Sean L. Seyler

Curriculum Vitae

Education

Dec 2017   **Ph.D., Physics**, *Arizona State University*, Tempe, AZ, *GPA – 4.0*.
Dissertation: *Computational Approaches to Simulation and Analysis of Large Conformational Transitions in Proteins*

May 2012   **M.Eng., Engineering Physics**, *Cornell University*, Ithaca, NY, *GPA – 4.19*.
Research project: *Modeling dynamic ionization and radiation transport in a numerical magnetohydrodynamic code*

May 2011   **B.S., Engineering Physics**, *Cornell University*, Ithaca, NY, *Cum Laude*.
Minor in Applied Mathematics

Research Experience

Jan 2018 – present   **Postdoctoral research scholar under Steve Pressé**, *Department of Physics, Arizona State University*, Tempe, AZ.
Unifying theoretical advances in nonequilibrium statistical physics with novel numerical methods to gain physical insight into nanoscale transport processes.

- Continuously developing a general numerical code for modeling generalized Langevin equations to study nonequilibrium transport (see current implementation of GLSimulator on BitBucket: `https://bitbucket.org/sseyler/glsimulator`)

- Applications to nanoscale transport, such as understanding molecular motor efficiency in the context of intracellular transport. I.e., how do enzymes and molecular motors leverage their aqueous environment to perform useful work?

- General interest in the theoretical connection between continuum and particle models, and how this relates to experimentally accessible observables.

Fall 2016 – Fall 2017   **Blue Waters Graduate Fellowship Research Project**, *Department of Physics, Arizona State University*, Tempe, AZ.
Developing a hybrid atomistic-continuum simulation approach for biomolecular systems.

- Implemented a numerical model for fluctuating hydrodynamics and a novel stochastic integration algorithm using a 3D Discontinuous Galerkin hydrodynamic Fortran simulation code (see HERMESHD on BitBucket: `https://bitbucket.org/sseyler/hermeshd`).

- Designed and implemented a numerical hybrid simulation scheme based on subdomain decomposition, using a continuum model of the solvent bath; employed the LAMMPS MD engine and the HERMESHD fluctuating hydrodynamics code.

- Applications to the physics of solute-solvent interactions between bio(macro)molecules (polypeptides in particular) and water.

- 50,000 node-hour allocation on the Blue Waters supercomputer at the University of Illinois at Urbana-Champaign; used for accelerating the development and testing of the hybrid code (and its various components).

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

- Studied the mechanisms and statistical physics of macromolecular conformational transitions
- Developed computational methods that mitigate rare-event (macromolecular transition path) sampling problem.
- Deployed path-sampling approaches to investigate kinetic transition pathways and aid free energy and rate calculations.
- Mentored 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.

Fall 2011 – Spring 2012	**M.Eng. Research**, *Department of Applied and Engineering Physics, Cornell University*, Ithaca, NY. 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 and Efficient Upwind Scheme), a numerical code used to simulate dense Z-pinch experiments in the Cornell Lab of Plasma Studies and the precursor to HERMESHD (HERMESHD on BitBucket: `https://bitbucket.org/sseyler/hermeshd`)
- Implemented a dynamic ionization state model for PERSEUS.
- Implemented a modular radiation transport model for PERSEUS.

Summer 2010 – Winter 2012	**Undergraduate Research**, *Lab of Plasma Studies, Cornell University*, Ithaca, NY. Studied applications of GPU programming to continuum numerical simulations 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 Fortran90 code for task-parallelization using CUDA Fortran.

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

Publications

2019 **SL Seyler** and S Pressé. Long-time persistence of hydrodynamic memory boosts microparticle transport. *Phys Rev Research*. Accepted for publication as a Rapid Communication (2019). Preprint available: arXiv:1906.04957 [physics.flu-dyn]

J Lee, **SL Seyler** and S Pressé. Hydrodynamic interaction facilitates the unsteady transport of two neighboring vesicles. *J Chem Phys*. **151**, 094108 (2019). doi:10.1063/1.5113880

2017 N Coudray, **SL Seyler**[*], R Lasala, Z Zhang, KM Clark, ME Dumont, A Rohou, O Beckstein and DL Stokes. Structure of the SLC4 transporter Bor1p in an inward-facing conformation. *Protein Sci*. **26**, 130–145 (2017). doi:10.1002/pro.3061. [*]First theorist on project

