Nicolas Boullé

Department of Mathematics
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Research interests

Numerical analysis, machine learning, operator learning

Employment

2024-date	**Assistant Professor in Applied Mathematics**, Imperial College London, UK. Department of Mathematics.
2022-2024	**Research Fellow**, University of Cambridge, UK. Isaac Newton Institute and Department of Applied Maths and Theoretical Physics.

Education

2018-2022	**DPhil in Numerical Analysis**, University of Oxford, UK. Supervised by Prof. Patrick Farrell and Prof. Alex Townsend.
2017-2018	**Visiting Research Student**, Cornell University, USA. Supervised by Prof. Alex Townsend.
2015-2017	**BSc and 1st year of MSc in Mathematics**, ENS Rennes, France.
2013-2015	**University foundation course in Mathematics**, Lycée Saint-Louis, France.

Research prizes

2024	**SIAM Activity Group on Linear Algebra Best Paper Prize**
2023	**IMA Lighthill-Thwaites Prize**, 2nd place.
2022	**STEM for Britain**, finalist.
2021	**IMA Leslie Fox Prize for Numerical Analysis**, 2nd prize.
2021	**G-Research PhD Prize**, 2nd place (£5000).

Research grants and fellowships

2026	**AIRR Compute opportunity: AI for Science**, UKRI, 200k GPU hours, Co-I.
2023-2028	**Scientific Artificial Intelligence (SciAI) Center**, Office of Naval Research, $11.3m, Imperial PI, personal support: $485k.
2022-2023	**INI-Simons Postdoctoral Research Fellowship**, Simons Foundation.

Research supervision

PhD students:

- Gustav Conradie (Cambridge, with Matthew Colbrook), 2024-date.

- Kelan Gray (Imperial, with Matthew Colbrook), 2025-date.

- Jack Ross (Imperial, with Martin Rasmussen), 2025-date.

- Oussama Zekri (ENSAE Paris, with Anna Korba), 2025-date.

PhD graduates:

- Christina Runkel (Cambridge, with Carola Schönlieb), 2021-2025.

Undergraduate and MSc students: 18 undergraduate research projects or MSc dissertations at Imperial College London, University of Cambridge, University of Oxford, and Cornell University.

Teaching

2025-date	**Lecturer for Mathematical Foundations of Machine Learning**, Imperial College London.
2025	**Lecturer for Finite Element**, AIMS Rwanda.
2019-2021	**TA/Tutor for Approximation of functions**, University of Oxford.
2019	**TA for Practical Numerical Analysis**, University of Oxford.

Professional activities

2025-date	**Editorial Board**, Numerical Functional Analysis and Optimisation.
2025-date	**Co-organizer of the Imperial-UCL CCMI seminar**
2026	**Scientific Committee**, 5th IMA Conference on Inverse Problems from Theory to Application
2025	**Program Committee**, International Conference on Scale Space and Variational Methods in Computer Vision 2025.
2024	**Co-organizer of a minisymposium**, SIAM Conference on Applied Linear Algebra Title: Operator Learning and Linear Algebra.
2023-2024	**Co-organizer of the Cambridge ACA seminar**
2023	**Co-organizer of a minisymposium**, 93rd GAMM Annual Meeting Title: Randomized algorithms in numerical linear algebra.
2021-date	**Referee for international journals and conferences**, including NeurIPS, ICML, ICLR, JMLR, JCP, and SISC (highlighted reviewer of ICLR 2022).
2021	**Co-organizer of a minisymposium**, SIAM Annual Meeting Title: Approximation theory of neural networks.

