The Alan Turing Institute

**Research Associate, Adjoint-accelerated Programmable Inference for large PDEs, Probabilistic Programming.**

## THE ALAN TURING INSTITUTE

There has never been a more significant time to work in data science and AI. There is recognition of the importance of these technologies to our economic and social future: the so-called fourth industrial revolution. The technical challenge of keeping our data secure and private has grown in its urgency and importance. At the same time, voices from academia, industry, and government are coming together to debate how these technologies should be governed and managed.
The Alan Turing Institute, as the UK's national institute for data science and artificial intelligence, plays an important part in driving forward advances in these technologies in order to change the world for the better.

The Institute is named in honour of Alan Turing, whose pioneering work in theoretical and applied mathematics, engineering and computing is considered to have laid the foundations for modern-day data science and artificial intelligence. The Institute's purpose is to make great leaps in data science and AI research to change the world for the better. Its goals are to advance world-class research and apply it to national and global challenges, build skills for the future by contributing to training people across sectors and career stages, and drive an informed public conversation by providing balanced and evidence-based views on data science and AI.

After launching in 2015 with government funding from EPSRC and five founding universities, the Institute has grown an extensive network of university partners from across the UK and launched a number of major partnerships with industry, public and third sector. Today it is home to more than 500 researchers, a rapidly growing team of in-house research software engineers and data scientists and a business team.

## BACKGROUND

### NEW PROBABILISTIC PROGRAMMING PILLAR

In 2022, the Alan Turing Institute signalled its intention to establish a portfolio of foundational AI research, which would complement the strengths of the institute around applications of AI and AI policy. An initial portfolio of research across three pillars, foundation models, game theory, and probabilistic programming, was launched in early 2023.

We are looking for a Research Associate to support and enable the delivery of the "Programmable Inference" theme within the Probabilistic Programming Pillar. Matthew Juniper and Hong Ge (both at the University of Cambridge) will direct this theme.

## ADJOINT-ACCELERATED PROGRAMMABLE INFERENCE FOR LARGE PDEs

The aim of this project is to extend Programmable Inference to large non-self-adjoint PDE problems, such as the Navier–Stokes equations.

These problems are challenging because:

- their function evaluations are expensive,
- they can contain many variable parameters,
- the forward problem must be carefully formulated in order for the inverse problem to be well-posed.

We will combine Matthew Juniper's group's expertise in adjoint-accelerated Bayesian Inference for PDEs (https://mpj1001.user.srcf.net/MJ_biography.html) with Hong Ge and the Machine Learning group's expertise in Programmable Inference using Turing.jl (https://mlg.eng.cam.ac.uk, https://turinglang.org). High impact examples of adjoint-accelerated Bayesian Inference applied *ad hoc* to practical problems are (i) assimilation of Flow-MRI data directly into CFD (https://doi.org/10.1017/jfm.2022.503) and (ii) assimilation of thermoacoustic data directly into low order models (https://doi.org/10.1016/j.jsv.2022.117096).

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During this project, the Research Associate will interact with both groups to generalise adjoint-accelerated Bayesian Inference within the Programmable Inference framework. We will disseminate flagship applications of Probabilistic Programming for PDEs through Turing Interest Groups and Special Interest Groups of the UK Fluids Network (www.fluids.ac.uk)

**Strand 1: Implementing Laplace's method in Turing.jl**

In current work with a stand-alone code, we have assimilated data into the Lotka–Volterra (L–V) problem using Bayesian Inference with Laplace's approximation. When data is sparse and noisy, this method seems to be superior to statistical methods such as SINDy (https://doi.org/10.1073/pnas.1517384113), which are currently gaining traction within the Fluid Dynamics community. The L–V problem is already implemented in some programmable inference codes (e.g., STAN, Turing.jl) using MCMC or HMC. STAN also implements Laplace's method, but only for ODEs.

The L–V problem will be our first toy problem to implement our existing algorithm within Turing.jl. We will start by formulating the L–V parameter estimation problem as an optimization problem, assuming Gaussian distributions for the prior and posterior. We will use first derivatives to converge to the MAP point with gradient-based optimization (BFGS). We will then use the Hessian around the MAP point to calculate the parameter uncertainties in three ways: (i) estimated from the BFGS algorithm during the optimization process, (ii) estimated from first derivatives only (Gauss-Newton), (iii) calculated precisely with the first and second derivatives of the model with respect to its parameters. We will compare Laplace's method with MCMC and HMC results.

