

PSAAPII PUBLICATIONS REPORT — AUGUST 2018

## XPACC: The Center for Exascale Simulation of Plasma-Coupled Combustion



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This report provides a listing of XPACC publications (page 2) and presentations (page 10).

## XPACC Presentations

- [1] I. V. Adamovich. Energy conversion in transient molecular plasmas: implications for plasma flow control and plasma assisted combustion. Plenary lecture at the 13th International Conference on Flow Dynamics, October, Sendai, Japan, 2016.
- [2] I. V. Adamovich. Energy conversion in transient molecular plasmas: implications for plasma flow control and plasma assisted combustion. Seminar at Ohio University, November, 2016.
- [3] I. V. Adamovich. Electric field measurements in atmospheric pressure electric discharges. Seminar at King Abdullah University of Science and Technology (KAUST), Jeddah, Saudi Arabia, November, 2017.
- [4] I. V. Adamovich. Electric field measurements in nanosecond pulse discharges in air and in hydrogen flame. Invited lecture at 6th International Symposium on Jet Propulsion and Power Engineering, Beihang University, Beijing, China, October, 2017.
- [5] I. V. Adamovich. Electric field measurements in nanosecond pulse discharges in air and in hydrogen flame. Invited talk at 14th International Conference on Flow Dynamics, Sendai, Japan, November, 2017.
- [6] I. V. Adamovich. Electric field measurements in nanosecond pulse discharges in air over solid and liquid dielectric surfaces. Invited talk at the 70th Gaseous Electronics Conference, Pittsburgh, PA, November, 2017.
- [7] I. V. Adamovich. Electric field measurements in plasmas by ps four-wave mixing and by ps second harmonic generation. Invited lecture at Electrical Engineering Institute of Chinese Academy of Sciences, Beijing, China, October, 2017.
- [8] I. V. Adamovich. Electric field measurements in surface discharges in atmospheric air over solid and liquid dielectrics. invited talk at XXXIII International Conference on Phenomena in Ionized Gases (ICPIG) Estoril / Lisbon, 2017.
- [9] I. V. Adamovich. Energy conversion in transient molecular plasmas: implications for plasma assisted combustion. Invited lecture at King Abdulla University of Science and Technology (KAUST) Research Conference: New Combustion Concepts, Jeddah, Saudi Arabia, 2017.
- [10] I. V. Adamovich. Electric field measurements in atmospheric pressure electric discharges. seminar at Tsinghua University, Beijing, China, 2018.
- [11] M. Anderson, D. Bodony, A. Brooks, M. Campbell, M. Diener, C. Evans, J. Freund, B. Gropp, J. Kress, S. Garcia, J. Larson, C. Mikida, L. Olson, T. Prabhu, M. Smith, L. Spies, T. Teixeira, and S. White. Developing fast code through high-level annotations center for exascale simulation of plasma-coupled combustion. SIAM CSE, Atlanta, GA, February 2017.
- [12] N. N. Beams, L. Olson, and J. B. Freund. A scalable fast method for N-body problems based on exact finite element basis screen functions. SIAM Conference on Computational Science and Engineering (CSE15), 2015.
- [13] Natalie Beams, Jonathan Freund, and Luke Olson. A scalable fast method for n-body problems based on exact finite element basis screen functions, February 2015. SIAM Conference on Computational Science and Engineering (CSE15).

