Stokes Preconditioning on a GPU

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Collaborators

- Prof. Dave Yuen
  - Dept. of Geology and Geophysics, University of Minnesota
- Dr. David May, developer of BFBT (in PETSc)
  - Dept. of Earth Sciences, ETHZ
- Felipe Cruz, developer of FMM-GPU
  - Dept. of Applied Mathematics, University of Bristol
- Prof. Lorena Barba
  - Dept. of Mechanical Engineering, Boston University

Outline

BFBT

BFBT preconditions the Schur complement using

$$S_b^{-1} = L_p^{-1} G^T K G L_p^{-1} \tag{1}$$

where L_p is the Laplacian in the pressure space.

Current Problems

The current BFBT code is limited by

- Bandwidth constraints
  - Sparse matrix-vector product
  - Achieves at most 10% of peak performance
- Synchronization
  - GMRES orthogonalization
  - Coarse problem
- Convergence
  - Viscosity variation
  - Mesh dependence

Alternative Proposal

Use a Boundary Element Method,

for the Laplace solves in BFBT,

accelerated by FMM.

Missing Pieces

- BEM discretization and assembly
  - Matrix-free operator application using the Fast Multipole Method
  - Overcomes bandwidth limit, 480 GF on an NVIDIA 1060C GPU
  - Overcomes coarse bottleneck by overlapping direct work
- Solver for BEM system
  - Same total work as FEM due to well-conditioned operator
  - Possibility of multilevel preconditioner (even better)
- Interpolation between FEM and BEM
  - Boundary interpolation just averages
  - Can again use FMM for interior

Direct Fast Method for Variable-Viscosity Stokes

- Complexity not currently precisely quantified
  - We would like a given number of flops/digit of accuracy
- Brute Force
  - Use BEM to compute layers between regions of constant viscosity
  - Better conditioned, but not direct
- Elegant method should be possible
  - The operator is pseudo-differential
  - “Kernel-independent” FMM exists

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Problems

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- Synchronization
- Convergence

Outline

2 What are the Problems?
- Bandwidth
- Synchronization
- Convergence

Bandwidth

Small bandwidth to main memory can limit performance

- Sparse matrix-vector product
- Operator application
- AMG restriction and interpolation

STREAM Benchmark

Simple benchmark program measuring sustainable memory bandwidth

- Protoypical operation is Triad (WAXPY): $\mathbf{w} = \mathbf{y} + \alpha\mathbf{x}$
- Measures the memory bandwidth bottleneck (much below peak)
- Datasets outstrip cache

Machine	Peak (MF/s)	Triad (MB/s)	MF/MW	Eq. MF/s
Matt's Laptop	1700	1122.4	12.1	93.5 (5.5%)
Intel Core2 Quad	38400	5312.0	57.8	442.7 (1.2%)
Tesla 1060C	984000	102000.0*	77.2	8500.0 (0.8%)

Table: Bandwidth limited machine performance

http://www.cs.virginia.edu/stream/

Analysis of Sparse Matvec (SpMV)

Assumptions

- No cache misses
- No waits on memory references

Notation

m Number of matrix rows

nz Number of nonzero matrix elements

V Number of vectors to multiply

We can look at bandwidth needed for peak performance

$$\left(8+\frac{2}{V}\right)\frac{m}{nz}+\frac{6}{V}\ \mathrm{byte/flop} \tag{2}$$

or achieveable performance given a bandwith BW

$$\frac{Vnz}{(8V+2)m+6nz}BW\ \mathrm{Mflop/s} \tag{3}$$

Towards Realistic Performance Bounds for Implicit CFD Codes, Gropp, Kaushik, Keyes, and Smith.

Improving Serial Performance

For a single matvec with 3D FD Poisson, Matt's laptop can achieve at most

$$\frac{1}{(8+2)\frac{1}{7}+6} \text{ bytes/flop}(1122.4 \text{ MB/s}) = 151 \text{ MFlops/s}, \tag{4}$$

which is a dismal 8.8% of peak.

Can improve performance by

- Blocking
- Multiple vectors

but operation issue limitations take over.

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Better approaches:

- Unassembled operator application (Spectral elements, FMM)
  - N data, N^2 computation
- Nonlinear evaluation (Picard, FAS, Exact Polynomial Solvers)
  - N data, N^k computation

Outline

2 What are the Problems?
- Bandwidth
- Synchronization
- Convergence

Synchronization

Synchronization penalties can come from

- Reductions
  - GMRES orthogonalization
  - More than 20% penalty for PFLOTRAN on Cray XT5
- Small subproblems
  - Multigrid coarse problem
  - Lower levels of Fast Multipole Method tree

