Saurabh S. Sawant, Ph.D.

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Summary

- **Expertise in diverse modeling techniques as a researcher:**
  - Nonequilibrium Green's function method for quantum transport.
    (e.g. modeling multiple channeled carbon nanotube field effect transistors)
  - Direct Simulation Monte Carlo method for solving Boltzmann transport equation
    (e.g. modeling shock-wave/boundary-layer interactions, thermal protection materials)
  - FDTD method for solving Maxwell's equations (e.g. S-parameter of transmission lines)
  - Modal order reduction (e.g. proper orthogonal decomposition), linear stability analysis.
- **Experience as a research software engineer:** 10+ years of experience in developing scalable software using C++, MPI, and GPUs for diverse scientific applications:
  - Developed a GPU-accelerated open-source software for modeling nanomaterials during postdoctoral work using C++17, templates, AMReX library.
  - Developed C++11, MPI software for kinetic modeling of hypersonic flows during PhD. (largest simulation: 60b particles, 4.5b cells, 20k MPI ranks, million node-hours.)
  - Select parallelized algorithms: adaptive mesh refinement, space-filling curve, ray-tracing, cut-cell volume computation, tall-&-skinny QR factorization, Broyden's method, block-tridiagonal matrix inversion, cloud-in-cell.
  - Understanding of traditional software design patterns (certificate), CI/CD using GitHub Actions. Software blog on CUDA kernel optimization, advanced design patterns.
- **Contributions to collaborative, interdisciplinary projects for over 7 years.**
- **Effective communicator.** (See talk at CS postdoc symposium 2023)
- **Mentored students individually and served as a Teaching Assistant for 3 years.**

Education

Ph.D. (with emphasis on **Computational Science**) *May 2022*
Department of Aerospace Engineering, University of Illinois Urbana-Champaign
Thesis: **The development of kinetic models and simulation methods to study molecular fluctuations, modal response, and shock-laminar separation bubble instabilities**
Advisor: Professor Deborah A. Levin
Cumulative GPA: 3.76 on a scale of 4

M.S. (with emphasis on **Computational Science**) *Dec. 2015*
Department of Aerospace Engineering, University of Illinois Urbana-Champaign
Thesis: **Development of AMR octree Direct Simulation Monte Carlo (DSMC) approach for shock dominated flows.**
Advisor: Professor Deborah A. Levin
GPA: 3.87 on a scale of 4

B.E. *Aug. 2011*
Department of Mechanical Engineering, Vidyavardhini's College of Engineering & Tech., Mumbai University, India.
Thesis: **Efficiency analysis of Aerospike nozzles.**
Advisor: Professor Dipak Choudhary
Class: First Class

Research Experience

Postdoctoral Scholar *Jan. 2022- Present*
Center for Computational Sciences and Engineering (CCSE)
Applied Mathematics and Computational Research Division (AMCRD)
Lawrence Berkeley National Laboratory, Berkeley, CA-94709, USA.
Supervisor: Dr. Andrew Nonaka

I contributed to a DOE-funded project, "Codesign and Integration of Nanosensors on CMOS," where we developed a CMOS chip with nanoscale photon sensors made of carbon nanotubes functionalized with quantum dots. My role involved development of computational tools for nanoscale modeling of realistic CNTFET configurations and microscale modeling of transmission lines for electromagnetic wave propagation on the chip.

