

Nicolas Boullé

Research interests

Numerical analysis, machine learning, computational physics

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

- 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 Matt Colbrook), 2024-present.
- Christina Runkel (Cambridge, with Carola Schönlieb), 2021-present.

Undergraduate and MSc students: Markus Dablander (2020), Franklin Deng, Jack Krew, Henry Smith (2021), Emily Zhang, Qile Jiang (2023), Gustav Conradie (2024), Yudi Cai, Penelope Forcioli, Moritz Hauschulz, Ade Olugboji, Lars Slettengren, Emre Ulusoy, Yaxuan Wang, Oussama Zekri, Zihan Zhou (2025).

Teaching

- 2025 **Lecturer for Mathematical Foundations of Machine Learning**, Imperial College London.
- 2021 **Tutor for Approximation of functions**, University of Oxford.
- 2020 **Tutor for Approximation of functions**, University of Oxford.
- 2019 **TA for Practical Numerical Analysis**, University of Oxford.
- 2019 **TA for Approximation of functions**, University of Oxford.

Professional activities

- 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.
- 2022 **Highlighted Reviewer of ICLR 2022**
- 2021-date **Referee for several journals and conferences, including NeurIPS, ICML, ICLR, JMLR, and SISC.**
- 2021 **Co-organizer of a minisymposium**, SIAM Annual Meeting
Title: Approximation theory of neural networks.

Submitted papers

- 30. O. Zekri and **N. Boullé**, *Fine-Tuning Discrete Diffusion Models with Policy Gradient Methods*, submitted.
- 29. C. Runkel, S. Xiao, **N. Boullé**, and Y. Chen, *Operator learning regularization for macroscopic permeability prediction in dual-scale flow problem*, submitted.
- 28. O. Zekri, A. Odonnat, A. Benechehab, L. Bleistein, **N. Boullé**, and I. Redko, *Large Language Models as Markov Chains*, submitted.
- 27. N. Bouziani and **N. Boullé**, *Structure-Preserving Operator Learning*, submitted.
- 26. **N. Boullé** and M. Colbrook, *Multiplicative Dynamic Mode Decomposition*, submitted.
- 25. D. Persson, **N. Boullé**, and D. Kressner, *Randomized Nyström approximation of non-negative self-adjoint operators*, submitted.

Publications

- 24. T. J.B. Liu, **N. Boullé**, R. Sarfati, and C. J. Earls, *Visualizing in-context probability trajectories of LLMs*, ICLR (2025).
- 23. R. Sarfati, T. J.B. Liu, **N. Boullé**, and C. J. Earls, *Lines of Thought in Large Language Models*, ICLR (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.

Academic visits and talks

Maxwell Institute , Edinburgh, UK.	November 2024
California Institute of Technology , Los Angeles, USA.	November 2024
University of British Columbia , Vancouver, Canada.	November 2024
Simon Fraser University , Vancouver, Canada.	November 2024
Oberwolfach workshop on Inverse Problems , Germany.	October 2024
Imperial-UCL Numerics Seminar , London, UK.	October 2024
CNRS Besançon , Besançon, France.	October 2024
I-X Imperial College London Seminar , London, UK.	October 2024
Firedrake 2024 Conference , Oxford, UK.	September 2024
Huawei Workshop , 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
Cornell University , USA.	June 2024
Grenoble AI for Sciences Workshop , keynote speaker, France.	May 2024
SIAM Conference on Applied Linear Algebra , Prize Lecture, France.	May 2024
Alan Turing Institute , online seminar.	May 2024
University of Bath , Numerical Analysis seminar, UK.	April 2024
One World Mathematics of Machine Learning , online seminar.	April 2024
Dynamics, Data and Deep learning workshop , invited speaker, UK.	March 2024
SCML2024 Conference , invited speaker, Japan.	March 2024
Inria Strasbourg , invited by Victor Michel-Dansac, France.	February 2024
University of Cambridge , M4DL Workshop.	January 2024
University of Birmingham , Applied Mathematics Seminar.	January 2024
Lawrence Livermore National Laboratory , DDPS Webinar.	December 2023
UCLouvain , invited by Estelle Massart, Belgium.	October 2023
Johns Hopkins University , online Postdoc Seminar.	September 2023
Maths4DL Conference , invited speaker, UK.	July 2023
29th Biennial Numerical Analysis Conference , UK.	June 2023
Brown University , invited by Brendan Keith, USA.	June 2023
British Applied Mathematics Colloquium , UK.	April 2023
UCL , Math4DL workshop.	March 2023
SIAM Conference on Computational Science and Engineering , Netherlands.	February 2023
KU Leuven , invited by Daan Huybrechts, Belgium.	February 2023
The Alan Turing Institute , Oden-Turing workshop.	January 2023
University of Cambridge , CIA seminar.	November 2022
The Alan Turing Institute , UK.	November 2022
University of Leicester , CMS Mathematics seminar.	November 2022
EPFL , invited by Daniel Kressner, Switzerland.	October 2022
Imperial College , Numerics & Acoustics Workshop.	September 2022
BIFD conference , Netherlands.	August 2022
Equadiff 15 conference , Czech Republic.	July 2022

University of Cambridge , invited by Carola Schönlieb.	June 2022
IMA Conference on Numerical Linear Algebra and Optimization , Birmingham.	June 2022
Householder Symposium on Numerical Linear Algebra , Italy.	June 2022
University of Oxford , Numerical Analysis seminar.	May 2022
ICLR 2022 conference , online.	April 2022
SIAM Conference on Uncertainty Quantification , online.	April 2022
Virtual study group , V-KEMS.	March 2022
STEM for Britain , UK House of Commons.	March 2022
Cornell University , invited by Alex Townsend, USA.	February 2022
PRISM Residential workshop , UK.	January 2022
SIAM UKIE Annual Meeting , online.	January 2022
University of Oxford , Junior Applied Mathematics Seminar.	October 2021
11th Montreal Industrial Problem Solving Workshop , online.	August 2021
SIAM Annual Meeting , online.	July 2021
British Early Career Mathematicians' Colloquium , online.	July 2021
20th IMA Leslie Fox Prize Event , online.	June 2021
21st Geilo Winter School , online.	January 2021
NeurIPS 2020 conference , online.	December 2020
University of Oxford , Numerical Analysis seminar.	November 2020
European Study Group with Industry 162 , University of Leeds.	July 2020
Simula Research Laboratory , visiting Marie Rognes, Norway.	August-September 2019
European Study Group with Industry 145 , University of Cambridge.	April 2019
University of Oxford , Numerical Analysis seminar.	October 2018
MIT , visiting Jonasz Słomka, USA.	April 2018
Cornell University , SCAN seminar, USA.	November 2017
Memorial University of Newfoundland , visiting Alex Bihlo, Canada.	September 2017