2016 RJ Gowers, M Linke, J Barnoud, TJE Reddy, MN Melo, **SL Seyler**, DL Dotson, J Domanski, S Buchoux, IM Kenney, and O Beckstein. MDAnalysis: a Python package for the rapid analysis of molecular dynamics simulations. *Proc of the 15th Python in Science Conf*. 102–109 (2016). doi:10.25080/majora-629e541a-00e

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DL Dotson, **SL Seyler**, M Linke, and O Beckstein. datreant: persistent, Pythonic trees for heterogeneous data. *Proc of the 15th Python in Science Conf.* 51–56 (2016). doi:10.25080/Majora-629e541a-007

2015 **SL Seyler**, A Kumar, MF Thorpe, and O Beckstein. Path Similarity Analysis: a Method for Quantifying Macromolecular Pathways. *PLoS Comput Biol.* **11**, e1004568 (2015). doi:10.1371/journal.pcbi.1004568

2014 **SL Seyler** and O Beckstein. Sampling large conformational transitions: adenylate kinase as a testing ground. *Mol Simul.* **40**, 10–11, 855-877 (2014). doi:10.1080/08927022.2014.919497

Fellowships, Scholarships, and Awards

2017 **College of Liberal Arts and Sciences Student Leader**—*Department of Physics, Arizona State University, College of Liberal Arts and Sciences (CLAS), Oct 2017*. The College of Liberal Arts and Sciences recognizes distinguished students throughout the College as CLAS Student Leaders.

Graduate Excellence Award—*Arizona State University, College of Liberal Arts and Sciences, Aug 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.

GPSA Outstanding Research Award—*Graduate & Professional Student Association, Arizona State University, Mar 2017*.

2016 **College of Liberal Arts and Sciences Student Leader**—*Department of Physics, Arizona State University, College of Liberal Arts and Sciences, Oct 2016*. The College of Liberal Arts and Sciences recognizes distinguished students throughout the College as CLAS Student Leaders.

Blue Waters Graduate Fellowship—*National Center for Supercomputing Applications, University of Illinois, Apr 2016*. 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.

Molecular Imaging Corporation Endowment—*Arizona State University, Department of Physics, Apr 2016*.

Education Committee Travel Award—*Biophysical Society, Feb 2016*. Awarded to help defray travel expenses to the Biophysical Society 60th Annual Meeting.

Lindau Nobel Laureate Meeting Young Researcher—*Council for the Lindau Nobel Laureate Meetings, Mar 2016*.

2015 **ASU Summer Graduate Fellowship**—*Arizona State University, Department of Physics, May 2015*. Supports a PhD student to work on their research during the summer months and also provides additional flexibility to, for instance, attend conferences.

Shirley Chan Student Travel Award—*American Physical Society, Division of Biological Physics, Jan 2015*.

2014 **Wally Stoelzel Physics Fellowship**—*Arizona State University, Department of Physics, May 2014*. 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.

2012 **David Delano Clark Award**—*Cornell University, Department of Applied and Engineering Physics, May 2012*. Awarded annually to a student in Engineering Physics for best M.Eng. project.

Henri S. Sack Memorial Award—*Cornell University, Department of Applied and Engineering Physics, May 2012*. Awarded for top academic performance among Engineering Physics M.Eng. students.

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Presentations

2019 **NCSA Blue Waters Symposium**, Sun River, OR, **Invited Talk**: *Hydrodynamics beyond Navier-Stokes: mass and energy transport in nanofluidic flows through the lens of the numerical model*. S. L. Seyler, June 3, 2019.

BioPhest Meeting, Arizona State University, Tempe, AZ, Talk: *Transport of sub-micron particles in liquids: hydrodynamic memory effects can boost efficiency*. S. L. Seyler and S. Pressé, March 30, 2019.

APS March Meeting, Boston, MA, Talk: *Hydrodynamic Brownian motion and nanoscale transport efficiency in liquids*. S. L. Seyler and S. Pressé, March 7, 2019.

2018 **APS March Meeting**, Los Angeles, CA, Talk: *Fluctuating Hydrodynamics in the 13-moment Approximation for Simulating Biomacromolecular Nanomachines*. S. L. Seyler, C. E. Seyler and O. Beckstein, March 8, 2018.

2017 **NCSA Blue Waters Symposium**, Sun River, OR, **Invited 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.

BioPhest Meeting, Arizona State University, Tempe, AZ, Talk: *Developing a hybrid atomistic-continuum method for simulating large-scale heterogeneous biomolecular systems* . S.L. Seyler, C. E. Seyler and O. Beckstein, April 22, 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 **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, 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**, 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.