- **GPU-accelerated Quantum Transport for Modeling Nanomaterials.**
  - Developed a 3D open-source framework ELEQTRONeX (**ele**ctrostatic-**q**uantum **tr**ansport **m**odeling **of** **n**anomaterials at **ex**ascale), built using **the AMReX library, modern C++, templates, MPI, and GPU-acceleration**.
    https://github.com/AMReX-Microelectronics/ELEQTRONeX
  - Quantum transport is modeled using MPI/GPU-parallelized **nonequilibrium Green's function** (NEGF) method, and self-consistency is achieved using an MPI/GPU-parallelized **Broyden's modified second algorithm**.
  - Conducted weak-scaling studies up to **512 NVIDIA A100 GPUs on NERSC's Perlmutter**, and used the solver to model field effect transistors with multiple carbon nanotubes in a single simulation to study their cross-talk.
  - **Recent Talk** Sawant *et al.*, ***245th ECS Meeting***, *B03-091, 28th May, 2024.*
- **Characterization of microscale transmission lines using the FDTD method.**
  - Developed a workflow to compute scattering ($\boldsymbol{S}$) parameters for transmission lines, implemented it in the open-source FDTD Maxwell solver, ARTEMIS, conducted weak-scaling studies up to 2048 A100 GPUs on Perlmutter.

Graduate Research Assistant *Aug. 2014- Dec. 2021*
Department of Aerospace Engineering
University of Illinois Urbana-Champaign, Champaign, IL-61801, USA
Advisor: Professor Deborah Levin

During M.S. & Ph.D., I have contributed to multiple projects in the field of hypersonics, funded by AFOSR, ONR, DoD, and NASA. A brief overview of these is provided below.

- **Development of an exascale particle-based DSMC solver.**
  - Developed a 3-D DSMC solver, SUGAR (Scalable Unstructured Gas-dynamic Adaptive mesh-Refinement), using C++11 & MPI, with features including adaptive mesh refinement (**AMR**) for octree grids, **ray-tracing**, **3D embedded boundaries** with a robust cut-cell algorithm, Morton-based **space-filling-curve** approach for **load balancing**, techniques for reducing communication.
  - Achieved ideal **strong scaling speed-up up to 4096 processors and 87% weak scaling efficiency** for 8192 processors in hypersonic flow simulations with shocks requiring AMR depth of 4 and 24 billion particles.
  - Achieved many grants totalling over two million node-hours on supercomputers such as NSF's Bluewaters, TACC's Stampede2, FRONTERA.
- **Kinetic modeling of hypersonic shock-wave/boundary-layer interactions.**

- Conducted challenging 3D DSMC simulations of Mach 7 Shock-wave/Boundary-layer interactions that required **60 and 4.5 billion computational particles and adaptively refined computational cells, respectively, using 20k processors and over a million node-hours**.
- Employed MPI-parallelized data-driven techniques like **proper-orthogonal decomposition** for noise reduction and dominant mode extraction. Implemented parallel **tall-and-skinny QR** factorization. (see description)
- Investigated 3D linear instabilities within a laminar separation bubble coupled with separation and detached shocks. This required analysis of **many terabytes of data**.

- **Kinetic Study of Low-Frequency Fluctuations in One-Dimensional Shock.**
  - Studied shock fluctuations in argon, revealing two-order lower frequency variations compared to freestream, with consistent Strouhal numbers ($St = 0.002 - 0.02$) across Mach 2-10.
  - Developed Lotka-Volterra two-energy-bin model, attributing shock frequency differences to bimodal energy density functions.
  - Derived analytical formula for bimodal energy distribution as non-central chi-squared (NCCS) distributions, establishing semi-analytical model to predict shock fluctuation frequencies.

- **Modeling of multi-scale thermal response of an AVCOAT-like thermal protection system.**
  - Carried out DSMC simulations of gas transport through the microstructure of an AVCOAT-like ablative heatshield and computed permeability and tortuosity of the structure.
  - Developed a random walk model from stochastic differential equations for coupled convection, conduction, and radiation through the microstructure.
  - Studied the thermal response of AVCOAT material with spatially varying thermophysical properties at high temperatures using the loosely-coupled DSMC-random walk model and compared it with finite-volume approaches.

- **Modeling of shock-induced dust lifting.**
  - Implemented capability to model dust particles in the open-source FLASH solver, used to model charged particle-fluid interactions by a junior graduate student.

