Algorithm Design for Large Scale Parallel FFT-Based Simulations on CPU-GPU Platforms
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Motivation
Extreme memory requirements and high communication overhead prevent scaling of large scale iterative simulations involving parallel FFTs to higher grid sizes, which is necessary for high resolution analysis.

An example is that of Moulinec Suquet’s Basic Scheme to compute local stress and strain fields in materials, a partial differential equation simulation that uses FFTs.

3D Hooke’s law:

Elliptical PDE:

MSC Basic Scheme is solved by convolution with Green’s function using FFT.

Increasing grid resolution is desirable. However, larger problem sizes must be run with parallelized code. This requires large parallel FFT computations which means high memory usage and all-all communication.

Memory requirement increases 32.4k times!

Goal: Overcome these limitations and run stress-strain simulations for larger problem sizes

Our solution: An algorithm and software co-design for heterogeneous platforms using irregular domain decomposition and local FFTs.

Background
Algorithm 1 MSC Basic Scheme

Original method by Moulinec and Suquet

Stress and strain fields in grain interiors are smooth. Hence we can treat these as separate domains.

99% energy of the space-domain Green’s function is concentrated at central peak. Hence, Green’s function can be truncated before convolution.

Proposed Method
The proposed MSC Alternate Scheme is a co-design of algorithm and software for heterogeneous platforms. It enables scaling of stress-strain simulations to large grids by overcoming high memory requirements and communication bottlenecks.

Smooth stress fields in grain interiors can be compactly represented with data models. This reduces communication overhead.

Grain boundaries are convolved at full resolution without approximations.

Convergence of our method:

Ideal model characteristics

Phase I: Successes
Computational aspects for prototype development: MATLAB-FORTRAN workflow

Next iteration

Runs FORTRAN code

Writes data in each iteration

Processes data in MATLAB

Smooth regions for data modeling:

Convergence of our method:

Mismatch in stress field in each iteration compared to MSC Basic Scheme:

Stress field slice in MSC Basic Scheme:

Stress field slice in MSC Alternate Scheme:

Phase II: Plans
Thrust 1: Algorithm improvement

• De-noise convolution output

• Reduce model error

• Extend to different datasets with irregular grains

Thrust 2: Deployment on heterogeneous system with Tesla K80

Thrust 3: Support and adapt to different accelerators and machines

Thrust 4: Extend to visco-plastic code [2] which includes deformation of crystals and studies cracking and fracture formation

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References