PSPFFT: Multi-threaded Parallel FFT-Based 3D Poisson Solver

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Introduction

- Many physics simulations require the solution of Poisson's equation
- Common example: Newtonian gravitational potential, potential of electric charge, spectral method
- We implement a method that employ Fourier transform to solve the discretized Poisson's equation on 3D system
- The solver, named PSPFFT ('Poisson Solver Parallel FFT') solves the equation globally on mesh block distributed across multiple processes on parallel computer
- It is suitable for large-scale parallel simulations

Poisson's Equation

- We need to solve

$$\nabla^2 \Phi(\mathbf{x}) = S(\mathbf{x})$$

with boundary condition $\Phi(\mathbf{x}) \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$

- Formal solution:

$$\Phi(\mathbf{x}) = \int d\mathbf{x}' G(\mathbf{x} - \mathbf{x}') S(\mathbf{x}')$$

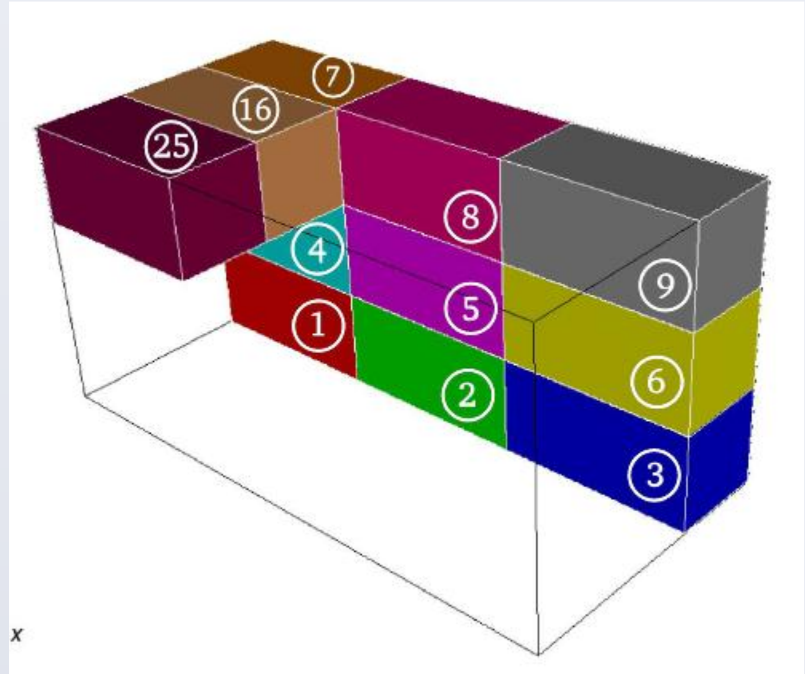
- By convolution theorem, evaluate the integral as:

$$\tilde{\Phi}(\mathbf{k}) = \tilde{G}(\mathbf{k}) \tilde{S}(\mathbf{k})$$

where $\tilde{\xi}(\mathbf{k})$ is the Fourier transform of $\xi(\mathbf{x})$

Mesh Decomposition

- Discrete Fourier transform is done with FFT
- $n\log(n)$ operation
- Optimized implementation provided by FFTW (can use other library)
- Not convenient for typical brick mesh decomposition

