Tree-based methods on GPUs

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Outline

Scientific Computing Challenge

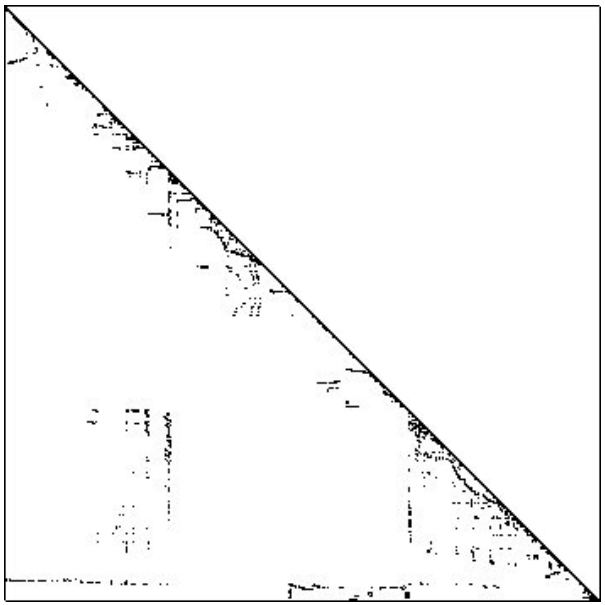
How do we create
reusable
implementations which are also
efficient?

Scientific Computing Insight

Structures are conserved,

but tradeoffs change.

Structure vs. Tradeoffs



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- Sparse matrix-vector product has a common structure
- Different storage formats are chosen based upon
  - architecture
  - PDE

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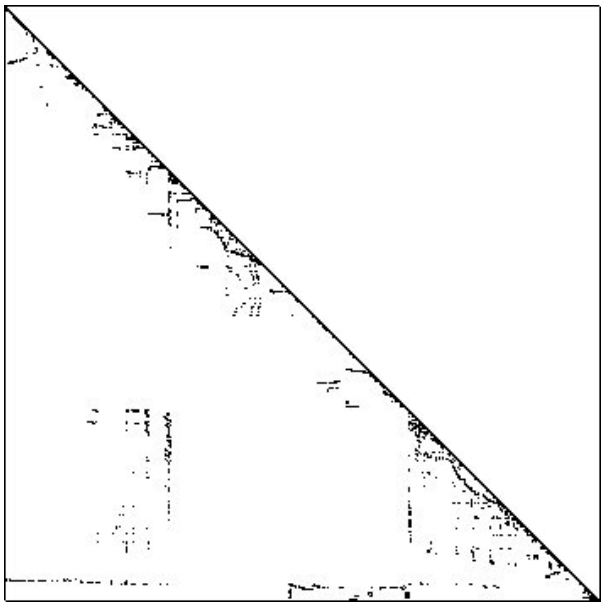

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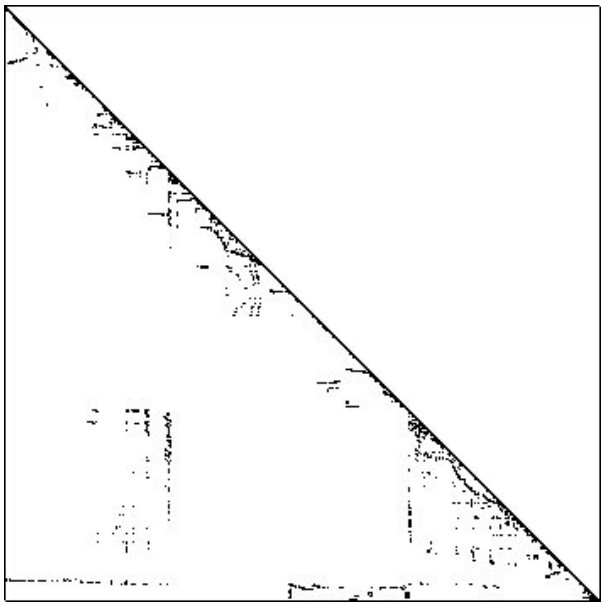

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$$A\,x = b$$

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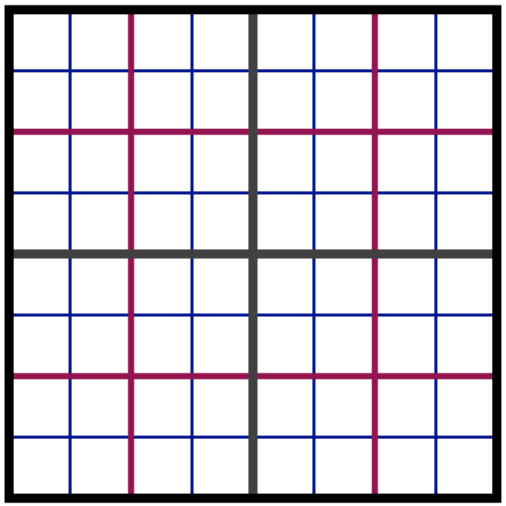

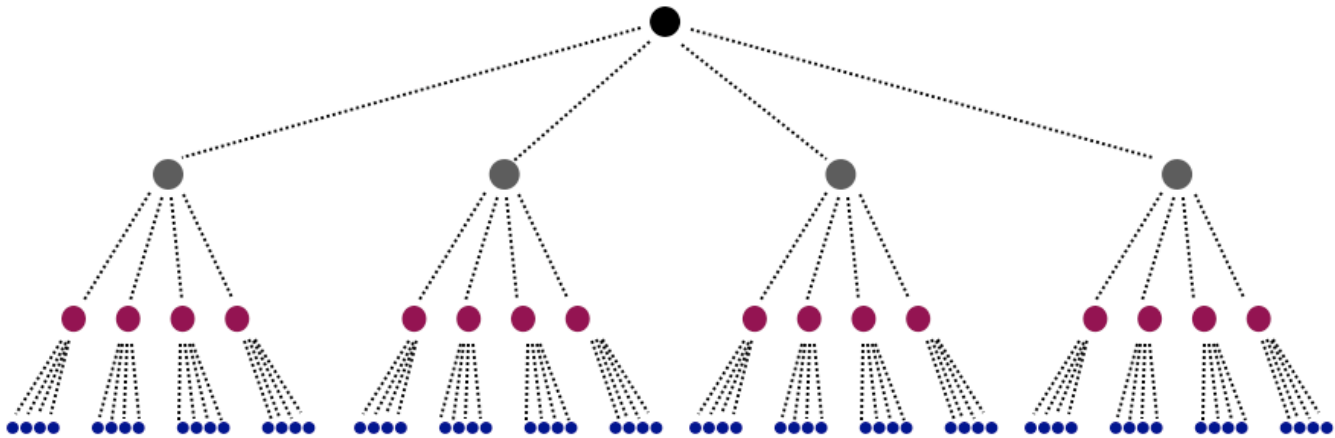

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- Hierarchical algorithms have a common structure
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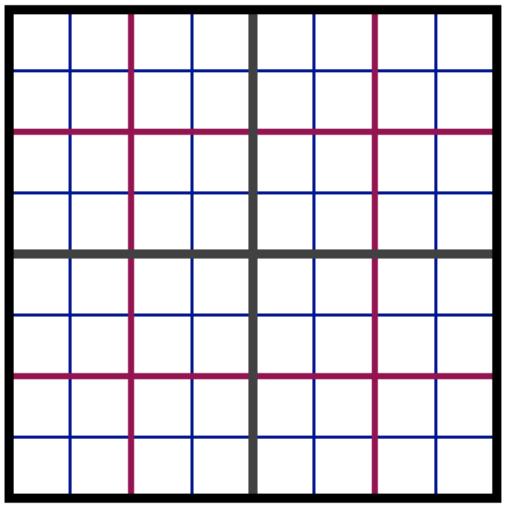

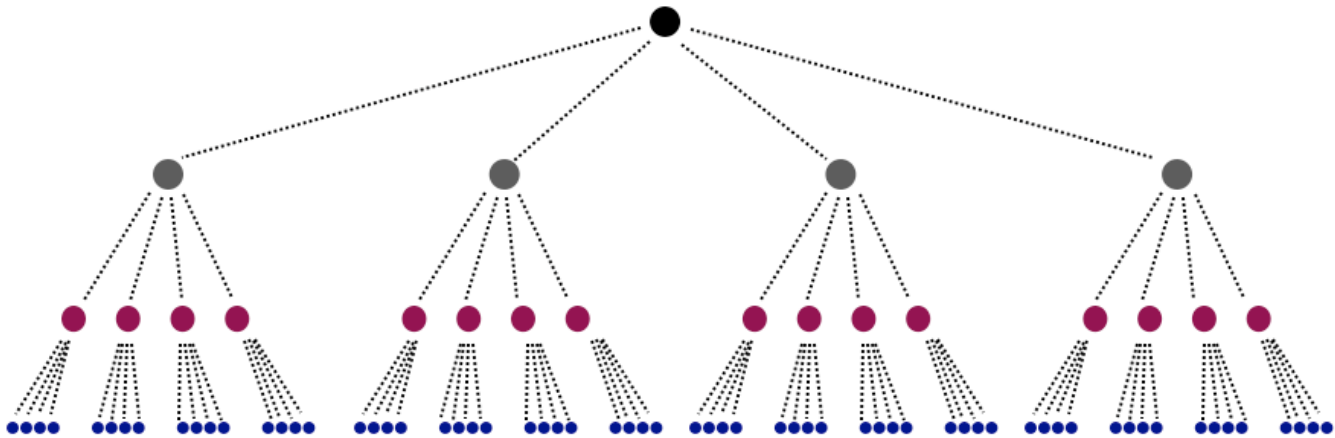

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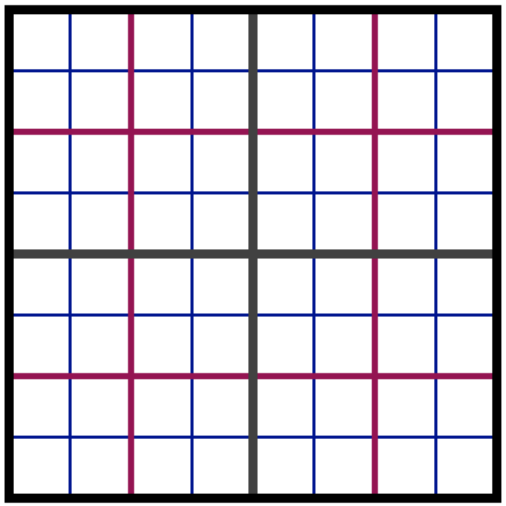

