

Sean L. Seyler

Curriculum Vitae

Education

- Dec 2017 **Ph.D., Physics**, Arizona State University, Tempe, AZ, GPA – 4.0.
Specialized in computational biophysics
- May 2012 **M.Eng., Engineering Physics**, Cornell University, Ithaca, NY, GPA – 4.19.
Specialized in magnetohydrodynamics simulation
- May 2011 **B.S., Engineering Physics**, Cornell University, Ithaca, NY, *Cum Laude*.
Minor in Applied Mathematics

Master of Engineering project

- Title *Modeling dynamic ionization and radiation transport in a numerical magnetohydrodynamic code*
- Supervisor Professor Bruce Kusse
- Description The aim of this project was to enhance a numerical Fortran code by adding radiation transport physics. The code, named PERSEUS (Physics of an Extended Relaxation System using an Efficient Upwind Scheme), is based on the extended magnetohydrodynamics (XMHD) model for simulating, in particular, high-energy-density and Hall plasmas. Radiative transport is modeled by hydrodynamic-like balance equations describing the flow of radiative energy and momentum; additionally, I implemented a dynamical model for the ionization state (originally a user-specified, static value in PERSEUS), which is necessary to accurately calculate radiative absorption and emission. I developed a modular approach so that the coupling of the radiative transport and dynamic ionization models to the rest of PERSEUS can be toggled easily. doi: 10.6084/m9.figshare.1619903

Publications

- 2017 Coudray, N., Seyler, S. L., Lasala, R., Zhang, Z., Clark, K. M., Dumont, M. E., Rohou, A., Beckstein, O. and Stokes, D. L. *Structure of the SLC4 transporter Bor1p in an inward-facing conformation*. Protein Science, **26**: 130–145. doi:10.1002/pro.3061 (2017).
- 2016 Gowers, R. J., Linke, M., Barnoud, J., Reddy, T. J. E., Melo, M. N., Seyler, S. L., Dotson, D. L., Domanski, J., Buchoux, S., Kenney, I. M., and Beckstein, O. *MDAnalysis: a Python package for the rapid analysis of molecular dynamics simulations*. Proc. of the 15th Python in Science Conf. (2016).

700 W University Dr Unit 117 – Tempe, AZ 85281 – USA

☎ +1 (607) 227 3374 • ✉ slseyler@asu.edu

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- 2015 Seyler, S. L., Kumar, A., Thorpe, M. F., and Beckstein, O. *Path Similarity Analysis: a Method for Quantifying Macromolecular Pathways*. PLoS Comput Biol. doi:10.1371/journal.pcbi.1004568 (2015). (see also: arXiv:1505.04807 [q-bio.QM])
- 2014 Seyler, S. L. and Beckstein, O. *Sampling large conformational transitions: adenylate kinase as a testing ground*. Mol. Simul. **40** (10-11), 855-877 (2014).

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Research Experience

- Jan 2018 – present **Postdoctoral researcher under Steve Pressé**, *Department of Physics, Arizona State University, Tempe, AZ.*
Studying the physical mechanisms underlying biological molecular motor function using numerical simulation combined with theoretical approaches.
- Fall 2016 – Fall 2017 **Blue Waters Graduate Fellowship Research**, *Department of Physics, Arizona State University, Tempe, AZ.*
Developing a hybrid atomistic-continuum simulation approach for biomolecular systems.
- Implementing a numerical model for fluctuating hydrodynamic equations and a compatible stochastic integration algorithm using a 3D Discontinuous Galerkin hydrodynamic Fortran simulation code (see HERMESHD on GitHub: <https://github.com/sseyler/HERMESHD>).
 - Exploring the feasibility and limitations of various hybrid atomistic-continuum coupling approaches/algorithms as applied to molecular dynamics (MD) simulations using common biomolecular force fields (e.g., CHARMM, AMBER, OPLS-AA).
 - Designing and implementing a numerical hybrid simulation scheme employing an appropriate MD engine for biomolecular simulation (e.g., NAMD, Gromacs, OpenMM) and the fluctuating hydrodynamics code; all-atom MD performed in a restricted subdomain—containing the solute and (some) explicit solvent—is coupled to the fluctuating hydrodynamics solver in the surrounding computational domain.
 - Studying the physics of solute-solvent interactions as applied to bio(macro)molecular solutes (polypeptides in particular) and water. Also interested in the general non-equilibrium behavior of fluctuating hydrodynamic systems, such as mass/momentum/energy transport in water-based electrolyte solutions.
 - An allocation on the Blue Waters supercomputer at the University of Illinois at Urbana-Champaign will be a central tool for accelerating the development and testing of the hybrid code (and its various components).
- Fall 2013 – Fall 2017 **Ph.D. Research**, *Department of Physics, Arizona State University, Tempe, AZ.*
Studying the protein structure-function connection using numerical simulation under Professor Oliver Beckstein.
- Studying the mechanisms and statistical physics of macromolecular conformational transitions
 - Developing computational methods that mitigate rare-event (macromolecular transition path) sampling problem.
 - Deploying path-sampling approaches to investigate kinetic transition pathways and aid free energy and rate calculations.
 - Mentoring an undergraduate (supervised by Dr. Beckstein) who is doing a research project on the atomistic and thermodynamic mechanisms driving the transport cycle of secondary active membrane transporter Mhp1 and the catalytic cycle of the enzyme adenylate kinase.

