# Fast Methods with Sieve

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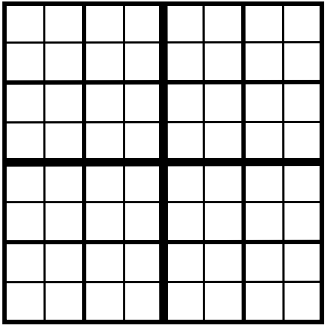
# Challenges

- Can we establish good interfaces for all levels of the hierarchy?
- Do we need language extensions for more sophisticated problems?
- What information is required from each component?
- Is inter-language programming effective?
- Can we develop a general framework for boundary conditions?

# Outline

# FMM in Sieve



- The Quadtree is a `Sieve`
  - with optimized operations
- Multipoles are stored in `Sections`
- Two `Overlaps` are defined
  - Neighbors
  - Interaction List
- Completion moves data for
  - Neighbors
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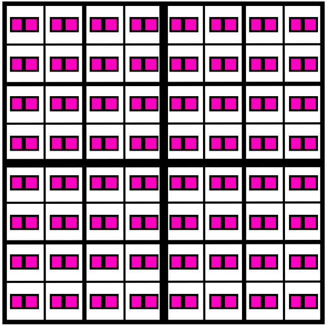

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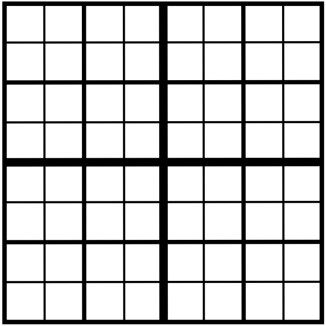

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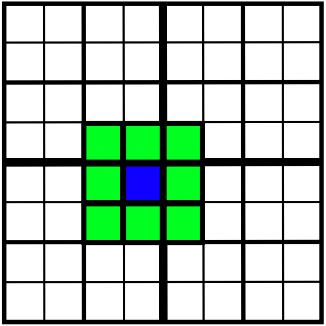

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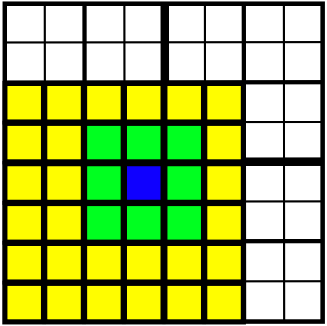

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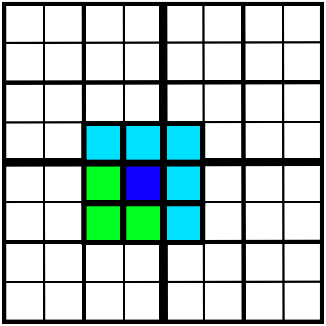

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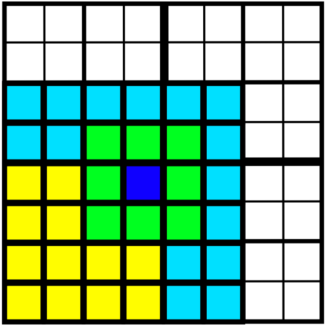

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# Quadtree Implementation

- We use binary scheme to label cells (or vertices)
- Relevant relations can be determined implicitly
  - `cone()`
  - neighbors
  - parent
  - interaction list
- When vertices are not used, we can directly connect cells
  - `cone()` becomes neighbor method

# Tree Interface

- `locateBlob(blob)`
  - Locate point in the tree
- `fillNeighbors()`
  - Compute the neighbor section
- `findInteractionList()`
  - Compute the interaction list cell section, allocate value section
- `fillInteractionList(level)`
  - Compute the interaction list value section
- `fill(blobs)`
  - Compute the blob section
- `dump()`
  - Produces a verifiable repesentation of the tree

# 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

# 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

# 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) + $n_I p^2$ (M2L) + $N_i p$ (L2P) + $3^d N_i^2$ (P2P)

    **Interior** $n_c p^2$ (M2M) + $n_I p^2$ (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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# Parallel Tree Interface

- `fillNeighbors()`
  - Compute neighbor overlap, and send neighbors
- `findInteractionList()`
  - Compute the interaction list overlap
- `fillInteractionList(level)`
  - Complete and copy into local interaction sections
- `fill(blobs)`
  - Now must scatter blobs to local trees
  - Uses `scatterBlobs()` and `gatherBlobs()`

# 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

# Parallel Evaluator Interface

- `initializeExpansions(local trees, blobInfo)`
  - Evaluate each local tree
- `upwardSweep(local trees, partition, root tree)`
  - Evaluate each local tree and then gather to root tree
- `downwardSweep(local trees, partition, root tree)`
  - Scatter from root tree and then evaluate each local tree
- `evaluateBlobs(local trees, blobInfo)`
  - Evaluate on all local trees
- `evaluate(tree, blobs, blobInfo)`
  - Identical

# Outline

# Recursive Parallel

- For large problems, a single root can be a bottleneck
- We can recursively assign roots to subtrees
  - Bandwidth to root is controlled
  - What about utilization?
- Root computation is similar to MG coarse solve