

Dmitri Schebarchov

Modeller. Analyst. 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 a track record in technical writing, presenting, teaching, and mentoring. Moved on from academia to a fintech startup developing market-based solutions to environmental and socio-economic problems.

Skillset

Modelling and computer simulation
Research software development
Data analysis and visualisation
Critical and analytical thinking
Technical writing and communication
Teaching, mentoring, and peer-review

Toolset

Python, Fortran, Bash, Linux command-line tools,
Perl, Julia, Java, Tcl/Tk, SQL, Octave/Matlab, Make.
NumPy, SciPy, Pandas, Matplotlib, Beautiful Soup,
NetworkX, F2Py, SQLite, BLAS/LAPACK.
GitHub, Google Docs/Sheets/Slides, LaTeX, Quarto,
VS Code, Obsidian, Inkscape, GIMP.

Experience

- 2019 – 23 *Senior Scientist @ Toha (www.toha.nz).*
Early full-time employee at Toha – fintech startup building a market-based system for environmental impact accounting, reporting, and investing. Main contributions:
- Developed agent-based models and system-dynamics simulations in Python.
- Deployed model demos and interactive analyses in Jupyter notebooks.
- Scraped data and monitored “carbon” markets, focusing on the NZ-ETS.
- Gathered market intelligence on cryptocurrencies and blockchain technology.
- Minted and transacted ERC-20 tokens on Ethereum’s Ropsten testnet.
- Wrote whitepapers and provided critical feedback on 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 core subroutines in the [TERMS](#) program.
- Wrote Python wrappers for Fortran subroutines using F2Py, and tried out Julia.
- 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 globally-used software ([GMIN](#), [OPTIM](#)).
- Supervised 3 student research projects and led multiple technical tutorials.
- 2010 – 12 *Postdoctoral Researcher @ Industrial Research Ltd, NZ.*
Pursued several concurrent projects involving high-performance computing.
- Conducted large-scale simulations of confined fluid flow on a supercomputer.
- Carried out quantum chemistry calculations using density functional theory.
- Developed code for “superatom” analysis and applied it on gigabytes of data.
- 2007 – 10 *PhD Student Researcher @ Victoria University of Wellington, NZ, and The MacDiarmid Institute for Advanced Materials and Nanotechnology.*
- Wrote a parallelised molecular dynamics code in Fortran and ran it on supercomputer.
- Implemented methods for analysing structure and dynamics of model nanoparticles.
- Built pipelines for data analysis and code compilation using shell-scripts and Make.
- Presented research outputs and published in leading peer-reviewed journals.

- 2004 – 06 *Summer Internships @ Industrial Research Ltd, NZ.*
- Ran atomistic simulations on a Linux cluster and analysed gigabytes of data.
- Constructed simpler mathematical models to explain simulation results.
- Used statistical methods to fit model parameters to simulation data.

Education

- 2007 – 10 PhD in Physics, Victoria University of Wellington, NZ. [Thesis: “Mechanisms in Carbon Nanotube Growth: Modelling and Molecular Dynamics Simulations.”](#)
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 15 research talks (three by invitation) at academic conferences (12 international).
- Delivered tens of technical and non-technical seminars in academic institutions worldwide.
- Tutored undergraduate students in physics and theoretical chemistry courses in NZ and UK.
- Co-supervised three undergraduate and two graduate students' research projects, which resulted in four peer-reviewed publications, three internal reports, and one MPhil thesis.
- Refereed tens of research articles for reputable academic journals, including *Phys. Rev. Lett.*
- MacDiarmid Young Scientist of the Year Award finalist in 2009.

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](#)

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)