DiRAC
High Performance
Computing Facility

Hewlett Packard
Enterprise

DiRAC placement opportunity: AI in multi-physics/multi-scale cosmological simulations

DiRAC will award one Innovation Placement in 2021 to explore the application of the HPE "SmartSim" AI library to cosmological simulations as a means to replace parameterised sub-grid physics models. The placement will be with Hewlett Packard Enterprise in collaboration with the University of Cambridge.

You have to be working on research that falls within the STFC remit in order to qualify for the placement; however, you can be funded by other organisations besides STFC, as long as the subject area is identifiable as being in Particle Physics, Astronomy & Cosmology, Solar Physics and Planetary Science, Astro-particle Physics, and Nuclear Physics.

To check your eligibility, please contact Mark Wilkinson (miw6@leicester.ac.uk).

You must get your supervisor's or PI's permission before applying for this placement. Participation in the placement scheme is allowed under UKRI's rules, but only with your supervisor/PI's consent.

We will do our best to be flexible; part time working can be arranged as long as the placement does not exceed 9 months.

This should be looked on as an opportunity to learn new skills and contribute outside of your research area.

The deadline for applications is 5pm on Monday 8th February 2021.

AI in multi-physics/multi-scale cosmological simulations with the HPE SmartSim library

In cosmological simulations, physical processes below the resolution limit of the simulation are typically included as simple parameterized approximations based on separate, high-resolution simulations of the smaller-scale processes. An example is the feedback from a black hole at the centre of a galaxy – this process is driven by interactions with timescales of minutes/hours and length scales of order 10^{10} metres, but the typical resolution limit of a galaxy formation simulation is at best 10^{17} metres (i.e. 7 orders of magnitude larger). To bridge these scales in a single simulation capable of properly capturing the physics will be beyond reach for the foreseeable future, and hence innovative methods that go beyond simple parametrizations are needed to push the current state-of-the-art.

One very promising way forward is to have high resolution simulations running alongside the main simulation with an AI engine learning how those models evolve and how to represent them within the larger-scale simulation in the most physically meaningful way. The successful use of these "surrogate" models requires both development of the AI engine and work on explainable AI to ensure that what is generated leads to physical insight for the researchers. These types of approaches are currently being developed in other fields as well, such as material engineering, which highlights their potentially very broad impact and great interdisciplinary potential.

HPE are developing a software library, SmartSim, to support the inclusion of machine-learning (ML) frameworks into numerical models for on-the-fly training, inference, and analysis. SmartSim facilitates this by overcoming systemic impediments including lack of interoperability between programming languages and dependence on file I/O. SmartSim shares data between C, C++, Fortran, and Python clients using an in-memory, distributed database cluster. The library also manages hardware allocations, orchestrates simulation and analytics workloads, and automates model ensembling. A Jupyter notebook can be connected to the system allowing interactive, online analysis and prototyping of ML models.

The overall aim of the placement is to explore the use of the SmartSim library in the context of cosmological simulations. In particular, you will construct a surrogate model with SmartSim to replace the sub-grid physics models currently included in simulations of the feedback from a black hole at the centre of a galaxy.

The specific goals are to:

1) Develop a working surrogate model for black hole feedback using the SmartSim library.
2) Quantify the benefits of the surrogate model in terms of physical realism and/or performance.
3) Create a step-by-step guide for other researchers who are considering the implementation of surrogate models using SmartSim.

You will be working with members of the Hewlett Packard AI Lab, who will provide access to the SmartSim library and support in its deployment within a cosmological simulation. In addition, you will work closely with the research group of Debora Sijacki at Cambridge who will provide access to the relevant simulation codes. With support from these colleagues, you will be expected to produce work of sufficient quality that it will suitable for publication in peer-reviewed journals.

A suitable candidate would have knowledge of C or C++ and at least working knowledge of Python (particularly NumPy, Pandas, Xarray). Knowledge of Machine Learning techniques (dimensionality reduction, data preparation, hyperparameter optimization), models (neural networks, random forests, autoencoders) and frameworks (Pytorch, TensorFlow) is a significant advantage. Previous experience with simulations for N-body, Molecular Dynamics or Computational Fluid Dynamics is preferred and some knowledge of the underlying physics in cosmological simulations would be useful. Experience with HPC systems, libraries and tools (Slurm, MPI) is useful but not required.

As the HPE team is not UK-based, the main mode of working for the placement is home working (or working at your home institution). Depending on the progress of the Covid-19 pandemic, a visit to the HP AI lab may be possible later in 2021.

- Who will you work with?
  - HPE Supervisors: Sam Partee and Sorin-Cristian Cheran
  - DiRAC Supervisors: Debora Sijacki (Cambridge)
- What should you do if you are interested?
  - Speak to your current supervisor and get their views BEFORE applying.
  - Contact Mark Wilkinson (miw6@leicester.ac.uk) if you need further information.
  - Send a CV and a 200-word statement on why you would want to do this placement to miw6@leicester.ac.uk and c.jenner@ucl.ac.uk by 5pm on Monday 8th February 2021.

Selection process: shortlisted candidates will be invited to attend a zoom interview with representatives from both DiRAC and HPE.