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Fall 2011 – **M.Eng. Research**, *Department of Applied and Engineering Physics, Cornell University*, Ithaca, NY.
Spring 2012

Research in computational magnetohydrodynamics and radiation transport under Professor Bruce Kusse.

- Studied basics of radiation hydrodynamics in the context of high-energy-density (HED) plasmas.
- Became proficient in using PERSEUS (Physics of an Extended-mhd Relaxation System using an Efficient Upwind Scheme), a numerical code used to simulate dense Z-pinch experiments in the Cornell Lab of Plasma Studies.
- Implemented a dynamic ionization state model for PERSEUS.
- Implemented a modular radiation transport model for PERSEUS.

Summer 2010 – **Undergraduate Research**, *Lab of Plasma Studies, Cornell University*, Ithaca, NY.

Winter 2012 Learned about GPU programming as applied to numerical simulation under Professor Pierre Gourdain.

- Learned basics of PERSEUS extended magnetohydrodynamics numerical simulation code.
- Studied basic principles of parallel computation, GPGPU programming, and CUDA Fortran.
- Modularized PERSEUS for task-parallelization using CUDA Fortran.

Summer 2009 – **Undergraduate Research**, *Department of Electrical and Computer Engineering, Cornell University*, Ithaca, NY.
Winter 2010

Studied basic scientific computing using Fortran under Professor Michael Kelley.

- Sorted and post-processed large data sets containing upper-atmospheric wind measurements.
- Developed working knowledge of Fortran and Mathematica for sorting and visualizing data.

Applied Skills

Programming Languages

Python	Experienced	<i>Regular use in research</i>
Fortran	Experienced	<i>Used in previous and some in current research with f2py</i>
Mathematica	Experienced	<i>Used in previous and some in current research</i>
Cython	Intermediate	<i>Used in research; self-taught</i>
C/C++	Intermediate	<i>One course and some research experience</i>
MATLAB	Intermediate	<i>Two undergraduate-level courses and research experience</i>
parallel prog.	Intermediate	<i>MPI, OpenMP, Python multiprocessing</i>
GPGPU prog.	Familiar	<i>CUDA/PyCUDA, OpenCL/PyOpenCL</i>
Java	Familiar	<i>Two undergraduate-level courses</i>

General Computing Skills

L ^A T _E X	Experienced	<i>Regular use in research</i>
Linux	Intermediate	<i>Regular use in research; building/install programs/modules</i>
Shell scripting	Intermediate	<i>Regular use in research</i>
Inkscape	Intermediate	<i>Regular use in figure-production in research</i>
GIMP	Familiar	<i>Occasional use in figure-production in research</i>
mencoder	Familiar	<i>Used in research to produce movies of simulations</i>

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Specialized Scientific Programming

VMD	Experienced	<i>Regular use in research</i>
Gromacs	Experienced	<i>Regular use in research</i>
NAMD	Experienced	<i>Regular use in research</i>
CHARMM	Experienced	<i>Regular use in research</i>
OpenMM	Familiar	<i>Occasional use in research</i>
supercomputing	Experienced	<i>Regular use in research; Stampede, Anton, Saguro</i>
Chimera	Basic	<i>Occasional use in research</i>

