Tree-based methods on GPUs

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Outline

FMM Applications for Geoscience

FMM can accelerate both integral and boundary element methods for:

- Laplace
- Stokes
- Elasticity

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Advantages

- Mesh-free
- $\mathcal{O}(N)$ time
- GPU and distributed parallelism
- Memory is greatly reduced in 3D for BEM

FMM Applications for Geoscience

Constant coefficient versions can precondition full equations:

- Work by Dave May at ETH
  - Solve Stokes
  - Scale identity by viscosity magnitude
- Advantages over MG
  - No grids have to be created
  - No iterative problems

Stokes Flow
Vorticity Formulation

In vorticity form, the Stokes equation conserves vorticity

$$\frac{\partial \omega}{\partial t} + u \cdot \nabla \omega = \frac{\mathrm{D}\omega}{\mathrm{D}t} = 0$$

and we can recover the velocity using the Biot-Savart law

$$\begin{aligned} u(x,t) &= \int (\nabla \times \mathbb{G})(x - x')\omega(x',t)dx' \\ &= \int \mathbb{K}(x - x')\omega(x',t)dx' = (\mathbb{K} * \omega)(x,t) \end{aligned}$$

where $\mathbb{G}$ is the Green function for the Poisson equation.

Stokes Flow
RBF Expansion

We expand the vorticity

$$\omega(x,t) \approx \omega_\sigma(x,t) = \sum_i^N \gamma_i \zeta_\sigma(x, x_i)$$

in a basis of radial functions

$$\zeta_\sigma(x,y) = \frac{1}{2\pi\sigma^2} \exp\left(\frac{-|x-y|^2}{2\sigma^2}\right)$$

resulting in the following kernel

$$\mathbb{K}_\sigma(x) = \frac{1}{2\pi|x|^2}(-x_2, x_1)\left(1 - \exp\left(-\frac{|x|^2}{2\sigma^2}\right)\right).$$

Stokes Flow
N-body Formulation

Thus the velocity evaluation is an *N*-body summation:

$$u_\sigma(x,t) = \sum_{j=1}^{N} \gamma_j \, \mathbb{K}_\sigma(x - x_j).$$

Fast Multipole Method

FMM accelerates the calculation of the function:

$$\Phi(x_i) = \sum_j K(x_i, x_j) q(x_j) \tag{1}$$

- 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

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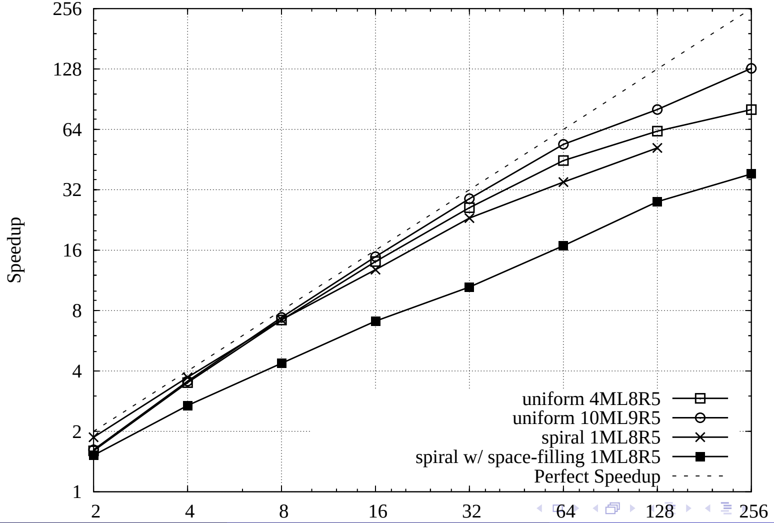
PetFMM

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

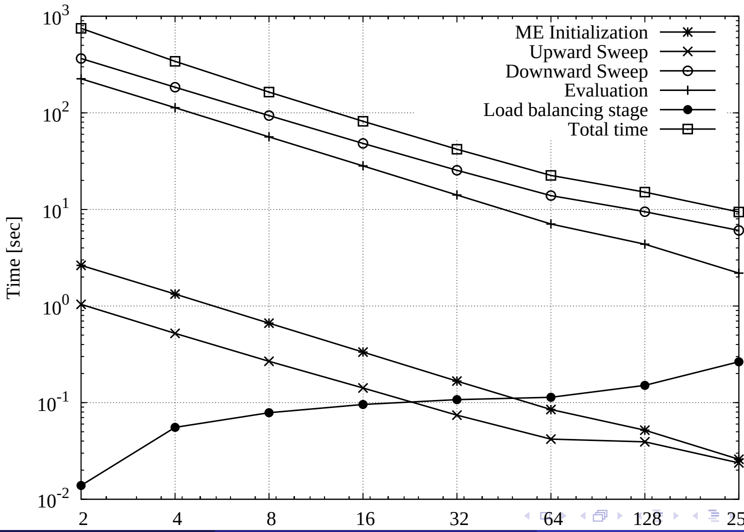
- Leverages PETSc
  - Same open source license
  - Uses Sieve for parallelism
- Extensible design in C++
  - Templated over the kernel
  - Templated over traversal for evaluation
- MPI implementation
  - Novel parallel strategy for anisotropic/sparse particle distributions
  - PetFMM–A dynamically load-balancing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

