ITER PHYSICS DEPARTMENT

Proposal for the Use of High Level Support Team resources

Abstract

Cluster systems built with general-purpose processors are superseded today by platforms built around a hybrid architecture, with nodes constituted by processors based on CPU cores and many-core accelerated devices (MIC) or graphical processing units (GPU). By being able to exploit the capabilities of these computers, we expect to be able to significantly enhance the computational capabilities of codes currently being executed on standard platforms. We therefore propose to carry out the necessary steps to port the GBS code, used to simulate plasma turbulence in the tokamak SOL, to hybrid architecture computers. In particular a mixed communication (OpenMP+MPI+OpenACC or Intel Offload OpenMP) will be implemented in GBS, first focusing on the parallel multigrid solver recently implemented in GBS. GBS will then be tested on the supercomputers based on hybrid architecture. By being able to exploit these computers, we expect GBS to perform full size simulations of SOL plasma turbulence in JET and ITER that are presently out of reach.

Project Title	*Moving the GBS code towards clusters based on a hybrid architecture*
Project Acronym (up to 8 characters)	*GBSHYB*

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Please duplicate the table above if Principal Investigators from more than one Research Unit

Requirements for the present largest run of the code

Total amount of CPU hours	1'000'000
Architecture(s) where application is already used	HELIOS, CRAY XE6, BlueGene/Q, and several other clusters
Number of CPUs	1024-2048
Memory requirements	500MB per core (+250MB with neutrals active)
Storage requirements	50GB
Pure MPI or mixed communication (OpenMP+MPI)	Pure MPI
Own code / 3rd party code	Own code
Code publicly available (yes/no)?	No
Library requirements	Lapack, FFTW, Pardiso, MUMPS, HDF5
Special requirements	
Site name(s) where application is already used	IFERC-CSC, CSCS, CADMOS, EPFL, NERSC
Expected usage of the IFERC computer (yes/no)?	Yes

Technical Improvement or adaptation work done so far

1. Do you apply in parallel for similar support from other institutions? No
2. Has your code/project already received support (especially as part of a previous HLST call) related to improvement of its computational capabilities? Yes.
   In a previous call the development of a flexible 2D domain decomposed parallel multigrid solver has been carried out and it has been implemented in GBS. This has avoided gathering the data into one single processor to invert the Poisson equations, allowing the full advancement of fluid equations on a decomposed domain and, furthermore, improving the parallel scalability of the code.

Request for work

a) Indicate nature (type) of HLST support being requested
   1. Porting the multigrid solver recently implemented in GBS to a mixed communication (OpenMP+MPI).
   2. Porting the multigrid solver to GPU/MIC architecture by changing the OpenMP directive into OpenACC and Intel Offload OpenMP.
   3. Coupling the multigrid solver to the GBS code.
   4. Testing the GBS code, now written with a mixed communication (MPI_+ OpenMP on the CPU + OpenACC for GPU or Intel offload OpenMP for MIC), on clusters based on hybrid architecture (MIC and GPU graphic accelerators).
   5. If time permits, porting the recently developed module for neutral dynamics implemented to the mixed communication.

b) Indicative level of support (in ppm[1]) 6ppm

Involvement of the project proponents

Indicate the effort (in ppm[1]) of the projects proponents to be given (in parallel to the HLST work) to the execution of the project
Staff from CRPP will participate in the implementation of the hybrid OpenMP +MPI parallelization of GBS. This is expected to account for 6 ppm.

Potential Impact

Indicate the estimated benefits that the HLST support activity will have on the software and physics modelling capabilities.

Thanks to the present project, the necessary steps to port the GBS code to hybrid-architecture clusters will be performed. As cluster systems built with general purpose processors are superseded today by platforms built around specialized multicore processors, the present project will allow to access today's most advanced supercomputers, attaining capabilities that are out of reach at the moment, in particular performing full size simulations of SOL plasma turbulence in JET and ITER.

