APMA 2822B: Default Final Project No 1

Assignment:

Write a code for solving 3D Poisson equation:

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z)=f(x,y,z).$$

As an exact solution you can use φ = sin(n*π*x)*cos(m*π*y)*sin(k*π*z). Here, n,m,k are integer values (for example 2 or 4) . x, y and z are in the range of 0 to 1

The function “f” can be calculated from the analytical differentiation of φ.

The operator for the 2^{nd} order derivatives in each dimension can be based on structured grid, finite difference discretization and 3 point stencil:

second derivative of φ in x-dimension can be computed from (φ(x-Δx)-2*φ(x)+ φ(x+Δx))/(Δx*Δx).

Other discretization methods are also acceptable (finite elements, spectral methods, etc.).

Use Dirichlet boundary conditions for φ at x=0 and x=1, use periodicity at boundaries at y=0, y=1, z = 0 and z=1 The values of φ on the boundaries can be computed from the analytical solution. You need to solve for interior grid points only.

The computational domain φ and the field “f” must be decomposed into an arbitrary number of partitions and each partition should be assigned to one process (mpi rank). Use at least 8 partitions.

The computations within a partition can be done on either GPU or CPU using shared memory parallelism.

Similarly, to our exercises in the class, you can start from an arbitrary solution, for example φ=0, and then iterate using Jacobi method to obtain the final solution. Jacobi method will result in a slow convergence – it is recommended to use red-black algorithm to accelerate the convergence or other methods of your choice.

For execution of the code in parallel with domain decomposition, you will need to design the Halo exchange of φ across the partition boundaries; for this purpose, use non-blocking communication via MPI_Isend and MPI_Irecv.

To compute the residual and error you will need to use MPI_Allreduce.

Specific tasks (to be reflected in the final report):

1. Provide a roof-line analysis for each step of the solver.
2. If you compute on GPUs (recommended) profile your code using the NVIDIA nsigh profiler or AMD's rocprof
3. Plot the residual and error as a function of iteration count.
4. Describe the architecture of Halo exchange.
5. Describe all optimization methods you have applied (for example use of share memory on GPU, use of CUDA streams, cache blocking, choice of memory allocator, etc).

Prepare to present your efforts and answer questions during the final presentation. Assume 12-15 minutes per presentation. Write a detailed report (4-10 pages).

Use Oscar or HPCFUND computer or any other computer providing multiple servers (nodes) and adequate computational power within a node.

Remember that your report and presentation is a demonstration of the knowledge you have acquired during the class.

Please let me know if you have any questions.