# Software Design for PDEs on GPUs

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# Collaborators

## Chicago Automated Scientific Computing Group:

- Prof. Ridgway Scott
  - Dept. of Computer Science, University of Chicago
  - Dept. of Mathematics, University of Chicago
- Peter Brune, (biological DFT)
  - Dept. of Computer Science, University of Chicago
- Dr. Andy Terrel, (Rheagen)
  - Dept. of Computer Science and TACC, University of Texas at Austin

# Collaborators

The PetFMM team:

- Prof. Lorena Barba
  - Dept. of Mechanical Engineering, Boston University
- Dr. Felipe Cruz, developer of GPU extension
  - Nagasaki Advanced Computing Center, Nagasaki University
- Dr. Rio Yokota, developer of 3D extension
  - Dept. of Mechanical Engineering, Boston University

# Collaborators

The PyLith Team:

- Dr. Brad Aagaard (PyLith)
  - United States Geological Survey, Menlo Park, CA
- Dr. Charles Williams (PyLith)
  - GNS Science, Wellington, NZ

# Main Point

To be widely accepted,

GPU computing must be transparent to the user,

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# Lessons from Clusters and MPPs

Failure

- Parallelizing Compilers
- Automatic program decomposition

Success

- MPI (Library Approach)
- PETSc (Parallel Linear Algebra)
- User provides only the mathematical description

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# Outline

# Thrust

Thrust is a CUDA library of parallel algorithms

- Interface similar to C++ Standard Template Library
- Containers (`vector`) on both host and device
- Algorithms: `sort`, `reduce`, `scan`
- Freely available, part of PETSc configure (`-with-thrust-dir`)
- Included as part of CUDA 4.0 installation

# Cusp

Cusp is a CUDA library for
sparse linear algebra and graph computations

- Builds on data structures in Thrust
- Provides sparse matrices in several formats (CSR, Hybrid)
- Includes some preliminary preconditioners (Jacobi, SA-AMG)
- Freely available, part of PETSc configure (`-with-cusp-dir`)

# VECCUDA

## Strategy: Define a new **Vec** implementation

- Uses Thrust for data storage and operations on GPU
- Supports full PETSc **Vec** interface
- Inherits PETSc scalar type
- Can be activated at runtime, `-vec_type cuda`
- PETSc provides memory coherence mechanism

# Memory Coherence

PETSc Objects now hold a coherence flag

| | |
|---|---|
| PETSC_CUDA_UNALLOCATED | No allocation on the GPU |
| PETSC_CUDA_GPU | Values on GPU are current |
| PETSC_CUDA_CPU | Values on CPU are current |
| PETSC_CUDA_BOTH | Values on both are current |

Table: Flags used to indicate the memory state of a PETSc CUDA **Vec** object.

# MATAIJCUDA

Also define new **Mat** implementations

- Uses Cusp for data storage and operations on GPU
- Supports full PETSc **Mat** interface, some ops on CPU
- Can be activated at runtime, `-mat_type aijcuda`
- Notice that parallel matvec necessitates off-GPU data transfer

# Solvers

## Solvers come for Free

Preliminary Implementation of PETSc Using GPU,

Minden, Smith, Knepley, 2010

- All linear algebra types work with solvers
- Entire solve can take place on the GPU
  - Only communicate scalars back to CPU
- GPU communication cost could be amortized over several solves
- Preconditioners are a problem
  - Cusp has a promising AMG

# Installation

PETSc only needs

```
# Turn on CUDA
--with-cuda
# Specify the CUDA compiler
--with-cudac='nvcc -m64'
# Indicate the location of packages
#  --download-* will also work soon
--with-thrust-dir=/PETSc3/multicore/thrust
--with-cusp-dir=/PETSc3/multicore/cusp
# Can also use double precision
--with-precision=single
```

# Example
## Driven Cavity Velocity-Vorticity with Multigrid

```
ex50 -da_vec_type seqcusp
  -da_mat_type aijcusp -mat_no_inode # Setup types
  -da_grid_x 100 -da_grid_y 100      # Set grid size
  -pc_type none -pc_mg_levels 1      # Setup solver
  -preload off -cuda_synchronize     # Setup run
  -log_summary
```

# Outline

# What are the Benefits for current PDE Code?

## Low Order FEM on GPUs

- Analytic Flexibility
- Computational Flexibility
- Efficiency

http://www.bitbucket.org/aterrel/flamefem

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# Outline

# Analytic Flexibility
## Laplacian

$$\int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) d\mathbf{x} \tag{1}$$

```
element = FiniteElement('Lagrange', tetrahedron, 1)
v = TestFunction(element)
u = TrialFunction(element)
a = inner(grad(v), grad(u))*dx
```

# Analytic Flexibility
## Laplacian

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# Analytic Flexibility
## Linear Elasticity

$$\frac{1}{4}\int_{\mathcal{T}} \left(\nabla\vec{\phi}_i(\mathbf{x}) + \nabla^T\vec{\phi}_i(\mathbf{x})\right) : \left(\nabla\vec{\phi}_j(\mathbf{x}) + \nabla\vec{\phi}_j(\mathbf{x})\right) d\mathbf{x} \tag{2}$$

```
element = VectorElement('Lagrange', tetrahedron, 1)
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a = inner(sym(grad(v)), sym(grad(u)))*dx
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# Analytic Flexibility
## Full Elasticity

$$\frac{1}{4}\int_{\mathcal{T}} \left(\nabla\vec{\phi}_i(\mathbf{x}) + \nabla^T\vec{\phi}_i(\mathbf{x})\right) : C : \left(\nabla\vec{\phi}_j(\mathbf{x}) + \nabla\vec{\phi}_j(\mathbf{x})\right) d\mathbf{x} \tag{3}$$

```
element  = VectorElement('Lagrange', tetrahedron, 1)
cElement = TensorElement('Lagrange', tetrahedron, 1,
                         (dim, dim, dim, dim))
v = TestFunction(element)
u = TrialFunction(element)
C = Coefficient(cElement)
i, j, k, l = indices(4)
a = sym(grad(v))[i,j]*C[i,j,k,l]*sym(grad(u))[k,l]*dx
```

Currently broken in FEniCS release

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# Outline

# Form Decomposition

Element integrals are decomposed into analytic and geometric parts:

$$\int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) d\mathbf{x} \tag{4}$$

$$= \int_{\mathcal{T}} \frac{\partial\phi_i(\mathbf{x})}{\partial x_\alpha} \frac{\partial\phi_j(\mathbf{x})}{\partial x_\alpha} d\mathbf{x} \tag{5}$$

$$= \int_{\mathcal{T}_{\text{ref}}} \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\xi_\gamma}{\partial x_\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} |J| d\mathbf{x} \tag{6}$$

$$= \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\text{ref}}} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} d\mathbf{x} \tag{7}$$

$$= G^{\beta\gamma}(\mathcal{T}) K^{ij}_{\beta\gamma} \tag{8}$$

Coefficients are also put into the geometric part.

# Form Decomposition

Additional fields give rise to multilinear forms.

$$\int_{\mathcal{T}} \phi_i(\mathbf{x}) \cdot \left(\phi_k(\mathbf{x}) \nabla \phi_j(\mathbf{x})\right) dA \tag{9}$$

$$= \int_{\mathcal{T}} \phi_i^\beta(\mathbf{x}) \left(\phi_k^\alpha(\mathbf{x}) \frac{\partial \phi_j^\beta(\mathbf{x})}{\partial x_\alpha}\right) dA \tag{10}$$

$$= \int_{\mathcal{T}_{\text{ref}}} \phi_i^\beta(\xi) \phi_k^\alpha(\xi) \frac{\partial \xi_\gamma}{\partial x_\alpha} \frac{\partial \phi_j^\beta(\xi)}{\partial \xi_\gamma} |J| dA \tag{11}$$

$$= \frac{\partial \xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\text{ref}}} \phi_i^\beta(\xi) \phi_k^\alpha(\xi) \frac{\partial \phi_j^\beta(\xi)}{\partial \xi_\gamma} dA \tag{12}$$

$$= G^{\alpha\gamma}(\mathcal{T}) K_{\alpha\gamma}^{ijk} \tag{13}$$

The index calculus is fully developed by Kirby and Logg in A Compiler for Variational Forms.

# Form Decomposition

Isoparametric Jacobians also give rise to multilinear forms

$$\int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) dA \tag{14}$$

$$= \int_{\mathcal{T}} \frac{\partial\phi_i(\mathbf{x})}{\partial x_\alpha} \frac{\partial\phi_j(\mathbf{x})}{\partial x_\alpha} dA \tag{15}$$

$$= \int_{\mathcal{T}_{\text{ref}}} \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\xi_\gamma}{\partial x_\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} |J| dA \tag{16}$$

$$= |J| \int_{\mathcal{T}_{\text{ref}}} \phi_k J_k^{\beta\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \phi_l J_l^{\gamma\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} dA \tag{17}$$

$$= J_k^{\beta\alpha} J_l^{\gamma\alpha} |J| \int_{\mathcal{T}_{\text{ref}}} \phi_k \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \phi_l \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} dA \tag{18}$$

$$= G_{kl}^{\beta\gamma}(\mathcal{T}) K_{\beta\gamma}^{ijkl} \tag{19}$$

A different space could also be used for Jacobians

# Weak Form Processing

```
from ffc.analysis import analyze_forms
from ffc.compiler import compute_ir

parameters = ffc.default_parameters()
parameters['representation'] = 'tensor'
analysis = analyze_forms([a,L], {}, parameters)
ir = compute_ir(analysis, parameters)

a_K = ir[2][0]['AK'][0][0]
a_G = ir[2][0]['AK'][0][1]

