Project Team INRIA:
HiePACS

Author of the post-doctoral research subject:
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Title of the post- doctoral research subject:
Fast tensor arithmetic for large scale computing and applications

Scientific priorities (cf strategic plan):

Computing tomorrow: Extreme-scale computing for data intensive science

Applications: materials physics, uncertainty quantification, biodiversity, machine learning

Scientific Research context (10-15 lines):
High-dimensional problems are encountered in many areas of practical interest like in stochastic equations, uncertainty quantification problems, quantum and vibrational chemistry, optimization, machine learning, ... Such problems have led to the introduction of numerical techniques such as variable reduction, reduced modeling, and randomized algorithms. However, the typical dimension of these problems makes unaffordable the existing standard techniques. In the last decades, the theoretical study [1, 2] of low-rank tensor methods has developed and reached a satisfactory level of maturity to be applied on such domains. A new approach particularly well suited is to seek a hierarchical low-rank tensor format that captures the algebraic structure of the system. The tensor train format [1] and their variants (QTT, …) are successfully used in many very different applications (chemistry, machine learning, approximation, boundary element method ...) and they proved to provide efficient and stable data sparse representation for extremely high-dimensional systems. However, accessible and general high-performance parallel software has not yet emerged despite its obvious and crucial need. We have started to develop new computational tools designed to achieve high-performance for high dimension problems on supercomputing platforms (Parallel Tensor Train Solver). This entails the development of specialized high-performance, more scalable, robust and further accurate algorithms than contemporary designs.

Post- doctoral researcher work description (10-15 lines):
The first stage will be dedicated to identify and implement tools to solve linear system with the tensor arithmetic in the context of either iterative solvers such as Krylov methods or eigenvalue solvers. Many questions have to be addressed namely 1) how we compute the rank of tensor and 2) what is the best stable algorithm to project the solution vector in the hierarchical format. In the second step we develop a parallel version of the previous algorithm to boost its performance. The test bed for the numerical validation and benchmark of these kernels will be the computation of vibrational spectra of molecules in dimension's space 12 ([4]) and 20. Other domains like biodiversity or machine learning will likely be considered as second application

domain. This research action falls within the upcoming research agenda of the HiePACS team with initiatives at the national and the European scale to foster collaboration and exchanges.

Required Knowledge and background:

Candidates should have a strong background in scientific computing with a PhD in computational sciences (applied mathematics, numerical linear algebra, numerical algorithms, …).

References (max 5):

[1] W. Hackbusch, *Tensor Spaces and Numerical Tensor Calculus*, vol. 42. Berlin, Heidelberg: Springer Berlin Heidelberg, 2012.

[2] T. G. Kolda and B. W. Bader, "Tensor Decompositions and Applications," *SIAM Review*, vol. 51, no. 3, pp. 455–500, 2009.

[3] J. Ballani, L. Grasedyck, and M. Kluge, "A Review on Adaptive Low-Rank Approximation Techniques in the Hierarchical Tensor Format," in *Extraction of Quantifiable Information from Complex Systems*, vol. 102, 2014, pp. 195–210.

[4] M. Rakhuba and I. Oseledets, "Calculating vibrational spectra of molecules using tensor train decomposition", in J. Chem. Phys. 145, 124101 (2016); https://doi.org/10.1063/1.4962420

[5] T. Huckle, K. Waldherr, and T. Schulte-Herbrüggen, "Computations in quantum tensor networks," *Linear Algebra and Its Applications*, vol. 438, pp. 750–781, 2013.

Keywords (max 5-6):

Tensor Train decomposition, high-dimensional, low rank approximation, eigensolver, linear solver.

Duration:

12 months or 16 months