Funded PhD subject:
Performance-portable support of complex discretizations at extreme scale in modern C++

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Keywords: parallel programming models, software engineering, modern C++, partitioned global address space, performance portability, GPU, extreme-scale parallelism

Context

Extreme-scale simulation codes are typically developed in C or FORTRAN, parallelized with MPI[7] and OpenMP[16]. This approach has proven very successful for code portability during the last decades; but with the advent of GPU-based supercomputers, codes have to be ported to a new architecture for which a rewrite from scratch is often required.

Lots of efforts have been devoted recently to design programming models targeting (performance) portability between CPU and GPU including `Kokkos` [18], OpenACC, RAJA[4], or SYCL[17] for example. Some also target distributed memory parallelism like Co-array Fortran[14], HPX[11], UPC[5, 6], UPC++[3], or XMP[15]. These models rely on the same abstractions that were present in previous models: (multi-dimensional) arrays and (parallel) loops. Numerical applications then build higher-level abstractions on top of these by taking into account the specifics of the hardware they target, hence limiting performance portability. Many concepts also remain implicit in the code so as not to pay a cost at execution; leading to issues with code maintainability and adaptability.

These issues can only be solved by directly providing higher-level abstractions to the numerical simulation codes. An interesting example is offered by `numpy`, `xarray` and `dask.Array` in Python. These libraries make it possible to express numerical computations in a very natural way thanks to the abstraction of mesh and data distribution they provide and to execute it on a variety of hardware architectures by adding just a few dedicated annotations. However, this ecosystem remains far from offering performances comparable with FORTRAN + OpenMP/MPI.

Goal

The goal of this PhD thesis is to evaluate if a solution based on C++ template metaprogramming can offer high-level (zero-cost) abstractions handling a large range of data discretization at compile time. The work will take place in the framework of the `ddc`[1] library and will be evaluated on the very demanding simulation code GYSELA[2][8, 12] that leverage the largest existing super computers and manipulates multiple complex discretizations of its high-dimension data along execution. The goal is to handle seamless replacement of discretization in code (*e.g.* structured uniform mesh to unstructured), while offering the best performance from each one. Another goal is to handle parallelism at all levels: distributed-memory parallelism similarly to PGAS languages, shared-memory parallelism on both CPU and GPU, but also SIMD parallelism.

[1] `https://ddc.mdls.fr`
[2] `https://gyselax.github.io/`

Work-plan

During the first phase of the work, the candidate will study the related bibliography (see an extract bellow), focusing on parallel programming models, and especially PGAS languages to get a good understanding of the involved concepts, understand the limitations of current approaches, and seize the benefits of existing softwares. In addition to academic publications, this first phase will be used to discover existing work in `ddc` and the needs identified as part of the rewrite of the GYSELA code.

Then, the work will focus on the conception of a programming model supporting the various features identified in the previous section. This work will start by focusing on single-node CPU and GPU parallelism before moving to multi-node distributed parallelism. The proposed concepts will be tested on academic cases using the usual evaluation criteria from the literature: portability, performance, lines of code, readability, etc.

Finally, the proposed solutions will be implemented in `ddc` and applied to the development of the next-generation production code GyselaX in collaboration with the team developing the code at CEA/IRFM, Cadarache and with collaborators working on performance optimization and portability in JAEA, Tokyo, Japan. They will be tested at scale on several supercomputers including systems amongst the most powerful in the world (Fugaku[3], Joliot-Curie[4], Adastra[5], ...) but also on testbeds of new GPU accelerators in the framework of collaborations with vendors such as Intel. All results will be submitted to international peer-reviewed conferences and journals, such as SuperComputing, IPDPS, Cluster, JPDC, etc. for publication. The candidate will also be encouraged to participate in the writing of a proposal to the C++ standard comittee about the solutions found.

Skills

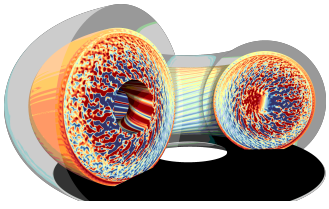
The successful candidate will master the following skills and knowledge:

- strong interest in programming models in general and parallel programming models in particular,
- proficiency and experience with modern C++ and template metaprogramming,
- motivation for team-work in an international environment.