K = a_K.A0.astype(numpy.float32)
G = a_G
```

# Computational Flexibility

We generate different computations on the fly,

and can change

- Element Batch Size
- Number of Concurrent Elements
- Loop unrolling
- Interleaving stores with computation

# Computational Flexibility
## Basic Contraction

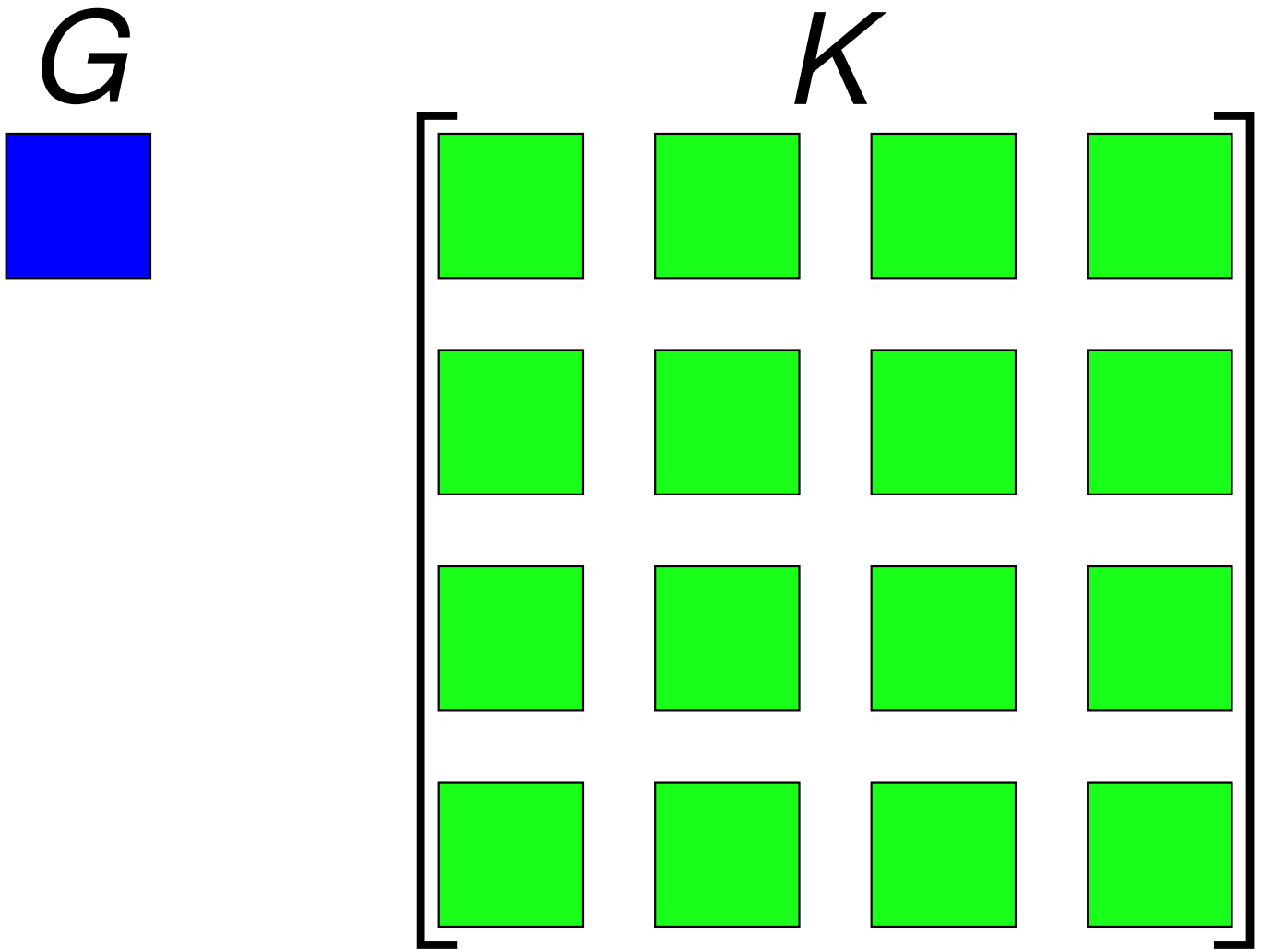


Figure: Tensor Contraction $G^{\beta\gamma}(\mathcal{T})K^{ij}_{\beta\gamma}$

