

Software Design for PDEs on GPUs

Matthew Knepley

Computation Institute
University of Chicago

Department of Molecular Biology and Physiology
Rush University Medical Center

Advanced Algorithms on GPUs
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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

The PetscGPU team:

- **Dr. Barry Smith**
 - Mathematics and Computer Science Division, ANL
- **Satish Balay**
 - Mathematics and Computer Science Division, ANL
- **Victor Minden**
 - Dept. of Mathematics, Tufts University

The PyLith Team:

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

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GPU computing must be
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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

- 1 PETS_c-GPU
- 2 FEM-GPU

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`)

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`)

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.

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

- 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

```
ex19 -da_vec_type seqcuda
      -da_mat_type aijcuda -mat_no_inode # Setup types
      -da_grid_x 100 -da_grid_y 100     # Set grid size
      -pc_type none -dmmg_nlevels 1     # Setup solver
      -preload off -cuda_synchronize    # Setup run
      -log_summary
```

Outline

1 PETSc-GPU

2 FEM-GPU

- Analytic Flexibility
- Computational Flexibility
- Efficiency

What are the Benefits for current PDE Code?

Low Order FEM on GPUs

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

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Analytic Flexibility

Laplacian

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

```
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

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

```

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

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

```

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

Analytic Flexibility

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- Analytic Flexibility
- **Computational Flexibility**
- Efficiency

Form Decomposition

Element integrals are decomposed into analytic and geometric parts:

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

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

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

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

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

Coefficients are also put into the geometric part.

Form Decomposition

Additional fields give rise to multilinear forms.

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

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

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

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

$$= \mathbf{G}^{\alpha\gamma}(\mathcal{T}) \mathbf{K}_{\alpha\gamma}^{ijk} \quad (13)$$

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

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

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

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

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