- **Development of a framework for stability analysis of internal shock structure.**
  - Formulated linear stability framework for studying modal analysis of planar shocks using Navier-Stokes equations as well as using more accurate Mott-Smith model to account for bimodality in shocks.
  - Solved generalized eigenvalue problem to predict modal response of 1-D shock structure against small-amplitude perturbations.

Achievements

Finalist for Research SLAM Talk Competition (LBNL) *2024*

Argonne Training Program on Extreme Scale Computing Certificate *2022*

FRONTERA Leadership Resource Allocation (over million node-hours) *2020-2022*

AE Outstanding Graduate Student Fellowship (UIUC) *2020*

MAVIS Future Faculty Fellows (MF3) Program (UIUC) *Fall 2019–2020*

Best Undergraduate Project *2011*

Teaching & Mentoring

Mentoring Experience during Postdoctoral Work *Summer 2024*
Student: Teo Lara, MIT (SULI Intern)
Project: Fast Self-Energy Calculations and Point Charge Implementation in ELEQTRONeX

Teaching Assistant during Graduate Studies
Department of Aerospace Engineering
University of Illinois Urbana-Champaign, Champaign, IL-61801, USA.

- **Incompressible Flows (AE 311)** *Spring 2020*
  Instructor: Professor Laura Villafane Roca
- **Aerospace Flight Mechanics (AE 202)** *Fall 2019*
  Instructor: Professor Huy Tran
- **Incompressible Flows (AE 311)** *Spring 2019*
  Instructor: Professor Theresa Saxton-Fox
- **Aerospace Propulsion (AE 433)** *Fall 2018*
  Instructor: Professor Joshua Rovey
- **Rocket Propulsion (AE 434)** *Spring 2018*
  Instructor: Professor Deborah Levin

Duties for last four TAs: Preparing homework and exam solutions, holding office hours, conducting python workshops, making sure that lectures are recorded for online students, and conducting lectures when instructor is traveling.

Journal Publications

Sawant, S. S., Léonard, F., Yao, J., & Nonaka, A. (Under review) **ELEQTRONeX: A GPU-Accelerated Exascale Framework for Non-Equilibrium Quantum Transport in Nanomaterials.** ***NPJ Computational Materials***. arXiv:2407.14633

Sawant, S. S., Yao, J., Jambunathan, R., & Nonaka, A. (2023) **Characterization of Transmission Lines in Microelectronic Circuits Using the ARTEMIS Solver.** ***IEEE Journal on Multiscale and Multiphysics Computational Techniques***, vol. 8, pp. 31-39. doi:10.1109/JMMCT.2022.3228281

Sawant, S. S., Theofilis, V., & Levin, D. A. (2022) **On the synchronisation of three-dimensional shock layer and laminar separation bubble instabilities in hypersonic flow over a double wedge.** ***Journal of Fluid Mechanics***, 941, A7. doi:10.1017/jfm.2022.276

Sawant, S. S., Levin, D. A., & Theofilis, V. (2022) **Analytical prediction of low-frequency fluctuations inside a one-dimensional shock.** ***Theoretical and Computational Fluid Dynamics.***, 36, 25-40. doi:10.1007/s00162-021-00589-5

Klothakis, A., Quintanilha, H., & Sawant S. S., Protopapadakis, E., Theofilis V., & Levin D. A. (2022) **Linear stability analysis of hypersonic boundary layers computed by a kinetic approach: a semi-infinite flat plate at $4.5 \leq M_\infty \leq 9$.** ***Theoretical and Computational Fluid Dynamics.***, 36, 117-139. doi:10.1007/s00162-021-00601-y

Sawant, S. S., Levin, D. A., & Theofilis, V. (2021) **A kinetic approach to studying low-frequency molecular fluctuations in a one-dimensional shock.** ***Physics of Fluids***, 33 (10), 104106. doi:10.1063/5.0065971