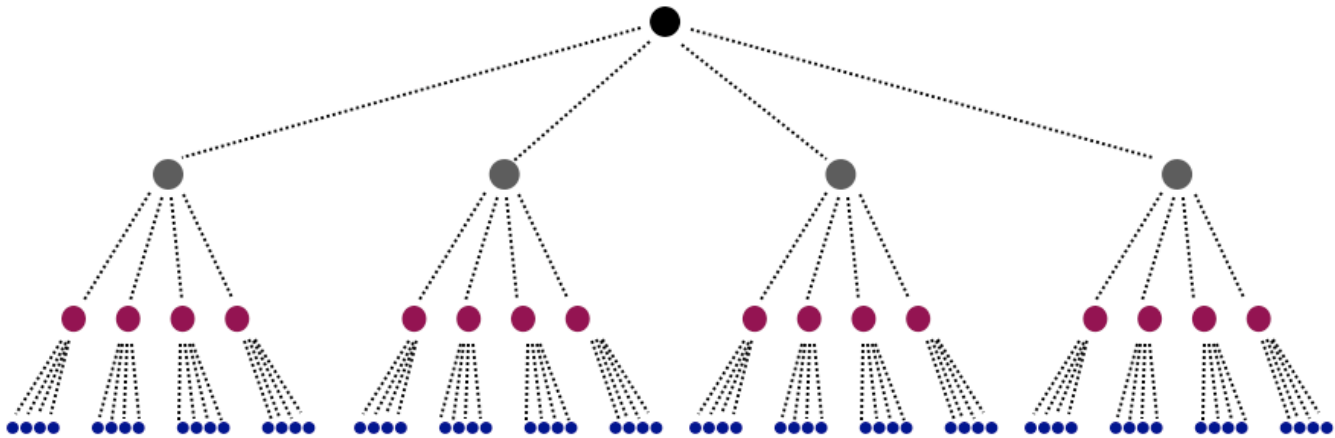

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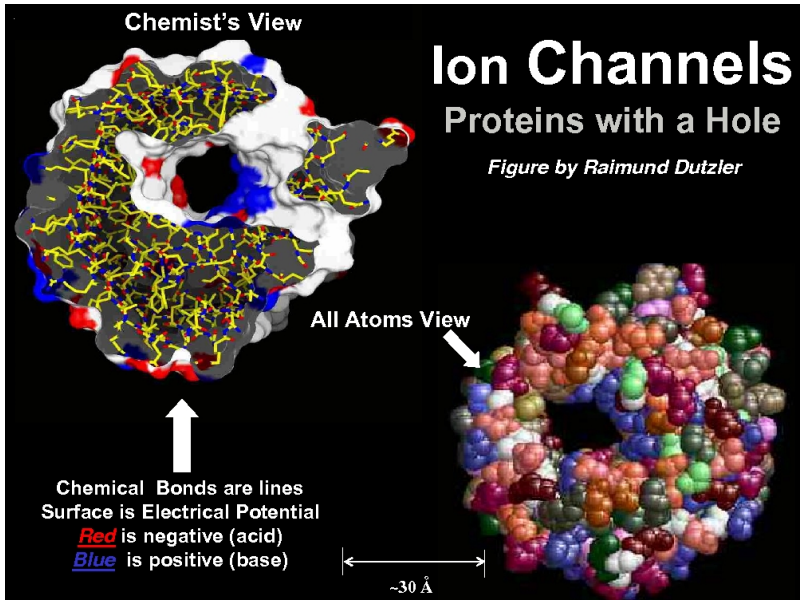
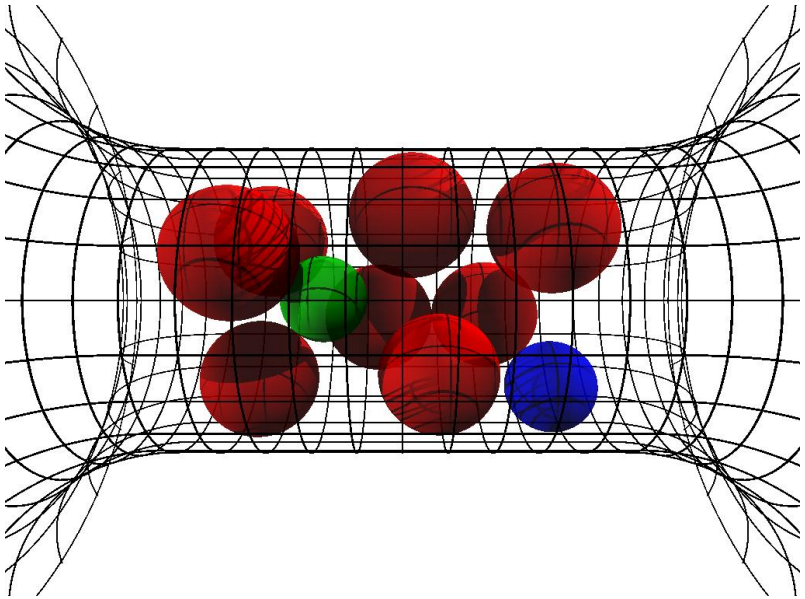


This is how biology works:

- For ion channels, Nature uses the same
  - protein building blocks
  - energetic balances
- Different energy terms predominate for different uses

Structure vs. Tradeoffs



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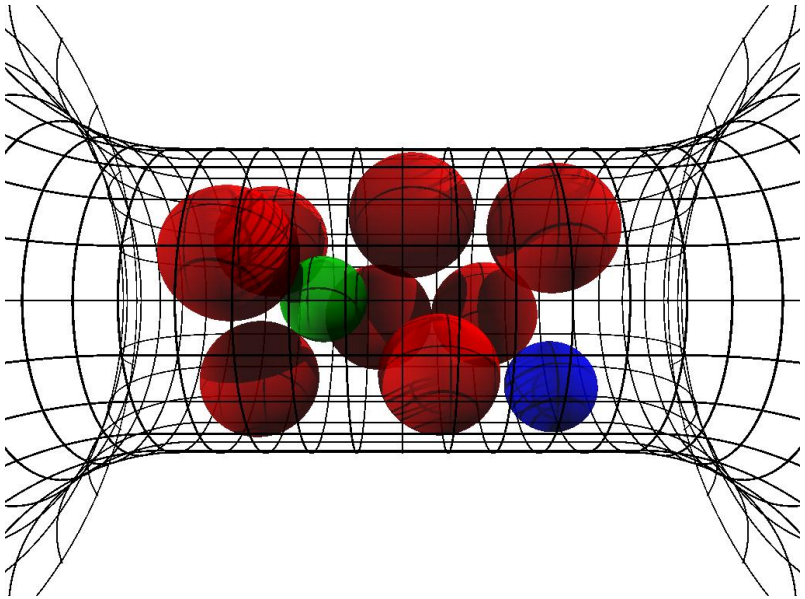

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Representation Hierarchy

Divide the work into levels:

- Model
- Algorithm
- Implementation

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Spiral Project:

- **D**iscrete **F**ourier **T**ransform (DSP)
- **F**ast **F**ourier **T**ransform (SPL)
- C Implementation (SPL Compiler)

Representation Hierarchy

Divide the work into levels:

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FLAME Project:

- Abstract LA (PME/Invariants)
- Basic LA (FLAME/FLASH)
- Scheduling (SuperMatrix)

Representation Hierarchy

Divide the work into levels:

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- Implementation

FEniCS Project:

- Navier-Stokes (FFC)
- Finite Element (FIAT)
- Integration/Assembly (FErari)

Representation Hierarchy

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Treecodes:

- Kernels with decay (Coulomb)
- Treecodes (PetFMM)
- Scheduling (PetFMM-GPU)

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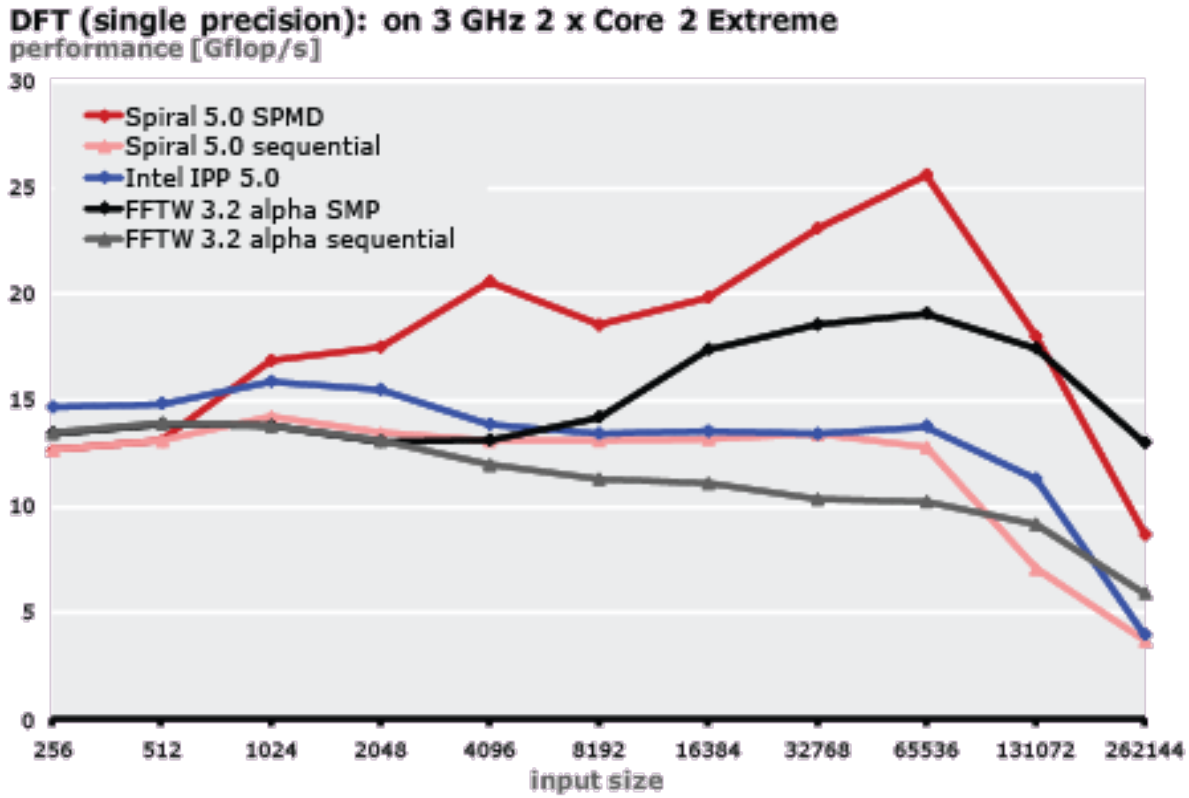
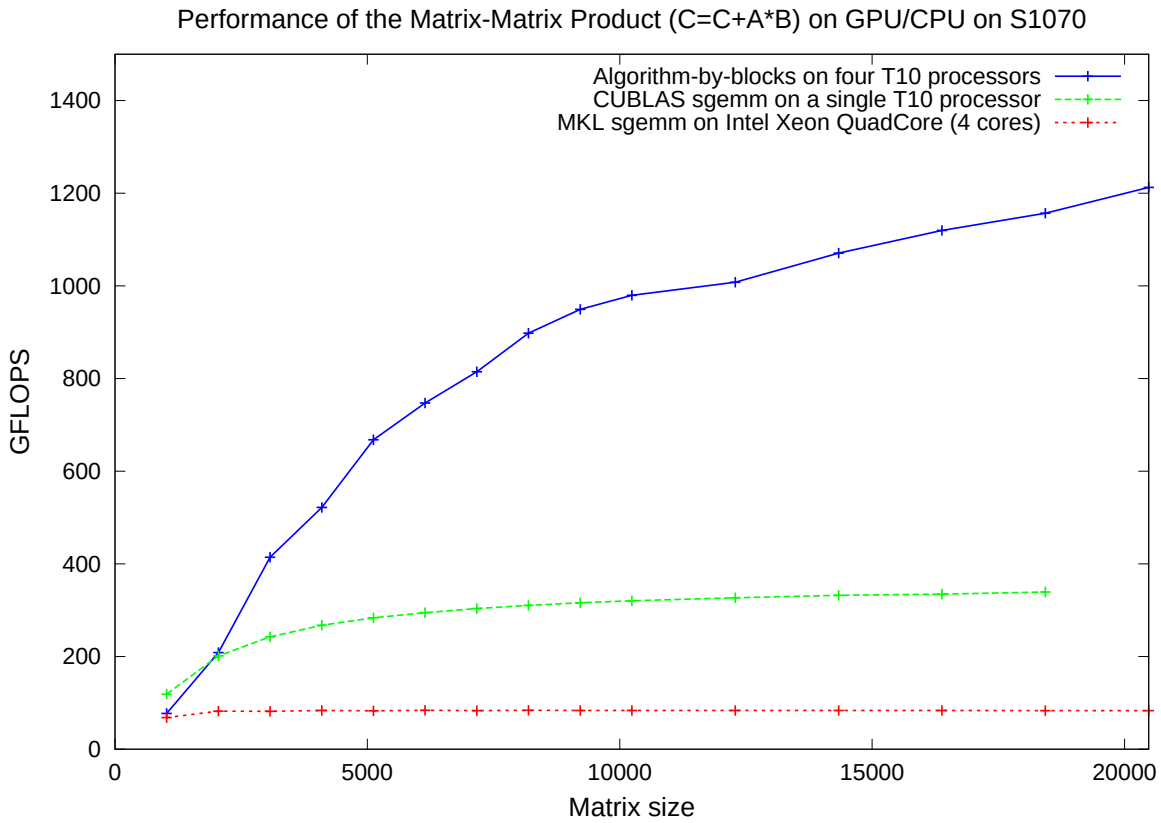
Each level demands a strong abstraction layer

