M2 Stage: AI-augmented iterative methods with applications to large-scale industrial fluid simulations

Research project

Scientific machine learning (SciML) has significantly enhanced traditional numerical methods by streamlining computational modeling and offering cost-effective surrogate models. However, SciML surrogates suffer from the absence of explicit error control and the lack of reliability in practice. This project aims to address this limitation by developing novel hybrid iterative methods that combine the efficiency of SciML with the reliability of standard numerical approaches. In particular, we will investigate how to enhance nonlinear solution strategies required for carrying out large-scale fluid simulations using SciML approaches.

Scientific environment

The candidate will join the international HAILSED Chair at ANITI and the IRIT Laboratory (APO team) at ENSEEIHT (Toulouse-INP). The HAILSED Chair, focused on hybridizing AI with large-scale numerical simulations for engineering design, offers valuable opportunities to collaborate with experts in (scientific) machine learning, applied mathematics, scientific computing, numerical simulation, and high-performance computing (HPC). The candidate will also actively collaborate with researchers and engineers from ICON, strengthening their scientific development and interdisciplinary research profile while ensuring that the developed hybrid algorithms have practical relevance in industrial settings.

Candidate's profile

The candidate should have a strong interest in computational science, scientific computing, scientific machine-learning, applied mathematics, or related fields. In addition, experience in the following areas would be highly beneficial:

- Programming in Python
- Practical deployment of (Sci)ML applications using PyTorch, TensorFlow, JAX, etc.
- Knowledge of numerical optimization and iterative methods for solving linear and nonlinear systems of equations (stationary iterative methods, Krylov methods, Newton's method)
- Knowledge of discretization methods for partial differential equations (PDEs)
- Basic understanding of fluid-flow simulations, including the governing equations (e.g., Navier-Stokes), boundary conditions, and numerical solution techniques
- Working proficiency in English

The application

Interested candidates are required to submit an application that includes the following:

1. A comprehensive CV

2. A motivation letter detailing the applicant's research interests and reasons for applying

Please send your complete application in one single PDF file to Alena Kopaničáková (alena.kopanicakova@toulouse-inp.fr). The call is open until the position is filled.

Related literature

1. Enrui Zhang, Adar Kahana, Alena Kopaničáková, Eli Turkel, Rishikesh Ranade, Jay Pathak, and George Em Karniadakis. Blending neural operators and relaxation methods in pde numerical solvers. *Nature Machine Intelligence*, pages 1–11, 2024

2. Alena Kopaničáková and George Em Karniadakis. Deeponet based preconditioning strategies for solving parametric linear systems of equations. *SIAM Journal on Scientific Computing*, 47(1):C151–C181, 2025

3. Alena Kopaničáková, Youngkyu Lee, and George Em Karniadakis. Leveraging operator learning to accelerate convergence of the preconditioned conjugate gradient method. *Machine Learning for Computational Science and Engineering*, 1(2):39, 2025