# Arnau Quera-Bofarull

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#### EDUCATION

University of Durham Durham, UK PhD in Astrophysics Oct. 2017 - July 2022 University of Heidelberg Heidelberg, Germany MSc in Physics Oct. 2015 - August 2017

University of Barcelona BSc in Physics

University of Barcelona Barcelona, Spain BSc in Mathematics Sep. 2010 - June 2015

Research Experience

#### Senior Research Associate

Feb 2022 – Present

Barcelona, Spain

Sep. 2010 - June 2015

Department of Computer Science, University of Oxford

Oxford, UK

- Pioneered differentiable agent-based models using PyTorch, Julia, and JAX.
- Created BlackBirds, a tool for gradient-assisted Bayesian calibration of differentiable simulators.
- Mentored MSc and PhD students in applying reinforcement learning to differentiable simulators.

Research Fellow Jun. 2023 – Present

Institute for New Economic Thinking, University of Oxford

Oxford, UK

Designed differentiable macro-economic agent-based models with PyTorch and Julia.

Research Affiliate May 2023 – Present MIT Media Lab Cambridge, USA

Utilized secure multi-party computation to develop privacy-preserving agent-based models.

Volunteer Researcher Oct 2020 - Sep 2022

United Nations Global Pulse

New York, USA

• Simulated the spread of COVID-19 in refugee camps using agent-based models.

PhD Researcher Mar 2020 – Sep 2022

Institute for Data Science, Durham University

Durham, UK

• Lead developer of June, a one-to-one agent-based model for simulating COVID-19 spread in England.

PhD Researcher Oct 2017 - Feb 2022

Institute for Computational Cosmology, Durham University

Durham, UK

Tsukuba, Japan

• Constructed Julia and Python code to perform simulations of black-hole outflows with radiation transfer.

Graduate Research Fellow

Dec 2019 - Mar 2020

Center for Computational Sciences, University of Tsukuba

• Modeled black-hole accretion discs via HPC simulations in Julia.

PhD Intern Apr 2019 – Jun 2019

Boeing Digital Aviation & Analytics

Frankfurt, Germany

Developed an end-to-end pipeline for process tracking in aircraft ground operations using Tensorflow.

PhD Intern Apr 2018 – May 2018 Ibex Innovations Sedgefield, UK

• Innovated a convolutional neural network for X-ray medical image segmentation.

#### BlackBirds | Python, PyTorch, Julia

April 2023 – Present

- Developed a library for the calibration of differentiable simulators using techniques such as variational inference with normalizing flows.
- Implemented forward and reverse automatic differentiation of simulators.
- Programmed support for multi-GPU training.
- Added cross-language support between Julia and PyTorch.

# June | Python, PyTorch, PyTorch Geometric, HPC

Mar 2020 - Present

- Developed a one-to-one synthetic population of England using heterogeneous data sources.
- Programmed an HPC simulator enabling the simulation of 56 million agents on computer clusters.
- Adapted the code to simulate epidemic spread in refugee camps in collaboration with the UN.
- Calibrated model to COVID-19 data using surrogate models and Bayesian history matching.
- Ported model to a tensorized differentiable framework, achieving 40,000x speed-up.
- Re-calibrated model using gradient-assisted calibration methods using BlackBirds.

# **XNet** | Python, Tensorflow

Apr 2018 – May 2018

- Collected data for X-ray image processing.
- Designed and implemented novel convolutional neural network architecture for X-ray image processing.
- Deployed model to company's (Ibex Innovations) production pipeline.

#### **TurnView** | Python, Tensorflow

Apr 2019 – Jun 2019

- Collected data from aircraft ground operations.
- Designed and implemented computer vision pipeline for tracking aircraft ground operations.
- Awarded best project award at internal Boeing conference.

# **Qwind** | Python, Julia, HPC

Oct 2017 – Jan 2022

- Developed Julia code to simulate magneto-hydrodynamics systems.
- Applied code to model black hole outflows to understand galaxy evolution processes.

# TECHNICAL SKILLS

Programming Languages: Python, Julia, C, Bash

Frameworks: PyTorch, Jax, Tensorflow, Pyro, Flux, SciML, Turing, CUDA

Developer Tools: Git, test-driven development, continuous integration (Github Actions), Slurm, MPI

Languages: English (Proficiency), Spanish (Native), Catalan (Native), German (Intermediate)

#### **Journal Publications**

- †2023 Arnau Quera-Bofarull, Joel Dyer, Anisoara Calinescu, J. Doyne Farmer, and Michael Wooldridge.

