

MACIEJ BUZE

Contact information

MARS: Mathematics for AI in Real-world Systems
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(last updated: July 2026)

SUMMARY

My research spans a wide range of topics at the intersection of **applied and computational mathematics** and **mathematical analysis** and is primarily inspired by **applications in materials science, physics and data science**. I use and develop tools in calculus of variations, bifurcation theory, numerical analysis, optimal transport, uncertainty quantification, approximation theory, scientific GPU computing, data analysis and machine learning. Current applications include atomistic modelling of matter with particular focus on crystalline materials, as well as bottom-up upscaling approaches to the modelling of plasticity, geometric modelling of microstructure in polycrystalline materials (with **industrial partner, Tata Steel**), quantifying uncertainties when modelling materials with machine-learning interatomic potentials, image processing and generation; barycentric data compression.

ACADEMIC APPOINTMENTS

Lancaster University, UK

- **Assistant Professor (Lecturer) in Mathematics and AI** **January 2025 – Present**
- A permanent post supported by a UKRI structural investment grant (E3: Expanding Excellence in England), awarded to establish a new applied mathematics and AI research group called MARS (Mathematics for AI in Real-world Systems).

Heriot-Watt University, UK

- **Visiting Assistant Professor** **August 2025 – Present**
- A honorary title in the School of Mathematical and Computer Sciences in recognition of my close research links with the School.

Heriot-Watt University, UK

- **Research Associate** **February 2023 – December 2024**
- A postdoctoral position at the School of Mathematical and Computer Sciences funded by EPSRC grant EP/V00204X/1 awarded to [Prof. Sir John Ball](#), [Dr David Bourne](#) and [Dr Lucia Scardia](#).

University of Birmingham, UK

- **Research Fellow** **February 2022 – January 2023**
- A postdoctoral position at the School of Mathematics funded by EPSRC grant EP/V038516/1 awarded to [Prof. Hong Duong](#).

Cardiff University, UK

- **Research Associate** **October 2019 – January 2022**
- A postdoctoral position at the School of Mathematics funded by EPSRC grant EP/S028870/1, awarded to [Prof. Angela Mihai](#).

EDUCATION

University of Warwick, UK

PhD in Mathematics and Statistics

October 2016 – January 2020

- Thesis advised by [Prof. Christoph Ortner](#) and [Dr Thomas Hudson](#).

University of Warwick, UK
MSc in Mathematics and Statistics
- Dissertation advisor: Prof. Christoph Ortner.

October 2015 - September 2016

University of Strathclyde, UK
BSc with Honours in Mathematics
- Dissertation advisor: Dr Andre Sonnet.

September 2011 - July 2015

PUBLICATIONS

12. D.P. Bourne, **M. Buze**, T. Gallouët, Q. Mérigot. (2026). *Polynomial diagrams for microstructure modelling*. Under review at Journal of Elasticity [[arXiv:2605.20816](#)].
11. F. Birks, I. Ghanem, L. Pastewka, J. Kermode, **M. Buze**. (2026). *Resolving Structural Avalanches in Amorphous Carbon with Arclength Continuation*. [Physical Review Letters](#), **136**, 206101.
10. J. Braun, **M. Buze**. (2025). *Incompleteness of Sinclair-type continuum flexible boundary conditions for atomistic fracture simulations*. [Multiscale Modeling & Simulation](#), **23**(2), 711-752.
9. **M. Buze** (2025). *Constrained Hellinger–Kantorovich Barycenters: Least-Cost Soft and Conic Multi-marginal Formulations*. [SIAM Journal on Mathematical Analysis](#), **57**(1), 495-519.
8. **M. Buze**, J. Feydy, K. Sedighiani, S.M. Roper, D.P. Bourne. (2024). *Anisotropic power diagrams for polycrystal modelling: Efficient generation of curved grains via optimal transport*. [Computational Materials Science](#), **245**, 113317. [[Python library PyAPD](#)].
7. **M. Buze**, M.H. Duong, (2023) *Entropic regularisation of unbalanced optimal transportation problems*, [[arXiv:2305.02410](#)].
6. **M. Buze**, T.E. Woolley, L.A. Mihai (2022). *A stochastic framework for atomistic fracture*, [SIAM Journal on Applied Mathematics](#), **82**(2):526–548.
5. **M. Buze** (2021). *Atomistic modelling of near-crack-tip plasticity*, [Nonlinearity](#), **34**(7):4503–4542.
4. **M. Buze**, J.R. Kermode (2021). *Numerical-continuation-enhanced flexible boundary condition scheme applied to mode-I and mode-III fracture*, [Physical Review E](#), **103**(3):033002.
3. **M. Buze**, T. Hudson, C. Ortner (2020). *Analysis of cell size effects in atomistic crack propagation*, [ESAIM: Mathematical Modelling and Numerical Analysis](#), **54**(6):1821–1847.
2. **M. Buze**, T. Hudson, C. Ortner (2019). *Analysis of an atomistic model for anti-plane fracture*, [Mathematical Models and Methods in Applied Sciences](#), **29**(13):2469–2521.
1. J. Braun, **M. Buze**, C. Ortner (2019). *The effect of crystal symmetries on the locality of screw dislocation cores*, [SIAM Journal on Mathematical Analysis](#), **51**(2):1108–1136.