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

$$= \mathbf{G}_{kl}^{\beta\gamma}(\mathcal{T}) \mathbf{K}_{\beta\gamma}^{ijkl} \quad (19)$$

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

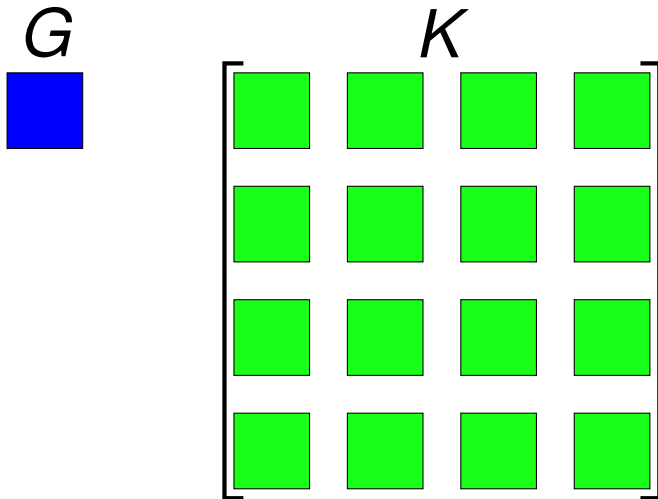


Figure: Tensor Contraction $G^{\beta\gamma}(T)K_{\beta\gamma}^{ij}$

Computational Flexibility

Basic Contraction

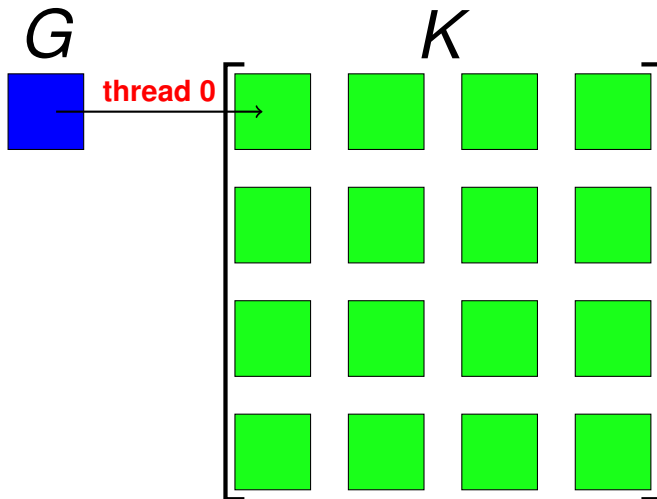


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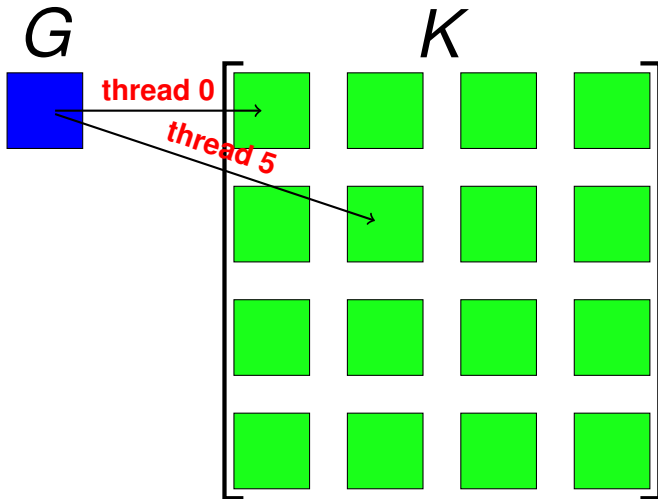


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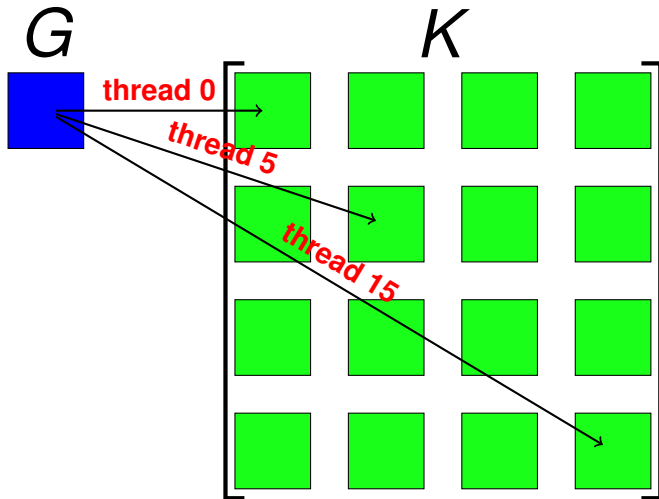


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Computational Flexibility

Element Batch Size

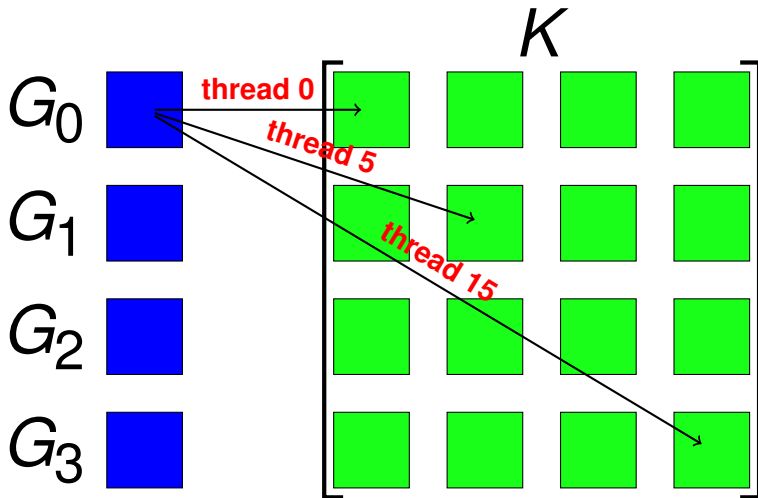


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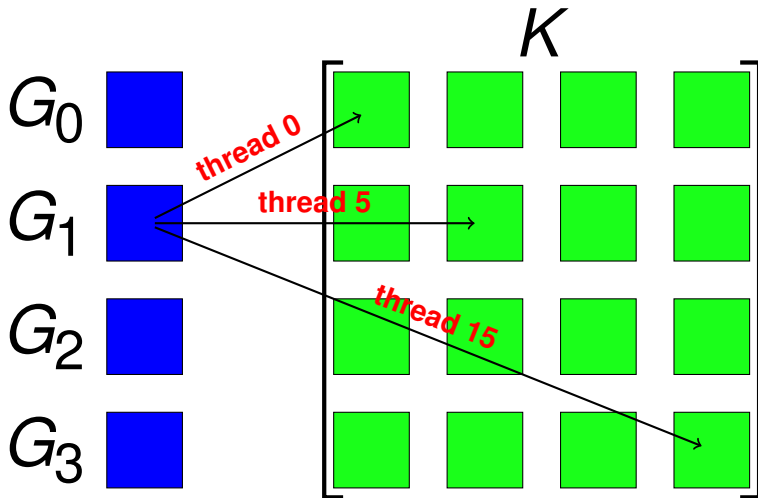


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Computational Flexibility

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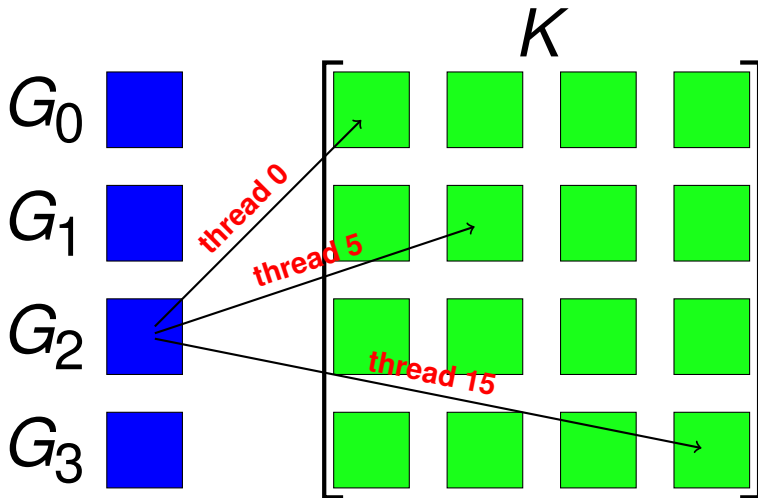


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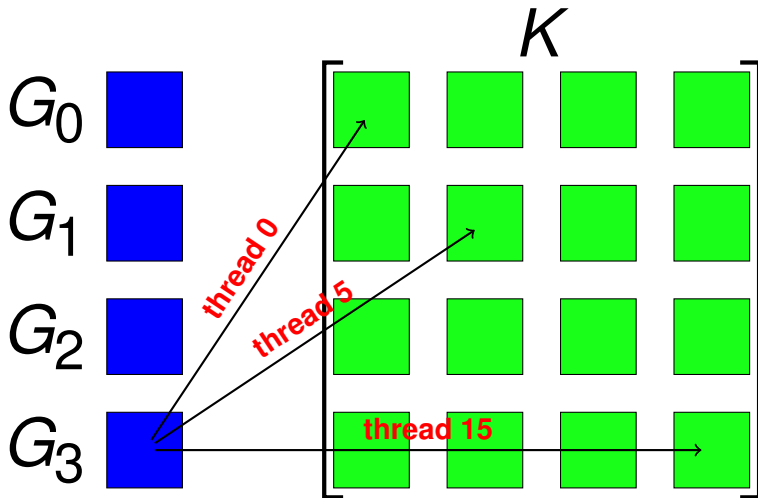
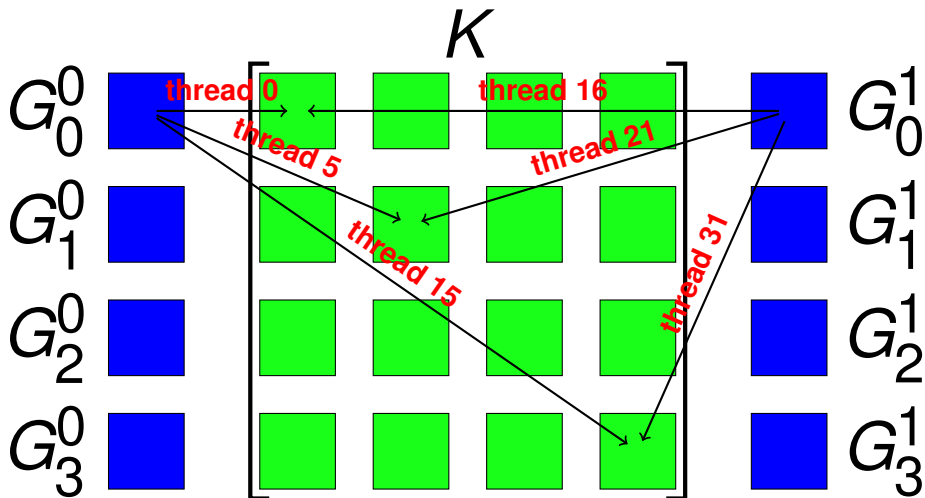


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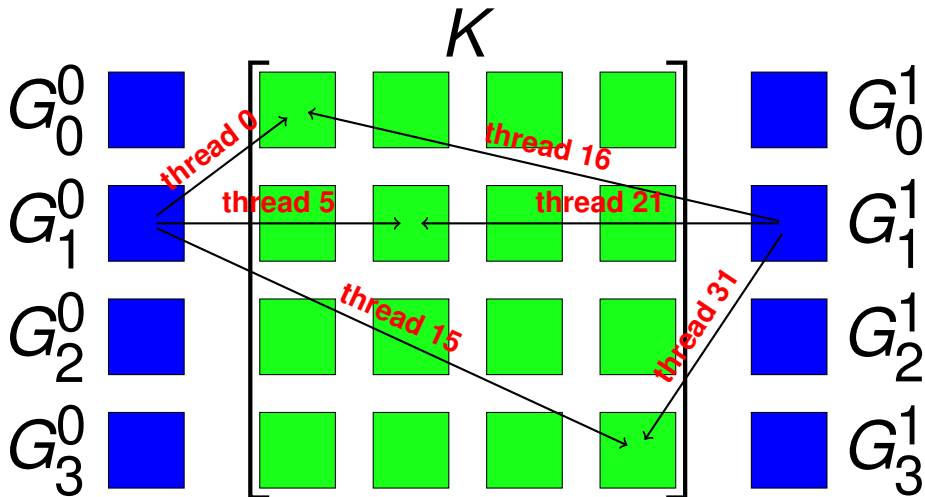
Computational Flexibility

Concurrent Elements



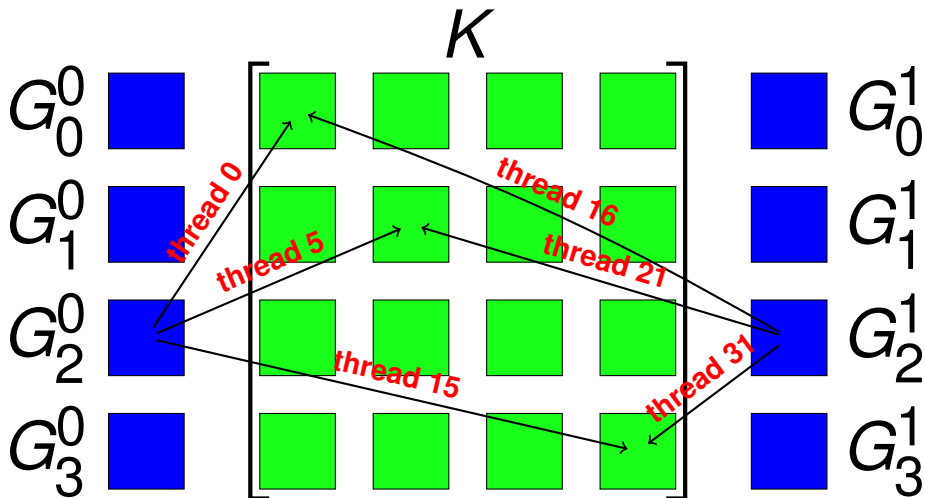
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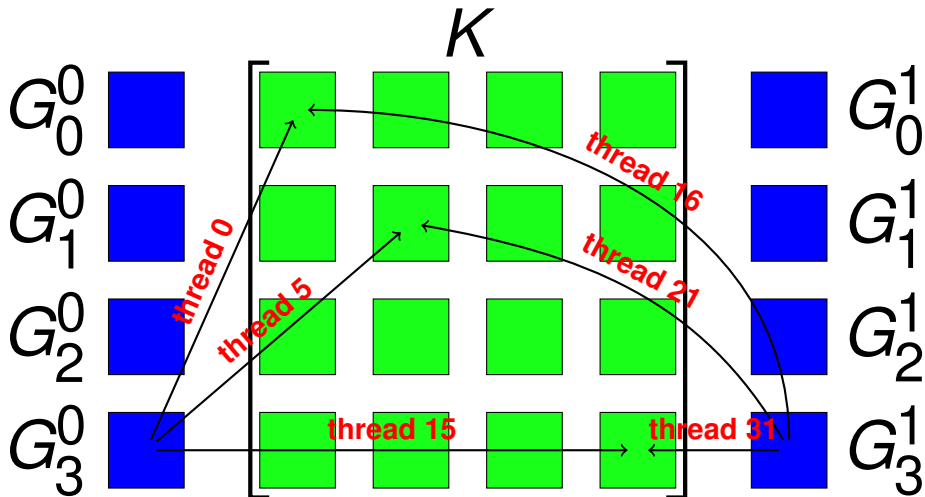
Computational Flexibility

Concurrent Elements



Computational Flexibility

Concurrent Elements



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;
```