Presentations

- 2017 **Blue Waters Symposium 2017**, Sun River, OR, Talk: *Developing a Hybrid Atomistic-Continuum Method for Simulating Large-scale Heterogeneous Biomolecular Systems*. S. L. Seyler, C. E. Seyler and O. Beckstein, May 17, 2017.
- 2016 **60th Annual Meeting of the Biophysical Society**, Los Angeles, CA, Platform Presentation: *Quantifying Macromolecular Transition Paths with Path Similarity Analysis*. S. L. Seyler, T. Colburn, A. Kumar, M. F. Thorpe, and O. Beckstein, March 2, 2016.
- 2015 **2015 APS 4CS Meeting**, Tempe, AZ, Contributed Talk: *Path Similarity Analysis: a Method for Quantifying Macromolecular Pathways*. S. L. Seyler, A. Kumar, M. F. Thorpe, and O. Beckstein, October 17, 2015.
- BioPhest Meeting 2015**, Arizona State University, Tempe, AZ, Talk: *Path Similarity Analysis: a method for quantifying macromolecular transition pathways*. S.L. Seyler, A. Kumar, M.F. Thorpe, and O. Beckstein, May 2, 2015.
- 2014 **BioPhest Meeting 2014**, University of Arizona, Tucson, AZ, Talk: *Quantifying conformational transitions: an application to simulations of apo adenylate kinase*. S. L. Seyler, A. Kumar, M. F. Thorpe, and O. Beckstein, April 26, 2014.
- 2013 **Invited Seminar**, University of Pittsburgh, Department of Biological Sciences: *Quantifying conformational transitions*. S. L. Seyler, A. Kumar, M. F. Thorpe, and O. Beckstein, November 7, 2013.
- 2013 APS 4CS Meeting**, Denver, CO, Contributed Talk: *An approach to quantifying conformational transitions*. S. L. Seyler, A. Kumar, M. F. Thorpe, and O. Beckstein, October 18, 2013.
- BioPhest Meeting 2013**, Arizona State University, Tempe, AZ, Talk: *Quantifying conformational transitions*. S. L. Seyler and O. Beckstein, April 20, 2013.

Posters

- 2017 **Blue Waters Symposium 2017**, Sun River, OR, Poster: *Developing a Hybrid Atomistic-Continuum Method for Simulating Large-scale Heterogeneous Biomolecular Systems*. S. L. Seyler, C. E. Seyler and O. Beckstein, May 16, 2017.
- 2015 **APS March Meeting 2015**, San Antonio, TX, Poster: *Quantifying macromolecular conformational transition pathways*. S. L. Seyler, A. Kumar, M. F. Thorpe, and O. Beckstein, March 4, 2015.

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Awards

- Aug 2017 **Graduate Excellence Award**—*Arizona State University, College of Liberal Arts and Sciences, 2016–2017*. The college recognizes outstanding graduate students who have been nationally acknowledged through funded fellowships, scholarships, travel and meeting awards. Eligible students receive funds to advance their research and are recognized at an annual ceremony.
- Mar 2017 **GPSA Outstanding Research Award**—*Graduate & Professional Student Association, Arizona State University*.
- Oct 2016 **2016 CLAS Student Leader**—*Arizona State University, College of Liberal Arts and Sciences*.
- Apr 2016 **2016–2017 Blue Waters Graduate Fellowship**. Provides PhD students with a year of support, an allocation of up to 50,000 node-hours on the powerful Blue Waters petascale computing system, and funds for travel to a Blue Waters-sponsored symposium to present research progress and results.
- Apr 2016 **Molecular Imaging Corporation Endowment**—*Arizona State University, Department of Physics*.
- Feb 2016 **Education Committee Travel Award**—*Biophysical Society*. Awarded to help defray travel expenses to the Biophysical Society 60th Annual Meeting.
- Mar 2016 **Lindau Nobel Laureate Meeting Young Researcher**—*Council for the Lindau Nobel Laureate Meetings*.
- May 2015 **ASU Summer Graduate Fellowship**—*Arizona State University, Department of Physics*. Supports a PhD student to work on their research during the summer months and also provides additional flexibility to, for instance, attend conferences.
- Jan 2015 **Shirley Chan Student Travel Award**—*American Physical Society, Division of Biological Physics*.
- May 2014 **Wally Stoelzel Physics Fellowship**—*Arizona State University, Department of Physics*. The Stoelzel Physics Scholarships are awarded by Mr. Wally Stoelzel in honor of Professor Allen Wager, former chair of the Department of Physics, and Ms. Glenna Curtis, former department secretary.
- May 2012 **David Delano Clark Award**—*Cornell University, Department of Applied and Engineering Physics*. Awarded annually to a student in Engineering Physics for best M.Eng. project.
- May 2012 **Henri S. Sack Memorial Award**—*Cornell University, Department of Applied and Engineering Physics*. Awarded for top academic performance among Engineering Physics M.Eng. students.

Employment

Academic

- Spring 2014 **Teaching Assistant**, *Department of Physics, Arizona State University, Tempe, AZ*. Full TA for calculus-based electricity and magnetism course for engineers (PHY 131).
 - Taught five recitation classes and held weekly office hours;
 - Graded weekly recitation worksheets and four exams;
 - 20 hours weekly.