MISCELLANEOUS

- S. Bagchi, I. Baghishov, **M. Buze**, et al (2023). *New Mathematics for the Exascale: Applications to Materials Science*. [White paper](#), Institute for Pure and Applied Mathematics, UCLA.

FUNDING

Workshop: Data-driven modelling of metallic materials across scales **6–8 May 2026**
Lancaster University, UK

Funding from (i) Lancaster Data Science and AI Institute: £5,000, (ii) MARS: £1,700.

Workshop: Computational Materials Science and Mathematics **10-14 November 2025**
at the Particle and Atomistic Scales, ICMS, Edinburgh, UK

Funding from (i) ICMS: £24,000, (ii) Edinburgh Mathematical Society: £3,000, (iii) Glasgow Mathematical Journal Trust: £2,000, (iv) MARS: £1,000.

Visiting Fellowship at Isaac Newton Institute
for Mathematical Sciences (INI), Cambridge, UK

10 July 2023 – 1 September 2023

Funding from INI: £3,000

Visiting Fellowship at the Institute for Pure and Applied Mathematics (IPAM), UCLA, Los Angeles, USA
Funding from IPAM: £12,000

13 March – 16 June 2023

Kanazawa University (KU) Visiting Scholarship, Japan
Funding from KU: £1,000

13 June – 19 July 2019

PHD STUDENT SUPERVISION

Catherine Needham (Lancaster, co-supervisor)

October 2026 - present

Tentative thesis title: *Machine learning for the quantum description of lanthanide and minor actinide chemistry.*

Funded by the Faculty of Science and Technology PhD in Natural Sciences competition.

Menna Shirras (Lancaster, co-supervisor)

October 2026 - present

Tentative thesis title: *Machine learning for the quantum description of uranyl chemistry.*

Funded by a competitive NDA grant (£82,334) with matched funding from the Saturn CDT (~£90,000).

Dawid Lipinski (Lancaster, main supervisor)

October 2025 - present

Tentative thesis title: *Optimal transport techniques in natural sciences and machine learning.*

Funding from MARS structural grant from UKRI.

Inayat Ullah (Lancaster, main supervisor)

October 2025 - present

Tentative thesis title: *Homotopy continuation methods in atomistic modelling of matter.*

Funding from MARS structural grant from UKRI.

Fraser Birks (Warwick, external co-supervisor)

October 2022 – Present

Tentative thesis title: *How amorphous carbon breaks: atomistic models and machine learning*

Funding from EPSRC CDT in Modelling of Heterogeneous Systems - HetSys

TEACHING

Lecturer for **MATH115: Geometry and Calculus**

2025/2026

Lancaster University, UK

Curriculum development for **BSc Hons in Mathematics, Artificial Intelligence, and Real-world Systems (MARS)** (new programme to start in 2026/2027)

2025/2026

Lancaster University, UK

Lecturer for **MATH400: Statistics in Practice**

2025/2026

Lancaster University, UK

Summer School on Deep Learning for Mathematical Imaging
University of Liverpool, UK

July 2024 & July 2025

Lecturer for **F17XB Mathematics for Engineers and Scientists 2**

2023/2024

Heriot-Watt University, UK

CONFERENCES

PAST INVITED TALKS (39 IN TOTAL, 10 IN THE LAST YEAR)