Invited and plenary talks

Chemnitz Summer School on Applied Analysis, invited speaker, Germany.	September 2026
ProbAI Workshop, invited speaker, UK.	September 2026
Workshop on Mathematics of data driven models, plenary speaker, Italy.	January 2026
Workshop on Applications of NA and ML, plenary speaker, Amsterdam, NL.	December 2025
Workshop on Infinite-dimensional ML, invited speaker, Zurich, Switzerland.	September 2025
Householder Symposium XXII, plenary speaker, Ithaca, USA.	June 2025
Huawei Lavender Summit, invited speaker, Bordeaux, France.	September 2024
Workshop on ML in infinite dimensions, invited speaker, Bath, UK.	August 2024
4th Symposium on ML and Dynamical Systems, invited speaker, Canada.	July 2024
Grenoble AI for Sciences Workshop, keynote speaker, France.	May 2024
SIAM Conference on Applied Linear Algebra, prize lecture, France.	May 2024
Dynamics, Data and Deep learning workshop, invited speaker, UK.	March 2024
SCML2024 Conference, invited speaker, Japan.	March 2024
Maths4DL Conference, invited speaker, UK.	July 2023

Submitted papers

37. G. Conradie, **N. Boullé**, J-C. Loiseau, S. L. Brunton, and M. J. Colbrook *Trustworthy Koopman Operator Learning: Invariance Diagnostics and Error Bounds*, submitted.

36. O. Zekri, T. Uscidda, **N. Boullé**, and A. Korba, *Generalized Discrete Diffusion from Snapshots*, submitted.

35. T. J.B. Liu, B. Zadeoglu, R. Sarfati, **N. Boullé**, and C. J. Earls, *Jacobian Scopes: token-level causal attributions in LLMs*, submitted.

34. **N. Boullé**, M. Colbrook, and G. Conradie, *Convergent Methods for Koopman Operators on Reproducing Kernel Hilbert Spaces*, submitted.

33. C. Runkel, S. Xiao, **N. Boullé**, and Y. Chen, *Operator learning regularization for macroscopic permeability prediction in dual-scale flow problem*, submitted.

32. O. Zekri, A. Odonnat, A. Benechehab, L. Bleistein, **N. Boullé**, and I. Redko, *Large Language Models as Markov Chains*, submitted.

31. N. Bouziani and **N. Boullé**, *Structure-Preserving Operator Learning*, submitted.

Publications

30. J. Bao, **N. Boullé**, T. J.B. Liu, R. Sarfati, and C. J. Earls, *Text-Trained LLMs Can Zero-Shot Extrapolate PDE Dynamics*, ICLR Workshop on AI & PDE - Oral (2026).

29. R. Sarfati, T. J.B. Liu, **N. Boullé**, and C. J. Earls, *What's in a prompt? Language models encode literary style in prompt embeddings*, EMNLP (2025).

28. J. Rowbottom, S. Fresca, P. Lio, C.-B. Schönlieb, and **N. Boullé**, *Multi-Level Monte Carlo Training of Neural Operators*, Comput. Methods Appl. Mech. Eng. (2026).

27. O. Zekri and **N. Boullé**, *Fine-Tuning Discrete Diffusion Models with Policy Gradient Methods*, NeurIPS (2025).

26. T. J.B. Liu, **N. Boullé**, R. Sarfati, and C. J. Earls, *Visualizing in-context probability trajectories of LLMs*, ICLR (2025).

25. R. Sarfati, T. J.B. Liu, **N. Boullé**, and C. J. Earls, *Lines of Thought in Large Language Models*, ICLR (2025).

24. **N. Boullé** and M. Colbrook, *Multiplicative Dynamic Mode Decomposition*, SIAM J. Appl. Dyn. Syst. (2025).

23. D. Persson, **N. Boullé**, and D. Kressner, *Randomized Nyström approximation of non-negative self-adjoint operators*, SIAM J. Math. Data Sci. (2025).

22. T. J.B. Liu, **N. Boullé**, R. Sarfati, and C. J. Earls, *LLMs learn governing principles of dynamical systems, revealing an in-context neural scaling law*, EMNLP - Oral (2024).

21. **N. Boullé**, D. Halikias, S. E. Otto, and A. Townsend, *Operator learning without the adjoint*, J. Mach. Learn. Res. (2024).

20. **N. Boullé** and M. Colbrook, *On the Convergence of Hermitian Dynamic Mode Decomposition*, Physica D (2024).