**Strand 2: Extending the methodology to increasingly challenging PDE problems.**

We will then extend the methodology described in strand 1 to increasingly challenging PDE problems: (i) 1D Heat equation, (ii) 2D Poisson equation, (iii) 1D steady Stokes flow (iv) 2D steady Stokes flow (v) 2D steady Navier–Stokes laminar flow (vi) 2D time-periodic Navier–Stokes laminar flow (vii) time-evolving nonlinear Burgers equation (1D in space, 1D in time) (viii) 2D unsteady (i.e. non-periodic) Navier–Stokes equation (ix) 3D unsteady Navier–Stokes. These PDE problems will be formed in continuous space with carefully constructed adjoints, which give the gradients of the model outputs with respect to the model parameters. This is somewhat similar to automatic differentiation but, by working in continuous space and considering the function spaces of the direct and adjoint solutions, the problem becomes better conditioned and therefore more numerically efficient than automatic differentiation of the PDEs.

**Strand 3: Disseminate software and develop flagship applications.**

We aim to reduce the barriers to entry of Probabilistic Programming for PDEs, so that Machine Learning researchers can extend their research to new disciplines, and Fluid Dynamics researchers can access recent developments in Probabilistic Programming. We will disseminate the following outputs: 1. Laplace's method implemented in Turing.jl for differentiable models. 2. Adjoint methods for PDE problems implemented in Turing.jl to replace automatic differentiation of PDEs when it enhances performance. 3. A set of open-source model problems for programmable inference applied to PDE problems across a range of complexity (strand 2). 4. Selected example problems in stand-alone Matlab and Python codes to reach a wider audience. 5. Inspiring outreach materials.

**ROLE PURPOSE**

The research associate will be based at the University of Cambridge or the Turing Institute and will be responsible for delivering strands 1 to 3 and supporting Matthew Juniper and Hong Ge with the overall delivery of the project. In addition, as an employee of the Alan Turing Institute (ATI), the research associates will have access to the ATI offices in London, where they can interact with the wider ATI community.

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**DUTIES AND AREAS OF RESPONSIBILITY**

- Publish and disseminate high-quality research papers and publications detailing research outputs and project case-studies while working closely with other members of the project team.
- Communicate or present research outputs to diverse stakeholders, through conferences, events, meetings, and press opportunities as appropriate.
- Keep on top of the state of the art in the relevant literature, in particular programmable inference, Bayesian inference, adjoint methods, and uncertainty quantification.
- Construct adjoint equations in continuous space and then discretize these problems for numerical implementation.
- Develop Turing.jl, as described in strands 1 to 3 and update its documentation accordingly.
- Work collaboratively with academic experts to write academic research papers.
- Disseminate the research output to the research community, e.g., by giving talks at international conferences.
- Present, disseminate and explain our work at internal and external events hosted by the ATI.
- Contribute to the life of the Institute and support a diverse and inclusive community through embracing the Turing values.

**OTHER DUTIES**

- Teaching may be required as part of collaboration work

Please note that job descriptions cannot be exhaustive, and the postholder may be required to undertake other duties, which are broadly in line with the above key responsibilities. This job description is written at a specific time and is subject to changes as the demands of the Institute and the role develop.