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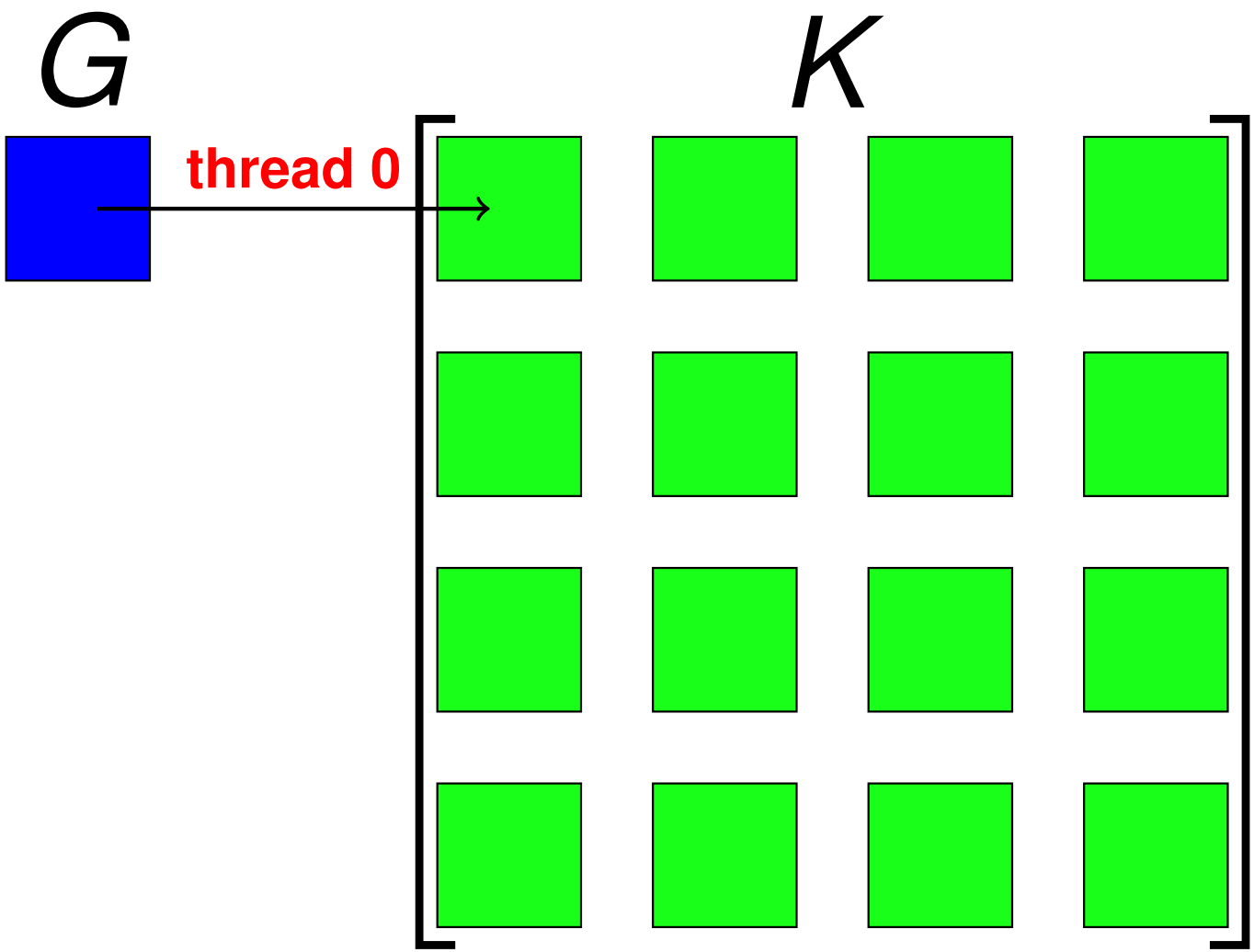


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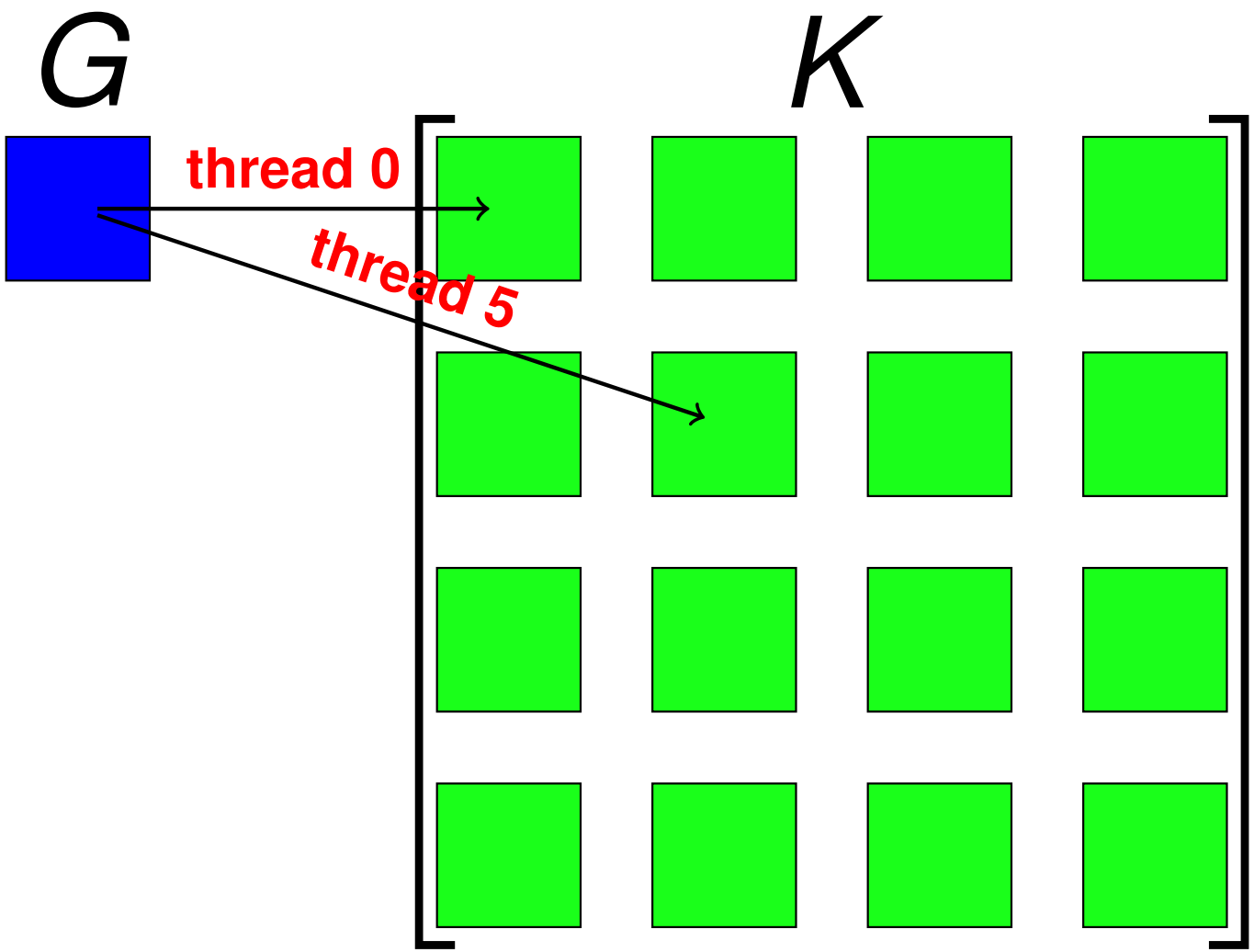


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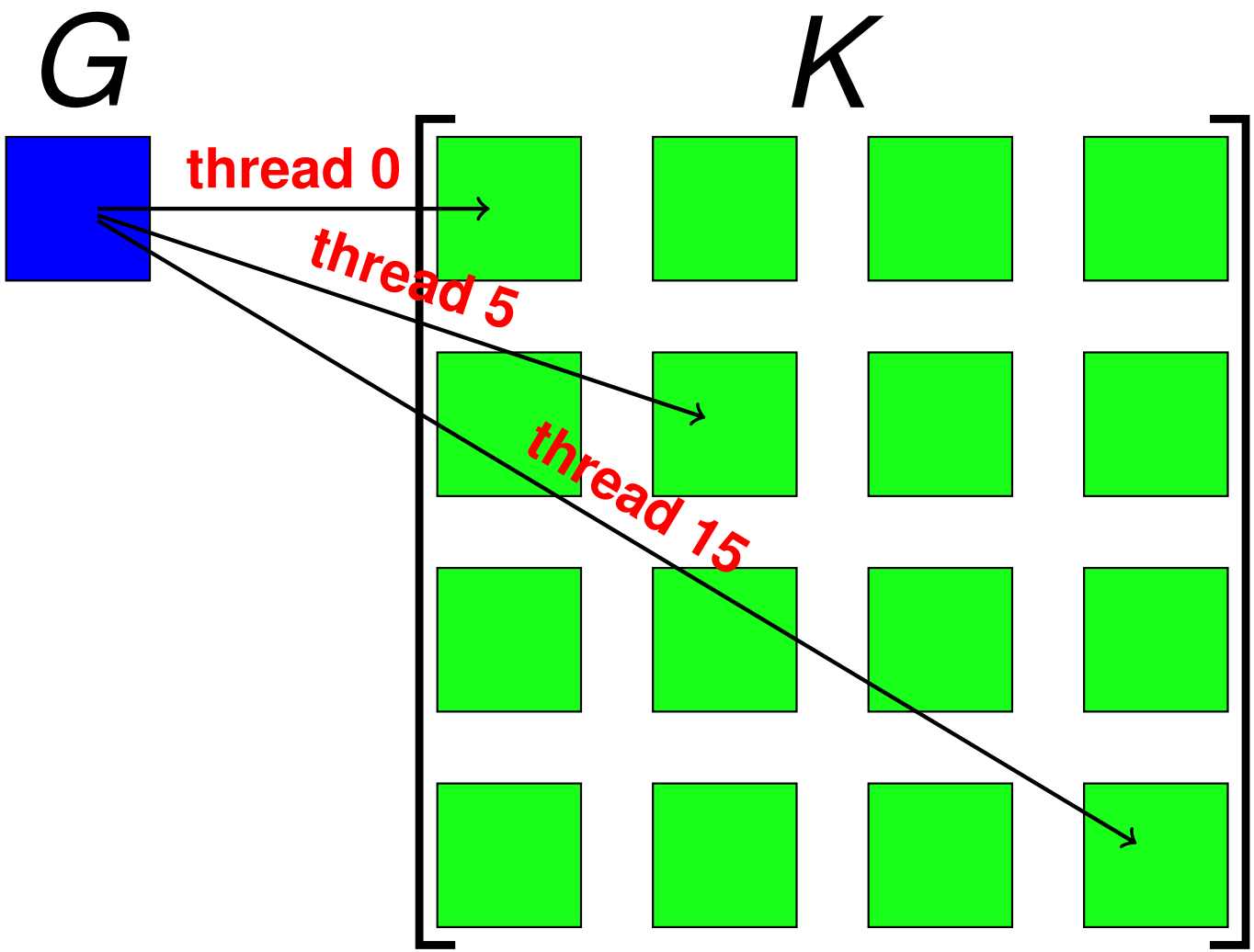


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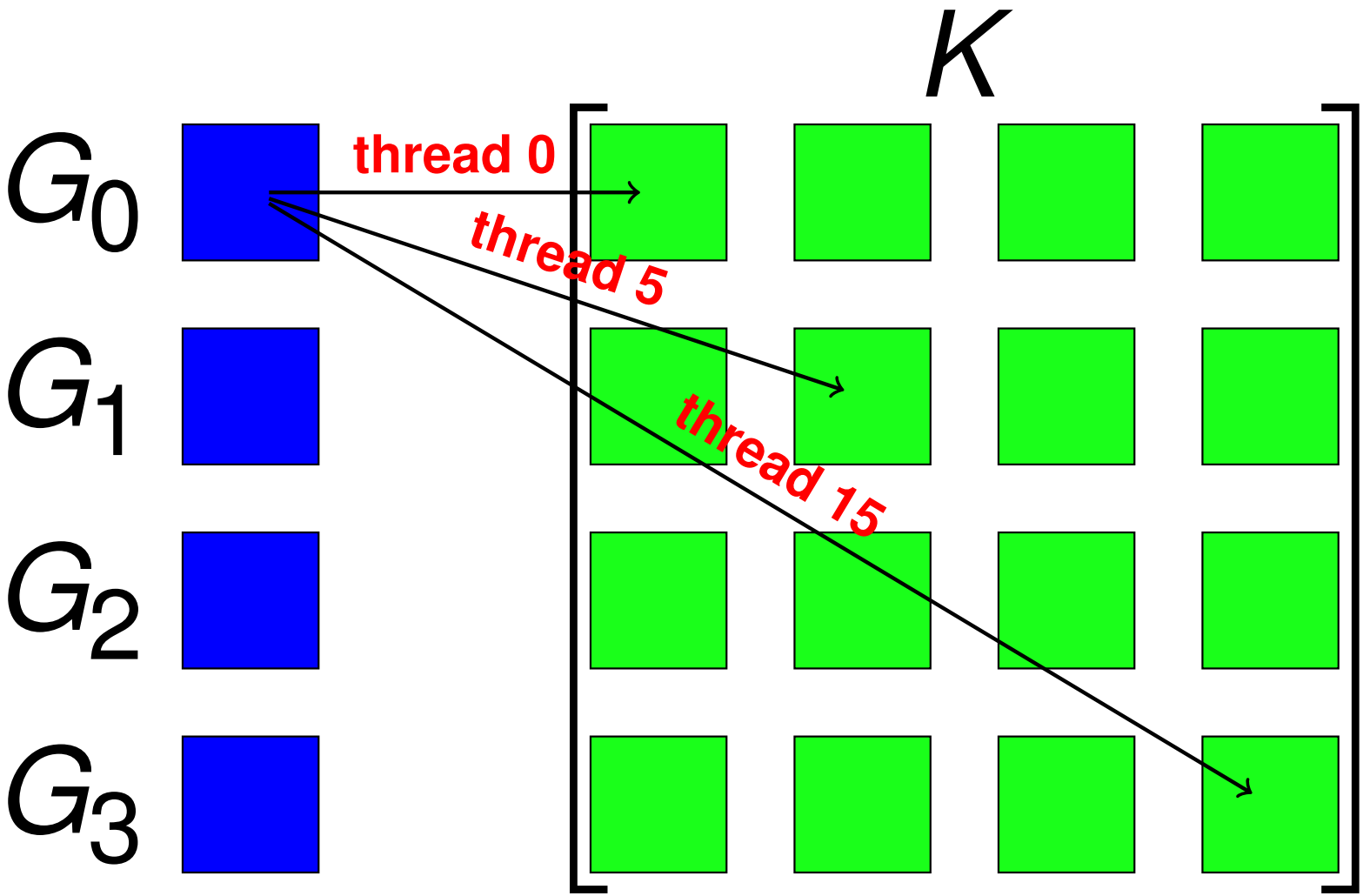