Spiral



- Spiral Team, http://www.spiral.net
- Uses an intermediate language, SPL, and then generates C
- Works by circumscribing the algorithmic domain

FLAME & FLASH



- Robert van de Geijn, http://www.cs.utexas.edu/users/flame
- FLAME is an Algorithm-By-Blocks interface
- FLASH/SuperMatrix is a runtime system

Outline

FMM Applications

FMM can accelerate both integral and boundary element methods for:

- Laplace
- Stokes
- Elasticity

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Advantages

- Mesh-free
- $\mathcal{O}(N)$ time
- Distributed and multicore (GPU) parallelism
- Small memory bandwidth requirement

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

FMM accelerates the calculation of the function:

$$\Phi(x_i) = \sum_j \frac{q_j}{|x_i - x_j|} \tag{1}$$

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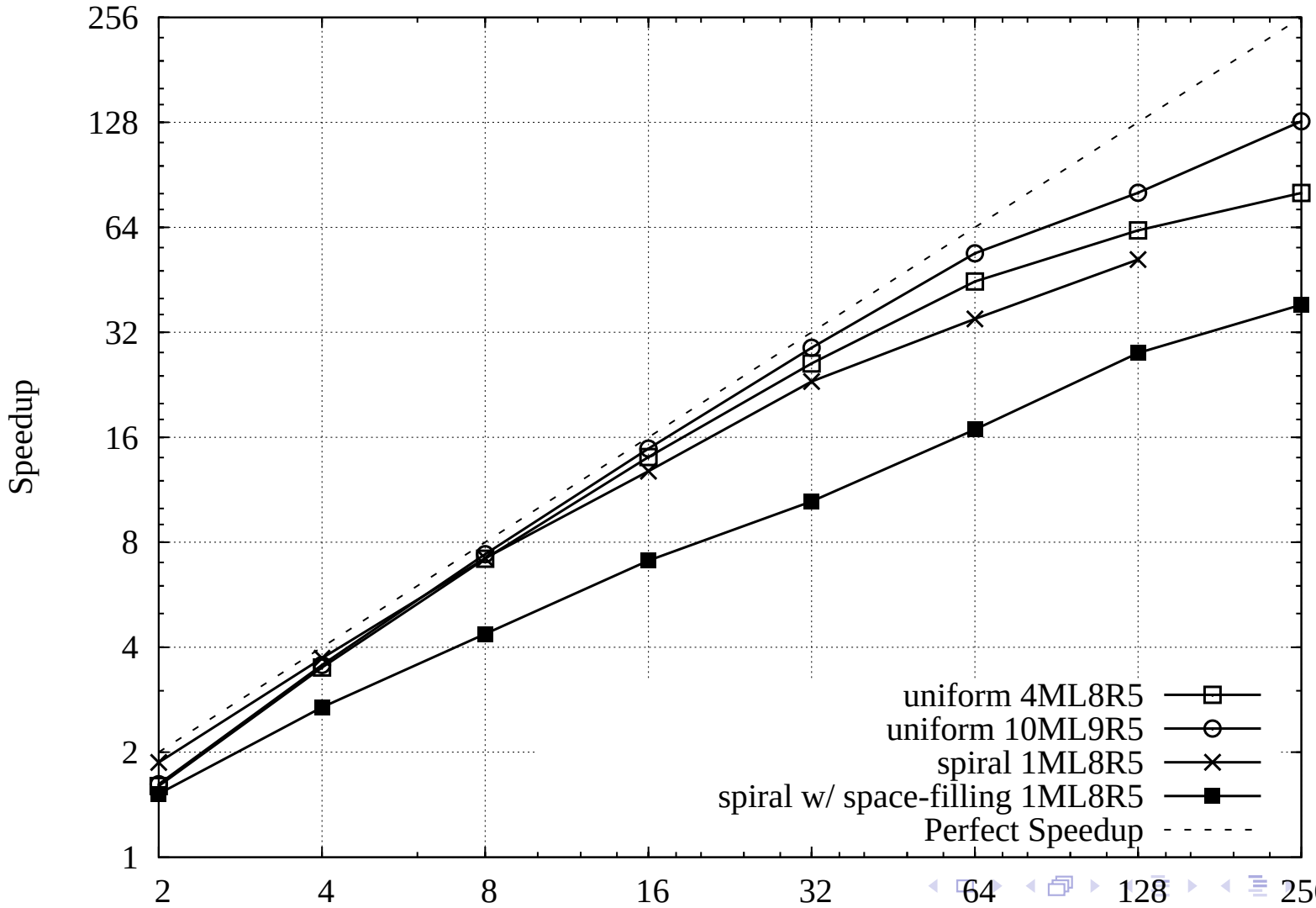
PetFMM

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

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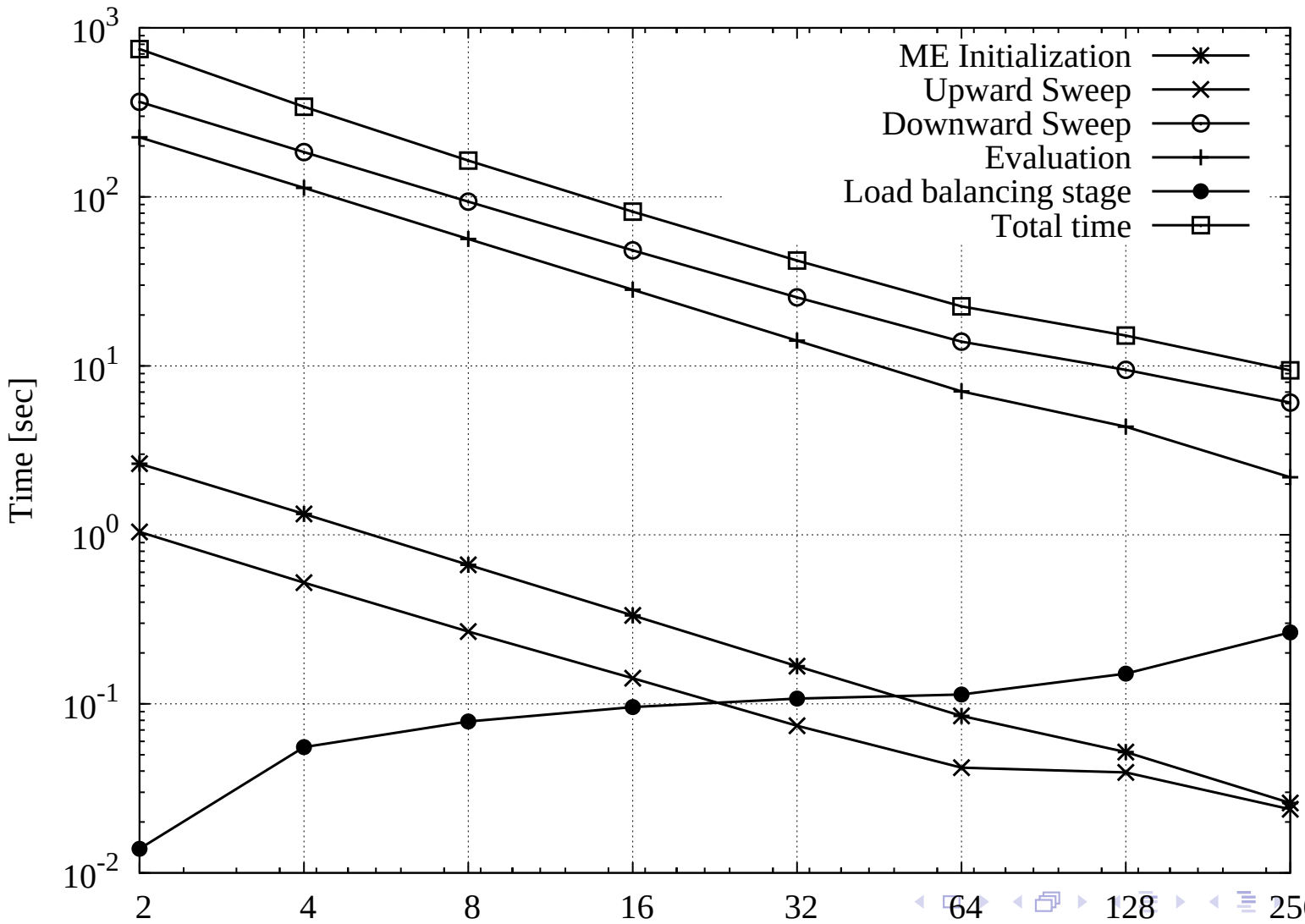

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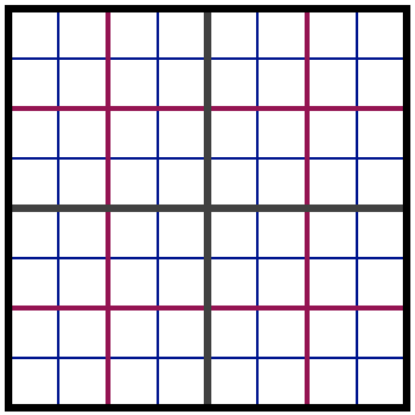
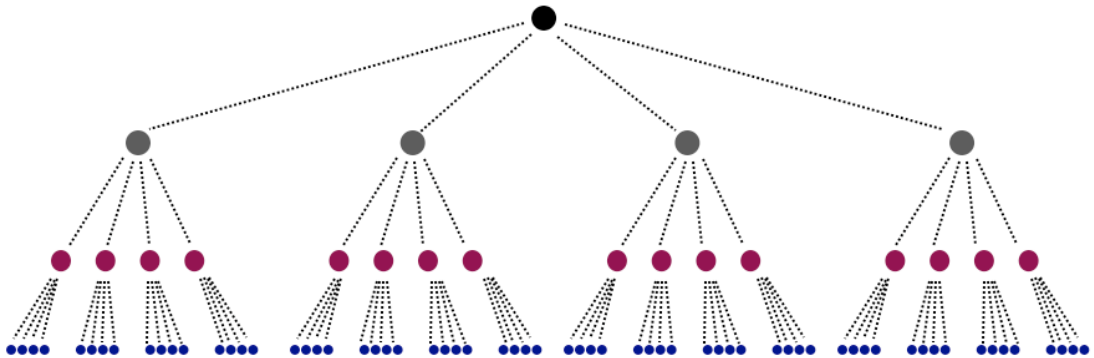
Spatial Decomposition

