Contact Dr. Lester Hedges

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http://lesterhedges.net

I am a computational physicist with research interests in soft matter, materials science, algorithm development, and data visualisation. I aim to exploit my training and expertise to solve complex data-driven problems.

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

8/2015-8/2016 Department of Physics, The University of Bath 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 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 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

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 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, 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)

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.

June 1, 2017

[†] denotes poster presentation.