# Computational Flexibility
## Element Batch Size

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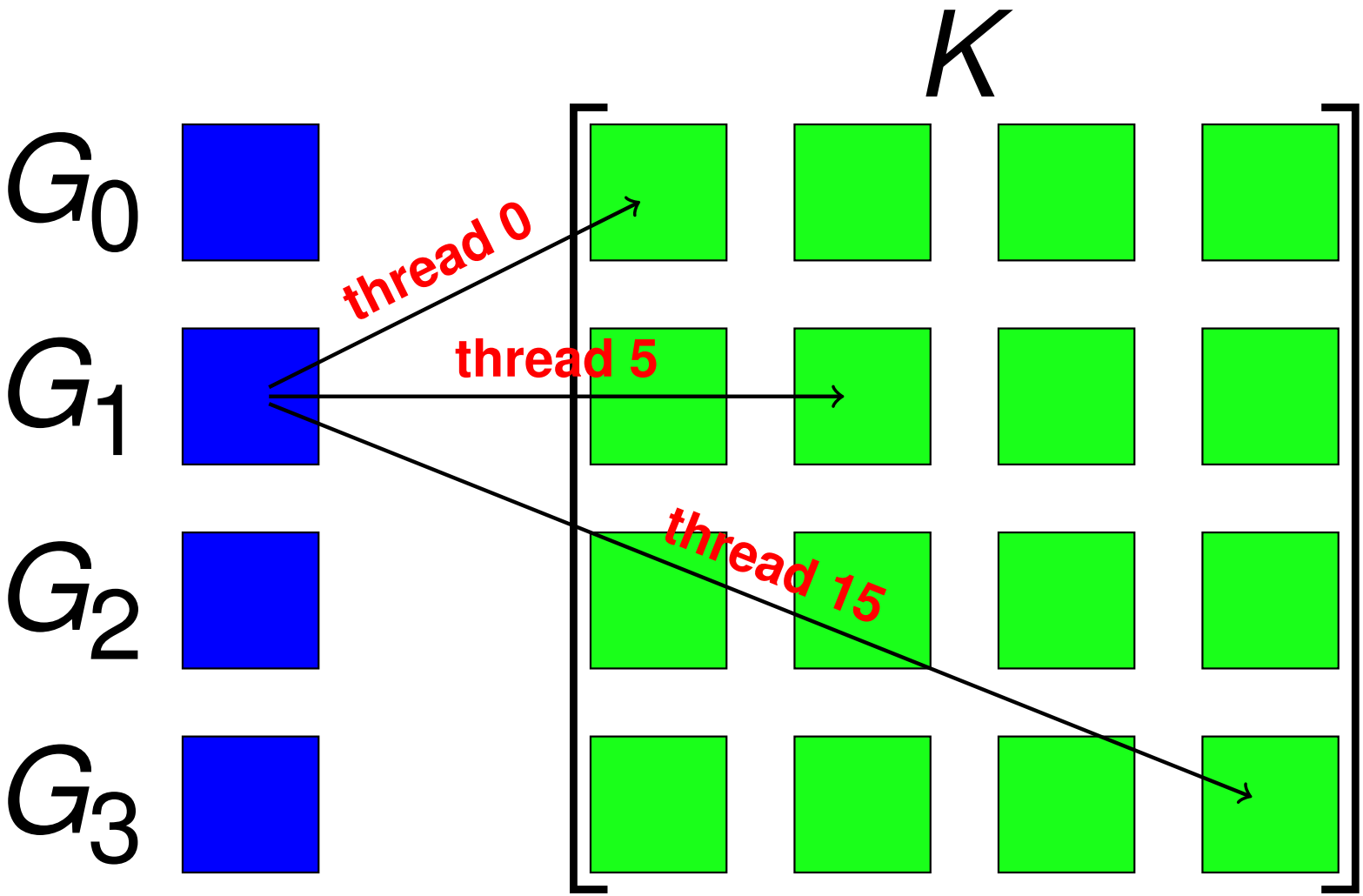


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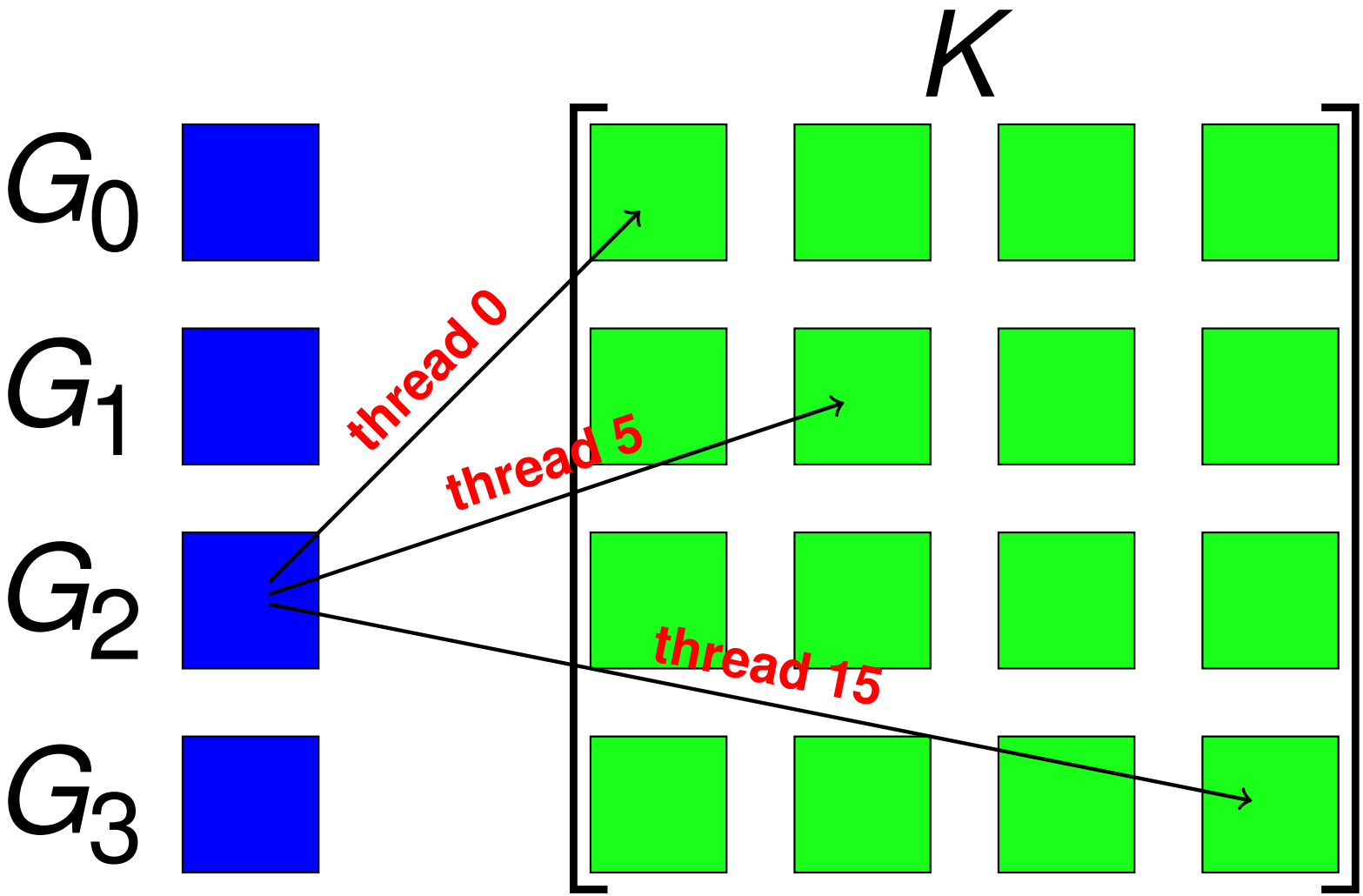


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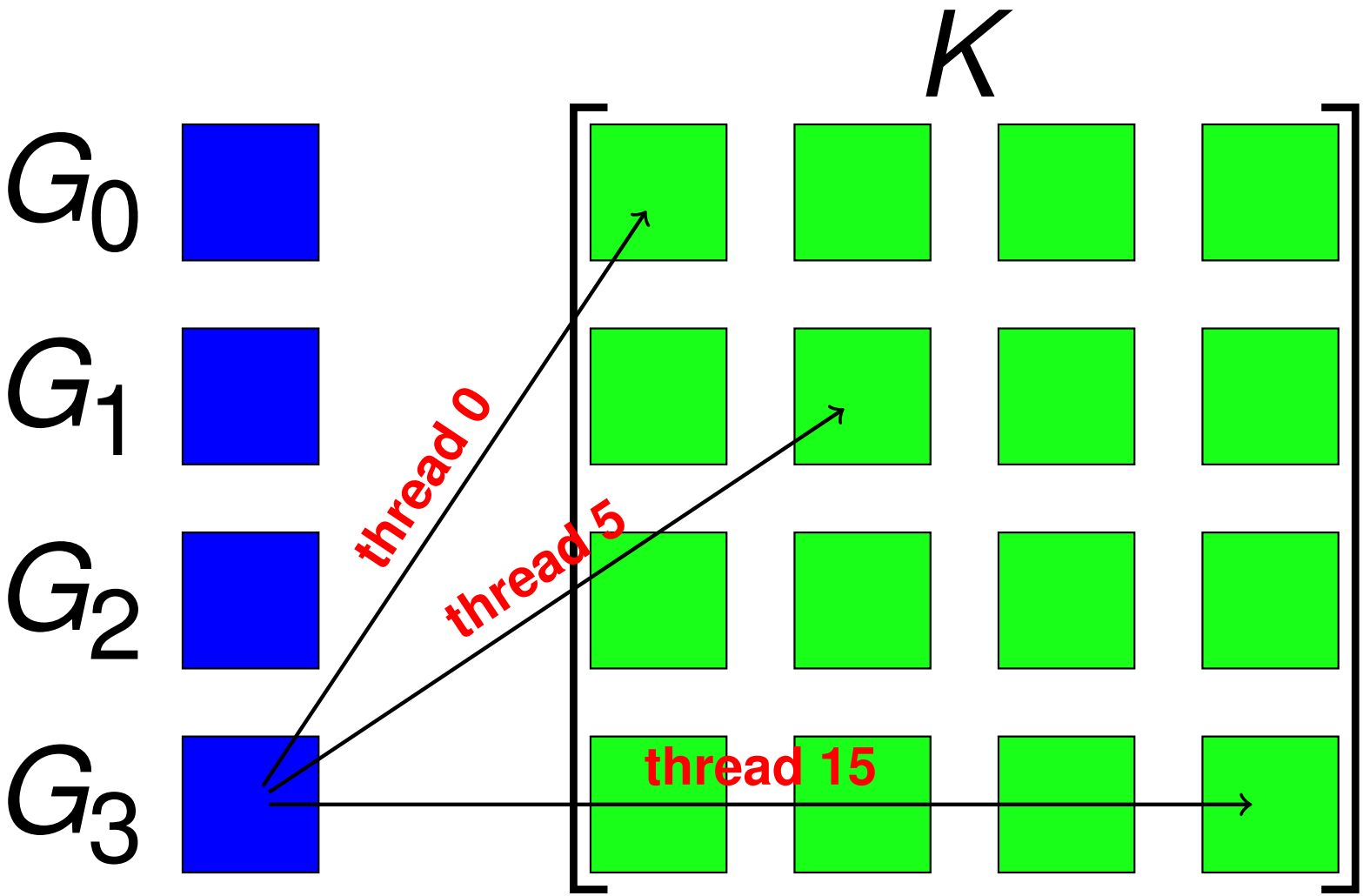


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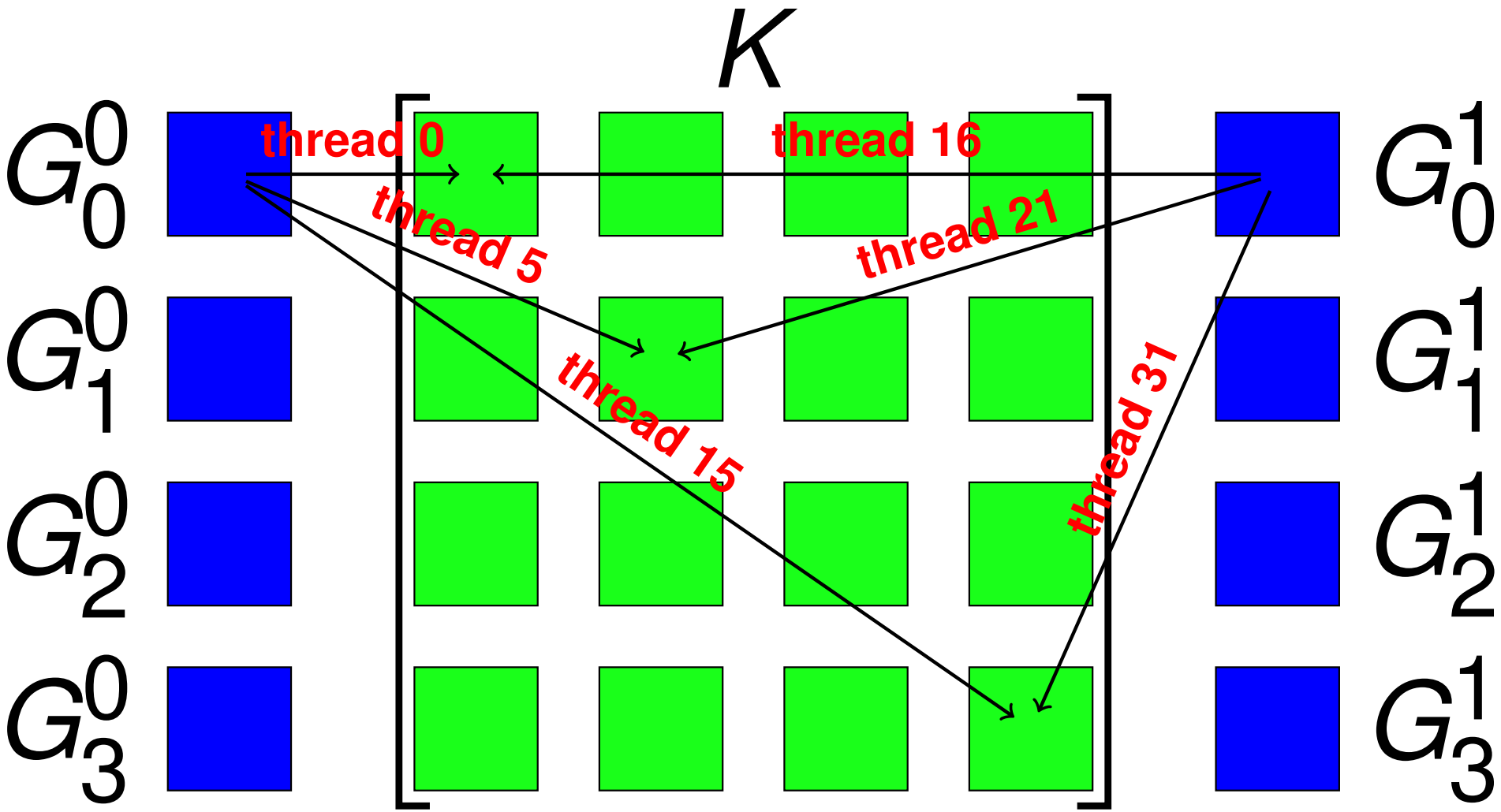
