Benjamin R. Gilbert

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Professional Summary

Engineer and software developer with a background in scientific computing. Experience solving problems in diverse computational science settings enables the application of novel techniques across domains. Skilled in the design and management of exploratory multi-year projects requiring flexibility, self-assessment mechanisms, and documentation suitable for publication. Proficient in presenting technical material to audiences with varying subject-matter expertise.

Technical Skills

Programming : C/C++, Fortran, Python, MATLAB, SQL, Bash, CUDA, Emacs Lisp, Tcl, LaTeX, UML

Tools : Unix/Linux, AWS, SVN, Git, SSH, Docker, Apptainer, slurm, PBS, GDB, GNU-Make, cmake, MySQL, PlantUML

Software : matplotlib, numpy, scipy, pandas, PyTorch, OpenMP, OpenMPI, Boost, Kokkos, HDF5, BLAS/LAPACK, CVODES, LAMMPS, HOOMD-blue, VMD, AutoCAD, Ansys Fluent, FEniCS, biopython, MAFFT, Clustal, BLAST, bowtie2, deepTools, SAMtools

Theoretical Training : *Mathematics* — Probability Theory, Stochastic Processes, Information Theory, Numerical Analysis, Linear Algebra, ODEs, PDEs, Optimization Theory, Complex Analysis, Spectral Theory | *Science & Engineering* — Biophysics, Systems Biology, Bioinformatics, Equil. and Nonequil. Statistical Physics and Thermodynamics, Transport and Kinetic Theory, Quantum Mechanics, Fluid and Solid Mechanics, Dynamical Systems Theory

Experience

Graduate/Postdoctoral Research Assistant | *Luthey-Schulten Group*, Dept. of Chemistry at UIUC *Jan 2020 – present*

- Used GPU-accelerated, hybrid stochastic-deterministic methods (C++, CUDA, python) to simulate whole-cell models of bacteria that capture the reaction and diffusion of ∼10,000 biochemical components at the cell-scale.
- Developed and authored computational models (C++, fortran, python) of chromosomes in bacteria.
  * Continuum polymer model (C++) to simulate motion of chromosomes at 10 base-pair resolution.
    · Developed and documented script-based C++ program to enable a variety of simulation protocols.
    · Programmed new OpenMP-accelerated Brownian dynamics integrator called using C++-API of LAMMPS.
    · Created novel representation for the replication states of circular chromosomes using binary trees.
  * Lattice polymer model (fortran) to generate chromosome geometries using Monte Carlo methods.
  * Created tools (python, fortran) to analyze replication-dependent chromosome conformation capture maps.
- Assisted PI in preparation of grant materials to acquire $30M+ in federal funding: *NSF DBI 2243257* - $29.78M (campus pre-proposal, proposal, and site-visit) | *NSF MCB 2221237* - $2.00M (proposal, annual reports) | *NSF MCB 1818344* - $1.50M (annual reports) | *NSF MCB 1840320* - $1.18M (annual reports).
- Collaborated with industrial and academic partners, both domestic and international.
- Presented research results to broader scientific community at domestic and international conferences.
- Mentored junior graduate and undergraduate student researchers.

Graduate Teaching Assistant | *Statistical Thermodynamics*, Dept. of Chemistry at UIUC *Fall 2019, Fall 2020*

- Prepared course materials, graded, and hosted office hours (*rated as excellent by students)*.

Graduate Research Assistant | *Stephani Group*, Dept. of Mechanical Science and Engineering at UIUC *Aug 2017 – Jun 2019*

- Generated 250GB+ databases of collisional cross-sections for state-specific CO+O reaction chemistry during Martian atmospheric reentry by running quasi-classical trajectory simulations on cluster at NASA Ames.
- Developed workflow to validate and merge databases, then fit functional forms to cross-sections with weighted least-squares (fortran with LAPACK) for implementation in DSMC simulations of gas kinetics.

Mechanical Engineering Intern | Page Southerland Page, Inc. in Austin, TX *May 2016 – Aug 2016*

- Reviewed building MEP plans in AutoCAD and implemented archived mechanical equipment specifications in Revit.

Education

University of Illinois at Urbana-Champaign (UIUC)	**PhD in Chemistry**	*Jan 2020 – Aug 2024*
University of Illinois at Urbana-Champaign (UIUC)	**MS in Mechanical Engineering**	*Aug 2017 – Aug 2019*
Texas Tech University (TTU)	**BS in Mechanical Engineering**	*Aug 2013 – May 2017*

Selected Publications (0000-0002-9344-5521)

B. R. Gilbert, Z. R. Thornburg, T. A. Brier, J. A. Stevens, F. Grünewald, J. E. Stone, S. J. Marrink, Z. Luthey-Schulten, **Dynamics of Chromosome Organization in a Minimal Bacterial Cell**, *Frontiers in Cell and Developmental Biology 2023*

J. A. Stevens, F. Grünewald, P.A. Marco van Tilburg, M. König, B. R. Gilbert, T. A. Brier, Z. R. Thornburg, Z. Luthey-Schulten, S. J. Marrink, **Molecular Dynamics Simulation of an Entire Cell**, *Frontiers in Chemistry 2023*

Z. R. Thornburg, D. M. Bianchi, T. A. Brier, B. R. Gilbert, T. M. Earnest, M. C.R. Melo, N. Safronova, J. P. Sáenz, A. T. Cook, K. S. Wise, C. A. Hutchison III, H. O. Smith, J. I. Glass, Z. Luthey-Schulten, **Fundamental Behaviors Emerge from Simulations of a Living Minimal Cell**, *Cell 2022*

B. R. Gilbert, Z. R. Thornburg, V. Lam, F.-Z. M. Rashid, J. I. Glass, E. Villa, R. T. Dame, Z. Luthey-Schulten, **Generating Chromosome Geometries in a Minimal Cell from Cryo-Electron Tomograms and Chromosome Conformation Capture Maps**, *Frontiers in Molecular Biosciences 2021*