- [14] D. J. Bodony. Advances in SBP-SAT-based methods for the prediction and control of compressible turbulent flows. Linköping University, Sweden.
- [15] D. J. Bodony. Advances in SBP-SAT-based methods for the prediction and control of compressible turbulent flows. Institute for Sound and Vibration Research, University of Southampton, UK.
- [16] P. S. Boehm, B. M. Goldberg, I. V. Adamovich, W. R. Lempert, and U. Czarnetzki. Laser-spectroscopic electric field measurements in a surface hugging fast ionization wave in pure hydrogen. 8th International Workshop on Microplasmas, Newark, NJ, May 11-14, 2015.
- [17] A. Brooks, M. Snir, and W. Gropp. Pickpocket: A guided allocation and data movement tool. Advanced Simulation and Computing Principal Investigators Meeting, May 2018.
- [18] D. Buchta, J. Capecelatro, and J. B. Freund. Adjoint-based ignition sensitivity in turbulent combustion. APS Topical Group on Shock Compression of Condensed Matter, St. Louis, MO, 2017.
- [19] J. Capecelatro, D. Bodony, and J. B. Freund. An adjoint-based search method for an ignition threshold. WCCM 2016 — World Congress on Computational Mechanics, Seoul, Korea, 2016.
- [20] J. Capecelatro, D. J. Bodony, and J. B. Freund. Adjoint-based sensitivity of flames to ignition parameters in non-premixed shear-flow turbulence. APS Division of Fluid Dynamics Annual Meeting, 2016.
- [21] J. Capecelatro, D. J. Bodony, and J. B. Freund. Adjoint-informed ignition characterization. 24th International Conference on Theoretical and Applied Mechanics, Montreal, Canada, 2016.
- [22] J. Capecelatro, D. J. Bodony, and J. B. Freund. Adjoint-based sensitivity of ignition in high-speed turbulent flows. 23rd AIAA Computational Fluid Dynamics Conference, Denver, CO, 2017.
- [23] J. Capecelatro and J. B. Freund. Adjoint-based sensitivity of ignition in non-premixed turbulent flows. SIAM Conference on Numerical Combustion, Orlando, FL, April 2017.
- [24] J. Capecelatro, W. Zhang, R. Fontaine, G. S. Elliott, and J. B. Bodony, D. J. ant Freund. Bypass transition of low-speed boundary layers using realistic sandpaper roughness. 68th Annual Meeting of the APS Division of Fluid Dynamics, Boston, MA., 2015.
- [25] S. Chung, S. D. Bond, E. C. Cyr, and J. B. Freund. Sensitivity analysis in particle-in-cell methods. Sandia National Laboratory, Albuquerque, NM, March 2017.
- [26] S. Chung, R. Vishnampet, D. J. Bodony, and J. B. Freund. Adjoint-based sensitivity of jet noise to near-nozzle forcing. American Physical Society-Division of Fluids Dynamics, Annual Meeting, 2017.
- [27] E. Cisneros-Garibay, C. Pantano, and J. B. Freund. Bayesian analysis of constrained equilibrium reduced kinetics model parameterization. SIAM Conference on Numerical Combustion, Orlando, FL, April 2017.

