

MATH 762 Homework 3 - Parallel computing

You have your choice of trying either an MPI or CUDA parallel computing example

SpectralMPI

Software installation

- Request an account on `killdevil.unc.edu`
- Download SpectralMPI from svn server

```
svn co http://mitran-lab.amath.unc.edu:8082/subversion/SpectralMPI/cd S
```
- Configure your environment to use gcc and OpenMPI

```
module initadd openmpi_gcc
```
- Go to the source code directory, download and install HDF4 support library

```
cd ./SpectralMPI/c  
wget http://www.hdfgroup.org/ftp/HDF/HDF_Current/bin/linux-x86_64/hdf-4.2.7-linux-x86_64.tar.gz  
tar zxvf hdf-4.2.7-linux-x86_64.tar.gz  
rm hdf-4.2.7-linux-x86_64.tar.gz  
ln -s hdf-4.2.7-linux-x86_64 hdf
```
- Download and install version 2.1.5 of FFTW

```
wget http://www.fftw.org/fftw-2.1.5.tar.gz  
tar zxvf fftw-2.1.5.tar.gz  
cd fftw-2.1.5  
make  
make install
```
- Modify the Makefile to reflect location of HDF and FFTW libraries

Tasks

1. Study the effect of hyperdiffusion ($n = 2$) versus normal diffusion ($n = 1$) for grid sizes of 128×128 and 512×512 .
2. Carry out a scaling study of performance with increasing number of CPUs for 512×512 , $N_{\text{CPU}} = 4, 8, 12, 16, 32, 64$.

Project ideas

1. Consider an additional vorticity source modeled physically as dependent on velocity magnitude leading to the equation

$$\theta_t = \psi_y \theta_x - \psi_x \theta_y + \nu \Delta \theta + a(\psi_x^2 + \psi_y^2)$$

2. Consider the interaction of vorticity with a phase-change model

$$\theta_t = \psi_y \theta_x - \psi_x \theta_y + \nu \Delta \theta - a \tau$$

$$\tau_t = \psi_y \tau_x - \psi_x \tau_y + \alpha \Delta \tau + b \theta.$$

qPAflow

Software installation

- Use your account on `pcoip01.its.unc.edu` and checkout a copy of the lattice Boltzmann code
`svn co http://mitran-lab.amath.unc.edu:8081/subversion/VirtualLung/qPAflow/`
- The lattice Boltzmann code is implemented in CUDA for GPU execution and called from a BEARCLAW application (refer to Homework 1 on BEARCLAW installation)
- Edit your `~/.bashrc` file
`export LBMLIB=$HOME/qPAflow/code/lib`

Example application

A simple example is flow in a pipe with square cross section

- `cd $HOME/qPAflow/code/examples/SquarePipe`

Tasks

1. Place a cubic obstacle in the channel and compute the resulting flow

Project ideas

1. Extend to multi-color (multiple species) Boltzmann
2. Include porous medium model