Autotuning for ultra-high performance computing with partitioned coupling

General context

Taking into account multiple and coupled physics is at the heart of many application requirements in fields as varied as, but not limited to, aeronautics, defense and biology. This is also strong area of expertise for CEA Energy Division, with multiple domains including fluid-structure interaction [1], neutronics coupled with thermal-hydraulics a/o thermal-mechanics [2] or severe accident modeling [3]. The emergence of exascale architectures opens the way to promising new levels of high-fidelity simulations, but also significantly increases the complexity of many software applications in terms of total or partial rewriting. Therefore, it specifically encourages partitioned coupling to limit development work. The idea is to search for each physics of interest in a necessarily reduced number of highly optimized software components, rather than making specific, possibly redundant developments in standalone applications.

Once the coupled multiphysics problem has been written with the expected levels of accuracy and stability, the proposed work concentrates on the coupling algorithms between applications assumed to be themselves exascale-compatible, to be solved efficiently at exascale. It is also worth noting that, in general, the couplings under consideration can present a high level of complexity, involving numerous physics with different level of feedback between them and various communications from exchanges of boundary conditions to overlapping domains. The current post-doctoral internship, to be carried out in the framework of the ExaMA collaborative project, is in particular dedicated to the identification and dynamic tuning of the relevant numerical parameters arising from the coupling algorithms and impacting the computational efficiency of the global simulation. Considered problems are in the general case time-evolving problems, with a significant number of time iterations, allowing using the first iterations to gather data and conduct the tuning.

Regarding software, the research is intended to be conducted within the ICoCo/C3PO low-intrusive open-source coupling framework [4], with data exchange through the MEDCoupling library [5]. To benefit from the synergies made possible by the ExaMA context, it is foreseen to mutualize autotuning techniques with related work addressing adaptive precision and validation in the Promise software environment [6].

Methodology and research directions

Two main topics can be identified in terms of computational efficiency specific to coupling frameworks: load balancing and scheduling on the one hand, and coupling algorithms and data transfers on the other hand. The proposed internship is dedicated to the second topic and aims at designing a strategy to automatically identify, rank and optimize the internal parameters impacting the cost of the coupling computational tasks. Such an autotuning approach is mandatory to provide the necessary versatility in the coupling tools to adjust to any multiphysics configuration with minimal *a priori* knowledge of its characteristics. Expected parameters to be tuned this way can be, without prejudging the findings of the proposed research, convergence criteria in the loops between physics, computing orders between physics, as well as possible multi-level convergence between groups of physics.

Practically, the work is intended to be based, in a first phase, on model apps mimicking the behaviour of several configurations of multiphysics coupling, in terms of computational cost of each physics and feedback between them, to design and test autotuning strategies for the automated discovery of a known optimal execution path. The second phase will consist in practical benchmarks between actual multiphysics tools on well chosen problems of interest, to quantify the performances and improve the strategies designed before. Fluid & structure (thermal-) mechanics and neutronics are primarily targeted physics for the tests, without excluding any additional coupling proving worthy of studying during the internship.

Location

CEA, IRESNE Institute, Cadarache center, France

Salary

The gross salary is approximately 3500 euros (including national health insurance and employment insurance).

Duration

1 year, renewable 1 year

Application

Candidates must have a PhD in Computer Science, Applied Mathematics or other relevant fields. Good programming skills are required.

Applications should be sent to Vincent Faucher (vincent.faucher@cea.fr). They should include:

- a curriculum vitae;
- a motivation letter;
- at least two referees with their e-mail addresses;
- links to PhD thesis and publications;
- links to software contributions.

Références

[1] Contribution to the multiphysical analysis of fuel assembly bow, PhD Stanislas de Lambert, CEA, Université Paris-Saclay, 2021

[2] Numerical optimization of a multiphysics calculation scheme, P. Cattaneo, R. Lenain, C. Patricot, The European Physical Journal Conferences 247(2):06008, 2021

[3] Solving coupled problems of lumped parameter models in a platform for severe accidents in nuclear reactors, L. Viot, L., Saas, & F. De Vuyst, International Journal for Multiscale Computational Engineering, 16(6), 555–577, 2018

[4] https://github.com/cea-trust-platform/icoco-coupling, https://sourceforge.net/projects/cea-c3po

[5] https://docs.salome-platform.org/7/dev/MEDCoupling/index.html

[6] S. Graillat, F. Jezequel, R. Picot, F. Fevotte, and B. Lathuiliere. Auto-tuning for floating-point precision with discrete stochastic arithmetic. Journal of Computational Science, 36:101017, 2019.