Contact Dr. Lester Hedges

lester.hedges@gmail.com (510) 926-5040 Oakland, CA http://lesterhedges.net

Computational physicist with research interests in soft matter, materials science, algorithm development, and data visualization.

Education

9/2004–12/2007 University of Nottingham, UK

PhD in Physics. Thesis: "Aspects of Dynamic Heterogeneity in Models of Super-

cooled Liquids"

9/2000–7/2004 University of Nottingham, UK

MSci in Physics. First-class honors. Salmon prize for undergraduate research.

Experience

1/2010-present

Molecular Foundry, Lawrence Berkeley National Laboratory with Dr. Steve Whitelam Postdoctoral researcher.

- Developed simple model systems and adapted advanced sampling algorithms to study nucleation and self-assembly.
- Collaborated with experimentalists and theorists as part of the Center for Nanoscale Control of Geologic CO₂ (DOE EFRC).
- Ran large-scale Monte Carlo simulations on high-performance computing clusters.
- Defined project goals for and mentored 2 summer interns.

1/2008-12/2009

College of Chemistry, UC Berkeley with Prof. David Chandler

Postdoctoral researcher.

- Developed fast, robust, and versatile molecular dynamics software for model supercooled liquids (faster than a standard physics library for specialized uses).
- Implemented novel algorithms to selectively access rare jammed configurations.
- Created smoothed animations of particle motions to aid spatial reasoning.

9/2004-5/2007

School of Physics and Astronomy, University of Nottingham, UK

Programming instructor.

- ullet Supervised 3 hrs/wk of introductory MATLAB workshops for classes of \sim 40 first-year Physics undergraduates.
- Provided individual assistance with debugging and programming fundamentals.

Languages and Tools

code/HPC C/C++, bash/zsh, awk, git, SGE/PBS, MPI, CMake, Doxygen, screen/tmux, MAT-

LAB/Octave, Python

viz/animation MEncoder, FFMpeg, POV-Ray, ImageMagick, gnuplot, Grace, VMD, PostScript,

OpenGL, Keynote, LATEX

physics/modeling Metropolis Monte Carlo, molecular dynamics, rare event sampling, phase diagrams,

structural analysis, rejection-free Monte Carlo, coarse-grained modeling

web HTML, CSS

Journal Publications

13. Microscopic Evidence for Liquid-liquid Separation in Supersaturated CaCO₃ Solutions

A.F. Wallace, L.O. Hedges, A.J. Fernandez-Martinez, P. Raiteri, S, Whitelam, G.A. Waychunas, J.D Gale, J.F. Banfield, and J.J DeYoreo Science, **341** 885 (2013)

12. Selective nucleation in porous media

L.O. Hedges and S. Whitelam Soft Matter, doi:10.1039/c3sm51946e (2013)

11. Uncovering the intrinsic size dependence of hydriding phase transformations in nanocrystals

R. Bardhan, L.O. Hedges, C.L. Pint, A. Javey, S. Whitelam, and J.J Urban Nature Materials, doi:10.1038/nmat3716 (2013)

10. Self-assembly of multicomponent structures in and out of equilibrium

S. Whitelam, R. Schulman, and L.O. Hedges Phys. Rev. Lett. **109**, 265506 (2012)

9. Patterning a surface so as to speed nucleation from solution

L.O. Hedges and S. Whitelam Soft Matter, **8**, 8624 (2012)

8. Preparation and relaxation of very stable glassy states of a simulated liquid

R.L. Jack, L.O. Hedges, J.P. Garrahan, and D. Chandler Phys. Rev. Lett. **107**, 275702 (2011)

7. Excitations are localized and relaxation is hierarchical in glass-forming liquids

A.S. Keys, L.O. Hedges, R.L. Jack, J.P. Garrahan, S.C. Glotzer, and D. Chandler Phys. Rev. X. 1, 021013 (2011)

6. Limit of validity of Ostwald's rule of stages in a statistical mechanical model of crystallization

L.O. Hedges and S. Whitelam J. Chem. Phys. **135**, 164902 (2011)

5. Dynamic order-disorder in atomistic models of structural glass formers

L.O. Hedges, R.L. Jack, J.P. Garrahan, and D. Chandler Science, **323** 1309 (2009)

4. Dynamic facilitation explains democratic particle motion of metabasin transitions

L.O. Hedges and J.P. Garrahan J. Phys. A **41** 3244006 (2008)

3. De-coupling of exchange and persistence times in atomistic models of glass formers

L.O. Hedges, L. Maibaum, J.P. Garrahan, and D. Chandler J. Chem. Phys. **127**, 211101 (2007)

2. Dynamic propensity in a kinetically constrained lattice gas

L.O. Hedges and J.P. Garrahan

J. Phys.: Condens. Matter 19 3244006 (2007)

1. Fast simulation of facilitated spin models

D.J. Ashton, L.O. Hedges, and J.P. Garrahan

J. Stat. Mech. P12010 (2005)

Open Source Projects

TaskFarmer A tool for running serial jobs with mpirun on HPC clusters. [sole developer]

LaTuXiT A command-line tool for producing cropped LATEX equations for use in figures and

presentations. [sole developer]

rectify/flux Monte Carlo generative art from the command-line. [sole developer]

Scientific Artwork

• Cover art, Biophysical Journal 105 (5), 2013

• Cover art, *PNAS 106 (36), 2009*

• Using *PostScript* for scientific visualization

Selected Presentations

• Size-scaling behavior of hydriding phase transformations in nanocrystals APS March Meeting (2012)

- Understanding the microscopic origins of multi-stage nucleation
 Computational Molecular Biology Group: Free University, Berlin (2011)
- Limit of validity of Ostwald's rule of stages in a model of solution crystallization APS March Meeting (2011)
- Homogeneous and heterogeneous nucleation in the Ising model †
 Berkeley Mini Stat-Mech Meeting (2011)
- Non-classical assembly pathways of anisotropic particles †
 Crystallization: from colloids to pharmaceuticals. CECAM, Lausanne (2010)
- Structure and relaxation of ideal glass states †
 Berkeley Mini Stat-Mech Meeting (2010)

Links to visualizations, personal projects, and tutorials here.

September 10, 2013

[†] denotes poster presentation.