In addition, the following will be considered a plus:

- knowledge and experience with GPU, parallel and high-performance computing,
- interest for applied mathematics and numerical simulation,
- experience with software engineering and library design.

Existing software

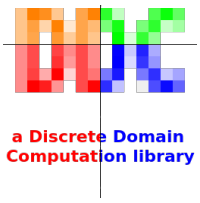


The 5D non-linear **gy**rokinetic, **se**mi-**La**grangian code **GYSELA** has been developed at CEA/IRFM for the last 20 years to study turbulence in Tokamak plasmas. The kinetic model couples the six dimensional Vlasov or Fokker-Planck equation for the distribution of particles, with Maxwell's equations for the electromagnetic field. Since turbulent fluctuations develop at much lower frequencies than the cyclotron motion, this can be reduced to the 5D *gyrokinetic* model (in addition to the time and species dimensions). Even with this dimensionality reduction however, gyrokinetic codes requires state-of-the-art high performance computing resources and GYSELA regularly use between 8 192 and 65 536 cores in parallel for multiple weeks simulations.

While GYSELA answers current needs of physicists very well, two changes will have to be be handled in the coming years. First, the regular toroidal mesh of GYSELA will have to be replaced with more complex meshes in order to handle the geometries of real Tokamaks. Second, with the arrival of Exascale, computational nodes become more and more heterogeneous often featuring GPUs. The code will have to be ported to these new compute architecture to keep using the most powerful

[3]Fugaku, top 1 supercomputer in Nov 2021 https://www.top500.org/system/179807/
[4]Joliot-Curie french supercomputer https://www.top500.org/system/179700/
[5]Adastra, upcoming supercomputer in France https://www.cines.fr/en/12600/

super-computers in the world. Many assumptions are made in the existing code that make these changes very complex, and a rewrite from scratch of the existing Fortran code into C++ is planned.



`ddc` is a C++ template meta-programming **d**discrete **d**omain **c**omputation library developed at Maison de la Simulation. `ddc` supports intensive computation over high-dimensional meshes. It provides multi-dimensional containers (based on `std::mdspan` [9] proposed for inclusion in the C++ standard), and supports iterators over geometric elements and type-safe array indexing. By giving a mesh semantic to algorithms, `ddc` eases working on fields mapped on sub-meshes, and switching between meshes; it supports writing generic mesh-independant algorithms, or optimized mesh-specific algorithms.

While similar to (and based on top of) other C++ template meta-programming libraries such as `Kokkos` or the standard library `std::mdspan` and the standard parallel algorithms, `ddc` offers a higher-level of abstraction and supports typed indices, preventing error when manipulating many different discrete dimensions. `ddc` is currently in the prototype phase and support for parallelism in the library is a work in progress.

Laboratory and collaborations

Maison de la Simulation (MdlS – `http://www.maisondelasimulation.fr/`) located on the Plateau de Saclay, is a joint laboratory of the alternative energies and atomic energy commission (CEA), the national center for scientific research (CNRS), Paris-Saclay University, and Versailles Saint-Quentin-en-Yvelines University. The laboratory groups activities around high performance computing (HPC): research in computer science and applied mathematics, engineering, and development for high-performance simulation applications. Of specific interest at MdlS are software engineering aspects of HPC, especially regarding separation of concerns, performance optimization and performance portability.

The **Institute for Magnetic Fusion Research** (IRFM – `http://irfm.cea.fr/`) located at the CEA research centre of Cadarache, is one of the 15 institutes that make up the fundamental research division in the alternative energies and atomic energy commission (CEA). For almost 60 years, its responsibility has been to carry out research on thermonuclear magnetically-confined fusion at the CEA in association with the Euratom fusion programme. In Tokamaks, matter is in a hot plasma state in interaction with a strong magnetic field, and controlling nuclear fusion requires to understand the mechanisms that govern heat confinement. Ion temperature gradient instabilities is an important mechanism whose understanding requires numerical simulation, this objective lead to the development of the GYSELA code.

Japan atomic energy agency (JAEA – `https://www.jaea.go.jp/english/`) is Japan top nuclear research agency. Amongst many others, it hosts researchers interested in the development of performance-portable simulation codes. IRFM and Maison de la Simulation have strong collaborations ongoing regarding these aspects for the design of the new-generation GYSELA code.

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