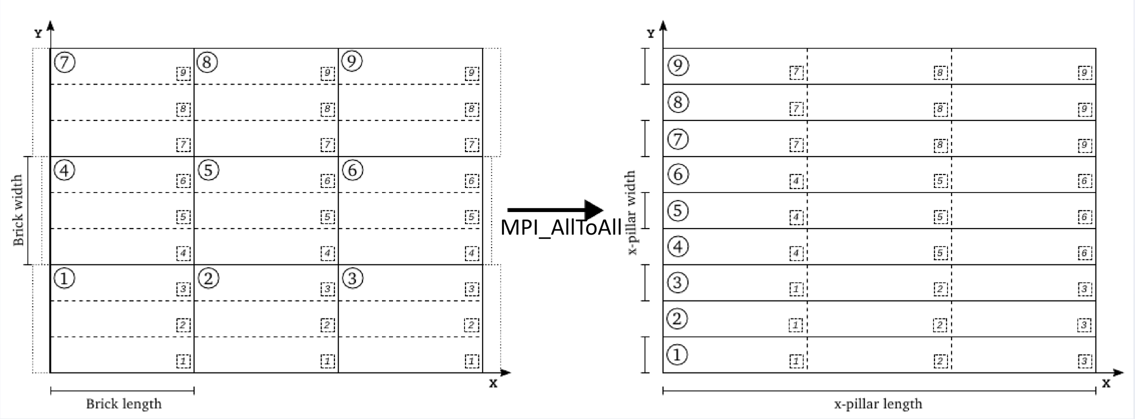


Code Description

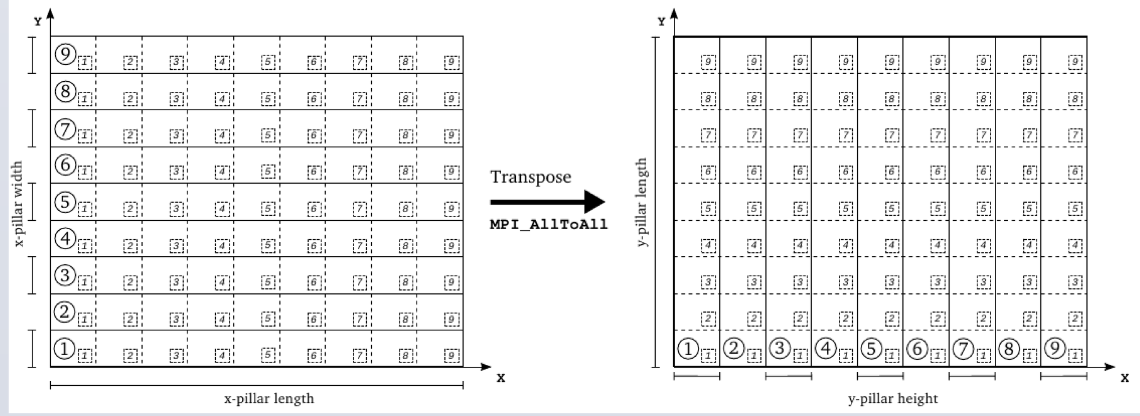
- PSPFFT is written in Fortran 2003 standard
- Follow object-oriented principle with abstraction, encapsulation, and polymorphism
- Currently uses FFTW, but usage is abstracted in one Fortran module such that other FFT libraries could be used without widespread code change
- Uses the latest FFTW Fortran interface and provides *façade* pattern for its *advanced* API
- Release will be available at **http://eagle.phys.utk.edu/pspfft**

Parallel Three-Dimensional FFT

- Transform 'bricks' to 'pillar' decomposition:



- Each MPI process performs multiple (*x-pillar width* times) 1D Fourier transform in parallel
- Multi-dimensional FFTs: sets of one-dimensional transform in each dimension
- Pillars decomposition has to be *transposed*
- Multiple MPI sub-communicators are created to transpose data in parallel