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





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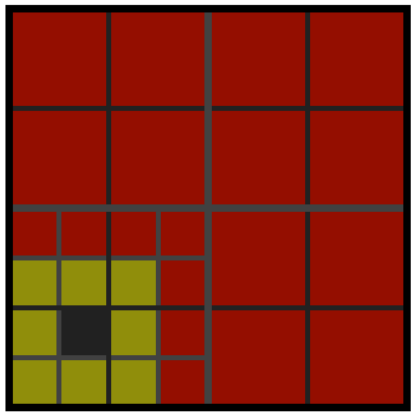
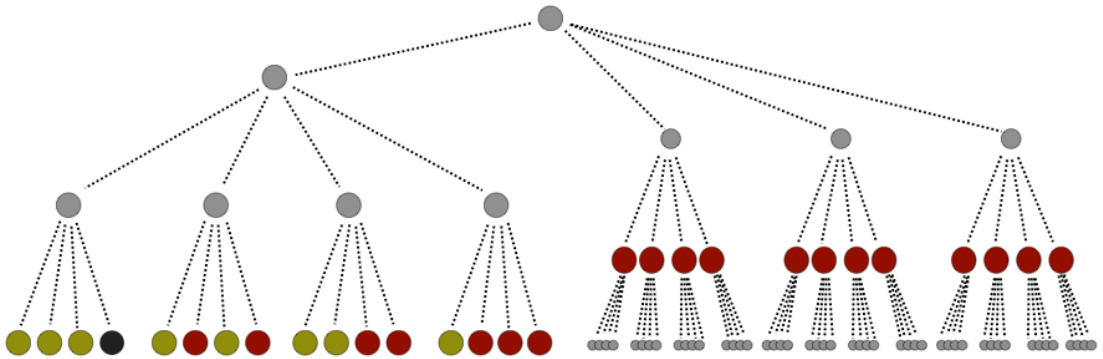
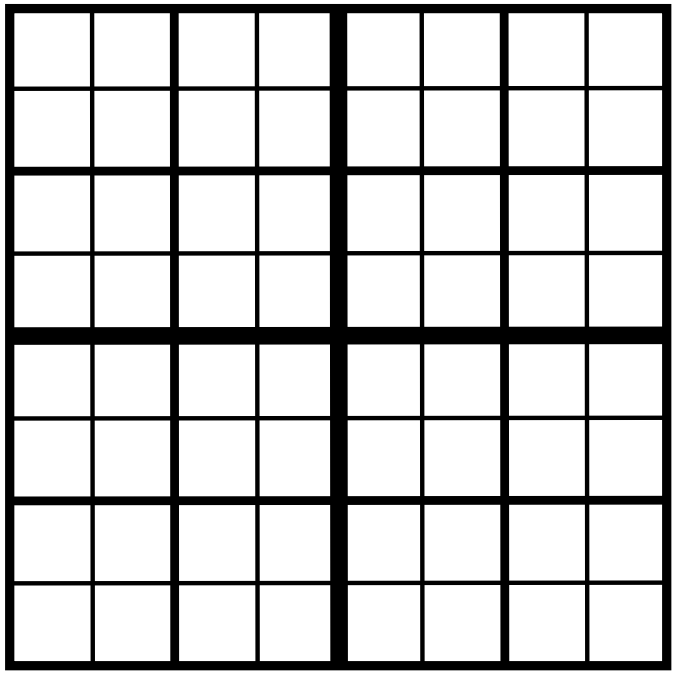




Neighbors are treated as *very near*.

FMM in Sieve



- The Quadtree is a `Sieve`
  - with optimized operations
- Multipoles are stored in `Sections`
- Two `Overlaps` are defined
  - Neighbors
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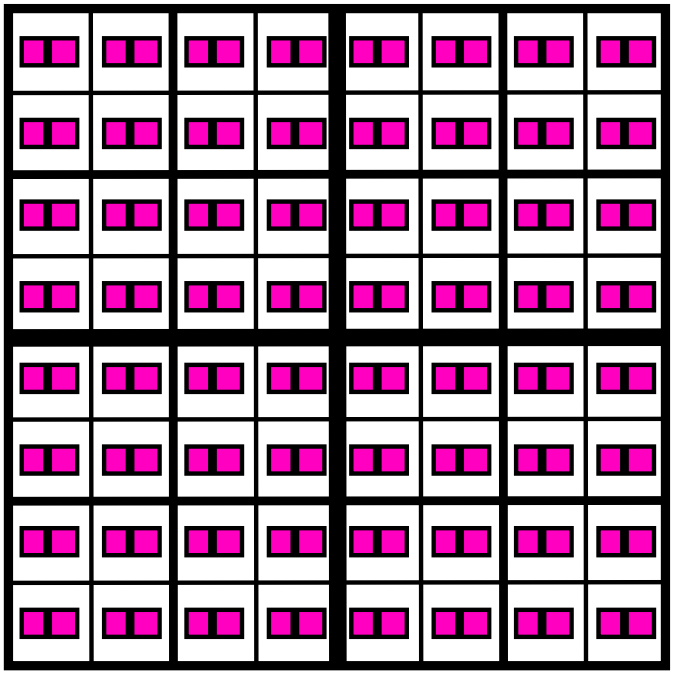

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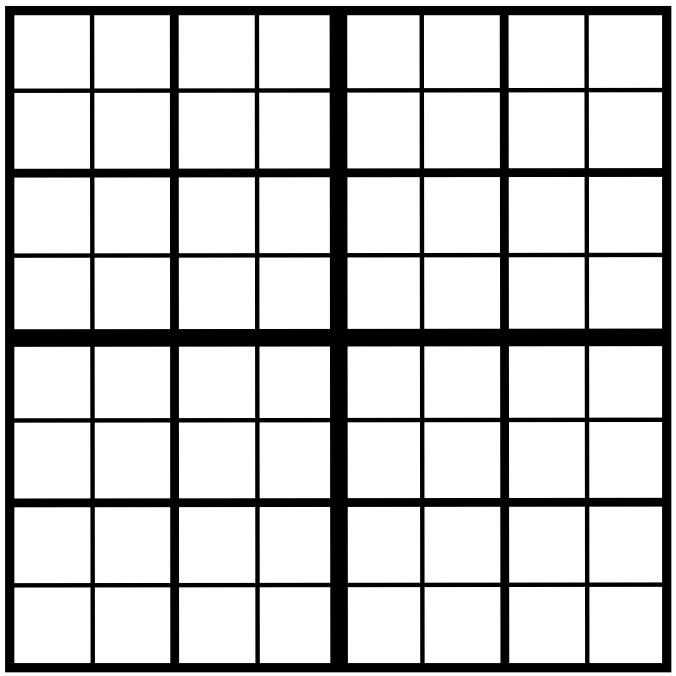

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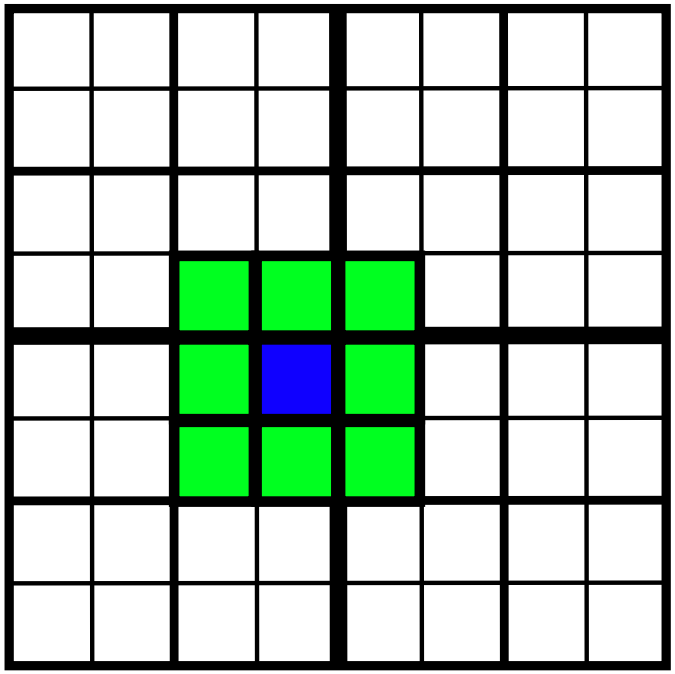

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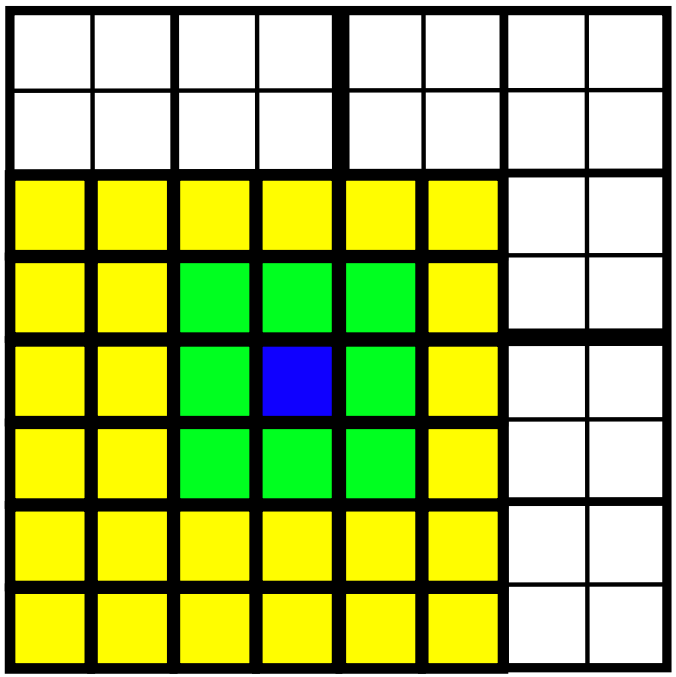