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| PERSON SPECIFICATION | | |
|---|---|---|
| **Skills and Requirements**<br>Post holders will be expected to demonstrate the following: | **Essential (E)**<br>**Desirable (D)** | **Tested at application (a)**<br>**Tested at interview (i)** |
| **Education/Qualification** | | |
| Research Associate level: PhD in Mathematics, Computer Science, Physics, Engineering, or a closely related discipline. | E | A |
| Research Assistant level: Near completion (thesis submitted) of a PhD or equivalent level of professional qualification in Mathematics, Computer Science, Physics, Engineering, or a closely related discipline | E | A |
| **Knowledge and Experience** | | |
| A solid background in one or more of the following: adjoint methods, Bayesian inference, uncertainty quantification, programmable inference. | E | A/I |
| Track record of the ability to initiate, develop and deliver high quality research aligned with the research strategy indicated by the PI and to publish in peer reviewed journals and conferences. | E | A |
| Track record of outstanding research and in delivering impact appropriate to career stage | E | A/I |
| Experience in publishing research papers, code libraries or technical reports and giving presentations or classes on technical subjects. | E | A/I |
| Ability to rapidly assimilate new computational and mathematical ideas and techniques on the job and apply them successfully. | E | A/I |
| Experience in design, development and implementation of research software tools and libraries | D | A/I |
| Experience of programming in Julia | D | A |
| Experience in using current software engineering tools for managing and coordinating distributed projects, such as git and github for distributed version control. | D | A/I |
| Ability to create and promote a collegial and collaborative approach to interdisciplinary research activities. | D | I |
| Evidence of participation within an organisation or discipline-related network to share knowledge and information in order develop practice or help others learn | D | A/I |
| **Communication** | | |
| Excellent verbal and written skills and a proven ability to communicate complex, specialist, or conceptual information/research findings clearly and persuasively to diverse audiences, including the ability to explain technical concepts to technical and nontechnical audiences. | E | A/I |
| Ability to write research reports and papers in styles accessible to both academic and lay audiences. | D | A |
| **Liaison and Networking** | | |
| Ability to collaborate successfully with colleagues in a multidisciplinary environment within the organisation/externally to share knowledge and information in order develop practice or help others learn | E | A/I |
| Willing to contribute to discussions and make decisions as part of a team, and across teams, providing support to others as required, with an approachable and flexible attitude towards work | E | A/I |
| **Decision Making** | | |
| Ability to lead one's own work, including planning and execution, and to prioritise work to meet deadlines | E | A/I |

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| Ability to independently make decisions which are low risk and that mainly affect themselves or a small number of people and are guided by regulation and practice | E | I |
| **Analysis and Research** | | |
| Ability to take the initiative, and carry out research independently or collaboratively under the guidance of the PI | E | I |
| Able to work with supervisors to plan, co-ordinate and implement research activity, including managing research resources | E | A/I |
| Ability to keep accurate and up to date knowledge of services available in own and related areas of work | E | A/I |
| **Other Requirements** | | |
| Commitment to EDI principles and to the Organisation values | E | I |

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**OUR VALUES**

The Alan Turing Institute is committed to equality diversity and inclusion and to eliminating discrimination. All employees are expected to embrace, follow and promote our EDI Principles and Our Values.


**APPLICATION PROCEDURE**

If you are interested in this opportunity, please click the apply button below. You will need to register on the applicant portal and complete the application form including your CV and covering letter. If you have questions about the role or would like to apply using a different format, please contact us on 020 3862 3536 or email recruitment@turing.ac.uk.

**CLOSING DATE FOR APPLICATIONS: Sunday 08 September 2024 at 23:59 (London UK, GMT)**

**TERMS AND CONDITIONS**

This full-time post is offered on a fixed term basis for 2 years. The annual salary is £44,180 - £49,966 plus excellent benefits, including flexible working and family friendly policies, https://www.turing.ac.uk/work-turing/why-work-turing/employee-benefits

Candidates who have not yet been officially awarded their PhD will be appointed as Research Assistant at a salary of £41,352 per annum.

**EQUALITY, DIVERSITY AND INCLUSION**

The Alan Turing Institute is committed to creating an environment where diversity is valued and everyone is treated fairly. In accordance with the Equality Act, we welcome applications from anyone who meets the specific criteria of the post regardless of age, disability, ethnicity, gender reassignment, marital or civil partnership status, pregnancy and maternity, religion or belief, sex and sexual orientation.

We are committed to building a diverse community and would like our leadership team to reflect this. We therefore welcome applications from the broadest spectrum of backgrounds.

We are committed to making sure our recruitment process is accessible and inclusive. This includes making reasonable adjustments for candidates who have a disability or long-term condition. Please contact us at adjustments@turing.ac.uk to find out how we can assist you.

***Please note all offers of employment are subject to obtaining and retaining the right to work in the UK and satisfactory pre-employment security screening which includes a DBS Check.***

***Full details on the pre-employment screening process can be requested from*** HR@turing.ac.uk***.***