Marayikkottu, V. A., Sawant, S. S., & Levin, D. A. (2021) **Study of particle lifting**

mechanisms in an electrostatic discharge plasma. ***International Journal of Multiphase Flows***, 137, 103564. doi:10.1016/j.ijmultiphaseflow.2021.103564

Sawant, S. S., Rao, P., Harpale, A., Chew, H. B., & Levin, D. A. (2019) **Multi-scale thermal response modeling of an AVCOAT-like thermal protection material.** ***International Journal of Heat and Mass Transfer***, 133, 1176-1195. doi:10.1016/j.ijheatmasstransfer.2018.12.182

Harpale, A., Sawant, S. S., Kumar, R., Levin, D. A., & Chew, H. B. (2018) **Ablative thermal protection systems: Pyrolysis modeling by scale-bridging molecular dynamics.** ***Carbon***, 130, 315-324. doi:10.1016/j.carbon.2017.12.099

Sawant, S. S., Tumuklu, O., Jambunathan, R., & Levin, D. A. (2018) **Application of adaptively refined unstructured grids in DSMC to shock wave simulations.** ***Computers & Fluids***, 170, 197-212. doi:10.1016/j.compfluid.2018.04.026

Refereed Conference Proceedings

Sawant, S. S., Tumuklu, O., Theofilis, V., & Levin, D. A. (2022). **Linear Instability of Shock-Dominated Laminar Hypersonic Separated Flows. In: Sherwin, S., Schmid, P., Wu, X. (eds)** ***IUTAM Laminar-Turbulent Transition.*** IUTAM Bookseries, vol 38. Springer, Cham. doi:10.1007/978-3-030-67902-6_57

Select Talks

Sawant, S. S., Léonard F., Yao, J., & Nonaka, A. (2024). **GPU-Enabled Exascale Quantum Transport Modeling of Carbon Nanotube Devices.** ***245th ECS Meeting (B03-091), San Francisco, CA, USA.***

Sawant, S. S., Léonard F., Yao, J., & Nonaka, A. (2023). **A Coupled Electrostatic - Quantum Transport Framework for Exascale Systems.** ***Intl. Workshop on Comput. Nanotech. (IWCN), Barcelona, Spain.*** Abstract pg. 84-85.

Sawant, S. S., Yao, J., Jambunathan, R., Léonard F., & Nonaka, A. (2019). **A Highly Scalable NEGF Solver for Modeling Time-Dependent Quantum Transport in Nanomaterials.** ***The APS March Meeting 2023, Las Vegas, Nevada, USA***.

Sawant, S. S., Yao, J., Jambunathan, R., Léonard F., & Nonaka, A. (2019). **Multiscale Modeling of Carbon Nanotube Field Effect Transistors (CNTFETs) for Photodetection.** ***Fourth CS-Area Postdoc Symposium, Lawrence Berkeley National Laboratory, Berkeley, USA***. Video of the talk.

Sawant, S. S., Tumuklu, O., Theofilis, V., & Levin, D. A. (2019). **Linear instability of shock-dominated laminar hypersonic separated flows.**, ***IUTAM Symposium on Laminar-Turbulent Transition 2019, London, UK***.

Sawant, S. S., Rao, P., Harpale, A., Chew, H. B., & Levin, D. A. (2019). **Multi-scale thermal response modeling of an AVCOAT-like thermal protection material.**, ***11th Ablation Workshop, University of Minnesota, Minneapolis, MN***.

Rao, P., Sawant, S. S., Harpale, A., Chew, H. B., & Levin, D. A. (2017). **Hybrid Walker Approach to Conduction-Radiation Coupling in Micro-Scale Ablation Modeling**, ***9th Ablation Workshop, Montana State University, Bozeman, MT***.

Sawant, S. S., Jambunathan R., and & Levin, D. A. (2018). **Multi-scale Gas Dynamic and Thermal Response Modeling of Ablative Thermal Protection Systems**, ***31st Rarefied Gas Dynamics Conference, Glasgow, Scotland***.