Muralidharan, P. Deymier, R. Fox, Z. Gao, T. J. O'Brien and M. Syamlal, *Presentation at ASCR AMR Annual Math PI meeting*, LLNL, May 22-24, **2007**.

52. "Wavelet-Based Multiscale Approach for Heterogeneous Chemically Reactive Flows: A Simple Case Study of Diffusion/Reaction Problem," with George Frantziskonis, Sudib Misra, Sreekanth Pannala, Srdjan Simunovic, Stuart Daw, Phani Nukala, Rodney O. Fox, Pierre Deymier, *Presentation at the SIAM CSE meeting*, Feb. 21, **2007**.

53. "Silicon CVD on powders in fluidized bed: Experimental and multifluid Eulerian modelling study," with Loïc Cadoret, Nicolas Reuge, Madhava Syamlal, Carole Coufort and Brigitte Caussat, poster at *Sixteenth European Conference on Chemical Vapor Deposition,* Den Haag (Scheveningen) - The Netherlands, September 16-21, **2007**.

54. "Silicon Chemical Vapor Deposition on Macro and Submicron Powders in a Fluidized Bed," with Loïc Cadoret, Nicolas Reuge, Madhava Syamlal, C. Rossingol, J. Dexpert-ghys, Carole Coufort and Brigitte Caussat, Proceedings of the *French National Symposium on Powder Science and Technology*, Ecole des Mines d'Albi (France), 23 – 25 May, **2007**.

55. "Coarse-Graining of Two-Fluid Models for Fluidized Gas-Particle Suspensions," with Yesim Igci, Sankaran Sundaresan, Tom O'Brien and Ronald W Breault, Proceedings of the *Fifth International Conference on CFD in the Process Industries*, December, Melbourne, Australia, **2006**.

56. "Simulations of Spouted Bed Dynamics in the Context of Coating Nuclear Fuel Particles," with Dhanunjay Boyalakuntla, Charles E. A. Finney and C. Stuart Daw, Proceedings of the *Fifth World Congress in Particle Technology*, Orlando, April 23-27, **2006**.

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58. "Experiences with the "Open Source Model" for Disseminating Information in Computational Gas-Solids Flow," with Madhava Syamlal, Thomas O'Brien, Sofiane Benyahia and Aytekin Gel, Proceedings of the *Fifth World Congress in Particle Technology*, Orlando, April 23-27, **2006**.

59. "Particle-Impact Sensor for Determining Mass Flux in a Spouted Bed," with Charles E. A. Finney, Duane D. Bruns, Jiandong Zhou, Stuart C. Daw and J. M. Lipkowitz, Proceedings of the *Fifth World Congress in Particle Technology*, Orlando, April 23-27, **2006**.

60. "Comparison of Frameworks for Next Generation Multiphase Flow Solver, MFIX. A Group Decision-Making Multiphase Flow Solver," with A. Gel, M. Syamlal, T. J. O'Brien and E. S. Gel, *Compframe 2005 Workshop*, Atlanta, GA, **2005**.
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http://www.compframe.org/compframe2005/CompFrame05_Program/talks/gel.pdf)

61. "Simulations of Spouted Beds for Coating TRISO Fuel Particles," with D. Boyalakuntla, C. E. A. Finney, J. H. Miller, R. A. Lowden and C. S. Daw, *AIChE Annual Meeting*, November, **2005**.

62. "Simulating the Hydrodynamics of Spouted Beds Using a Continuum Formulation," with D. S. Boyalakuntla, C. E. A. Finney and C. S. Daw, *AIChE Annual Meeting*, November, **2005**.

63. "Hydrodynamic Correlations with Experimental Results from Cold Mockup Spouted Beds for Advanced Fuel Particle Coating," with J. Zhou, D. D. Bruns, C. E. A. Finney and C. S. Daw, *AIChE Annual Meeting*, November, **2005**.

64. "A Hybrid Lagrangian-Eulerian Approach in Simulating Gas-Solid Flows Consisting of Multiple Solid Phases," with S. Boyalakuntla, C. S. Daw, S. Benyahia, T. J. O'Brien, and M. Syamlal, *AIChE Annual Meeting*, November, **2005**.

65. "Computational validation of the Glicksman scaling laws using gas/solids fluidized bed simulations," with S. Benyahia, C. E. A. Finney, M. Syamlal, C. S. Daw, and T. J. O'Brien, *AIChE Annual Meeting*, November, **2005**.

66. "Open-Source Development of a Gas/Particle Flow Problem Solving Environment," with T. J. O'Brien, M. Syamlal, M. Prinkey, P. Nicolleti, A. Gel and S. Benyahia, *AIChE annual meeting*, Austin, TX, November 7-12, **2004**.

67. "Monte Carlo Method for LNT Aging," with W. A. Shelton and C. S. Daw, Poster at 7th CLEERS workshop, Detroit Diesel, Detroit, June 16-17, **2004**.

68. "Coated Particle Fuel for Advanced Gas Reactors," with R. Lowden, J. Hunn, J. McLaughlin, J. Kelly, C. S. Daw and C. E. A. Finney, Annual Meeting of the American Ceramic Society, Indianapolis, Indiana, April 21, **2004.**

69. "Multiscale Studies of Catalyst-Assisted Carbon Nanotube Growth," with J. C. Wells, B. Sumpter, Q. M. Zhang, J. Z. Zhang, R. F. Wood, *Artificially Structured Nanomaterials: Formation and Properties*, Gatlinburg, TN, USA, October 10-13, **2003**.

70. "Simulation of Gas-particle Flows in a Vertical Riser with a Square Cross Section," with T. O'Brien, A. T. Andrews and S. Sundaresan, *AIChE Annual Meeting*, San Francisco, CA, USA, November 16-21, **2003**.