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, Arizona State University, Tempe, AZ, Talk: *Quantifying conformational transitions*. S. L. Seyler and O. Beckstein, April 20, 2013.

Posters

2017 **NCSA Blue Waters Symposium**, 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**, 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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Activities, Initiatives, and Outreach

Ad hoc reviewer (journals)	Archives of Biochemistry and Biophysics (invited), Proteins (supervised), Journal of the American Chemical Society (supervised)
Mentor	Mentee: Mikayla Carlson (ASU biochemistry graduate student) – current – working on understanding hunting behavior and dynamics of Bdellivibrio, a predatory bacterium.
Mentor	Mentee: Taylor Colburn (ASU physics undergraduate in physics) – 2015 –2019 – helped develop Dynamic Importance Sampling MD as applied to explicit solvent MD simulations; testing its viability on the Mhp1 membrane transporter protein.
Member	American Physical Society (APS), Biophysical Society (BPS)

Applied Skills

Programming Languages

Python	Expert	*Regularly used in research*
Fortran	Expert	*Regularly used in research, including f2py*
Mathematica	Experienced	*Regularly used in research*
Cython	Proficient	*Regularly used in research*
C/C++	Competent	*Occasionally used in research*
MATLAB	Competent	*Occasionally used in research*
parallel prog.	Proficient	*Regular research use; MPI/mpi4py, OpenMP, Python multiprocessing*
GPGPU prog.	Competent	*Occasional research use; CUDA/PyCUDA, OpenCL/PyOpenCL*
Java	Familiar	*Two undergraduate-level courses*

Scientific Computing – general software

LaTeX	Proficient	*Regularly used in research*
Linux	Proficient	*Regularly used in research; building/install programs/modules*
Bash	Proficient	*Regularly used in research*
Inkscape	Competent	*Regularly used for publication-quality figures*
GIMP	Familiar	*Occasionally used for publication-quality figures*

Scientific Computing – specialized software

VMD	Proficient	*Regularly used in research*
Gromacs	Proficient	*Regularly used in research*
NAMD	Proficient	*Regularly used in research*
CHARMM	Proficient	*Regularly used in research*
OpenMM	Competent	*Occasionally used in research*
Chimera	Familiar	*Occasionally used in research*

Other 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).

- o Taught five recitation classes and held weekly office hours;
- o Graded weekly recitation worksheets and four exams;
- o 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)

- o Assisted with equipment setup and provided student assistance;
- o 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

- o TA grader for homework and exams;
- o Responsible for implementing a satisfactory grading scheme;
- o 12 hours per week.

Vocational

Fall 2013 – present	**Private Tennis Instruction**, *Self-employed*, Tempe, AZ. o 5 hours weekly, private, semi-private, and group lessons
Summer 2010	**Head Tennis Instructor**, *Ithaca Youth Bureau*, Ithaca, NY.

- o Head instructor of Ithaca Youth Bureau summer tennis camp
- o Worked with beginner to intermediate players from ages 5 to 17
- o 15 hours per week

Summer 2009	**Head Tennis Coach**, *Ithaca Junior Team Tennis*, Ithaca, NY.

- o Coached a team of 12 kids (ages 13 -17) for the Junior Team Tennis league in Ithaca, NY
- o Ran weekday practices; put in 15 hours per week
- o Led team to second place finish in regional tournament held in Rochester, NY

2008 – 2010	**Front Desk Monitor/Instructor**, *Reis Tennis Center*, Ithaca, NY.

- o Was a full-time instructor for Cornell University Tennis Camp (summers of '08 – '10)
- o Instructed several 1-2 hour tennis clinics (players of all ages and abilities)
- o Currently fill in open hours as a desk monitor and occasionally work part-time weeks

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Notable Coursework

Graduate Courses

PHY 598	Simul. Approaches to Biophysics	PHY 531	Electrodynamics
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

- Member of the Cornell Club Tennis team for 3.5 years

- Member of the Arizona State Club Tennis team for 3.5 years; co-president ('14–'15 season), team captain (spring 2016)

- Captain of the Ithaca High School Varsity Tennis team (junior/senior, '06 and '07)

- Quarterfinalist in the 2007 NYSPHAA Championship Tournament held at Billie Jean King National Tennis Center in Flushing, NY

Hockey

- Assistant captain of the Ithaca High School Boys Varsity Hockey team during senior year ('06–'07)

- State tournament MVP and a member of the IHS NYSPHAA State Championship team (2007)

Cycling

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

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