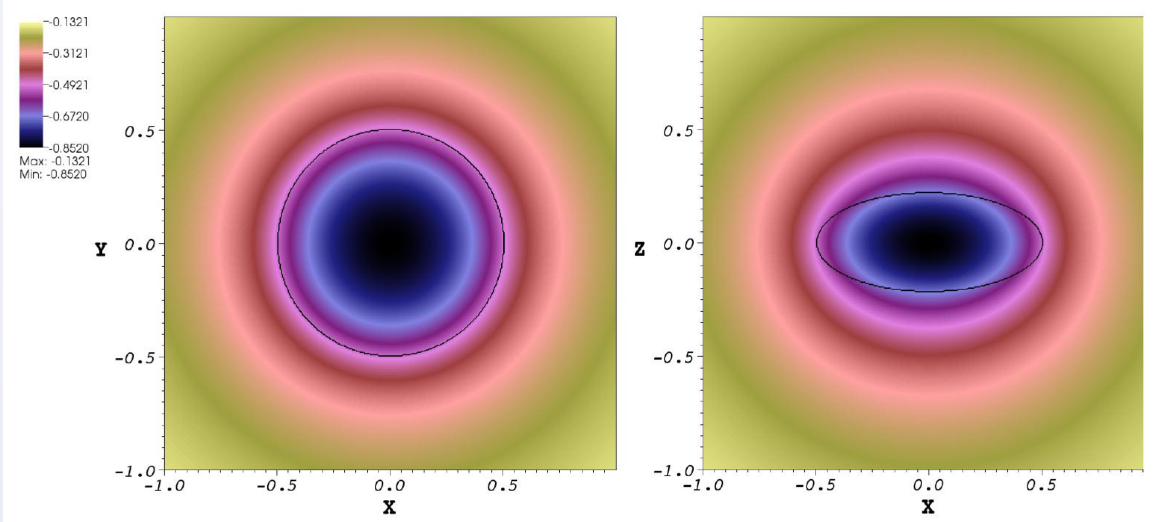


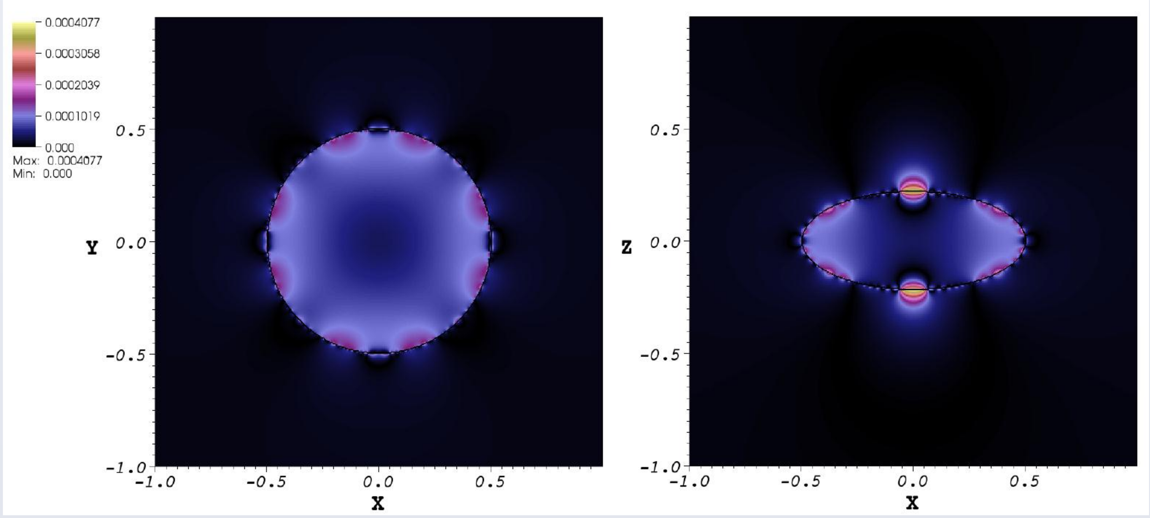
Multi-Threading using OpenMP

- Multiple numbers of 1D transform in each MPI process can be done in parallel using a team of threads
- Each thread is completely independent transform → linear scaling within an MPI process
- Thread-safe FFTW plan is required

