Mark Evan Fornace, PhD

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California Institute of Technology:
Postdoctoral scholar, Biology & Biological Engineering (1/22-)
Doctor of Philosophy, Chemistry (10/13-12/21. Cumulative GPA 4.1) Thesis: *Computational methods for simulating and parameterizing nucleic acid secondary structure thermodynamics and kinetics.*

Selected coursework: statistical physics, quantum chemistry, nuclear chemistry, thermodynamics of natural systems (also served as TA in quantum chemistry, introduction to bioengineering)

Projects:

- Unified dynamic programming framework for nucleic acid secondary structure analysis: recursions, evaluation algebras, operation orders (enhanced physical models [coaxial and dangle stacking], dramatic speedups [20-120x for test tube analysis], scalability [e.g., 30,000 nt complexes])
- Computational parametrization of equilibrium and kinetic nucleic acid secondary structure models via molecular dynamics simulation and Gaussian process regression (repeatable computational framework replacing patchwork multi-decade experimental parameterization process)
- Efficient stochastic algorithms for simulation of nucleic acid hybridization kinetics (complexity reduction, enabling simulation of systems of practical interest with order-of-magnitude speedups)
- Automated coarse-graining of nucleic acid hybridization kinetics for complex and test tube ensembles (automatic generation of low-dimensional kinetic models governing large molecular systems)
- Non-negative least squares algorithms for spectral unmixing of fluorescent images of mRNA expression with hybridization chain reaction (HCR) (enable robust multiplexed bioimaging using fluorophores with strongly overlapping excitation and emissions spectra)
- Convolution-based methods for single molecule dot detection and colocalization in images of fluorescent HCR expression (enable single-molecule imaging in whole-mount vertebrate embryos)
- Re-architecture, improvement, and cloud-based implementation of NUPACK, a growing software suite for the analysis and design of nucleic acid structures, devices, and systems (NUPACK web app (www.nupack.org) usage in 2021: 180,000 user sessions, 2,700,000 screen minutes, 3,500,000 page views)
- Embedded mean field theory for ab initio multiscale electronic structure calculations using density functional theory (DFT) (principled cost reduction by calculating energetic terms using different density functionals, basis sets, and Coulombic repulsion treatments)

University of Chicago:
Bachelor of Science in Chemistry (9/09-5/13. Cumulative GPA 3.74. Major GPA 3.84)
Bachelor of Science with Honors in Geophysical Sciences

Selected coursework: organic chemistry, physical chemistry, inorganic chemistry, computational chemistry, biological diversity, ecology and evolution, numerical analysis

Research experience:

- Pierce lab, Caltech (2015-, PI: Niles Pierce, PhD)
- Miller lab, Caltech (2013-2015, PI: Thomas F. Miller III, PhD)

- Origins lab, University of Chicago (2011-2013, PI: Nicolas Dauphas, PhD)
- Plasma mass spectrometry lab, University of Maryland (2011, PI: Bill McDonough, PhD)

Subject matter expertise:

- Computational biology: nucleic acid analysis and design, fluorescent image analysis
- Computational chemistry: statistical mechanics, molecular dynamics, electronic structure
- Machine learning: Markov chains, Gaussian processes, dynamic programming algorithms

Computational skills:

- Experienced programming in C++17 and Python 3; working knowledge of Docker, MPI, OpenMP, git, zsh/bash/csh, C, Fortran, Mathematica, MATLAB, LaTeX
- Past experience using Kubernetes, OpenStack, PBS-based clusters (government and academic), and AWS cloud computing services (EC2, CloudWatch, and S3)

Research artifacts:

- NUPACK 4 hybrid cloud web application (alpha.nupack.org)
- NUPACK 4 C++/Python module (nupack.org/downloads) with extensive user guide
- Public Github contributions: dask-jetstream XSEDE Jetstream scheduling using dask and Kubernetes, lilwil C++ unit testing framework

Publications:

- Fornace†, M. E., Gonzalvo i Ulla†, M., Cheng, L., Miller III, T. F., Pierce, N. A. (N.D.) Computational parameterization of equilibrium and kinetic nucleic acid secondary structure models. *In prep.*
- Fornace, M. E., Tao, D., Pierce, N. A. (N.D.) Efficient stochastic simulation of nucleic acid hybridization trajectories. *In prep*.
- Schulte, S. J., Fornace, M. E., Hall, J., Pierce, N. A. (N. D.) Spectral imaging of orthogonal hybridization chain reactions enables 10-plex quantitative RNA and protein imaging in thick autofluorescent samples. *In prep.*
- Fornace†, M. E., Huang†, J., Newman†, C. T., Porubsky, N. J., Pierce, M. B., Pierce, N. A. (2022) NUPACK: analysis and design of nucleic acid structures, devices, and systems. *ChemRxiv* 10.26434/chemrxiv-2022-xv98l.
- Fornace†, M. E., Porubsky†, N. J., & Pierce, N. A. (2020). A Unified Dynamic Programming Framework for the Analysis of Interacting Nucleic Acid Strands: Enhanced Models, Scalability, and Speed. *ACS Synthetic Biology*, *9*(10), 2665-2678.
- Choi, H. M., Schwarzkopf, M., Fornace, M. E., Acharya, A., Artavanis, G., Stegmaier, J., Cunha, A., & Pierce, N. A. (2018). Third-generation in situ hybridization chain reaction: multiplexed, quantitative, sensitive, versatile, robust. *Development*, *145*(12), dev165753.
- Fornace†, M. E., Lee†, J., Miyamoto†, K., Manby, F. R., & Miller III, T. F. (2015). Embedded mean-field theory. *Journal of chemical theory and computation*, *11*(2), 568-580.
- Heard, A., Dauphas, N., Hinz, I., Johnson, J., Blanchard, M., Alp, E., Hu, M., Zhao, J., Lavina, B., Fornace, M.E., Hu, J., Baptiste, B. (2022). Isotopic constraints on the nature of primary precipitates in Archean-early Paleoproterozoic iron formations from determinations of the iron phonon density of states of greenalite, and 2L- and 6L-ferrihydrite. *Submitted to ACS Earth and Space Chemistry.*
- Blanchard, M., Dauphas, N., Hu, M. Y., Roskosz, M., Alp, E. E., Golden, D. C., Sio, C. K., Tissot, F.L.H., Zhao, J., Gao, L., Morris, R. V., Fornace, M., Floris, A., Lazzeri, M., & Balan, E. (2015). Reduced partition function ratios of iron and oxygen in goethite. *Geochimica et Cosmochimica Acta*, *151*, 19-33.
- Dauphas, N., Kobayashi, H., Fornace, M., & Tang, H. (2013). Chronological and dynamical constraints on the accretion of Mars. In *Lunar and Planetary Science Conference* (No. 1719, p. 1305).

†Co-first authors.