## Concurrent Elements



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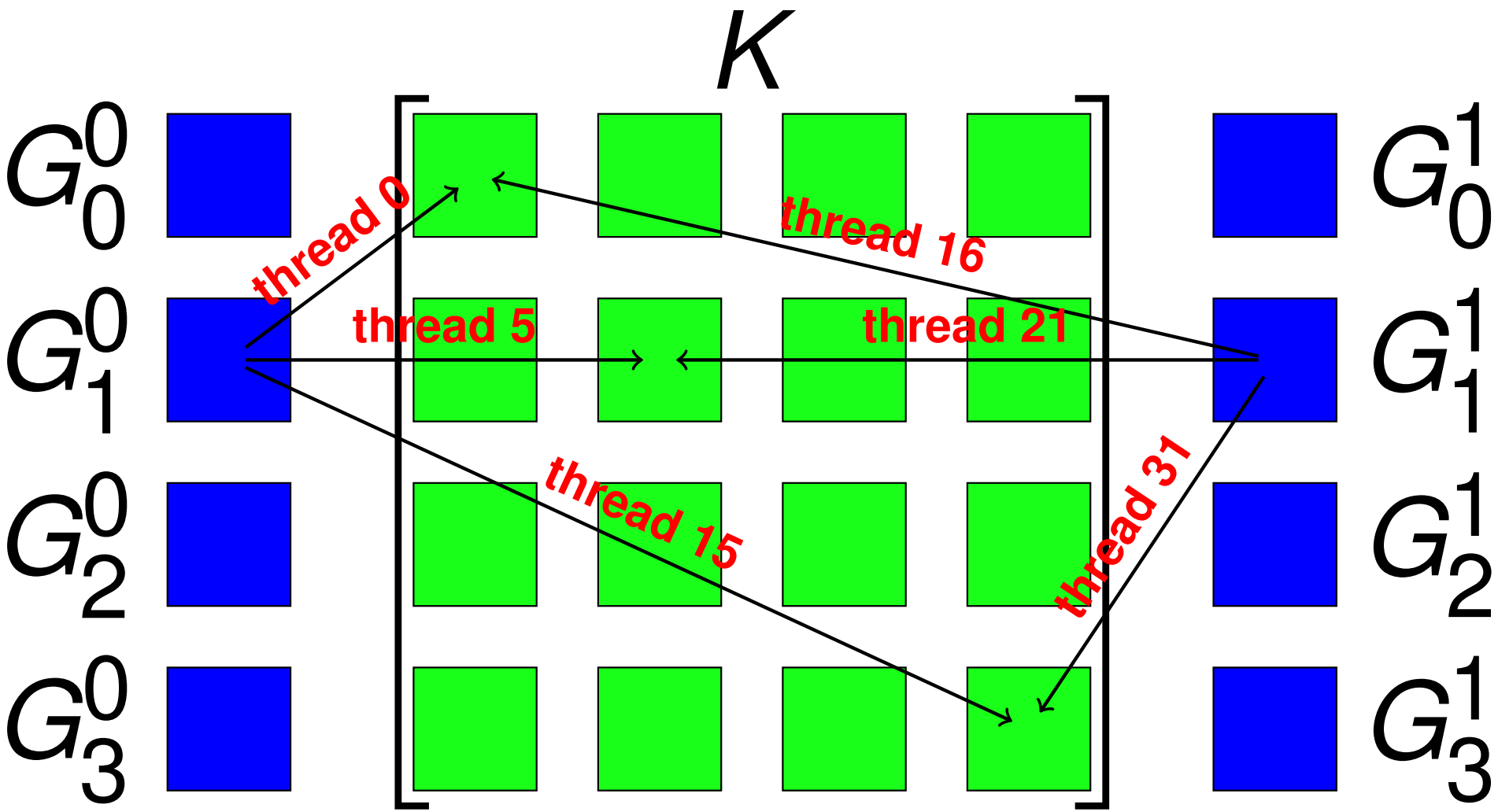

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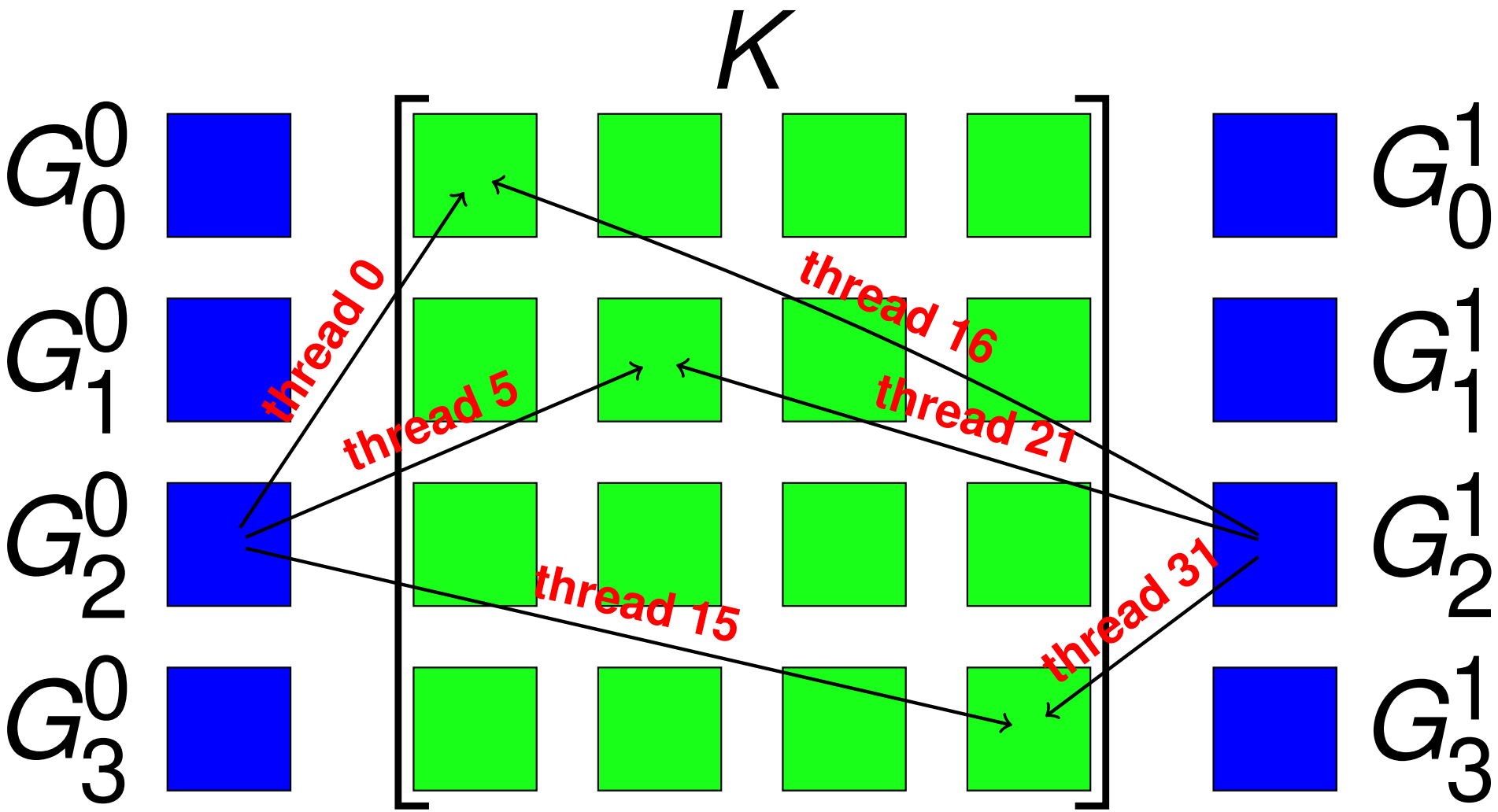

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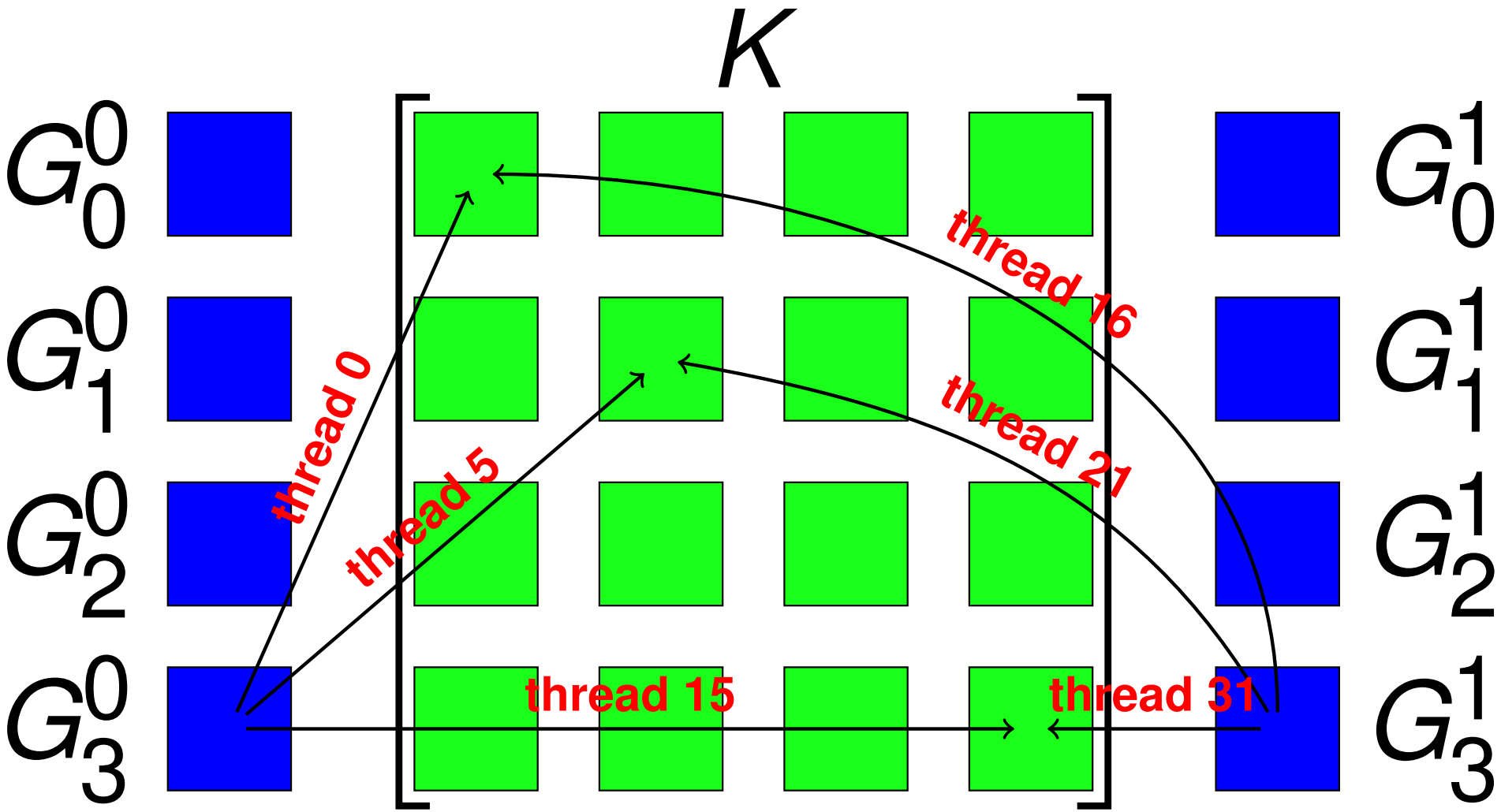


# Computational Flexibility
## Loop Unrolling