- [28] Matthias Diener. Using OpenMP offloading in Charm++. 16th Annual Workshop on Charm++ and its Applications, April 2018.
- [29] G. S. Elliott. Designing experiments and laser diagnostics for validating computational models. Invited Talk, The Ohio State University, 2017.
- [30] G. Carl Evans. Vector Seeker: Finding vector potential. XPACC Deep Dive Presentation, February 2015.
- [31] J. B. Freund. XPACC: The center for exascale simulation of plasma-coupled combustion. AFOSR MURI Review: Fundamental Mechanisms, Predictive Modeling, and Novel Aerospace Applications of Plasma Assisted Combustion, Washington, DC, October 2013.
- [32] J. B. Freund. Adjoint-based sensitivity and jet noise. University of Wisconsin, Madison, Feb. 2015, 2015.
- [33] J. B. Freund. PSAAP2@Illinois: The center for exascale simulation of plasma-coupled combustion. Sandia National Lab, Jan. 2015, 2015.
- [34] J. B. Freund. PSAAP2@Illinois: The center for exascale simulation of plasma-coupled combustion. Los Alamos National Lab, Jan. 2015, 2015.
- [35] J. B. Freund. PSAAP2@Illinois: The center for exascale simulation of plasma-coupled combustion. Lawrence Livermore National Lab, March 2015, 2015.
- [36] J. B. Freund. The center for exascale simulation of plasma-coupled combustion. AFOSR Program Review, guest lecture, June 2016.
- [37] J. B. Freund. PSAAP2@Illinois: XPACC, and efforts on adjoint-based sensitivity. Los Alamos National Lab, December, 2016.
- [38] J. B. Freund. PSAAP2@Illinois: XPACC, and efforts on adjoint-based sensitivity. Lawrence Livermore National Lab, November, 2016.
- [39] J. B. Freund. PSAAP2@Illinois: XPACC, and efforts on adjoint-based sensitivity. Sandia National Lab, October, 2016.
- [40] J. B. Freund. Adjoint-based ignition sensitivity in turbulent combustion. Workshop on UQ and Data-Driven Modeling, Austin, TX, March, 2017.
- [41] J. B. Freund. PSAAP2@Illinois: The center for exascale simulation of plasma-coupled combustion. University of Minnesota, December 2017, 2017.
- [42] J. B. Freund and R. H. Ewoldt. Quantitative rheological model selection. APS DFD Annual Meeting, 2014.
- [43] J. B. Freund and R. H. Ewoldt. Rheological model selection: Bayesian assessment of good fits versus credible models. Society of Rheology Annual Meeting, Philadelphia, PA, 2014.
- [44] J. B. Freund and R. H. Ewoldt. Field sensitivity to rheological parameters. American Physical Society-Division of Fluids Dynamics, Annual Meeting, 2017.
- [45] Simon. Garcia De Gonzalo. Preliminary results for H-MxPA on compute interior derivatives. IMPACT Group meeting of May 5 , 2015.

- [46] B. Goldberg, I. Shkurenkov, I. Adamovich, and W. Lempert. Electric field measurements in a nanosecond pulse discharge by picosecond CARS / 4-wave mixing. 67th Gaseous Electronics Conference, November 2-7, 2014, Raleigh, NC, USA, 2015.
- [47] B. Goldberg, I. Shkurenkov, I. V. Adamovich, and W. R. Lempert. Electric field measurements in AC double dielectric barrier discharge overlapped with ns pulse discharge. 68th Gaseous Electronics Conference, October 12-16, 2015, Honolulu, HI, 2015.
- [48] H. T. Johnson, K. Das, and J. B. Freund. Molecular dynamics modeling of focused ion beam material removal. Université Grenoble-Alpes, Grenoble, France, 2015.
- [49] P. Kim, M. Panesi, and J. B. Freund. Adjoint-based sensitivity of jet noise to near-nozzle forcing. American Physical Society-Division of Fluids Dynamics, Annual Meeting, 2017.
- [50] A. Kloeckner. Loo.py: transformation-based code generation for GPUs and CPUs. ACM SIGPLAN International Workshop on Libraries, Languages, and Compilers for Array Programming (co-located with ACM PLDI), June 2014.
- [51] Andreas Kloeckner. Domain-specific languages to manycore and GPU: building high-performance tools with Python. International Conference on Python for Education and Scientific Computing (SciPy India), December 2015.
- [52] Andreas Kloeckner. Loo.py: From Fortran to performance via transformation and substitution rules. ACM SIGPLAN International Workshop on Libraries, Languages, and Compilers for Array Programming (co-located with ACM PLDI), June 2015.
- [53] Andreas Kloeckner. Don't implement: Declarative programming for PDE solvers, July 2016.
- [54] Andreas Kloeckner. High performance with Python: Architectures, approaches, and applications. 15th Annual Conference on Scientific Computing with Python (SciPy 2016), July 2016.
- [55] Andreas Kloeckner. Loopy: heterogeneous code generation for array computations. WEST, January 2016.
- [56] Andreas Kloeckner. Array program transformation with Loo.py by example: high-order finite elements. Third ACM SIGPLAN International Workshop on Libraries, Languages, and Compilers for Array Programming, June.
- [57] Andreas Kloeckner and Matt Wala. Heterogeneous high-order DG for hyperbolic PDEs: Methods and tools. International Workshop 'Fast High-Order Discontinuous Galerkin Methods for Future Architectures' (Sponsored by DFG Priority Programme 1648 SPPEXA), 2017.
- [58] Andreas Kloeckner and Matt Wala. User interfaces to performance: Kernel transformation with loopy. Dagstuhl Seminar 17431: 'Performance Portability in Extreme Scale Computing: Metrics, Challenges, Solutions', 2017.
- [59] J. L. Larson. 3-D sparse and stride-1 vectorized matrix-vector multiplication. Hwulgans archive of IMPACT Group meeting presentations, February 2015.