PetFMM CPU Performance

Strong Scaling



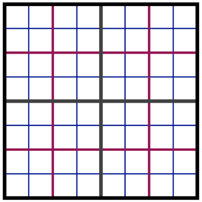
PetFMM CPU Performance
Strong Scaling

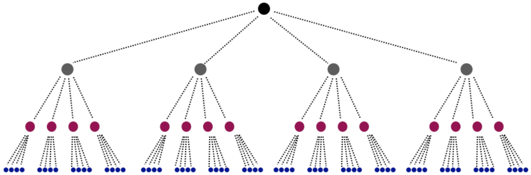


Outline

Spatial Decomposition

Pairs of boxes are divided into *near* and *far*:





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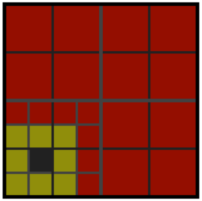

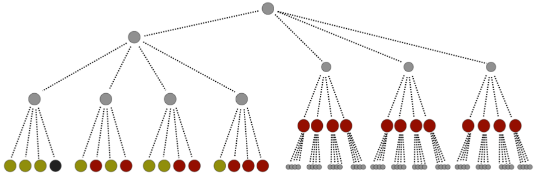

Neighbors are treated as *very near*.

Outline

FMM Sections

FMM requires data over the Quadtree distributed by:

- box
  - Box centers, Neighbors
- box + neighbors
  - Blobs
- box + interaction list
  - Interaction list cells and values
  - Multipole and local coefficients

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Notice this is multiscale since data is divided at each level

Outline

Greengard & Gropp Analysis

For a shared memory machine,

$$T = a\frac{N}{P} + b\log_4 P + c\frac{N}{BP} + d\frac{NB}{P} + e(N,P) \qquad (2)$$

1. Initialize multipole expansions, finest local expansions, final sum
2. Reduction bottleneck
3. Translation and Multipole-to-Local
4. Direct interaction
5. Low order terms

A Parallel Version of the Fast Multipole Method,
L. Greengard and W.D. Gropp, *Comp. Math. Appl.*, **20**(7), 1990.

Outline

GPU vs. CPU

A GPU looks like a big CPU with no virtual memory:

- Many more hardware threads encourage concurrency
- Makes bandwidth limitations even more acute
- *Shared memory* is really a user-managed cache
- *Texture memory* is also a specialized cache
- User also manages a very small code segment

GPU vs. CPU

Power usage can be very different:

Platform	TF	KW	GB/s	Price ($)	GF/$	GF/W
IBM BG/P	14	40.00	57.0*	1,800,000	0.008	0.35
IBM BlueGene	280	5000	???	350,000,000	0.0008	0.55
NVIDIA C1060	1	0.19	102.0	1,475	0.680	5.35
ATI 9250	1	0.12	63.5	840	1.220	8.33

Table: Comparison of Supercomputing Hardware.

GPU programming in General

- What design ideas are useful?
- How do we customize them for GPUs?
- Can we show an example?

Break Operations Into Small Chunks

Usually called modularity

- Also called *orthogonality* or *separation of concerns*
- Allows reduction of complexity
    - eXtreme programming
- Just concerned with functionality

Break Operations Into Small Chunks
GPU Differences

We now have to worry about code size!

- 16K total for NVIDIA 1060C board
    - Instructions can be a significant portion of memory usage
- Have to split operations which logically belong together
- Also allows aggregation of memory access
    - Computation can be regrouped
- Needs tools to manage many small tasks

Break Operations Into Small Chunks

Example

Reduction over a dataset

- For instance, computation of finite element integrals
- Break into *computation* and *aggregation* stages
- Model this by:
  - Maximum flop rate stage
  - Bandwidth limited stage

Break Operations Into Small Chunks
Example

Reduction over a dataset

- For instance, computation of Multipole-to-Local transform
- Break into *computation* and *aggregation* stages
- Model this by:
  - Maximum flop rate stage
  - Bandwidth limited stage

Reorder for Locality

Exploits “nearby” operations to aggregate computation

- Can be *temporal* or *spatial*
- Usually exploits a cache
- Difficult to predict/model on a modern processor

Reorder for Locality
GPU Differences

We have to manage our “cache” explicitly

- The NVIDIA 1060C shared memory is only 16K for 32 threads
- We must also manange “main memory” explicitly
  - Need to move data to/from GPU
- Must be aware of limited precision when reordering
- Can be readily modeled
- Need tools for automatic data movement (marshalling)

Reorder for Locality
Example

Data-Aware Work Queue

- A work queue manages many small tasks
  - Dependencies are tracked with a DAG
  - Queue should manage a single computational phase (supertask)
- Nodes also manage an input and output data segment
  - Specific classes can have known sizes
  - Can hold main memory locations for segments
- Framework manages marshalling:
  - Allocates contiguous data segments
  - Calculates segment offsets for tasks
  - Marshalls (moves) data
  - Passes offsets to supertask execution