```
/* G K contraction: unroll = full */
E[0] += G[0] * K[0];
E[0] += G[1] * K[1];
E[0] += G[2] * K[2];
E[0] += G[3] * K[3];
E[0] += G[4] * K[4];
E[0] += G[5] * K[5];
E[0] += G[6] * K[6];
E[0] += G[7] * K[7];
E[0] += G[8] * K[8];
```

# Computational Flexibility
## Loop Unrolling

```
/* G K contraction: unroll = none */
for(int b = 0; b < 1; ++b) {
  const int n = b*1;
  for(int alpha = 0; alpha < 3; ++alpha) {
    for(int beta = 0; beta < 3; ++beta) {
      E[b] += G[n*9+alpha*3+beta] * K[alpha*3+beta];
    }
  }
}
```

# Computational Flexibility
## Interleaving stores

```
/* G K contraction: unroll = none */
for(int b = 0; b < 4; ++b) {
  const int n = b*1;
  for(int alpha = 0; alpha < 3; ++alpha) {
    for(int beta = 0; beta < 3; ++beta) {
      E[b] += G[n*9+alpha*3+beta] * K[alpha*3+beta];
    }
  }
}
/* Store contraction results */
elemMat[Eoffset+idx+0]  = E[0];
elemMat[Eoffset+idx+16] = E[1];
elemMat[Eoffset+idx+32] = E[2];
elemMat[Eoffset+idx+48] = E[3];
```

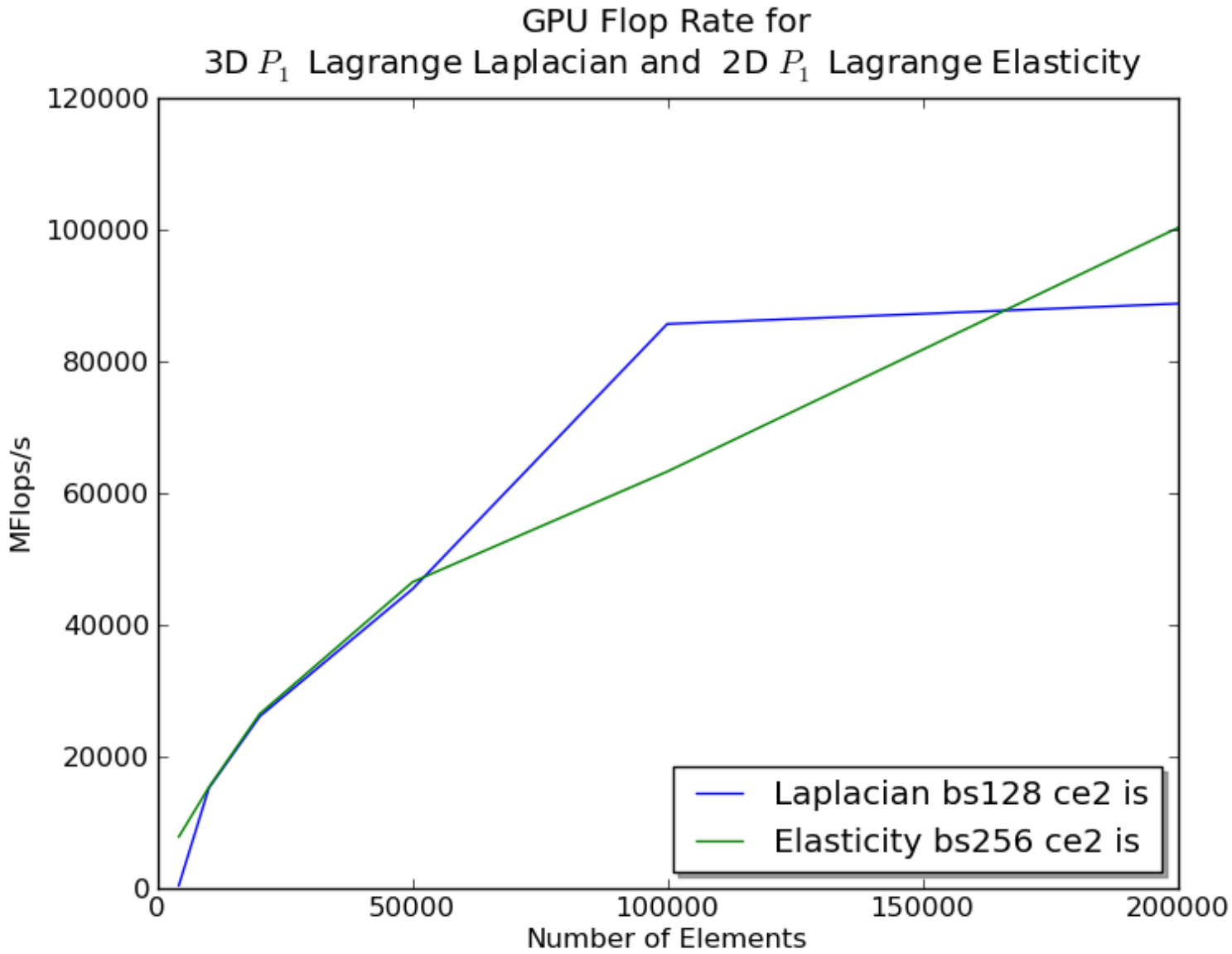
# Computational Flexibility
## Interleaving stores