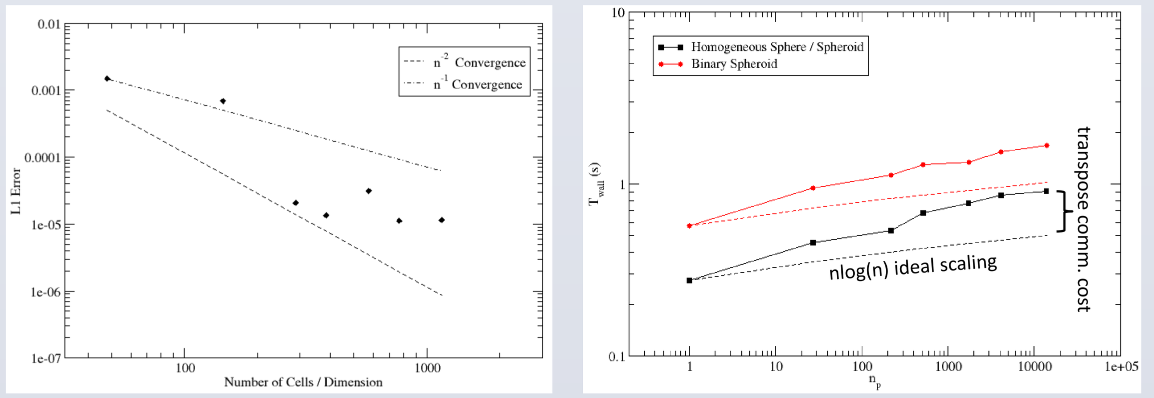
Results and Test Problems

- $\Phi(x)$ of homogeneous spheroid (and its relative error distribution)

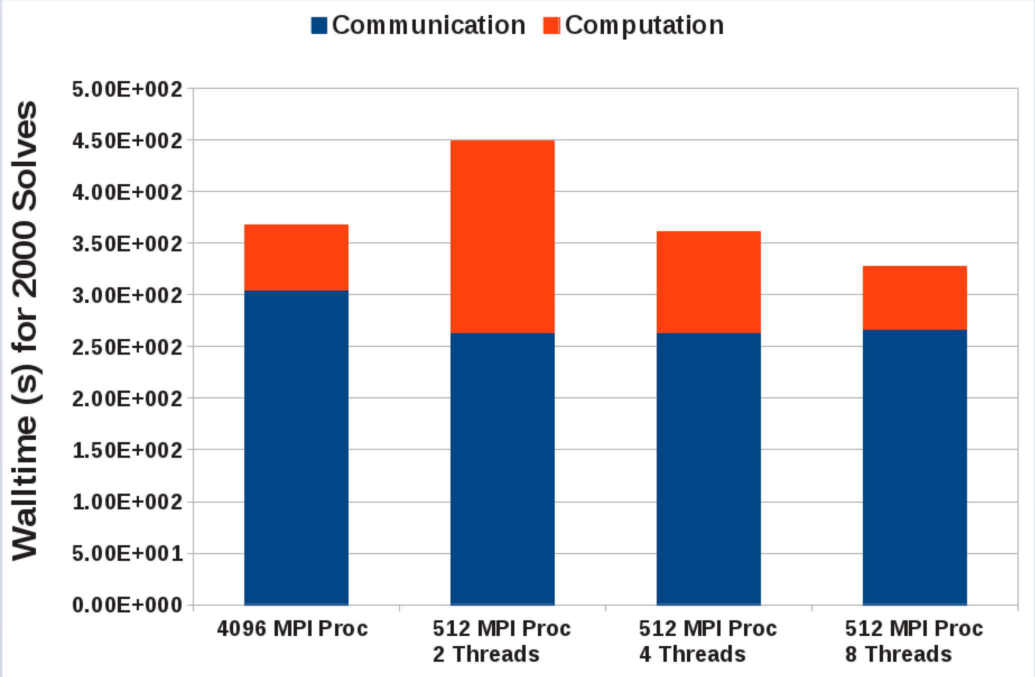




- Error convergence & weak scaling:



- MPI with OpenMP comparison:



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