Parallelization on a Hybrid Architecture of GBS, a Simulation Code for Plasma Turbulence at the Edge of Fusion Devices

C. Wersal, T.M. Tran, P. Emonts, F.D. Halpern, R. Jorge, J. Morales, P. Paruta, P. Ricci, F. Riva
École Polytechnique Fédérale de Lausanne (EPFL), Swiss Plasma Center (SPC), CH-1015 Lausanne, Switzerland

Introduction

GBS is a simulation code to evolve plasma turbulence in the edge of fusion devices. It solves 3D fluid equations for electrons and ions, Poisson’s and Ampere’s equations, and a kinetic equation for neutral atoms.

The GBS code

Two fluid drift-reduced Braginskii equations, \( \frac{k_B^2}{\Omega_p^2} \gamma^2 = \frac{k_B^2}{\Omega_p^2} \gamma^2 \), differ in \( \gamma^2 < \gamma^2 \omega \)

Amperé’s equation from Ohm’s law, \( \nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mathbf{e} \times \mathbf{E} \)

Stencil based parallel multigrid implemented in GBS. The elliptic equations are separable in the parallel direction leading to independent 2D solutions for each x-y plane.

The Poisson and Ampere equations

Poisson equation with Boussinesq approximation, \( \nabla^2 \phi \approx \omega \), or without, \( \nabla^2 \phi \approx \Omega \approx \gamma \nabla \phi \)

Stencils used for parallelization using the Crunge Kutta method. GBS uses a 3D Cartesian MPI communicator decomposing the computational 3D domain. OpenMP directives have been included recently.

The kinetic equation for neutral atoms

\( \frac{\partial n_i}{\partial t} + \nabla \cdot (\mathbf{v}_i n_i) = 0 \)

Method of characteristics to obtain the formal solution of \( h_i \)

Two assumptions: neutral losses \( \propto \) turbulence and Amp, neutrals \( \propto \) plasma, leading to a 2D steady state system for each x-y plane

Linear integral equation for neutral density obtained by integrating \( h_i \) over \( v \)

Spatial discretization leading to a linear system of equations

\( \mathbf{n}_i = \mathbf{r}_i - \sum_{i=1}^{n} k_i^{(1)} \mathbf{v}_i \mathbf{n}_i \)

This system is solved for neutral density, \( n_i \), and neutral particle flux at the boundaries, \( \mathbf{r}_i \), with the threaded LAPACK solver.

Scalability of MPI+OpenMP GBS

- Hybrid MPI+OpenMP with MPI_THREAD_FORKED (MPI calls only by thread 0)
- Basic OpenMP directives: parallel, do, single, master, barrier, simd
- Simple clauses: schedule(static), collapse
- Scalings performed on the Helios Supercomputer system at IFERC-CSC, two 8-core Sandy-brige processors and 64 GB memory on each node, InfiniBand network

Parallel Multigrid Solver with OpenACC

- Initialize the array TYPED grid_3d, grid_1 (levels) including grids, stencils, and solution arrays on the host and offload to the GPU before MG iterations start.
- No support for derived types with ALLOCATABLE members in OpenACC-2D: only shallow-copy of such derived types
- Extension of Cray Fortran: deep-copy with the compiler switch -fpseudo=deep-copy
- Offloading during MG iterations:
  - Residual norm and normalization scheme (16 Bytes) used in the stopping criteria
  - For multi-node multi-gpu version, additional offload of 2D boundary (10 buffers) for ghost cells exchange
- Run on a Cray XC30 (Piz Daint at CSCS) equipped with one 8-core Xeon ES-2670@2.6GHz and one NVIDIA Tesla K20X per node

3x speed-up from a single GPU (8 cores) to a single GPU

Good speed-up in the strong scaling for two GPUs, but saturation above four GPUs

In GBS the x-y planes are located closest in the 3D MPI communicator, so only two GPUs are involved in the 2D parareal solver, and parallel scalability up to 2-4 GPUs is sufficient.

Super-linear speed-up for the CPU parareal solver, probably due to inefficient cache use

The increase of execution time in the weak scaling is mainly due to the increase in exchange time (offloading and MPI communication)

Large problem size necessary for efficient use of many GPUs

Summary and Outlook

- The hybrid MPI+OpenMP parallelization implemented recently in GBS leads to performance improvements for the fluid equations in the code.
- The optimal distribution of processors between MPI and OpenMP depends on the chosen problem and platform. The scalability on many-core platforms (Xeon Phi) to be evaluated.
- Adind MPI+OpenMP multigrid Poisson solver developed as a first step in porting GBS to mixed CPU+GPU architectures.
- The fluid equations evaluation of GBS still to be ported to MPI+OpenACC. CPUs will be used for MPI ghost cell exchange and diagnostics output, while the main computation is to be carried out on the GPUs.

This work has been carried out within the framework of the EURospherion Consortium and has received funding from the European research and training programme 2014-2018 under grant agreement no 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

christoph.wersal@epfl.ch

PASC16 Platform for Advanced Scientific Computing Conference, Lausanne, Switzerland, 08-10 June 2016