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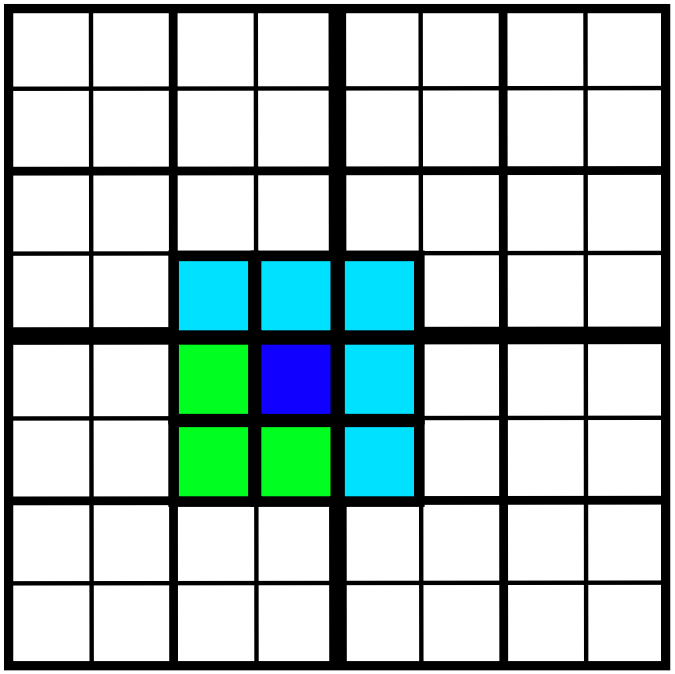

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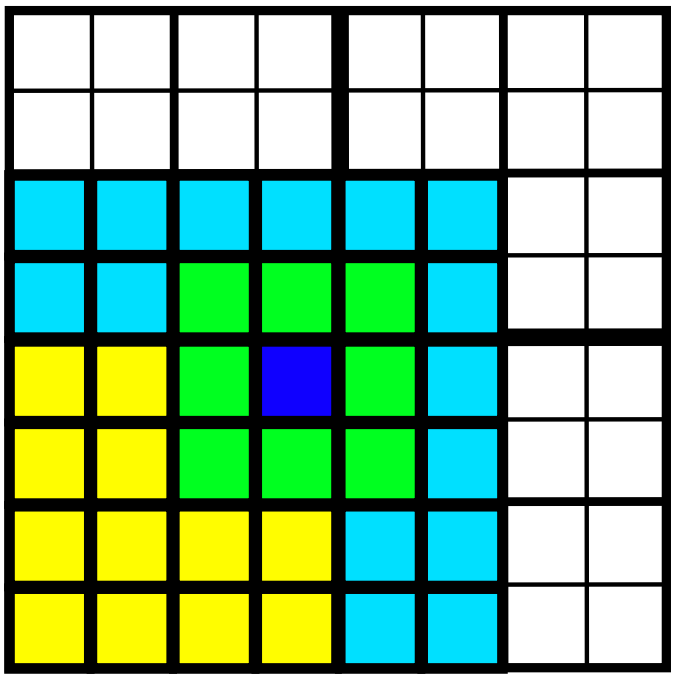

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FMM Sections

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

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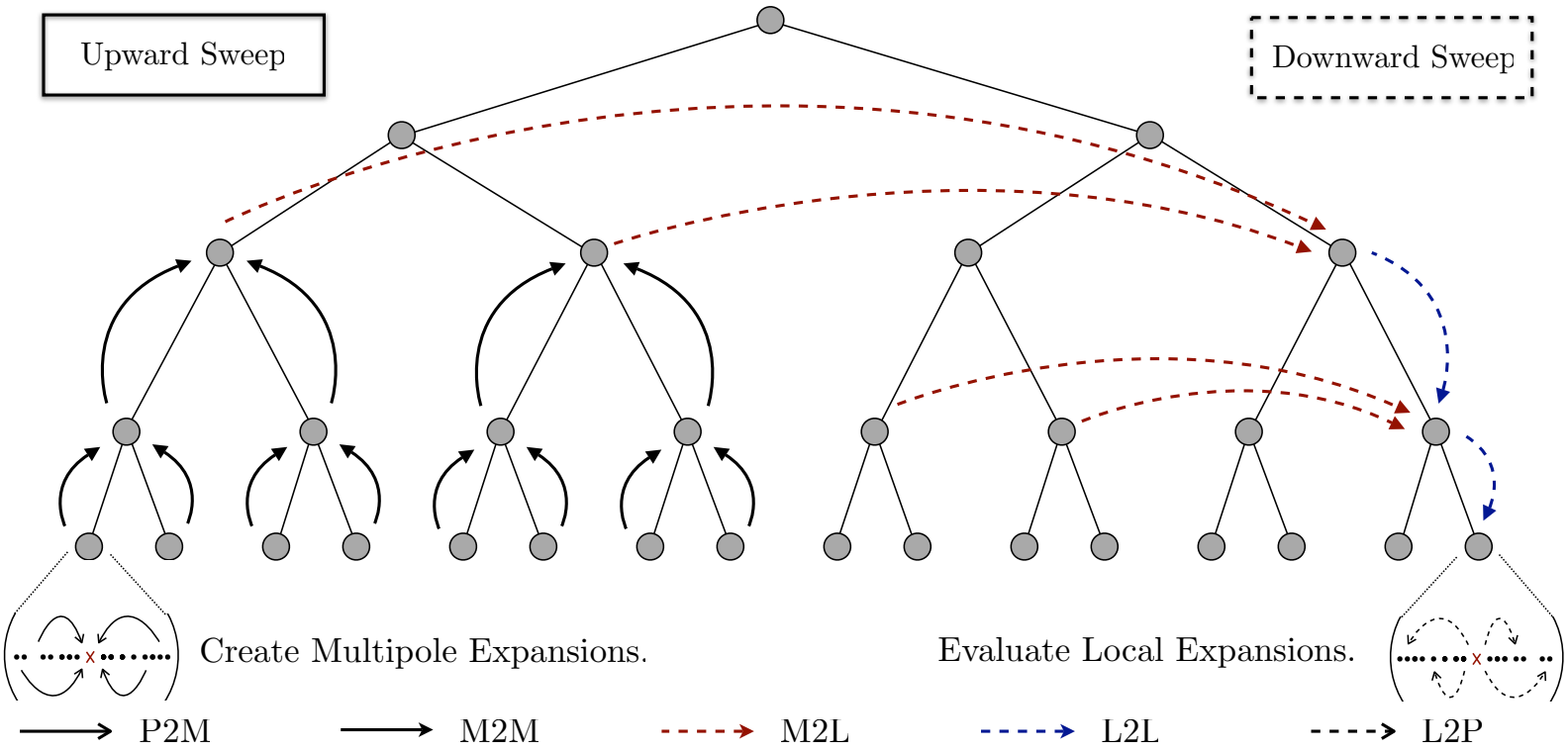
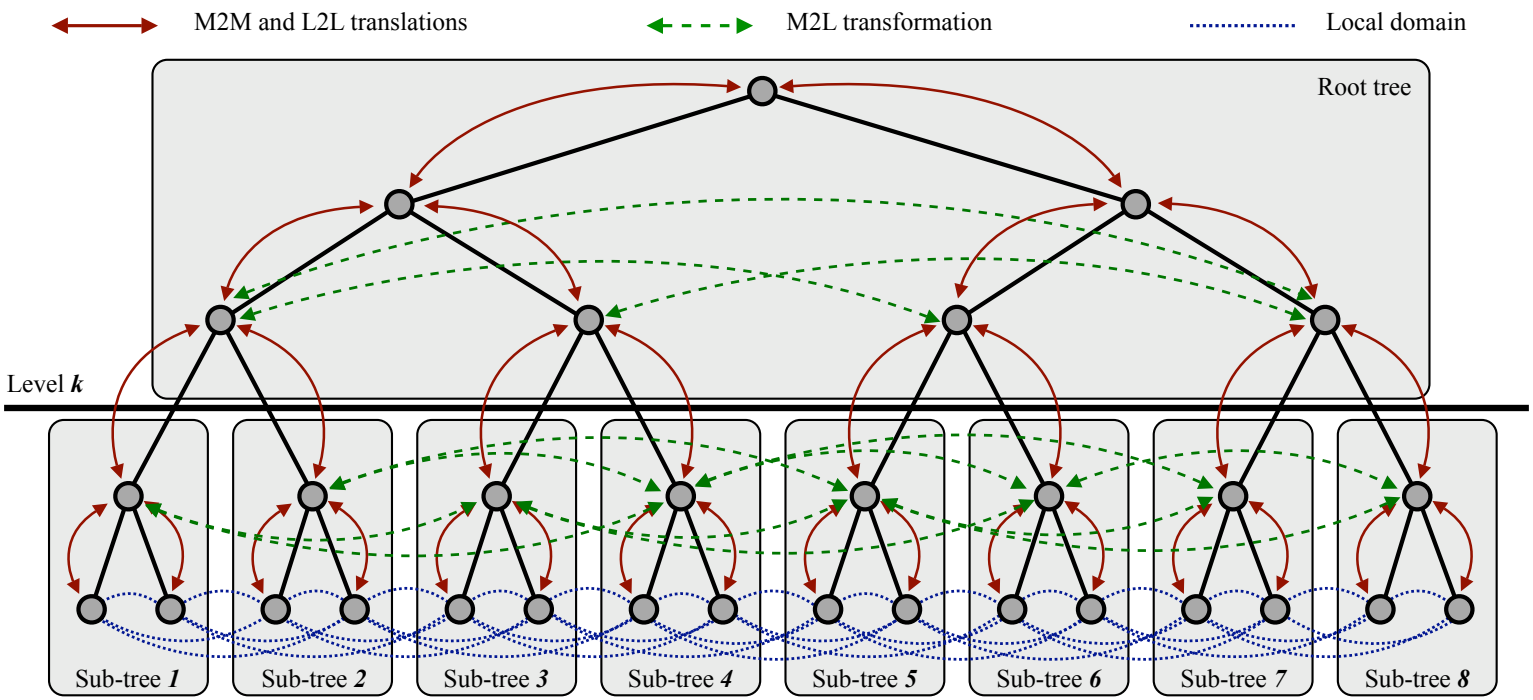
FMM Control Flow



Kernel operations will map to GPU tasks.

FMM Control Flow
Parallel Operation



Kernel operations will map to GPU tasks.

Outline

Evaluator Interface

- `initializeExpansions(tree, blobInfo)`
  - Generate multipole expansions on the lowest level
  - Requires loop over cells
  - $O(p)$
- `upwardSweep(tree)`
  - Translate multipole expansions to intermediate levels
  - Requires loop over cells and children (support)
  - $O(p^2)$
- `downwardSweep(tree)`
  - Convert multipole to local expansions and translate local expansions on intermediate levels
  - Requires loop over cells and parent (cone)
  - $O(p^2)$

Evaluator Interface

- `evaluateBlobs(tree, blobInfo)`
  - Evaluate direct and local field interactions on lowest level
  - Requires loop over cells and neighbors (in section)
  - $O(p^2)$
- `evaluate(tree, blobs, blobInfo)`
  - Calculate the complete interaction (multipole + direct)

Kernel Interface

Method	Description
`P2M(t)`	Multipole expansion coefficients
`L2P(t)`	Local expansion coefficients
`M2M(t)`	Multipole-to-multipole translation
`M2L(t)`	Multipole-to-local translation
`L2L(t)`	Local-to-local translation
`evaluate(blobs)`	Direct interaction

- `Evaluator` is templated over `Kernel`
- There are alternative kernel-independent methods
  - kifmm3d

Outline

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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.

