Dmitri Schebarchov

Modeller. Scientist. Developer.

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All-round computational modeller with PhD in physics and extensive experience in simulation-based research, including methods development and data analysis. Thoughtful communicator with numerous peer-reviewed articles and teaching experience. Left academia for a fintech startup to model socio-economic systems, looking to explore the effects of market design and policy choices.

Experience

2019 – 23 *Senior Scientist @ Toha (www.toha.nz).*
Early full-time employee at Toha – NZ-based start-up building a platform for environmental impact accounting, reporting, and investing. Main responsibilities:
- Developing system dynamics- and agent-based simulation models in Python.
- Co-designing the tokenomics for Toha's potential adoption of blockchain tech.
- Monitoring and analysing "carbon" markets, including the NZ-ETS.
- Contributing to the writing and critical analysis of Toha's early business plans.

2018 – 19 *Postdoctoral Researcher @ Victoria University of Wellington, NZ.*
Project: Numerical modelling of light scattering by systems of particles.
- Engineered and implemented the core Fortran routines in the TERMS program.
- Co-developed software using F2Py, Python, Julia, and GitHub.
- Designed, delivered, and assessed 9 lectures on atomistic simulation (Phys343).

2013 – 17 *Postdoctoral Researcher @ The University of Cambridge, UK.*
Project: Theoretical structure prediction of nanoalloys for catalytic applications.
- Devised, implemented, and benchmarked cutting-edge optimisation algorithms.
- Contributed to the development of a globally-used software (GMIN, OPTIM).
- Supervised 3 student research projects and led multiple technical tutorials.

2010 – 12 *Postdoctoral Researcher @ Industrial Research Ltd, NZ.*
Several concurrent projects involving high-performance computing.
- Conducted large-scale simulations of confined fluid flow on BlueGene/L.
- Carried out electronic structure calculations using density functional theory.
- Analysed data and developed Fortran software for electronic structure analysis.

2004 – 06 *Summer internships @ Industrial Research Ltd, NZ.*
- Ran atomistic simulations on Linux-based clusters and analysed the data.
- Constructed simple thermodynamic models to explain simulation results.

Skills	Languages	Tools/Libraries
Modelling and simulation	Fortran,	Linux, Jupyter, Git, SVN, LaTeX,
Research software development	Python,	Quarto, Valgrind, NumPy, SciPy,
Data analysis and visualisation	Bash,	Matplotlib, Pandas, F2Py,
Critical and analytical thinking	Perl, Julia,	NetworkX, SQLite, LAPACK,
Technical and academic writing	Java, Tcl/Tk,	Octave/Matlab, VS Code,
Teaching and supervision	SQL.	Inkscape, LAMMPS, VASP.

Education

2007 – 10	PhD in Physics, Victoria University of Wellington, NZ. Thesis: *"Mechanisms in Carbon Nanotube Growth: Modelling and Molecular Dynamics Simulations."* - Implemented a parallelised molecular dynamics software in Fortran with MPI. - Implemented software for kinetic Monte Carlo simulation and structure analysis. - Completed 4 research projects, with two in the US on a Fulbright scholarship.
2006	BSc(Hons) First Class in Physics, VUW, NZ.
2002 – 05	BSc/BCA in Physics, Mathematics and Economics, VUW, NZ.

Awards

2012	RSNZ Hatherton Award - for best paper in physical sciences, earth sciences or mathematics and information sciences by a New Zealand University PhD.
2010	VUW PhD Completion Award.
2008	Fulbright Graduate Student Award.
2006	Mike Collins Scholarship and VUW Graduate Award.
2001	Ballinger Scholarship and Dux of Rongotai College.

Achievements

- Co-authored 34 peer-reviewed articles (24 as first-author) with overall H-index of 19 (on Google Scholar), including 4 *Phys. Rev. Lett.*, 3 *Nanoscale*, 1 *Nano Lett.*, and 1 *ACS Nano*.
- Presented 14 research talks (three by invitation) at academic conferences (12 international).
- Delivered tens of technical and non-technical seminars in academic institutions worldwide.
- Reviewed tens of research articles for reputable academic journals: *Phys. Rev. Lett.*, *Phys. Rev. E, Phys. Rev. Materials, Eur. Phys. Lett., J. Chem. Phys., J. Phys. Chem. Lett., J. Phys. Chem. C, Langmuir, J. Stat. Phys.*, etc.
- Co-developed the TERMS program (URL: https://nano-optics.ac.nz/terms/) and contributed to the Wales group software (URL: http://www-wales.ch.cam.ac.uk/software.html).
- MacDiarmid Young Scientist of the Year Award finalist in 2009.

Teaching and supervision

- Designed, delivered, and assessed a 9-lecture module titled "Atomistic modelling and simulation" for PHYS 343 at VUW in 2018.
- Co-supervised two graduate and three undergraduate student research projects, which led to four publications in leading peer-reviewed journals.
- Supervised 3rd year undergraduate students for theoretical chemistry courses in Cambridge: Theoretical Techniques (A4), Symmetry (B7), Statistical Mechanics (B6); 2015-17.
- Supervised 100-, 200-, and 300-level physics labs and marked assignments for 1st year math courses (calculus, linear algebra, and discrete mathematics) at VUW, 2004-07.

Media and outreach

- Ambassador for FutureInTech – a NZ Government-funded initiative to promote careers in technology, engineering and science. (2011-2012)
- "Modelling Carbon Nanotubes" on Our Changing World, Radio NZ, 2011. URL: http://www.radionz.co.nz/national/programmes/ourchangingworld/audio/2501131/modelling-carbon-nanotubes

Extended professional visits

Oct – Nov '15	Department of Mathematics, University of Tennessee, Knoxville. Developed locally exhaustive transition-state searching, with Prof. Tim Schulze.

Oct ‘12	Institute for Pure & Applied Mathematics (IPAM), University of California, Los Angeles. Participated in the programme “Materials Defects: Mathematics, Computation, and engineering”.
Jul ‘11	Institute of Scientific Computing, Technische Universität Dresden. Developed a Phase-Field Crystal model of fluid flow at a solid boundary for self-consistent prediction of slip, with Prof. Axel Voigt and Rainer Backofen.
Jan – Jun ‘09	Center of Integrated Nanomechanical Systems, University of California, Berkeley. Developed models for simulating nanotube cap lift-off, with Prof. Jeffrey Grossman and Dr. Elif Ertekin.
Aug – Dec ‘08	Department of Mathematics, University of Tennessee, Knoxville. Kinetic Monte Carlo simulation of crystal-melt interfaces, with Prof. Tim Schulze.

Referees (information available on request)