71. "Simulations of Reacting Fluidized Beds Using an Agent Based Bubble Model," with C. S. Daw and J. S. Halow, *Chemical Reaction Engineering IX; Chemical Reactor Engineering - Meeting The Challenges For New Technology*, Quebec City, Quebec, Canada, June 29 - July 4, **2003**.

72. "Multiscale Simulations of Carbon Nanotube Nucleation and Growth: Continuum Calculations," with R. F. Wood, *Annual APS March Meeting 2003*, Austin, TX, March 3-7, **2003**.

73. "Multiscale Simulations of Carbon Nanotube Nucleation and Growth: Mesoscopic Continuum Calculations," with R. F. Wood, *NASA/Rice University Workshop on SWNT Growth Mechanisms*, Guadalupe River Ranch and Spa, Boerne, Texas, Feb. 28 - March 3, **2003**.

74. "Loosely Coupled Multiscale Modeling of Growth of Carbon Nanotubes," with R. F. Wood, B. Sumpter, D. Noid, J. C. Wells, Z. Zhang, *2003 SIAM Conference on Computational Science and Engineering*, San Diego, February 10-13, **2003**.

75. "Agent-Based Model for Bubbling Fluidized Beds," with C. S. Daw, and J. S. Halow, *2003 SIAM Conference on Computational Science and Engineering*, San Diego, February 10-13, **2003**.

76. "MFIX Simulations: Square CFB and ANL Flower Bed," ***Invited talk** at Second Workshop on Granular Flow and Kinetics*, Argonne National Laboratory, Argonne, Illinois, January 19-21, **2003**.

77. "Low-Order Bubble Dynamics Model for Gas-Fluidized Beds - A Case Study of Ozone Decomposition," with C. S. Daw and J. S. Halow, *7th Experimental Chaos Conference*, San Diego, Poster, August 25-29, **2002**.

78. "Near Real-Time Simulations of Fluidized Bed Reactors Using a Low-Order Bubble Model," with C. S. Daw and J. S. Halow, *GRC conference on Granular & Granular-Fluid Flow*, Holderness School, Plymouth, NH, Poster, June 30 - July 5, **2002**.

79. "MFIX - 3-D parallel multi-phase CFD code for Reacting Fluidized Beds," with T. O' Brien and M. Syamlal, *GRC conference on Granular & Granular-Fluid Flow*, Holderness School, Plymouth, NH, Poster, June 30 - July 5, **2002**.

80. "Near Real-time Simulations of Large Fluidized Beds with a Low Order Bubble Model," with C. S. Daw and J. S. Halow, Session 199b, *AIChE Annual Meeting*, Reno, Nevada, November 4-9, **2001**.

81. "Parallelization of MFIX: A Multiphase CFD Code for Modeling Fluidized Beds," with E. D'Azevedo, M. Syamlal, A. Gel, M. Prinkey, and T. O'Brien, Session CP15, *Tenth SIAM Conference on Parallel Processing for Scientific Community*, Portsmouth, Virginia, March 12-14, **2001**.

82. "Large-Eddy Simulation of Reacting Sprays," with W. J. Henry, W.-W. Kim and S. Menon, *3rd ASME/JSME Joint Fluids Engineering Conference,* San Francisco, California, July 18-23, **1999**.

83. "Parallel simulations of turbulent reacting sprays," with S. Menon, W.-W. Kim, V. K. Chakravarthy and W. J. Henry, *AIAA Plasmadynamics and Lasers Conference, 30th,* Norfolk, VA, AIAA Paper 99-3438, June 28-July 1, **1999**.

84. "On LEM/LES methodology for two-phase flows," with S. Menon, AIAA Paper No. 99-2209, *AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit, 35th,* Los Angeles, CA, June 20-24, **1999***.*

85. "Large-Eddy Simulation of Turbulent Fuel Sprays," with S. Menon, W.-W. Kim, V. K. Chakravarthy, and W. J. Henry, *1999 DoD High Performance Computing Modernization Program Conference,* Monterey, California, June 7-10, **1999**.

86. "Subgrid Combustion Simulations of Reacting Two-Phase Shear Layers," with S. Menon, AIAA Paper No. 98-3318, *34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit,* Cleveland, Ohio, July **1998**.

87. "Parallel Simulation of Turbulent Reacting Two-phase Flows," with S. Menon, W.-W. Kim, T. M. Smith and S. Arunajatesan, AIAA Paper No. 98-2928, *29th AIAA Plasma Dynamics and Lasers Conference,* Albuquerque, New Mexico, June **1998**.

88. "Parallel Simulations of Reacting Turbulent Two-Phase Flows," with S. Menon, S. Arunajatesan, W.-W. Kim and T. M. Smith, *DoD User Group Meeting,* Rice University, Houston, Texas, June **1998**.

89. "Large Eddy Simulations of Two-Phase Turbulent Flows," with S. Menon, AIAA Paper No. 98-0163, *36th AIAA Aerospace Sciences Meeting and Exhibit*, Reno Hilton, Reno, Nevada, January **1998**.

90. "Subgrid Two-phase Combustion Modeling for Large-Eddy," with S. Menon, *50th APS/DFD Meeting*, San Francisco, November **1997**.

91. "Subgrid Modeling of Unsteady Two-Phase Turbulent Flows," with S. Menon, AIAA Paper No. 97-3113, *33rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit*, Seattle, July **1997**.

92. "Numerical Design of a Liquid Fueled Combustor," with R.K. Thulasiram and S. Menon, AIAA Paper No. 97-3317, *33rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit*, Seattle, July **1997**.

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