- [60] J. L. Larson. XPACC status update: 1) vector optimization of the SAT\_FAR\_FIELD path in NS\_BC with grid pencils, and 2) a ‘parallel profile’ of NS\_BC does not exist. IMPACT: Group Meeting Archive, Feb 2016.
- [61] K. Mackay, J. B. Freund, and H. T. Johnson. Hydrogen recombination rates on silica from atomic scale simulations. Materials Research Society, Boston, MA, November 2016.
- [62] K. K. Mackay, J. B. Freund, and H. T. Johnson. Hydrogen recombination rates on silica from reactive force fields and transition state theory. Materials Research Society Fall Meeting, Boston, 2016.
- [63] L. Massa and J. B. Freund. Fluid-plasma-combustion coupling effects on the ignition of a fuel jet. APS Division of Fluid Dynamics Annual Meeting, 2016.
- [64] M. Natarajan, J. B. Freund, and D. J. Bodony. Actuator and sensor placement for controlling high-speed jet noise. SIAM Conference on Computational Science and Engineering (CSE15), 2015.
- [65] M. Natarajan, J. B. Freund, and D. J. Bodony. Global-mode based linear feedback control of a supersonic jet for noise reduction. APS Division of Fluid Dynamics Annual Meeting, 2016.
- [66] M. Panesi. Construction of non-equilibrium hydrodynamics models for atmospheric entry plasmas. Pasadena, October 2015.
- [67] M. Panesi. NLTE radiative and collisional processes in high enthalpy flows. University of California, Los Angeles, August 2015.
- [68] M. Panesi. Non-equilibrium aerothermodynamics: Construction of non-equilibrium models. University of Queensland, Australia, June 2015.
- [69] M. Panesi. Non-equilibrium aerothermodynamics: Construction of non-equilibrium models. University of New South Wales, Canberra, Australia, June 2015.
- [70] M. Panesi. Reduced order models for dissociating and recombining flows. Texas A&M, College Station, TX, 2015.
- [71] C. Pantano. A novel application of flame hole dynamics to consistent turbulent non-premixed combustion modeling. NASA AMES, Moffett Field, CA, July 2013.
- [72] C. Pantano. XPACC: Computational modeling of plasma-coupled combustion. AFOSR MURI Review: Fundamental Mechanisms, Predictive Modeling, and Novel Aerospace Applications of Plasma Assisted Combustion, Washington, DC, October 2013.
- [73] C. Pantano. A novel application of flame hole dynamics to consistent turbulent nonpremixed combustion modeling. Sandia National Laboratory, Albuquerque, NM, February 2014.
- [74] C. Pantano. A novel application of flame hole dynamics to consistent turbulent non-premixed combustion modeling. California Institute of Technology, Pasadena, CA, January 2015.