Outline

PetFMM-GPU

We break down sweep operations into `Tasks`

- Cell loops are now tiled
- Tasks are queued
- We can form a DAG since we know the dependence structure
- Scheduling is possible

This asynchronous interface can enable

- Overlapping direct and multipole calculations
- Reorganizing the downward sweep
- Adaptive expansions

GPU Classes

`Section`

- `size()` returns the number of values
- `getFiberDimension(cell)` returns the number of cell values
- `restrict/update()` retrieves and changes cell values
- `clone/extract()` converts between CPU and GPU objects

`Evaluator`

- `initializeExpansions()`
- `upwardSweep()`
- `downwardSweepTransform()`
- `downwardSweepTranslate()`
- `evaluateBlobs()`
- `evaluate()`

GPU Classes

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`Task`

- Input data size
- Output data size
- Dependencies (future)

`TaskQueue`

- Manages storage and offsets
- `evaluate()`

Tasks

`Upward Sweep Task`

- cell block

in cell and child centers, child multipole coeff

out cell multipole coeff

`Downward Sweep Transform Task`

- cell block

in cell and interaction list centers, interaction list multipole coeff

out cell temp local coeff

`Downward Sweep Expansion Task`

- cell block

in cell and parent centers, cell temp local coeff, parent local coeff

out cell local coeff

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Tasks

`Upward Sweep Task`

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out cell multipole coeff

`Downward Sweep Reduce Task`

- cell block

in interaction list temp local coefficients

out cell temp local coefficients

`Downward Sweep Expansion Task`

- cell block

in cell and parent centers, cell temp local coeff, parent local coeff

out cell local coeff

Transform Task

Shifts interaction cell multipole expansion to cell local expansion

- Add a task for each interaction cell
- All tasks with same origin are merged
- Local memory:
  - 2 (p+1) blockSize (Pascal) + 2 p blockSize (LE) + 2 p (ME)

8 terms	4416 bytes
17 terms	9096 bytes

- Execution
  - 1 block per ME
  - Each thread reads a section of ME and the MEcenter
  - Each thread computes an LE separately
  - Each thread writes LE to separate global location

Reduce Task

Add up local expansion contributions from each interaction cell

- Add a task for each cell
- Local memory:
  - 2*terms (LE)

8 terms	64 bytes
17 terms	136 bytes

- Execution
  - 1 block per output LE
  - Each thread reads a section of input LE
  - Each thread adds to shared output LE

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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CPU vs GPU

Sample run for 250,000 vortex particles in an 8 level tree

Section	Time(s)	
	PyCUDA	Laptop C++
Setup	0.55	0.00
InitExpansions	10.74	0.93
UpSweep	0.36	5.02
DownSweepEnqueue	0.09	—
GPUOverhead	2.97	—
DownSweepM2LTrns	2.08	363.21
DownSweepM2LRed	0.45	—
DownSweepL2L	0.36	4.11

Notice that once direct evaluation is moved to the GPU, Python can easily outperform C++.

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3 Multicore Implementation
- Complexity Analysis
- Redesign

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Question

What is the optimal number of particles per cell?

- Greengard & Gropp
  - Minimize time and maximize parallel efficiency
  - $B_{opt} = \sqrt{\frac{c}{d}} \approx 30$
- Gumerov & Duraiswami
  - Follow GG, but also try to consider memory access
  - $B_{opt} \approx 91$, but instead, they choose 320
  - Heavily weights the N^2 part of the computation
- We propose to cover up the bottleneck with direct evaluations

Problem
Missing Concurrency

We can balance time in direct evaluation with idle time for small grids.

- The direct evaluation takes time $d\frac{NB}{p}$
- Assume a single thread group works on the first L tree levels

Thus, we need

$$B \geq \frac{b}{d}\frac{4^{L+1}p}{N} \tag{4}$$

in order to cover the bottleneck. In an upcoming publication, we show that this bound holds for all modern processors.

Problem
Missing Bandwidth

We can restructure the M2L to conserve bandwidth

- Matrix-free application of M2L
- Reorganize traversal to minimize bandwidth

Old	Pull in 27 interaction MEs, transform to LE, reduce
New	Pull in cell ME, transform to 27 interaction LEs, partially reduce

Matrix-Free M2L

The M2L transformation applies the operator

$$M_{ij} = -1^{i} t^{-(i+j+1)} \binom{i+j}{j} \tag{5}$$

Notice that the t exponent is constant along perdiagonals. Thus we

- divide by t at each perdiagonal
- calculate the C_{ij} by the recurrence along each perdiagonal
- carefully formulate complex division (STL fails here)

What's Important?

Interface improvements bring concrete benefits

- Facilitated code reuse
  - Serial code was largely reused
  - Test infrastructure completely reused
- Opportunites for performance improvement
  - Overlapping computations
  - Better task scheduling
- Expansion of capabilities
  - Could now combine distributed and multicore implementations
  - Could replace local expansions with cheaper alternatives