```
n = 0;
for(int alpha = 0; alpha < 3; ++alpha) {
  for(int beta = 0; beta < 3; ++beta) {
    E += G[n*9+alpha*3+beta] * K[alpha*3+beta];
  }
}
/* Store contraction result */
elemMat[Eoffset+idx+0] = E;
n = 1; E = 0.0; /* contract */
elemMat[Eoffset+idx+16] = E;
n = 2; E = 0.0; /* contract */
elemMat[Eoffset+idx+32] = E;
n = 3; E = 0.0; /* contract */
elemMat[Eoffset+idx+48] = E;
```

# Outline

2 FEM-GPU
- Analytic Flexibility
- Computational Flexibility
- Efficiency

# Performance
## Peak Performance



# Performance

Price-Performance Comparison of CPU and GPU
3D $P_1$ Laplacian Integration

| Model | Price ($) | GF/s | MF/s$ |
|---|---|---|---|
| GTX285 | 390 | 90 | 231 |
| Core 2 Duo | 300 | 2 | 6.6 |

# Performance

## Price-Performance Comparison of CPU and GPU 3D $P_1$ Laplacian Integration

| Model | Price ($) | GF/s | MF/s$ |
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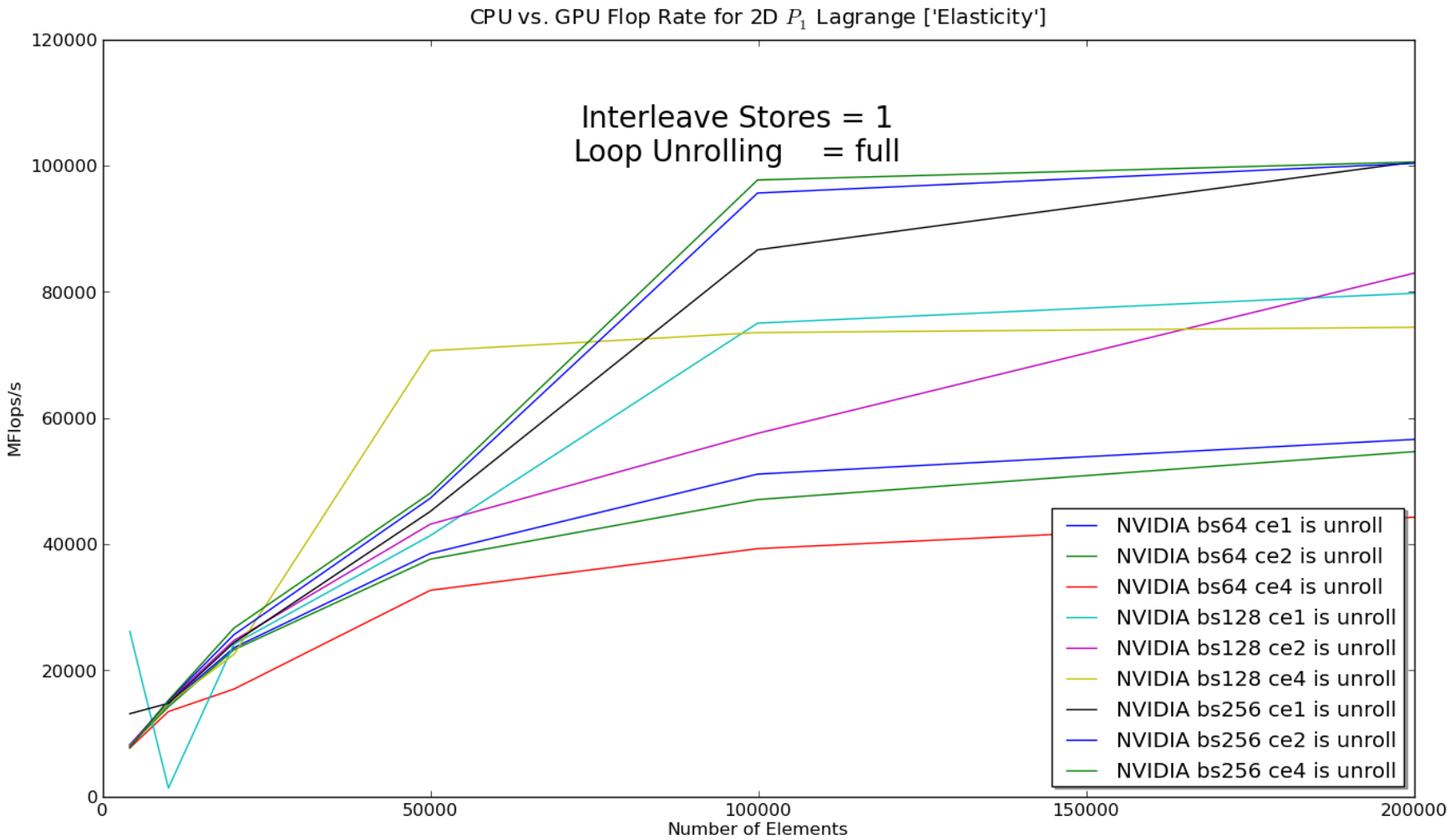
| GTX285 | 390 | 90 | 231 |
| Core 2 Duo | 300 | 12* | 40 |

* Jed Brown Optimization Engine

# Performance
## Influence of Element Batch Sizes



# Explaining performance

- Increase shared memory and work/thread until you top out
  - Occupancies go down or level out as performance goes up
- Does not work without interleaved stores
  - Scheduler can switch to kernels who are computing
  - Larger number of smaller computations makes better fit
- Should I worry about detailed explanations for performance?
  - Sensible decompositions, coupled with exploration
  - FLAME methodology

# Automated Tuning System

Components of our performance evaluation system:

- Generate set of kernels using:
  - Loop slicing, store reordering, etc.
  - Loop invariants ala FLAME
  - High level constructs ala Rheagen and FEniCS
- Store results and metadata in HDF5 using PyTables
  - Thousands of tests for this talk
- Interrogate and plot with Matplotlib
- Eventually couple to build system
  - FFTW, Spiral, FLAME

# Why Should You Try This?

Structured code generation,

can allow easy integration
of novel hardware

and reconcile user physics
with system traversals.

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# 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:

$$\Phi(x_i) = \sum_j K(x_i, x_j) q(x_j) \tag{20}$$

- 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

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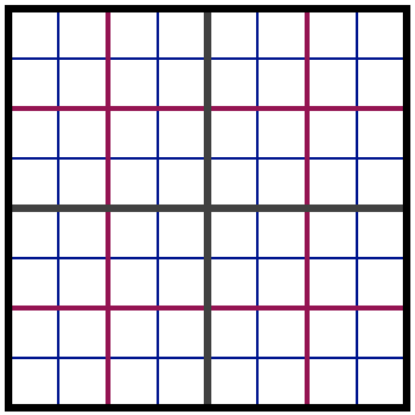
# PetFMM

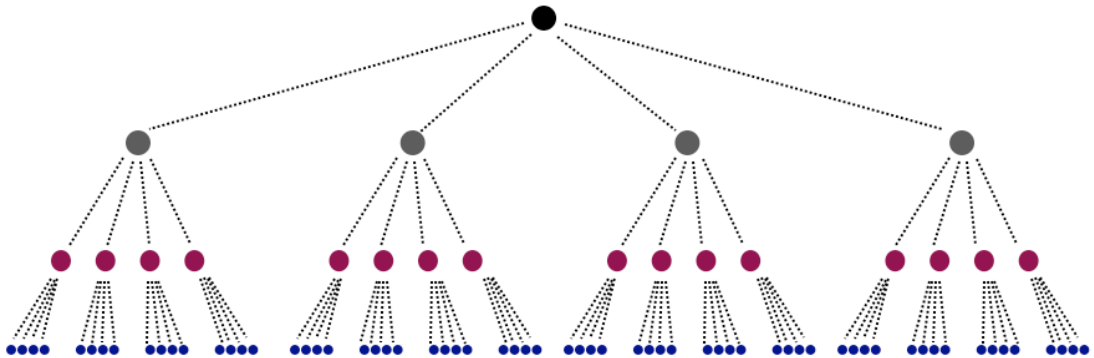
PetFMM is an freely available implementation of the
Fast Multipole Method
http://barbagroup.bu.edu/Barba_group/PetFMM.html

- 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

# Spatial Decomposition

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





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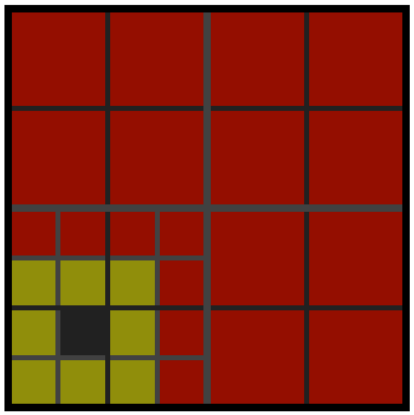
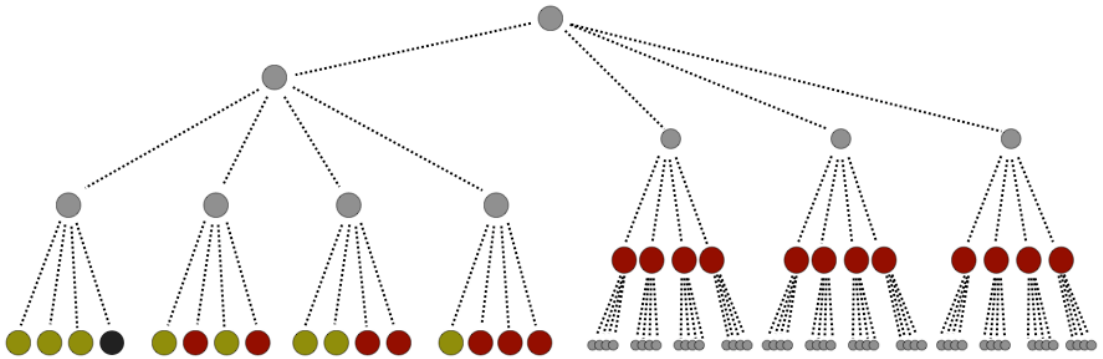
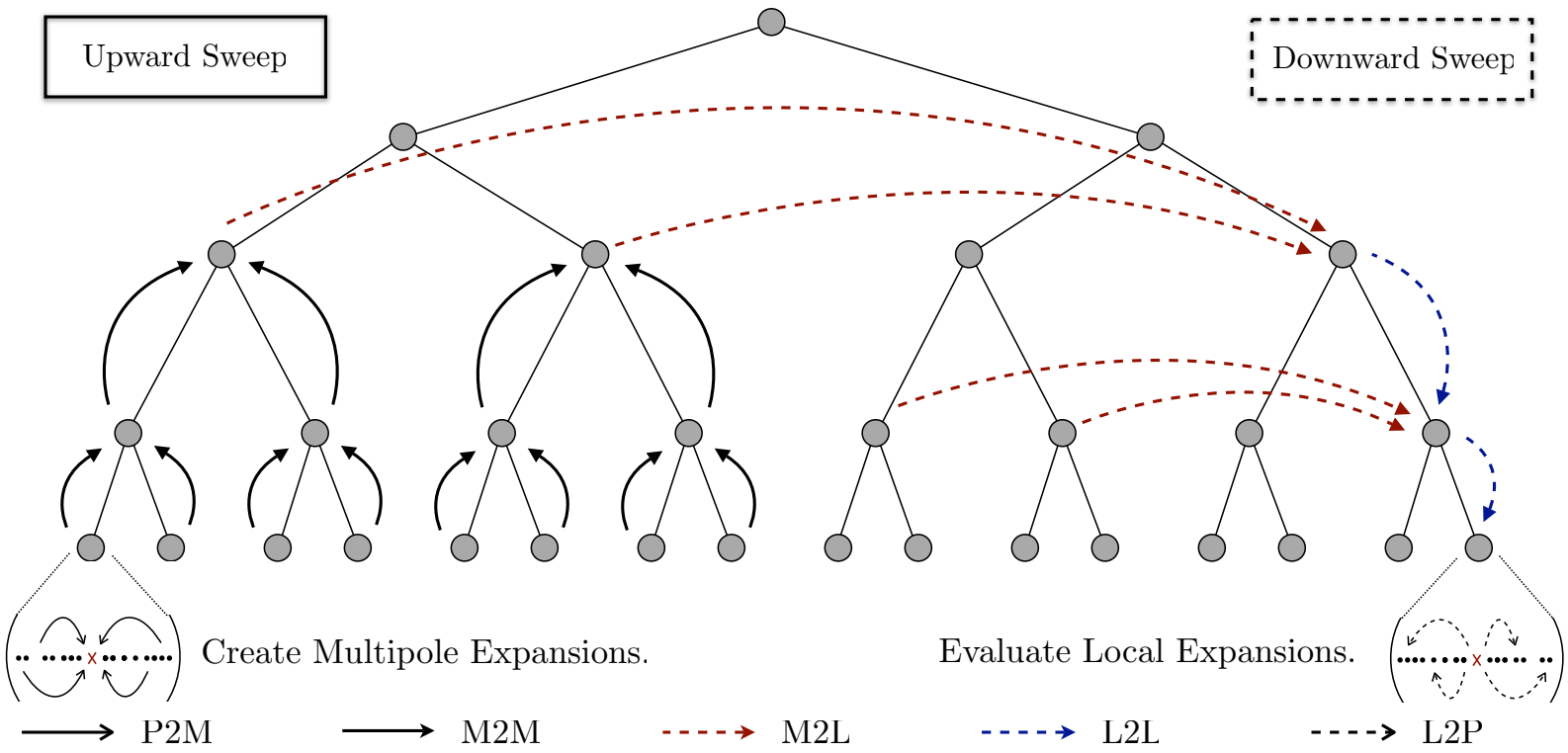




Neighbors are treated as *very near*.

# Functional Decomposition

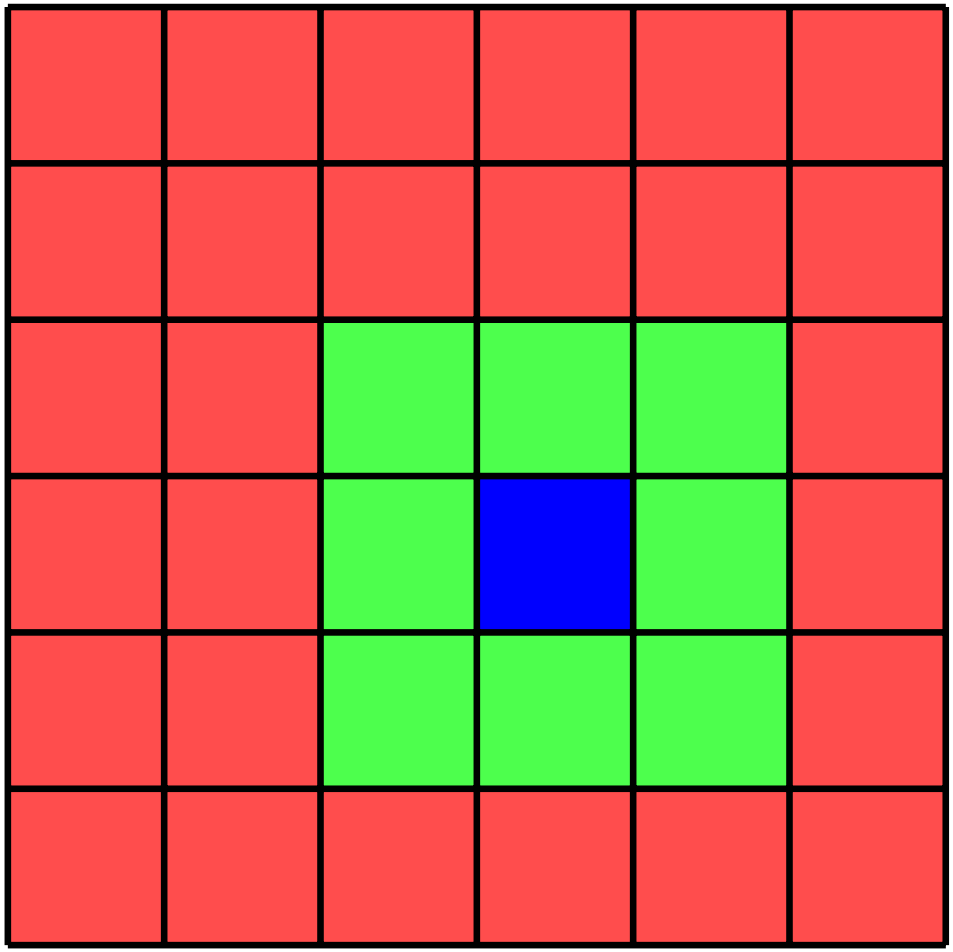


# Outline

# Multipole-to-Local Transformation

## Re-expands a multipole series as a Taylor series

- Up to 85% of time in FMM
  - Tradeoff with direct interaction
- Dense matrix multiplication
  - $2p^2$ rows
- Each interaction list box
  - $\left(6^d - 3^d\right) 2^{dL}$
- $d = 2, L = 8$
  - 1,769,472 matvecs