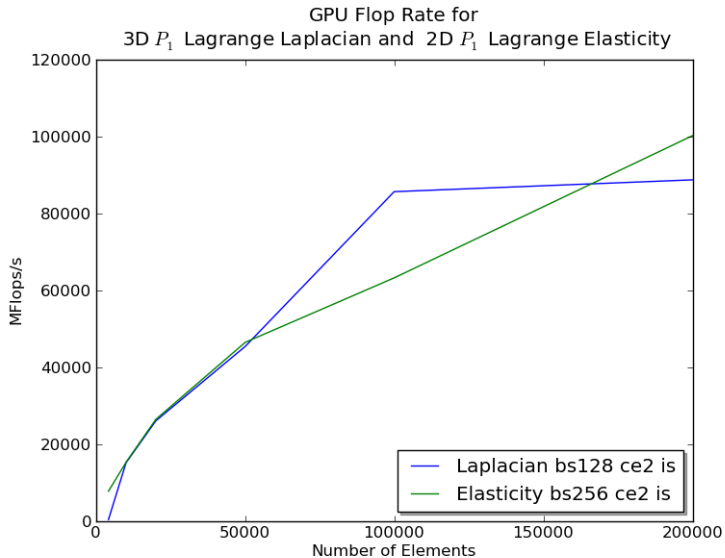
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- **Efficiency**

