CEMRACS 2023 mini-project proposal

Title: Physics Informed Neural Network to reduce data storage of gyrokinetic plasma turbulence simulations

Contact: Emmanuel Franck
Institution or company: INRIA
Email: emmanuel.franck@inria.fr
Phone number:

Scientific supervisors: D. Zarzoso (CNRS), V. Grandgirard (CEA), L. Navoret (Université de Strasbourg), E. Franck (INRIA), F. Almuhisen (CEA)

1. Context

Nuclear fusion aims at producing on Earth the energy of the stars, by confining the fuel (called plasma). However, a fusion plasma is a complex system, characterised by instabilities developing on disparate spatio-temporal scales which, in nonlinear regimes, can lead to turbulent transport. It is well-known that turbulence can limit the performance of fusion devices. Therefore, understanding, predicting and controlling turbulence and the induced transport and losses of particles is of prime importance for nuclear fusion and represents an extremely challenging research activity for the ITER project. In tokamak, plasmas are characterized by low collisionality regimes, so that conventional fluid models are questionable and kinetic descriptions are more appropriate. In such kinetic descriptions of plasmas, the six dimensional evolution equation for the distribution function -Vlasov or Fokker-Planck equations- is solved for each species, coupled to the self-consistent equations for the electromagnetic fields, namely Maxwell's equations. Fortunately, as far as turbulent fluctuations are concerned, they develop at much lower typical frequencies than the high frequency cyclotron motion. Therefore, this 6D problem (3D in space and 3D in velocity) can be reduced to a 5D (3D in space and 2D in velocity), known as the gyrokinetic model. But even with this dimensionality reduction, the development process leading to a 5D gyrokinetic code reveals extremely challenging and requires state-of-the-art high performance computing (HPC). There exist about a dozen of gyrokinetic codes in the world, five being European.

The 5D GYSELA [1] (for GYrokinetic SEmi-LAgrangian) code is developed at IRFM/CEA for 20 years through national and international collaborations with a strong interaction between physicists, mathematicians and computer scientists. The code is optimized up to 500k cores and uses frequently from 16k to 64k cores for simulations which often run during several weeks. The annual time consumption on supercomputing facilities is currently of 150 million of core-hours. Because of the multi-scale physics at play and because of the duration of discharges, we already know that ITER core-edge simulations will require exascale HPC capabilities. The GYSELA code produces very large amounts of data. A typical 5D mesh contains several hundreds of billions of points, which leads to 5D distribution functions of the order of 2 TB to be followed at each time iteration. Given 10,000 to 100,000 iterations for each simulation, it is not conceivable to store the time evolution of the distribution functions. In the end, out of the Petabytes of data manipulated during a GYSELA simulation, only a few Terabytes are saved due to storage capacity limits. This data reduction is based on saving at fixed time steps a number of mainly 3D fluid quantities. Knowing that there is a growing gap between CPU performance and I/O bandwidth on large-scale systems, this post-hoc approach is already very constraining and will become even more so.

In this framework, the use of Artificial intelligence (AI) techniques might provide to optimize the storage of information. Specifically, Physics Informed Neural Networks (PINN) [2] techniques could be good candidates for reducing the amount of information stored. Indeed, in recent years, physics-based learning has been proposed in many areas of scientific computing due to its ability to easily integrate data-driven methods and domain-specific theoretical knowledge, allowing for the training of better performing neural network models that conform to physical laws, even in the face of data scarcity.

2. **Description and objectives**
   The first tests on simplified 2D Vlasov-Poisson problems are encouraging [3] but show that there are still many obstacles to overcome in order to apply to gyrokinetic equation systems. The objective of this project is to test PINN methods on more complex problems, both in terms of higher dimensionality and more complex operators (including for example collision operators) keeping in mind the final objective of exploring the capabilities of PINN neural networks for gyrokinetic applications like the GYSELA code.

3. **Proposed methodology**
   1. The first step will be to take in hand the PINN method on the 2D wave-particle problems (namely Landau damping and bump-on-tail instabilities) studied in [3]. The Python scripts developed for this purpose will be provided as starting point.
   2. Try to improve the PINN approach proposed in [3] which shows some limitations. A first idea will be to compare with the recent CAN-PINN approach [4] or variants.
   3. Apply the methods successfully tested in step 2 to a more complex Vlasov-Poisson 2D problem used for kinetic simulations of the plasma sheath [5]. This implies to take into account a collision operator and steep temperature gradients for which non-equidistant meshes are required.
   4. If there is time left, PINN methods can be applied to higher dimensional problems such as 4D drift-kinetic problems [6].

4. **Software requirements**
   The required simulation database will be created with the Gyselalibxx tools https://github.com/gyselax/gyselalibxx/ developed in C++.
   Python (Keras, TensorFlow and the standard libraries for scientific computation).

5. **References**

[1] V. Grandgirard et al, CPC, vol. 207, 35-68, 2016 , https://doi.org/10.1016/j.cpc.2016.05.007.

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[4] P-H Chiu et al, *CAN-PINN: A Fast Physics-Informed Neural Network Based on Coupled-Automatic-Numerical Differentiation Method*, https://doi.org/10.48550/arXiv.2110.15832.

[5] E. Bourne et al., *Non-Uniform Splines for Semi-Lagrangian Kinetic Simulations of the Plasma Sheath*, https://hal.science/cea-03748016/.

[6] V. Grandgirard et al, 217, 395–423, 2006, https://doi.org/10.1016/j.jcp.2006.01.023.