19. **N. Boullé** and A. Townsend, *A Mathematical Guide to Operator Learning*, Handbook of Numerical Analysis (2024).

18. **N. Boullé**, A. Herremans, and D. Huybrechs, *Multivariate rational approximation of functions with curves of singularities*, SIAM J. Sci. Comput. (2024).

17. **N. Boullé**, D. Halikias, and A. Townsend, *Elliptic PDE learning is provably data-efficient*, PNAS (2023).

16. F. Laakmann and **N. Boullé**, *Bifurcation analysis of a two-dimensional magnetic Rayleigh-Bénard problem*, Physica D (2024).

15. H. Praveen, **N. Boullé**, and C. Earls, *Principled interpolation of Green's functions learned from data*, Comput. Methods Appl. Mech. Eng. (2023).

14. **N. Boullé**, I. Newell, P. E. Farrell, and P. G. Kevrekidis, *Two-Component 3D Atomic Bose-Einstein Condensates Supporting Complex Stable Patterns*, Phys. Rev. A (2023).

13. **N. Boullé**, S. Kim, T. Shi, and A. Townsend, *Learning Green's functions associated with parabolic partial differential equations*, J. Mach. Learn. Res. (2022).

12. **N. Boullé**, P. E. Farrell, and M. E. Rognes, *Optimal control of Hopf bifurcations*, SIAM J. Sci. Comput. (2023).

11. **N. Boullé**, P. E. Farrell, and A. Paganini, *Control of bifurcation structures using shape optimization*, SIAM J. Sci. Comput. (2022).

10. **N. Boullé** and A. Townsend, *A generalization of the randomized singular value decomposition*, ICLR (2022).

9. **N. Boullé**, C. J. Earls, and A. Townsend, *Data-driven discovery of Green's functions with human-understandable deep learning*, Sci. Rep. (2022).

8. **N. Boullé**, V. Dallas, and P. E. Farrell, *Bifurcation analysis of two-dimensional Rayleigh–Bénard convection using deflation*, Phys. Rev. E (2022).

7. A. Ellingsrud, **N. Boullé**, P. E. Farrell, and M. E. Rognes, *Accurate numerical simulation of electrodiffusion and osmotic water movement in brain tissue*, Math. Med. Biol. (2021).

6. **N. Boullé** and A. Townsend, *Learning elliptic partial differential equations with randomized linear algebra*, Found. Comput. Math. (2022).

5. **N. Boullé**, E. G. Charalampidis, P. E. Farrell, and P. G. Kevrekidis, *Deflation-based identification of nonlinear excitations of the three-dimensional Gross–Pitaevskii equation*, Phys. Rev. A (2020).

4. **N. Boullé**, Y. Nakatsukasa, and A. Townsend, *Rational neural networks*, NeurIPS (2020).

3. E. G. Charalampidis, **N. Boullé**, P. E. Farrell, and P. G. Kevrekidis, *Bifurcation analysis of stationary solutions of two-dimensional coupled Gross–Pitaevskii equations using deflated continuation*, Commun. Nonlinear Sci. Numer. Simulat. (2020).

2. **N. Boullé** and A. Townsend, *Computing with functions in the ball*, SIAM J. Sci. Comput. (2020).

1. **N. Boullé**, V. Dallas, Y. Nakatsukasa, and D. Samaddar, *Classification of chaotic time series with deep learning*, Physica D (2020).

Technical reports

3. **N. Boullé**, J. Słomka, and A. Townsend, *An optimal complexity spectral method for Navier–Stokes simulations in the ball*, arXiv:2103.16638, 2021.

2. D. Barton, **N. Boullé**, E. Campillo-Funollet, C. Hall, S. Ruangdech, and Y. Zhou, *Compressing aerodynamic hazard data* (with Zenotech), ESGI 162, 2020.

1. E. Campillo-Funollet, **N. Boullé**, M. Ebeling-Rump, A. Pichler, A. Farid, M. P. Goodridge, H. Lee, B. Lyu, and M. Sejeso, *Uncertainty in seismic inverse problems* (with BP), ESGI 145, 2019.