- [75] P. Popov, D. Buchta, M. Anderson, and J. B. Freund. Ignition prediction in a hydrogen jet in turbulent crossflow by a laser-induced breakdown. American Physical Society-Division of Fluids Dynamics, Annual Meeting, 2017.
- [76] Tarun Prabhu and William Gropp. DAME: A runtime-compiled engine for derived datatypes. EuroMPI'15, Bordeaux, France, 2015.
- [77] A. Reisner, L. Olson, and J. D. Moulton. Improving the performance of line relaxation in boxmg. Copper Mountain Conference on Iterative Methods, March 2018.
- [78] A. Reisner, L. N. Olson, and J. D. Moulton. Preparing robust structured multigrid for exascale, 2017. Copper Mountain Conference on Multigrid Methods.
- [79] Andrew Reisner and Luke Olson. Multilevel solvers for high resolution electric field calculations, March 2015. Seventeenth Copper Mountain Conference on Multigrid Methods.
- [80] Andrew Reisner, Luke Olson, and David Moulton. Progress on improving the parallel scalability of BoxMG. Fourteenth Copper Mountain Conference on Iterative Methods, March 2016.
- [81] J. Retter. Behavior of a hydrogen-air dielectric-barrier-discharge burner. University of Illinois at Urbana-Champaign, Department of Mechanical Science and Engineering, Urbana, IL, November 2017.
- [82] Jonathan E. Retter, Nick Glumac, Gregory S. Elliott, and Sean P. Kearney. Spatially correlated temperature, oxygen, and fuel measurements in a plasma-assisted hydrogen diffusion flame by one-dimensional fs/ps rotational CARS imaging. Gordon Research Seminar on Laser Diagnostics in Combustion, 2017.
- [83] B. Shields. Adaptive numerical solution of advancing and retreating edge flames in a new configuration. SIAM Conference on Numerical Combustion, Orlando, FL, April 2017.
- [84] B. Shields, J. B. Freund, and C. Pantano. Numerical solution of an edge flame boundary value problem. APS Division of Fluid Dynamics Annual Meeting, 2016.
- [85] K. Tang, L. Massa, J. Wang, and J. B. Freund. A least-squares, adaptive uncertainty propagation approach for a plasma-coupled combustion system. WCCM 2016 — World Congress on Computational Mechanics, Seoul, Korea, 2016.
- [86] R. Vishnampet, D. J. Bodony, and J. B. Freund. An exact and dual-consistent formulation for high-order discretization of the compressible viscous flow equations. APS DFD Annual Meeting, 2014.
- [87] R. Vishnampet, D. J. Bodony, and J. B. Freund. An exact and consistent adjoint method for high-fidelity unsteady compressible flow simulations. SIAM Conference on Computational Science and Engineering (CSE15), 2015.
- [88] J. Wang, D. Buchta, and J. B. Freund. Vorticity generation and jetting caused by a laser-induced optical breakdown. American Physical Society-Division of Fluids Dynamics, Annual Meeting, 2017.
- [89] S. White. Introducing over-decomposition to existing applications: A case study with PlasComCM and Adaptive MPI. Charm++ Workshop, Urbana, IL, May 2015.

- [90] Sam White. Adaptive MPI: Overview and potential collaborations. The 5th Joint Laboratory on Extreme Scale Computing Workshop, Lyon, France, June 2016.
- [91] Sam White. Adaptive MPI: Overview and recent work. The 14th Annual Workshop on Charm++ and its Applications, Urbana, IL, April 2016.
- [92] Sam White. Charm++ and Adaptive MPI. The 2016 Workshop on Exascale Software Technologies, Albuquerque, NM, January 2016.
- [93] Z. Yin, C. Winters, V. Petrishchev, W. R. Lempert, and I. V. Adamovich. OH and H number density distributions in near-surface nanosecond pulse discharges at a liquid / vapor interface. 22nd International Symposium on Plasma Chemistry (ISPC), Antwerp, Belgium, 2015.
- [94] W. Zhang, J. L. Larson, D. J. Bodony, and L. A. Wilson. ECSS experience: Preparing a production MPI code for hybrid execution. National Science Foundation XSEDE[14] Conference, Atlanta, GA, July 2014.

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