[1] Note that 1ppy=12ppm

Detailed Project Description (max. 1-2 pages)

GBS (Global Braginskii Solver) [1] is an initial value code for the drift-reduced Braginskii equations proposed in [2]. Both the plasma equilibrium and the fluctuations are evolved as the result of the interplay between a plasma source, located in proximity of the last closed magnetic flux surface and mimicking the plasma flux from the core region, the radial turbulent transport, and the plasma losses at the limiter or divertor plates. Therefore, GBS simulations evolve self-consistently both the plasma profile and its fluctuations. Simulations are performed taking into account finite aspect ratio effects, with a toroidal limiter that can be placed at any poloidal angle. The code is mainly used to explore scrape-off layer (SOL) turbulence considering realistic tokamak parameters, focusing on the dependence of the plasma turbulence on magnetic shear, plasma beta, plasma shape, plasma size, and boundary conditions. Code developments are now in progress with the goal of describing more complex magnetic geometries.

In order to efficiently simulate SOL turbulence characterized by $k_{\|} \ll k_{\perp}$, the fluid equations are discretized using a second order accurate field-aligned finite-difference scheme. The $\mathbf{E}\times\mathbf{B}$ advective terms are treated using the Arakawa advection scheme, while the parallel convective terms are discretized with a second-order centered-difference method. Time is advanced using a standard explicit Runge-Kutta stepping. The performed benchmarks have included a rigorous verification carried out with the method of manufactured solutions.

The code is currently scientifically exploited on several HPC platforms, including HELIOS, with a parallelization based on a pure MPI. Thanks to the efficient parallelization, GBS can now perform simulations of the TCV and C-Mod tokamaks with realistic parameters. However, full size simulations of JET and ITER are still out of reach, but they might become possible by exploiting today's most advanced supercomputers or the clusters that will become available in the foreseen future. As cluster systems built with general-purpose processors are superseded today by platforms built around specialized multicore processors, we propose to carry out the necessary steps to port GBS to a hybrid architecture computer.

As a matter of fact, since GBS is based on a highly vectorizable numerical scheme (finite differences), it is an ideal candidate for this exercise. This requires implementing a mixed communication OpenMP+MPI, by revising the overall architecture of the GBS. We therefore propose to perform the following steps.

1. Porting the parallel multigrid solver recently implemented in GBS to a mixed communication (OpenMP+MPI). This is necessary to solve Poisson and Ampère equations that are required to approach the drift-reduced Braginskii model.
2. Porting the multigrid solver to GPU/MIC architecture by changing the OpenMP directive into OpenACC and Intel Offload OpenMP.
3. Coupling the multigrid solver to the GBS code. The idea is to have a part of GBS that runs on the CPU, in addition to the accelerated version of the multigrid. This part of the code should probably be optimized with OpenMP.
4. As a result, GBS will be written with a mixed communication (MPI + OpenMP on the CPU + OpenACC for GPU or Intel offload OpenMP for MIC). We then propose to test GBS on clusters based on hybrid architecture (MIC and GPU graphic accelerators). We will consider in particular exploiting the MIC processors that have recently been installed

on the Helios supercomputer and on the Piz Daint (Cray XC-30) supercomputer at the Swiss National Supercomputing Center, which is based on a hybrid GPU/CPU architecture.

5. If time permits, the recently developed module for neutral dynamics implemented in GBS to the mixed communication will also be ported to the hybrid computer architecture. This module requires approaching the inversion of a full matrix resulting from the discretization of an integral equation.

We finally note that, if the implementation of the new OpenMP-4 becomes mature enough, we will have parallelization made with MPI + OpenMP running on both CPU and accelerated devices.

References

[1] P. Ricci, F.D. Halpern, S. Jolliet, J. Loizu, A. Mosetto, A. Fasoli, I. Furno, C. Theiler, Simulation of plasma turbulence in scrape-off layer conditions: the GBS code, simulation results, and code validation, submitted to Plasma Physics and Controlled Fusion (2012).
[2] A. Zeiler, J.F. Drake, and B. Rogers, Phys. Plasmas 4, 2134 (1997)