Contact

Dr. Lester Hedges
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I am a research software engineer with over 10 years of experience working in the field of statistical physics. I have interests in soft matter, materials science, algorithm development, and data visualisation.

Education

9/2004–12/2007 *University of Nottingham, UK*
PhD in Physics. Thesis: "Aspects of Dynamic Heterogeneity in Models of Supercooled Liquids"

9/2000–7/2004 *University of Nottingham, UK*
MSci in Physics. First-class honours. Salmon prize for undergraduate research.

Experience

8/2017– *Advanced Computing Research Centre with Dr. Christopher Woods*
Research software engineer
- Writing an interopability layer to enable robust and portable workflows for biomolecular simulation.

8/2015–8/2016 *Department of Physics, The University of Bath / School of Engineering, The University of Cardiff with Dr. Rob Jack and Dr. Alicia Kim*
Research officer
- Developed a theoretical and numerical methodology for a stochastic level-set method.
- Wrote a fast and flexible C++ library for level-set topology optimisation.

10/2014–4/2015 *Department of Physics, The University of Bath with Prof. Nigel Wilding*
Research officer
- Developed a C++ software library for the simulation of lock and key colloids.
- Implemented overlap finding algorithms and simple effective potentials for novel particle shapes.

1/2010–6/2014 *Molecular Foundry, Lawrence Berkeley National Laboratory with Dr. Steve Whitelam*
Postdoctoral researcher / Project scientist
- Developed model systems and advanced sampling algorithms to study nucleation and self-assembly.
- Worked as part of the Center for Nanoscale Control of Geologic CO_2 (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 specialised 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
- Supervised 3 hrs/wk of introductory MATLAB workshops for classes of ∼40 first-year Physics undergraduates.
- Provided individual assistance with debugging and programming fundamentals.

Languages and Tools

code/HPC	C/C++, Bash/Zsh, Awk, Git, CI (Travis), SGE/PBS/Slurm, MPI, Make/CMake, Doxygen, Screen/Tmux, MATLAB/Octave, Python
viz/animation	MEncoder, FFMpeg, POV-Ray, ImageMagick, Gnuplot, Grace, VMD, PostScript, OpenGL, Keynote, LaTeX
physics/modeling	Monte Carlo methods, molecular dynamics, finite-element method, level set method, rare event sampling, phase diagrams, structural analysis, overlap/collision detection, coarse-grained modeling
web	HTML, CSS

Journal Publications

17. *Stochastic level-set method for shape optimisation*
L.O. Hedges, R.L. Jack, and H. Alicia. Kim
J. Comp. Phys. **348**, 82–107 (2017)

16. *Crystallization and arrest mechanisms of model colloids*
T.K. Haxton, L.O. Hedges, and S. Whitelam
Soft Matter, **11**, 9307 (2015)

15. *Growth of equilibrium structures built from a large number of distinct component types*
L.O. Hedges, R.V. Mannige, and S. Whitelam
Soft Matter, **10**, 6404 (2014)

14. *Self-assembly at a nonequilibrium critical point*
S. Whitelam, L.O. Hedges, and J.D. Schmit,
Phys. Rev. Lett., **112** 155504 (2014)

13. *Microscopic evidence for liquid-liquid separation in supersaturated $CaCO_3$ 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, **9**, 9763 (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, **12**, 905 (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

LibVMMC	A C++ library to implement the "virtual-move" Monte Carlo algorithm for approximating the dynamical evolution of systems of strongly interacting overdamped particles. [sole developer]
LibSLSM	A C++ implementation of a stochastic level-set method. [sole developer]
AABB.cc	Dynamic AABB trees in C++. Adapted from parts of the *Box2D* physics engine. [sole developer]
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]
cxx-template	A simple template and build system for small C++ libraries. [sole developer]
rectify/flux	Monte Carlo generative art from the command-line. [sole developer]

Scientific Artwork

- Cover art, *Soft Matter 41, 9729-9948, 2013*
- Cover art, *Biophysical Journal 105 (5), 2013*
- Cover art, *PNAS 106 (36), 2009*
- Using *PostScript* for scientific visualisation

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)

† denotes poster presentation.

Other interests

3/2016–present *Bradford on Avon Community Agriculture*
Volunteer
- Helped plant, maintain, and harvest a wide range of organic fruit and vegetables.
- Co-organised several volunteer days and pick-your-own events.
- Designed and maintained the website, ran the news feed.

Links to visualizations, personal projects, and tutorials here.

August 12, 2017