Outline

2. What are the Problems?
   - Bandwidth
   - Synchronization
   - Convergence

Convergence

Convergence of the BFBT solve depends on

- Viscosity constrast (slightly)
- Viscosity topology
- Mesh

Convergence of the AMG Poisson solve depends on

- Mesh

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Boundary Element Method

The Poisson problem

$$\Delta u(\mathbf{x}) = f(\mathbf{x}) \quad \text{on } \Omega \tag{5}$$

$$u(\mathbf{x})\,|_{\partial\Omega} = g(\mathbf{x}) \tag{6}$$

Boundary Element Method

The Poisson problem (Boundary Integral Equation formulation)

$$C(\mathbf{x})u(\mathbf{x}) = \int_{\partial\Omega} F(\mathbf{x},\mathbf{y})g(\mathbf{y}) - G(\mathbf{x},\mathbf{y})\frac{\partial u(\mathbf{y})}{\partial n} dS(\mathbf{y}) \quad (5)$$

$$G(\mathbf{x},\mathbf{y}) = -\frac{1}{2\pi}\log r \quad (6)$$

$$F(\mathbf{x},\mathbf{y}) = \frac{1}{2\pi r}\frac{\partial r}{\partial n} \quad (7)$$

Boundary Element Method

Restricting to the boundary, we see that

$$\frac{1}{2}g(\mathbf{x}) = \int_{\partial\Omega} F(\mathbf{x},\mathbf{y})g(\mathbf{y}) - G(\mathbf{x},\mathbf{y})\frac{\partial u(\mathbf{y})}{\partial n} dS(\mathbf{y}) \tag{5}$$

Boundary Element Method

Discretizing, we have

$$-Gq = \left(\frac{1}{2}I - F\right) g \tag{5}$$

Boundary Element Method

Now we can evaluate u in the interior

$$u(\mathbf{x}) = \int_{\partial\Omega} F(\mathbf{x},\mathbf{y})g(\mathbf{y}) - G(\mathbf{x},\mathbf{y})\frac{\partial u(\mathbf{y})}{\partial n} dS(\mathbf{y}) \tag{5}$$

Boundary Element Method

Or in discrete form

$$u = Fg - Gq \tag{5}$$

Boundary Element Method

The sources in the interior may be added in using superposition

$$\frac{1}{2}g(\mathbf{x}) = \int_{\partial\Omega} F(\mathbf{x},\mathbf{y})g(\mathbf{y}) - G(\mathbf{x},\mathbf{y})\left(\frac{\partial u(\mathbf{y})}{\partial n} - f\right) dS(\mathbf{y}) \tag{5}$$

Outline

3 Can we do Better?
- BEM Formulation
- BEM Solver
- Interpolation

BEM Solver

The solve has two pieces:

- Operator application
    - Boundary solve
    - Interior evaluation
    - Accomplished using the Fast Multipole Method
- Iterative solver
    - Usually GMRES
    - We use PETSc

Operator Application

Using the Fast Multiple Method,
the Green's functions (F and G) can be applied:

- in $\mathcal{O}(N)$ time
- using small memory bandwidth
- in the interior and on the boundary
- with much higher serial and parallel performance

Fast Multipole Method

FMM accelerates the calculation of the function:

$$\Phi(x_i) = \sum_j K(x_i, x_j) q(x_j) \tag{6}$$

- Accelerates $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$ time
- The kernel $K(x_i, x_j)$ must decay quickly from (x_i, x_i)
  - Can be singular on the diagonal (Calderón-Zygmund operator)
- Discovered by Leslie Greengard and Vladimir Rohklin in 1987
- Very similar to recent wavelet techniques

Fast Multipole Method

FMM accelerates the calculation of the function:

$$\Phi(x_i) = \sum_j \frac{q_j}{|x_i - x_j|} \tag{6}$$

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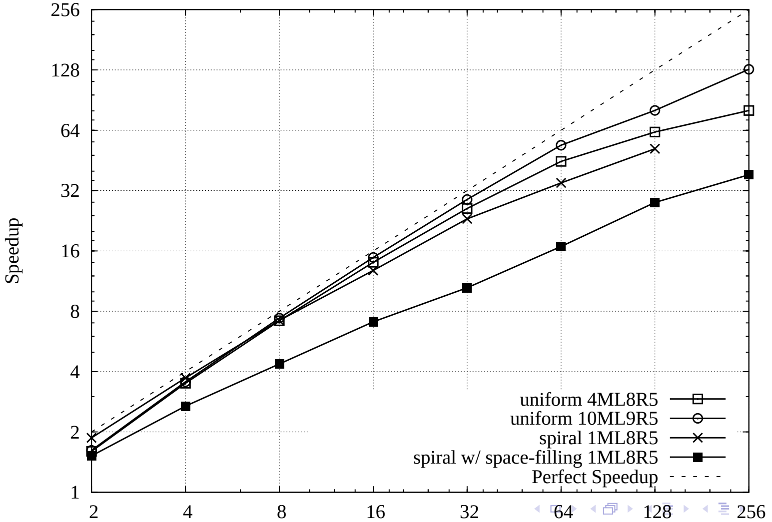
PetFMM CPU Performance
Strong Scaling