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

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

or achieveable performance given a bandwith BW

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

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

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

FLASH Design

FLASH enables multicore computing through FLAME

- LA interface is identical to FLAME
- FLAME executes operates immediately
- FLASH queues operations, and
- Executes queues on user call (does nothing in FLAME)

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Cholesky Factorization

```
FLA_Part_2x2(A, &ATL, &ATR,
                &ABL, &ABR, 0, 0, FLA_TL);
while(FLA_Object_length(ATL) < FLA_Object_length(A)) {
  FLA_Repart_2x2_to_3x3(
    ATL, ATR, &A00, &A01, &A02,
              &A10, &A11, &A12,
    ABL, ABR, &A20, &A21, &A22, 1, 1, FLA_BR);
  FLASH_Chol(FLA_UPPER_TRIANGULAR, A11);
  FLASH_Trsm(FLA_LEFT,FLA_UPPER_TRIANGULAR,FLA_TRANSPOSE,
             FLA_NONUNIT_DIAG, FLA_ONE, A11, A12);
  FLASH_Syrk(FLA_UPPER_TRIANGULAR, FLA_TRANSPOSE,
             FLA_MINUS_ONE, A12, FLA_ONE, A22);
  FLA_Cont_with_3x3_to_2x2(
    &ATL, &ATR, A00, A01, A02,
                A10, A11, A12,
    &ABL, &ABR, A20, A21, A22, FLA_TL);
}
FLA_Queue_exec();
```

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

`Section`

- `size()` returns the number of values
- `getFiberDimension(cell)` returns the number of cell values
- `restrict/update()` retrieves and changes cell values
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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

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, cell multipole coeff

out interaction list temp local coefficients

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Tasks

`Upward Sweep Task`

- cell block

in cell and child centers, child multipole coeff

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++.

Outline

Outline

Greengard & Gropp Analysis

For a shared memory machine,

$$T = a\frac{N}{P} + b\log_4 P + c\frac{N}{BP} + d\frac{NB}{P} + e(N,P) \tag{5}$$

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.

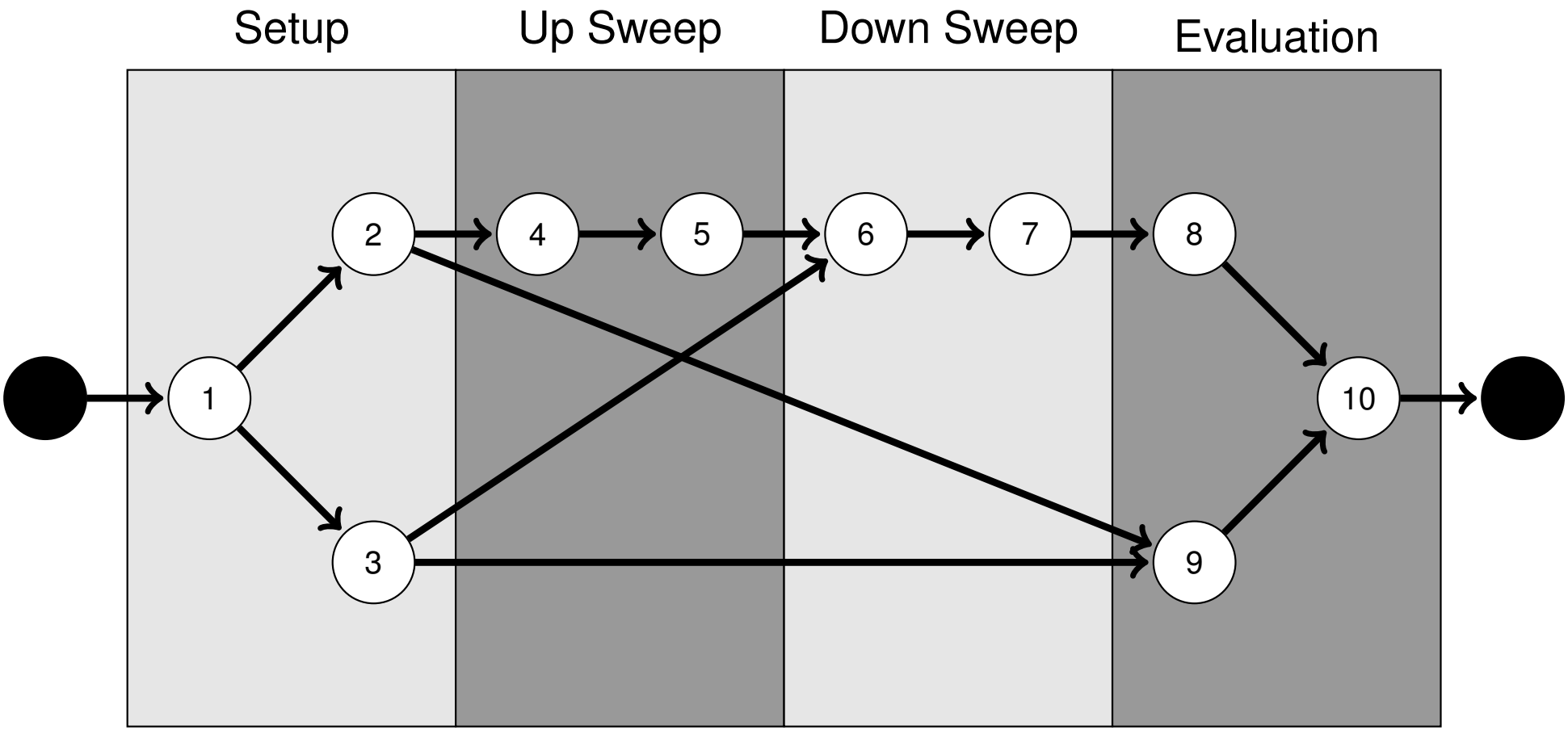
Outline

Question

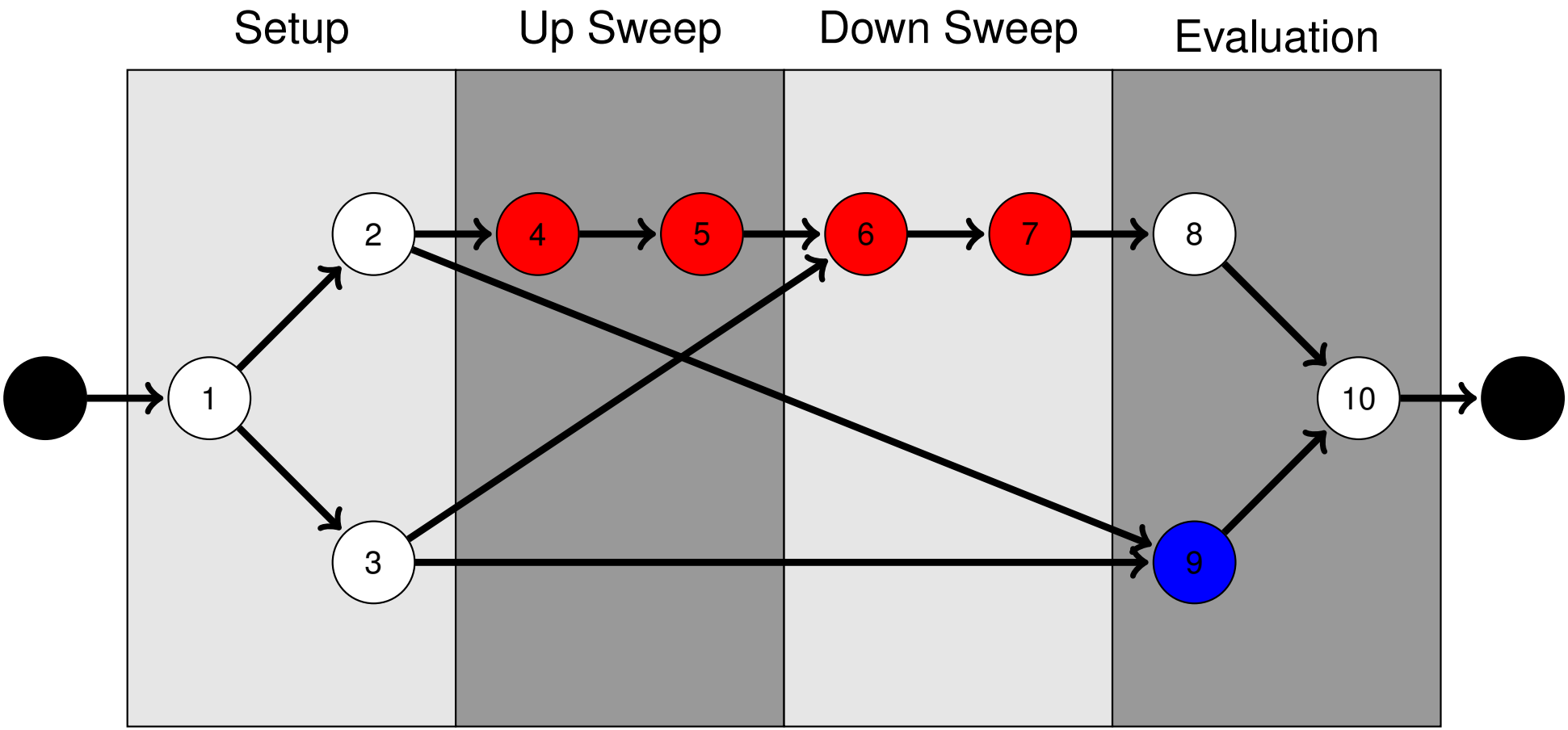
What is the optimal number of particles per cell?

- 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

PetFMM Stages



PetFMM Stages



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

$$B \geq \frac{b}{d}\frac{4^{L+1}p}{N} \tag{6}$$

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

$$M_{ij} = -1^i t^{-(i+j+1)} \binom{i+j}{j} \tag{7}$$

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)

Outline

Parallel Tree Implementation

- Divide tree into a root and local trees
- Distribute local trees among processes
- Provide communication pattern for local sections (overlap)
  - Both neighbor and interaction list overlaps
  - Sieve generates MPI from high level description

Parallel Tree Implementation

How should we distribute trees?

- Multiple local trees per process allows good load balance
- Partition weighted graph
  - Minimize load imbalance and communication
  - Computation estimate:

    Leaf $N_i p$ (P2M) + $n_l p^2$ (M2L) + $N_i p$ (L2P) + $3^d N_i^2$ (P2P)

    Interior $n_c p^2$ (M2M) + $n_l p^2$ (M2L) + $n_c p^2$ (L2L)

  - Communication estimate:

    Diagonal $n_c(L - k - 1)$

    Lateral $2^d \frac{2^{m(L-k-1)}-1}{2^m-1}$ for incidence dimesion m
- Leverage existing work on graph partitioning
  - ParMetis

Parallel Tree Implementation

Why should a good partition exist?

Shang-hua Teng, Provably good partitioning and load balancing algorithms for parallel adaptive N-body simulation, SIAM J. Sci. Comput., **19**(2), 1998.

- Good partitions exist for non-uniform distributions
  - 2D $\mathcal{O}\left(\sqrt{n}(\log n)^{3/2}\right)$ edgecut
  - 3D $\mathcal{O}\left(n^{2/3}(\log n)^{4/3}\right)$ edgecut
- As scalable as regular grids
- As efficient as uniform distributions
- ParMetis will find a nearly optimal partition

Parallel Tree Implementation

Will ParMetis find it?

George Karypis and Vipin Kumar, Analysis of Multilevel Graph Partitioning, Supercomputing, 1995.