# GPU M2L
## Version 0

## One thread per M2L transform

- Thread block (TB) transforms one Multipole Expansion (ME) for each Interaction List (IL) box — 27 times
- $p = 12$
- Matrix size is 2304 bytes
- Plenty of work per thread (81 Kflops or 36 flops/byte)
- **BUT**, 16K shared memory only holds 7 matrices

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Memory limits concurrency!

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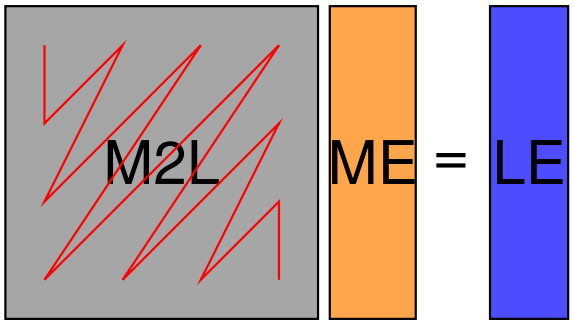
## Version 1

## Apply M2L transform matrix-free

$$\mathrm{m2l}_{ij} = -1^i \binom{i+j}{j} t^{-i-j-1} \tag{21}$$

- Traverse matrix by perdiagonals
- Same work
- No memory limit on concurrency
- 8 concurrent TBs per MultiProcessor (MP)
- $27 \times 8 = 216$ threads, **BUT** max is 512



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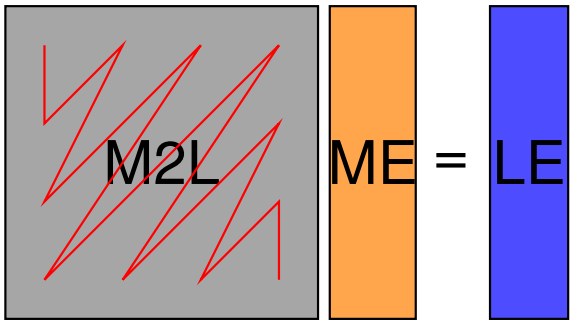

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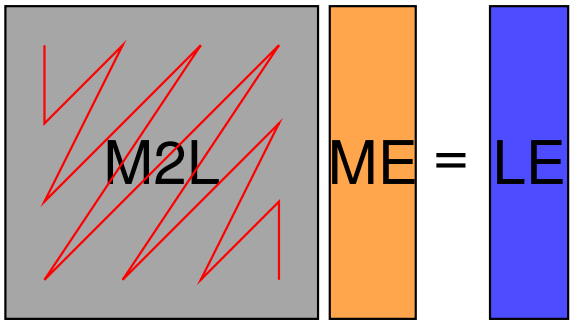

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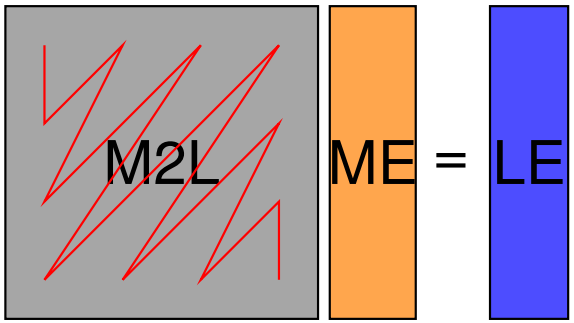

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Additional problems: Not enough parallelism for data movement

- Move 27 LE to global memory per TB
- $27 \times 2p = 648$ floats
- With 32 threads, takes 21 memory transactions

# GPU M2L
## Version 2

One thread per *element* of the LE

$$\mathrm{m2l}_{ij} = -1^i \binom{i+j}{j} t^{-i-j-1} \tag{22}$$

- Each thread does a dot product
- Cannot use diagonal traversal, more work
- Avoid branching
  - Each row precomputes $t^{-i-1}$
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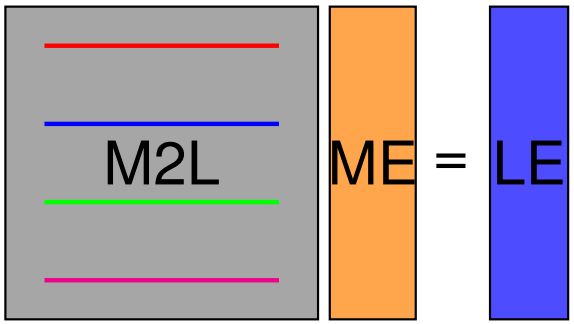
- Loop unrolling
- No thread synchronization



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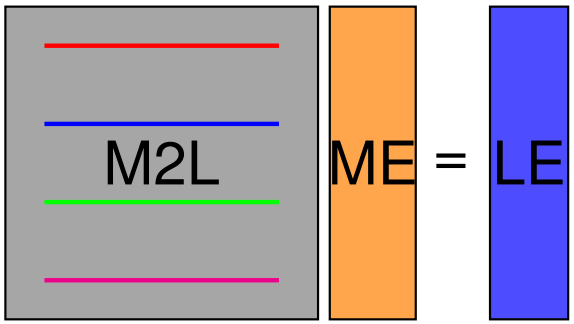

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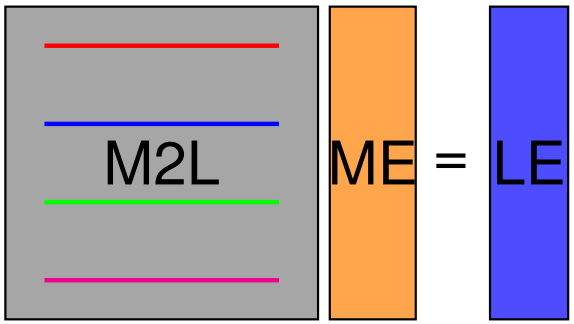

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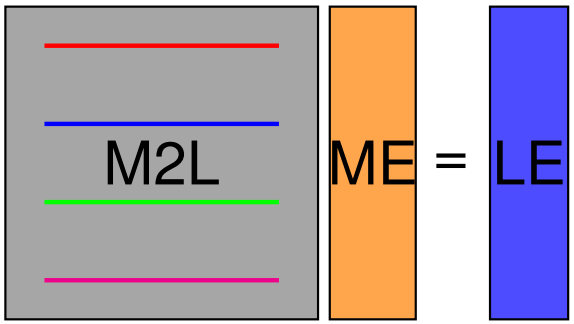

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Examine memory access

# Memory Bandwidth

Superior GPU memory bandwidth is due to both

bus width and clock speed.

| | CPU | GPU |
|---|---|---|
| Bus Width (bits) | 64 | 512 |
| Bus Clock Speed (MHz) | 400 | 1600 |
| Memory Bandwidth (GB/s) | 3 | 102 |
| Latency (cycles) | 240 | 600 |

Tesla always accesses blocks of 64 or 128 bytes

# GPU M2L
## Version 3

## Coalesce and overlap memory accesses

Coalescing is

- a group of 16 threads
- accessing consective addresses
  - 4, 8, or 16 bytes
- in the same block of memory
  - 32, 64, or 128 bytes

# GPU M2L
## Version 3

### Coalesce and overlap memory accesses

Memory accesses can be overlapped with computation when

- a TB is waiting for data from main memory
- another TB can be scheduled on the SM
- 512 TB can be active at once on Tesla

# GPU M2L
## Version 3

Coalesce and overlap memory accesses

Note that the theoretical peak (1 TF)

- MULT and FMA must execute simultaneously
- 346 GOps
- Without this, peak can be closer to 600 GF

480 GFlops

25x Speedup of Downward Sweep

# Design Principles

M2L required all of these optimization steps:

- Many threads per kernel
- Avoid branching
- Unroll loops
- Coalesce memory accesses
- Overlap main memory access with computation

# How Will Algorithms Change?

- Massive concurrency is necessary
  - Mix of vector and thread paradigms
  - Demands new analysis
- More attention to memory management
  - Blocks will only get larger
  - Determinant of performance