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- Fall 2012 **Teaching Assistant**, *Department of Physics, Arizona State University, Tempe, AZ.*
 Full TA for calculus-based electricity and magnetism course for engineers (PHY 131).
 - Taught five recitation classes and held weekly office hours;
 - Graded weekly recitation worksheets and four exams;
 - 20 hours weekly.
- Fall 2011 **Lab Teaching Assistant**, *Department of Applied and Engineering Physics, Cornell University, Ithaca, NY.*
 Part-time TA for a laboratory section in Computer Instrumentation Design (AEP 2640)
 - Assisted with equipment setup and provided student assistance;
 - 4 hours weekly.
- Fall 2010 **Teaching Assistant**, *Department of Applied and Engineering Physics, Cornell University, Ithaca, NY.*
 Grader for a course in Lasers and Photonics (AEP 110), an introductory course on the qualitative and basic quantitative aspects of lasers, photonics, and related optical phenomena
 - TA grader for homework and exams;
 - Responsible for implementing a satisfactory grading scheme;
 - 12 hours per week.

Vocational

- Fall 2013 – present **Private Tennis Instruction**, *Employer, Tempe, AZ.*
 General description no longer than 1–2 lines.
 - 5 hours weekly, private, semi-private, and group lessons
- Summer 2010 **Head Tennis Instructor**, *Ithaca Youth Bureau, Ithaca, NY.*
 General description no longer than 1–2 lines.
 - Head instructor of Ithaca Youth Bureau summer tennis camp
 - Worked with beginner to intermediate players from ages 5 to 17
 - 15 hours per week
- Summer 2009 **Head Tennis Coach**, *Ithaca Junior Team Tennis, Ithaca, NY.*
 General description no longer than 1–2 lines.
 - Coached a team of 12 kids (ages 13 -17) for the Junior Team Tennis league in Ithaca, NY
 - Ran weekday practices; put in 15 hours per week
 - Led team to second place finish in regional tournament held in Rochester, NY
- 2008 – 2010 **Front Desk Monitor/Instructor**, *Reis Tennis Center, Ithaca, NY.*
 General description no longer than 1–2 lines.
 - Was a full-time instructor for Cornell University Tennis Camp (summers of '08 – '10)
 - Instructed several 1-2 hour tennis clinics (players of all ages and abilities)
 - Currently fill in open hours as a desk monitor and occasionally work part-time weeks
- Summer 2006 **Construction volunteer**, *Community Recreation Center, Ithaca, NY.*
 General description no longer than 1–2 lines.
 - Worked several 7-10 hour weeks
 - Assisted with construction of new locker room for Ithaca High School Boys Varsity Hockey team
 - Did mostly construction labor - moving cinder blocks, concrete, sand, painting, furnishing

Notable Coursework

Graduate Courses

PHY 598 Simul. Approaches to Biophysics

PHY 531 Electrodynamics

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PHY 521	Classical & Continuum Mechanics	PHY 542	Topics in Biophysics
TAM 5780	Nonlinear Dynamics and Chaos	PHYS 6752	Quantum Mechanics I
TAM 6100	Methods of Applied Mathematics I	CHEM 7940	Quantum Mechanics II
TAM 6100	Methods of Applied Mathematics II	CHEM 7960	Statistical Mechanics
MAE 6010	Foundations of Fluid Mechanics I	PHYS 7653	Statistical Physics II
MAE 6020	Foundations of Fluid Mechanics II	ORIE 5600	Financial Engineering with Stochastic Calculus (audit)

Economics, Business, and Related Courses

ECON 2300	International Trade and Finance	AEM 3230	Managerial Accounting
ECON 3010	Intermediate Microeconomics	ORIE 3150	Financial & Managerial Accounting
ECON 3020	Intermediate Macroeconomics	CEE 3040	Uncertainty Analysis in Engineering
ECON 3670	Game Theoretic Methods	ENGRC 3500	Engineering Communications
AEM 2400	Marketing		

Extracurricular Interests and Achievements

- Tennis
 - o Member of the Cornell Club Tennis team for 3.5 years
 - o Member of the Arizona State Club Tennis team for 3.5 years; co-president ('14-'15 season), team captain (spring 2016)
 - o Captain of the Ithaca High School Varsity Tennis team (junior/senior, '06 and '07)
 - o Quarterfinalist in the 2007 NYSPHAA Championship Tournament held at Billie Jean King National Tennis Center in Flushing, NY

- Hockey
 - o Assistant captain of the Ithaca High School Boys Varsity Hockey team during senior year ('06-'07)
 - o State tournament MVP and a member of the IHS NYSPHAA State Championship team (2007)

- Cycling
 - o I enjoy both road biking and mountain biking for exercise and sport

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