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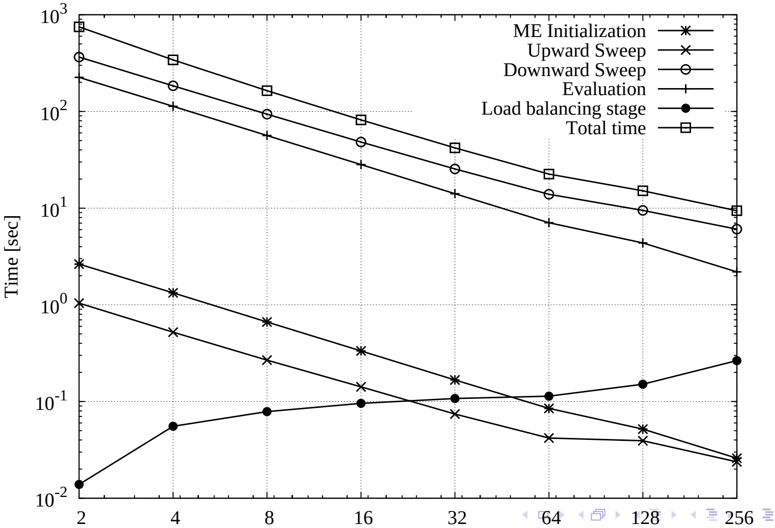
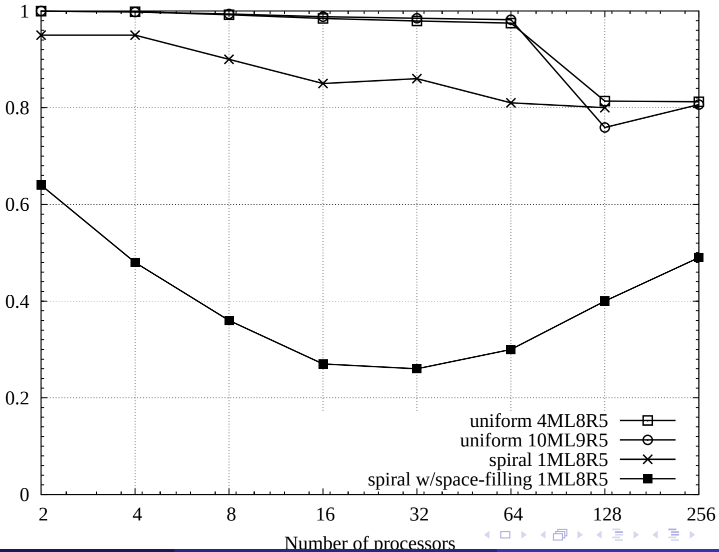


PetFMM Load Balance



GPU Performance

- In our C++ code on a CPU, M2L transforms take 85% of the time
  - This does vary depending on N
- New M2L design was implemented using PyCUDA
  - Port to C++ is underway
- We can now achieve 500 GF on the NVIDIA Tesla
  - Previous best performance we found was 100 GF
- We will release PetFMM-GPU in the new year

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PetFMM

PetFMM is an freely available implementation of the
Fast Multipole Method
http://barbagroup.bu.edu/Barba_group/PetFMM.html

- Leverages PETSc
  - Same open source license
  - Uses Sieve for parallelism
- Extensible design in C++
  - Templated over the kernel
  - Templated over traversal for evaluation
- MPI implementation
  - Novel parallel strategy for anisotropic/sparse particle distributions
  - PetFMM–A dynamically load-balancing parallel fast multipole library
  - 86% efficient strong scaling on 64 procs
- Example application using the Vortex Method for fluids
- (coming soon) GPU implementation

Convergence

BEM Laplace operator is well-conditioned

- $\kappa = \mathcal{O}(N_B) = \mathcal{O}(\sqrt{N})$
    - Dijkstra and Mattheij
- Thus the total work is in $\mathcal{O}(N_B^2) = \mathcal{O}(N)$
    - Same as MG
- Regular integral operators require only two multigrid cycles
    - Multigrid of the 2nd kind by Hackbush

Outline

3 Can we do Better?
- BEM Formulation
- BEM Solver
- Interpolation

FEM $\longleftrightarrow$ BEM

FEM $\longrightarrow$ BEM

- FEM boundary conditions can be directly used in BEM
- May require a `VecScatter`

FEM $\longleftarrow$ BEM

- BEM can evaluate the field at any domain point
- Cost is linear in the number of evaluations using FMM
- Can accomodate both
  - pointwise values, and
  - moments by quadrature

Outline

Outline

4 Advantages and Disadvantages
- Bandwidth
- Convergence

Bandwidth and Serial Performance

- Provably low bandwidth
  - Shang-Hua Teng, SISC, 19(2), 635–656, 1998
- Key advantage over algebraic methods like FFT
  - Similar to wavelet transform
- Amenable to GPU implementation
  - Also highly concurrent

Outline

4. Advantages and Disadvantages
   - Bandwidth
   - Convergence

Convergence and Synchronization

- BEM matrices are better conditioned
  - However, FEM has better preconditioners
  - Without better preconditioners, might see more synchronization
  - Underexplored
- FMM can avoid bottleneck at lower levels
  - Overlap direct work with lower tree levels
  - Can provably eliminate bottleneck

Debatable Advantages

- Small memory
  - FEM can be done matrix-free
- Opens door to using Stokes operator for PC
  - We currently do not know what to do here

Outline

1. 5 Slide Talk
2. What are the Problems?
3. Can we do Better?
4. Advantages and Disadvantages
5. What is Next?

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