- Workshop: Data-driven modelling of metallic materials across scales
Lancaster University, UK (organiser) 6–8 May 2026
- Interface of Mathematics and ML for Applications in Material Science
University of Glasgow, UK 30 March 2026
- Warwick Maths and Metals Meeting: a Future Leader's Fellowship Finale
University of Warwick, UK 23–27 March 2026
- Dagstuhl Seminar: Generalized Voronoi Diagrams and Applications, Germany 1–5 December 2025

- Applied Maths Seminar, University of Warwick, UK 21 November 2025
- Computational Materials Science and Mathematics
at the Particle and Atomistic Scales, ICMS, Edinburgh, UK 10-14 November 2025
- Joint MARS & Pioneer Centre for AI workshop, Copenhagen, Denmark 6-7 October 2025
- MARS Launch Event: a talk and chairing a panel discussion
Lancaster University, UK 16 September 2025
- The Third Joint SIAM/CAIMS Annual Meetings, Montreal, Canada July 28 - 1 August 2025
- British Maths & Applied Maths Colloquium, University of Exeter, UK 23-26 June 2025
- Lancaster AI Reading Group, Lancaster University, UK 21 May 2025
- Oberwolfach Workshop: Singularities in Discrete Systems, Germany 4-9 May 2025
- Condensed Matter Physics Seminar, Lancaster University, UK 11 April 2025
- Kanazawa University Analysis Seminar, Japan 18 December 2024
- New Math for the Exascale: Appl. to Materials Science Reunion Conference, LA 8-13 December 2024
- Multiscale Mechanics and Artificial Microstructures, ICMS, Edinburgh, UK 2-3 December 2024
- Scottish-Basque Meeting on Analysis, ICMS, Edinburgh, UK 28-30 October 2024
- Seminar at Laboratoire d'informatique Gaspard Monge, Université Gustave Eiffel, Paris 26 June 2024
- Maxwell Analysis Day, ICMS, Edinburgh, UK (organiser on behalf of Heriot-Watt) 27 March 2024
- Workshop on Optimal Transport: from Theory to Applications
Humboldt University of Berlin, Germany (contributed presentation) 11-15 March 2024
- Centre for Mathematical Imaging Techniques Seminar, University of Liverpool, UK 28 February 2024
- Analysis Seminar, University of Strathclyde, UK 5 December 2023
- Workshop on Polycrystals, ICMS, Edinburgh, UK 27 October 2023
- Applied Maths Seminar, University of Glasgow, UK 19 October 2023
- Joint Edinburgh–Heriot-Watt Applied and Computational Maths Seminar, UK 4 October 2023
- Seminar talk at Newton Institute during my fellowship (see Funding), Cambridge, UK 26 July 2023
- Three seminar talks at IPAM during my fellowship (see Funding), UCLA, USA March-June 2023
- Workshop on Increasing the Length, Time, and Accuracy of Materials Modeling
Using Exascale Computing, IPAM, UCLA, USA 31 March 2023
- Numerical Analysis and Scientific Computation Seminar, Besançon, France 8 November 2022
- Applied Maths Seminar, University of Warwick, UK 28 October 2022
- Computational Methods in Applied Mathematics, TU Wien, Austria 29 August - 2 September 2022
Minisymposium: Multiscale methods for materials and molecules
- Error control in first-principles modelling, CECAM, Lausanne, Switzerland 20-24 June 2022
- Applied Maths Seminar, University of Birmingham, UK 12 February 2022
- Fluids and Materials Seminar, University of Bristol, UK 3 February 2022
- Warwick – Jiao Tong Workshop: QM/MM Methods and Other Multiscale
Boundary Conditions for Atomistic Material Simulation, online 22 June 2020
- Applied and Computational Maths Seminar, Cardiff University, UK 29 October 2019
- CoMFoS19: Mathematical Aspects of Continuum Mechanics, Kanazawa, Japan 15-16 July 2019
- Colloquium, Faculty of Mathematics and Physics, Kanazawa University, Japan 17 June 2019
- SIAM Conference on Computational Science and Engineering 25 February – 1 March 2019
Spokane, USA. Minisymposium: Multiphysics and Multiscale Problems in Comp. Science and Eng.
- The 12th AIMS Conference on Dynamical Systems, Differential Equations and
Applications, Taipei, Taiwan. Special Session: Mathematics and Materials: Models and Applications. 5-9 July 2018

PROFESSIONAL MEMBERSHIPS

- Edinburgh Mathematical Society
- Lancaster Data Science and AI Institute (DSAIL)
- Society for Industrial and Applied Mathematics (SIAM)