2018-00404 - Post-doctoral - Study and design of pipelined Block Krylov linear solvers

Niveau de diplôme exigé : Thèse ou équivalent
Fonction : Post-Doctorant

A propos du centre ou de la direction fonctionnelle

An important force which has continued to drive HPC has been to focus on frontier milestones which consist in technical goals that symbolize the next stage of progress in the field. In the 1990s, the HPC community sought to achieve computing at a teraflop rate and currently we are able to compute on the first leading architectures at a petaflop rate. Generalist petaflop supercomputers are available and some communities are already in the early stages of thinking about what computing at the exaflop level would be like early 2020. For application codes to sustain a petaflop and more in the next few years, hundreds of thousands of processor cores or more will be needed, regardless of processor technology. Currently, a few HPC simulation codes easily scale to this regime, and major code development efforts are critical to achieve the potential of these new systems. Scaling to a petaflop and more will involve improving physical models, mathematical modelling, super scalable algorithms that will require paying particular attention to acquisition, management and visualization of huge amounts of scientific data.

In this context, the purpose of the HiePACS project is to perform efficiently frontier simulations arising from challenging research and industrial multiscale applications. The solution of these challenging problems require a multidisciplinary approach involving applied mathematics, computational and computer sciences. In applied mathematics, it essentially involves advanced numerical schemes. In computational science, it involves massively parallel computing and the design of highly scalable algorithms and codes to be executed on future petaflop (and beyond) platforms. Through this approach, HiePACS intends to contribute to all steps that go from the design of new high-performance more scalable, robust and more accurate numerical schemes to the optimized implementations of the associated algorithms and codes on very high performance supercomputers.

Contexte et atouts du poste

Scientific context :

The HiePACS team at Inria Bordeaux-Sud Ouest has been studying and developing Krylov linear solvers and associated software packages for the past few years with a recent emphasis on block Krylov methods enabling to solve multiple right-hand sides simultaneously [3]. Such linear systems arise in many large scientific and industrial applications, such as in radar cross section calculation in electromagnetism, wave scattering and wave propagation in acoustics, various source locations in seismic and parametric studies in general. These numerical methods exhibit attractive computational features in term of memory access; basically BLAS-3 type of operations compared to rather BLAS-1 calculation for their single right-hand side counterpart. Furthermore on the route to exa-scale, scalable algorithms should either remove global synchronisations or be redesigned to overlap these global synchronisations with other numerical calculation as pointed out for instance in the latest strategic research agenda of ETP4HPC [4]. Those global synchronisations are mainly involved when imposing orthogonality conditions in the construction of the search spaces, features very much suited to ensure the convergence and accuracy of the computed solutions. Consequently extending the ideas of numerical pipelining introduced for single right-hand side [5] to block solvers appears scientifically timely.

Supervision: The postdoc will work closely with Emmanuel Agullo and Luc Giraud (HiePACS project-team). Some meetings with other Inria teams (current or potential users of the MaPhyS and PaStiX software) will be organized as well to fully assess the decision made in the numerical and implementation design.

Mission confiée

The design of novel algorithms for exascale platforms require to develop novel algorithms that remove or hide the global synchronisations

Principales activités
The objective of this post-doctoral project is twofold. First, extend the numerical pipelining ideas from single right-hand side solver [6, 7] to the multiple-right-hand side framework for GMRES variants. The general ideas consist in redesigning the algorithms so that the global synchronizations involved in the orthonormalization process of the search space can be asynchronously computed while the calculation of the Krylov solver progresses. This task will start by a careful review and analysis of the recent papers published on this topic. It will be followed by the study of the possible ways to extend these ideas first to regular Block GMRES, possible extensions to more advanced numerical solution techniques with inexact breakdowns and spectral deflation at restart might also be considered [4].

In order to assess that the numerical choices allow for large calculations at scale. The second expected contribution is the implementation of these new numerical schemes in our software package Fabulous [1]. The performance validation at scale will be performed via the integration of these new solvers in either MaPhys [2] or PaStiX [3] in application contexts through our collaborations with our industrial partners, namely Airbus, CEA or Total, as well as other Inria teams we collaborate with, namely Magique3D and Nachos.

References:

[1] Fabulous package (hyperlink) - https://gitlab.inria.fr/solverstack/fabulous

Compétences

This position is intended for candidates with a strong background in computational sciences, preferably holding a PhD in applied mathematics or computer science, with some knowledge in numerical linear algebra. A knowledge/experience of parallel programming would also be appreciated.

Avantages sociaux

- Subsidised catering service
- Partially-reimbursed public transport

Rémunération

2653€ / month (before taxes)