- Good partitions exist for non-uniform distributions
  - 2D $C_i = 1.24^i C_0$ for random matching
  - 3D $C_i = 1.21^i C_0$?? for random matching
- 3D proof needs assurance that averge degree does not increase
- Efficient in practice

Parallel Tree Implementation
Advantages

- Simplicity
- Complete serial code reuse
- Provably good performance and scalability

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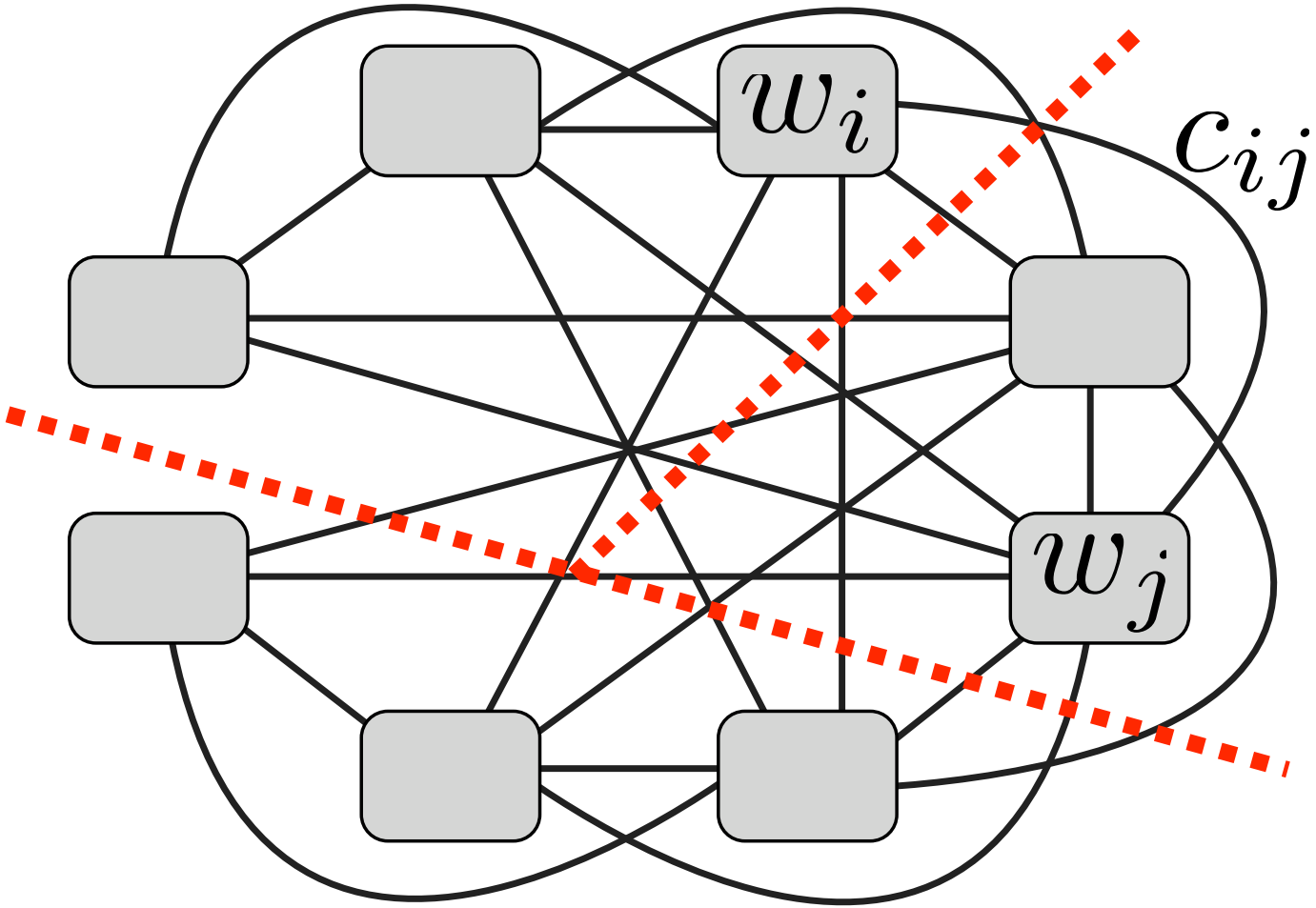
Distributing Local Trees

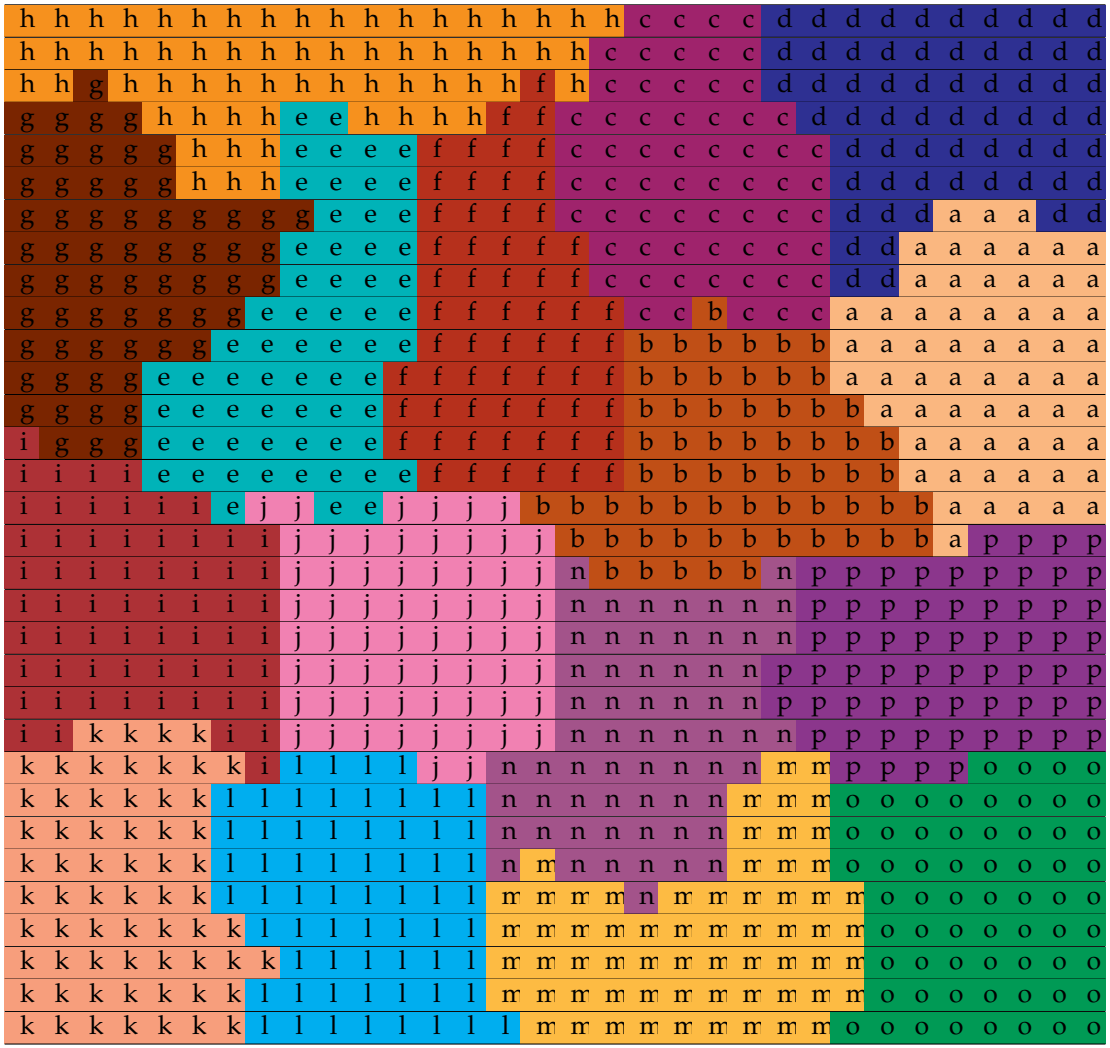
The interaction of locals trees is represented by a weighted graph.



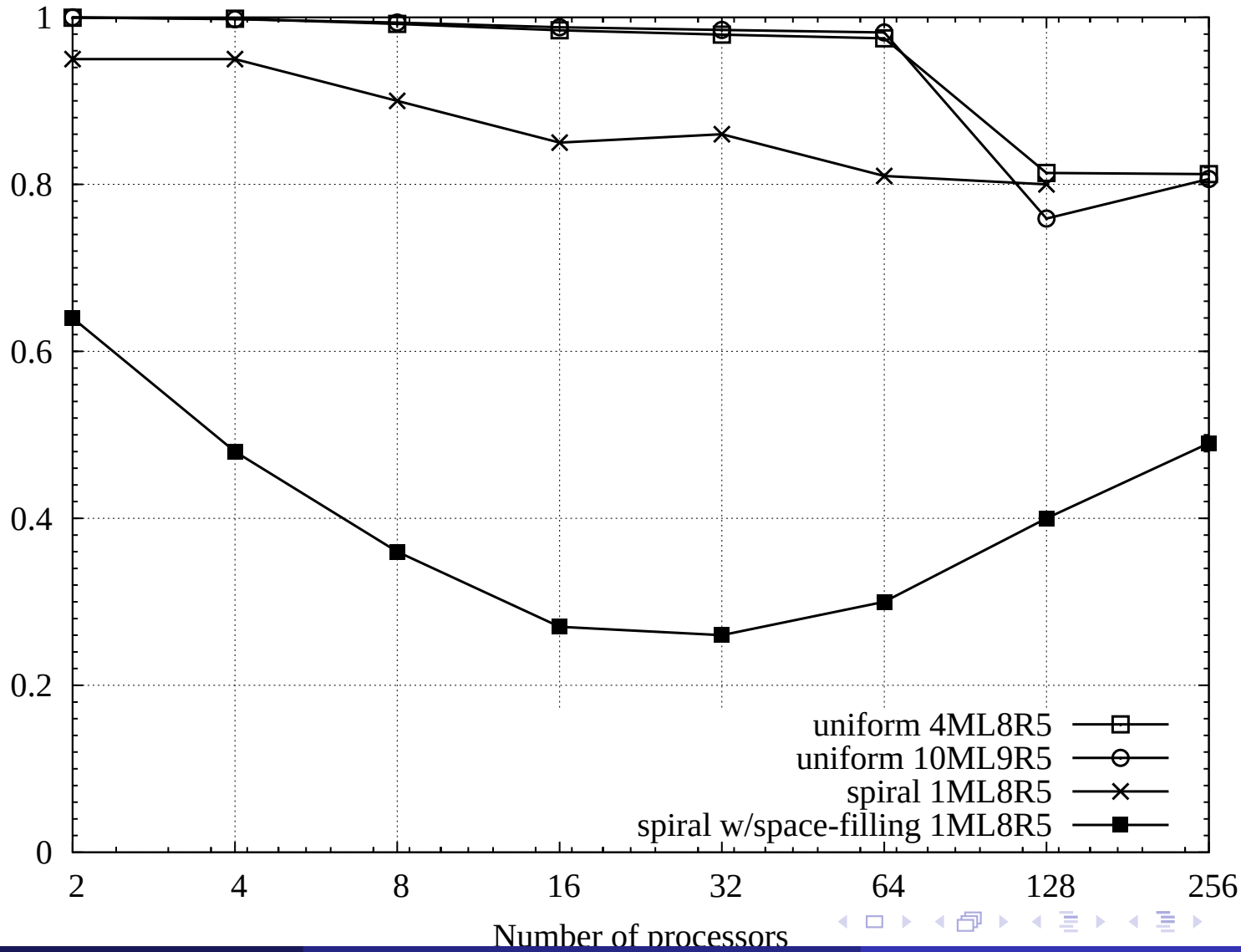
This graph is partitioned, and trees assigned to processes.

