Distributed Dimensionality Reduction for Large-Scale Physical Simulations
Internship + PhD offer

Supervision:

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Context. While artificial intelligence is growing at a fast pace, the bulk of the world's computing power remains targeted at modeling and predicting physical phenomena, such as climate models, weather forecasting, or nuclear physics. These simulations are run on highly parallel supercomputers on which both the hardware and the software are optimized for the task at hand. While the computing power of each processing unit is still increasing, the communication networks and the storage capabilities in these clusters do not follow such fast trends. As a result, computing nodes produce outputs faster than what can be stored or sent to process elsewhere: These **simulations are IO bound**.

To reduce the communication burden, a promising venue is **is situ computations**, meaning that most of the data is processed locally by the nodes, and only meaningful aggregates are stored or sent over the network. However, this is a difficult problem in general since meaningful information for the global simulation depends on the other nodes' output. The goal of this internship is to **leverage machine learning techniques to bypass IO bottlenecks in the context of physics simulation on high-performance computing (HPC) clusters**. This work is thus placed in a broader "Machine Learning for Science" context, which aims at using ML to solve key problems arising in traditional sciences. More specifically, we will focus on distributed dimensionality reduction techniques, which critically reduce the communication and storage needed to retain most of the information.

Methods. As specified above, the project will first focus on dimensionality reduction techniques, and in particular the standard PCA method. To fit the requirements imposed by the HPC setting, we will consider distributed incremental PCA methods [8], that work with streaming data split over many computing nodes. An important consideration in our context is that, unlike classical data stream, the data is not *i.i.d.* on the nodes, but stems from the domain partitioning imposed by the physic of the problem. The two main objectives are the following:

- **Benchmark existing methods:** This will require a thorough state-of-the-art review, as well as defining the relevant metrics for evaluating data compression in physics simulations (communication/computation time/cost, quality of the solution...). The benchmark will be realized with benchopt [3] and will benefit from the distributed coding expertise of both supervisors.

- **Designing new efficient methods:** To account for the structure of physic simulations, we propose to investigate how to efficiently leverage the inter-node communication to improve existing distributed PCA methods [5, 4]. The convergence of the proposed methods will be analyzed and we will provide tight convergence bounds.

While the initial focus will be on PCA, more advanced compression methods will be considered throughout the project, in particular with spatial compression [1, 2], mesh-based wavelets [7], or auto-encoders [6].

Environment. The internship will take place at Inria Grenoble, in the Thoth team for at most 6 months (April-September 2024). This is a large team focused on machine learning, and in particular computer vision. Particular topics of interest include visual comprehension, hyperspectral imaging, numerical and parallel optimization, and unsupervised learning. A particular emphasis is put on interdisciplinary projects. The internship will include frequent visits to the

[MIND team](#), at Inria Saclay. Full-time in Saclay can also be discussed, but the preferred location is Inria Grenoble. The two supervisors are young Inria researchers, with a strong track record in optimization and machine learning.

This project also takes place in the PEPR NumPEx, an initiative to improve the use of supercomputers for physical simulations. The results from the internship and the follow-up PhD will thus be integrated into the software stack for these applications. This internship thus provides the unique opportunity to discuss with scientists from other fields and to improve their workflows through IA research. Interaction with scientists developing computational simulations in various fields will be encouraged, in particular with the Gysela code, which is part of the ITER project.

Requirements. We seek candidates strongly motivated by challenging research topics in machine learning for science. Applicants should have a strong mathematical background with knowledge of numerical optimization and machine learning. With regards to software engineering, proficiency in `Python` is expected and preliminary experience in a distributed computation library is a plus. Note that funding for PhD is already available, so we are seeking a strongly motivated candidate who would like to continue on this topic with a PhD.

References

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