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

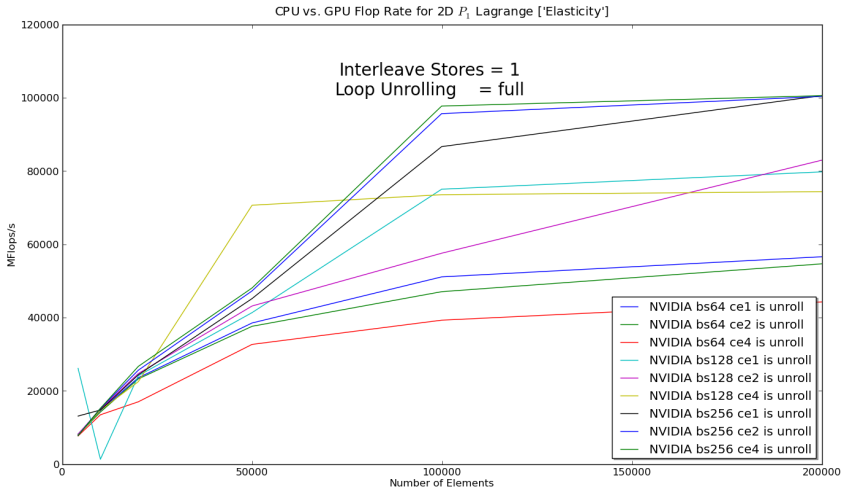
Price-Performance Comparison of CPU and GPU 3D P_1 Laplacian Integration

Model	Price (\$)	GF/s	MF/s\$
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* Jed Brown Optimization Engine

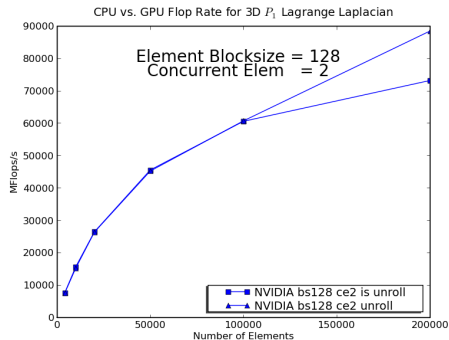
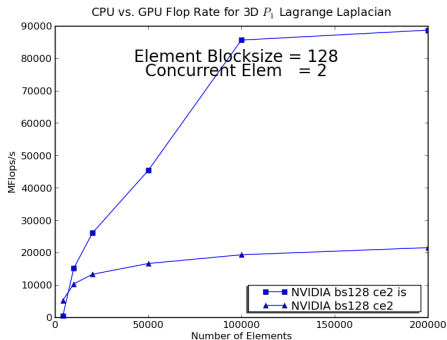
Performance

Influence of Element Batch Sizes



Performance

Influence of Code Structure



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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