Local Tree Distribution

Here local trees are assigned to processes:

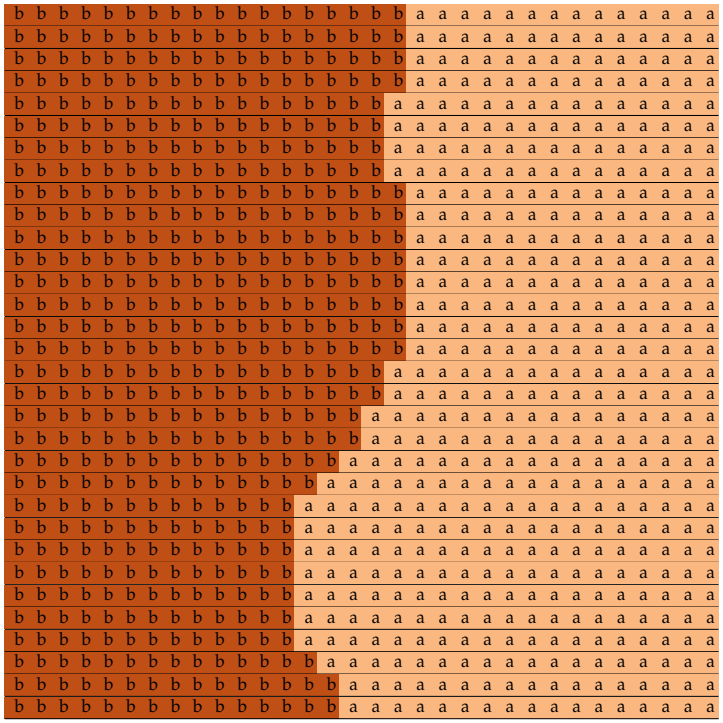


PetFMM Load Balance

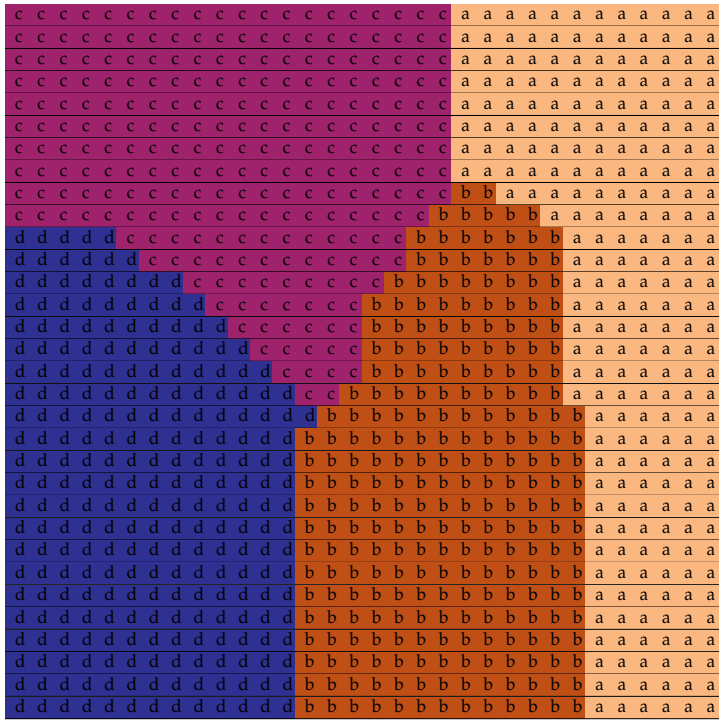


Local Tree Distribution

Here local trees are assigned to processes for a spiral distribution:



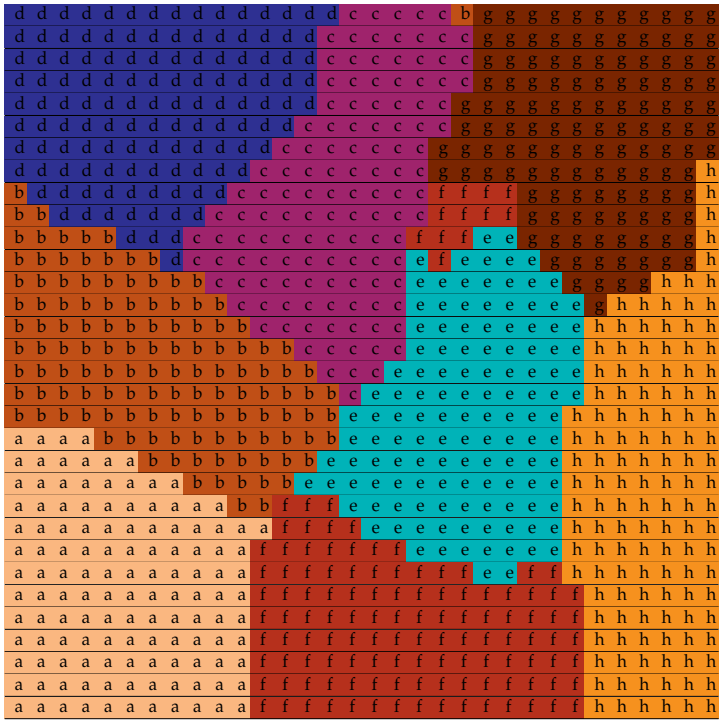
(a) 2 cores



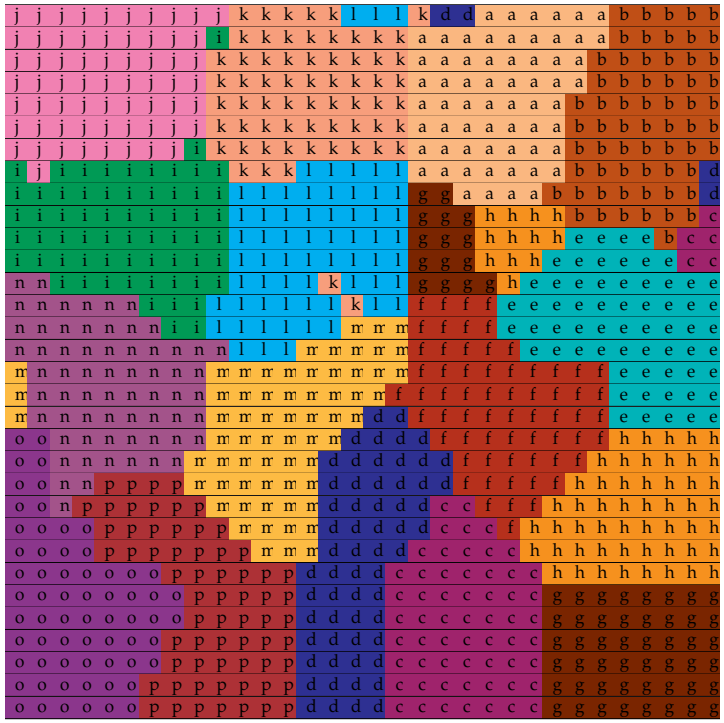
(b) 4 cores

Local Tree Distribution

Here local trees are assigned to processes for a spiral distribution:



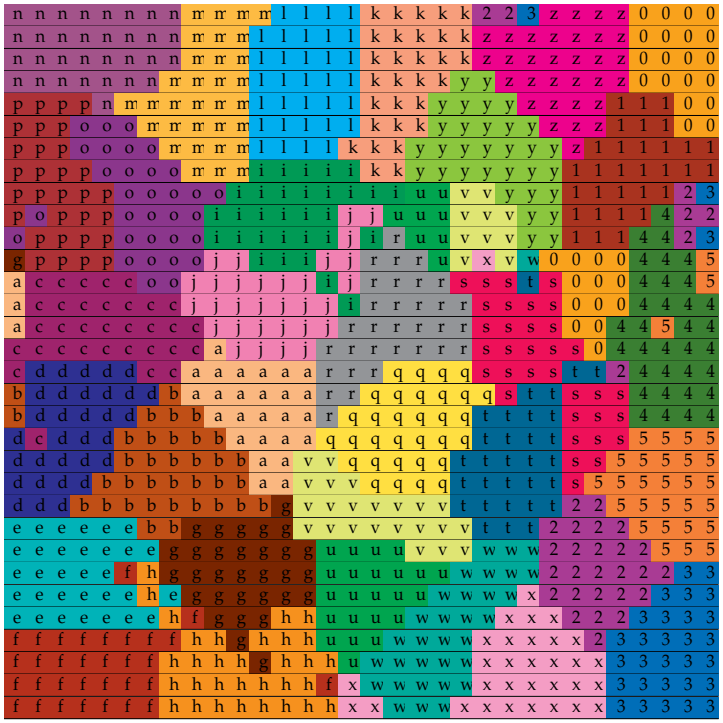
(c) 8 cores



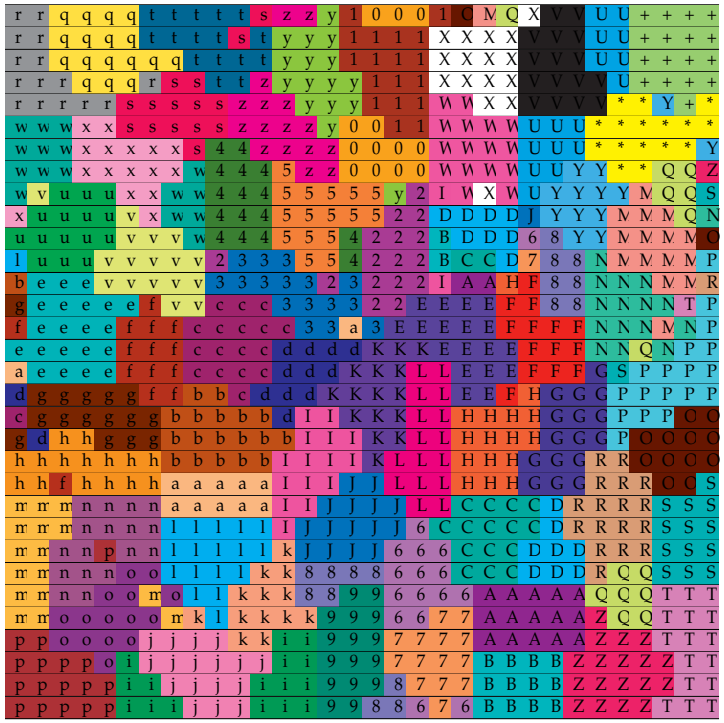
(d) 16 cores

Local Tree Distribution

Here local trees are assigned to processes for a spiral distribution:



(e) 32 cores



(f) 64 cores

Parallel Data Movement

1. Complete neighbor section
2. Upward sweep
   1. Upward sweep on local trees
   2. Gather to root tree
   3. Upward sweep on root tree
3. Complete interaction list section
4. Downward sweep
   1. Downward sweep on root tree
   2. Scatter to local trees
   3. Downward sweep on local trees

GPU Interaction

Since our parallelism is hierarchical

- Local (serial) tree interface is preserved
- GPU code can be reused locally without change
- Multiple GPUs per node can also be used

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