  Blackbirds: Black-box inference for differentiable simulators. *Journal of Open Source Software*, 8(89):5776, 2023
- 2022 I. Vernon, J. Owen, J. Aylett-Bullock, C. Cuesta-Lazaro, J. Frawley, A. Quera-Bofarull, A. Sedgewick, D. Shi, H. Truong, M. Turner, J. Walker, T. Caulfield, K. Fong, and F. Krauss. Bayesian emulation and history matching of JUNE. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 380(2233):20220039, October 2022
- 2022 I. Vernon, J. Owen, J. Aylett-Bullock, C. Cuesta-Lazaro, J. Frawley, A. Quera-Bofarull, A. Sedgewick, D. Shi, H. Truong, M. Turner, J. Walker, T. Caulfield, K. Fong, and F. Krauss. Bayesian emulation and history matching of JUNE. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 380(2233):20220039, October 2022
- †2022 Arnau Quera-Bofarull, Chris Done, Cedric G Lacey, Mariko Nomura, and Ken Ohsuga. Qwind3: UV line-driven accretion disc wind models for AGN feedback. *Monthly Notices of the Royal Astronomical Society*, 518(2):2693–2711, January 2023
- 2022 Joseph Aylett-Bullock, Robert Tucker Gilman, Ian Hall, David Kennedy, Egmond Samir Evers, Anjali Katta, Hussien Ahmed, Kevin Fong, Keyrellous Adib, Lubna Al Ariqi, Ali Ardalan, Pierre Nabeth, Kai von Harbou, Katherine Hoffmann Pham, Carolina Cuesta-Lazaro, Arnau Quera-Bofarull, Allen Gidraf Kahindo Maina, Tinka Valentijn, Sandra Harlass, Frank Krauss, Chao Huang, Rebeca Moreno Jimenez, Tina Comes, Mariken Gaanderse, Leonardo Milano, and Miguel Luengo-Oroz. Epidemiological modelling in refugee and internally displaced people settlements: Challenges and ways forward. BMJ Global Health, 7(3):e007822, March 2022
- †2021 Joseph Aylett-Bullock, Carolina Cuesta-Lazaro, Arnau Quera-Bofarull, Anjali Katta, Katherine Hoffmann Pham, Benjamin Hoover, Hendrik Strobelt, Rebeca Moreno Jimenez, Aidan Sedgewick, Egmond Samir Evers, David Kennedy, Sandra Harlass, Allen Gidraf Kahindo Maina, Ahmad Hussien, and Miguel Luengo-Oroz. Operational response simulation tool for epidemics within refugee and IDP settlements: A scenario-based case study of the Cox's Bazar settlement. *PLOS Computational Biology*, 17(10):e1009360, October 2021
- †2020 Joseph Aylett-Bullock, Carolina Cuesta-Lazaro, Arnau Quera-Bofarull, Miguel Icaza-Lizaola, Aidan Sedgewick, Henry Truong, Aoife Curran, Edward Elliott, Tristan Caulfield, Kevin Fong, Ian Vernon, Julian Williams, Richard Bower, and Frank Krauss. June: Open-source individual-based epidemiology simulation.

  Royal Society Open Science, 8(7):210506, 2021
- †2020 Arnau Quera-Bofarull, Chris Done, Cedric Lacey, Jonathan C. McDowell, Guido Risaliti, and Martin Elvis. Qwind code release: A non-hydrodynamical approach to modelling line-driven winds in active galactic nuclei. *Monthly Notices of the Royal Astronomical Society*, 495(1):402–412, June 2020
- †2018 Carolina Cuesta-Lazaro, Arnau Quera-Bofarull, Robert Reischke, and Björn Malte Schäfer. Gravitational corrections to light propagation in a perturbed FLRW universe and corresponding weak-lensing spectra. Monthly Notices of the Royal Astronomical Society, 477(1):741–754, June 2018

# Conference Proceedings

†2024 A. Quera-Bofarull and et al. Private agent-based models [under review]. In *International Conference on Autonomous Agents and Multiagent Systems*, 2024

- †2024 A. Quera-Bofarull and et al. Population synthesis as scenario generation for simulation-based planning under uncertainty [under review]. In *International Conference on Autonomous Agents and Multiagent Systems*, 2024
- †2023 J. Dyer, A. Quera-Bofarull, A. Chopra, J. Dyone Farmer, A. Calinescu, and M. Wooldridge. Gradient-assisted calibration for financial agent-based models. In 4th ACM International Conference on AI in Finance, 2023
- †2023 A. Quera-Bofarull, J. Dyer, A. Calinescu, and M. Wooldridge. Some challenges of calibrating differentiable agent-based models. In *ICML Differentiable Almost Everything Workshop*, 2023
- †2023 A. Quera-Bofarull, A. Chopra, A. Calinescu, M. Wooldridge, and J. Dyer. Bayesian calibration of differentiable agent-based models. In *ICLR AI4ABM Workshop*, 2023
- †2023 A. Quera-Bofarull, A. Chopra, J. Aylett-Bullock, C. Cuesta-Lazaro, A. Calinescu, R. Raskar, and M. Wooldridge. Don't simulate twice: one-shot sensitivity analyses via automatic differentiation. In *International Conference on Autonomous Agents and Multiagent Systems*, 2023
- 2023 A. Chopra, A. Rodríguez, J. Subramanian, A. Quera-Bofarull, B. Krishnamurthy, A. Prakash, and R. Raskar. Differentiable agent-based epidemiology. In *International Conference on Autonomous Agents and Multiagent Systems*, 2023
- †2019 Joseph Bullock, Carolina Cuesta-Lázaro, and Arnau Quera-Bofarull. XNet: A convolutional neural network (CNN) implementation for medical x-ray image segmentation suitable for small datasets. In *Medical Imaging 2019: Biomedical Applications in Molecular, Structural, and Functional Imaging*, volume 10953, pages 453–463. SPIE, March 2019