GPUs in Computational Science

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RUSH UNIVERSITY
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Collaborators

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Outline

1. Introduction
2. Tools
3. FEM on the GPU
4. PETSc-GPU
5. Conclusions

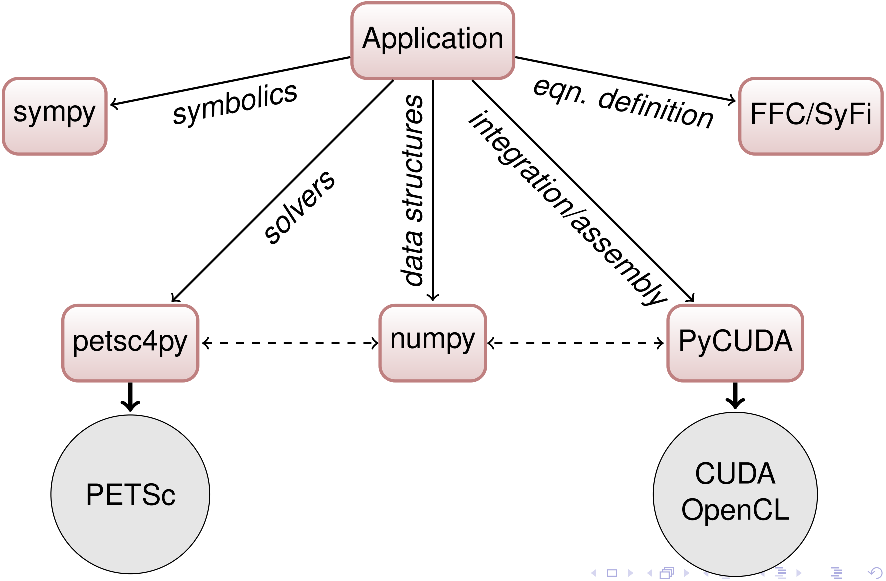
New Model for Scientific Software

Simplifying Parallelization of Scientific Codes by a Function-Centric Approach in Python

Jon K. Nilsen, Xing Cai, Bjorn Hoyland, and Hans Petter Langtangen

- **Python** at the application level
- **numpy** for data structures
- **petsc4py** for linear algebra and solvers
- **PyCUDA** for integration (physics) and assembly

New Model for Scientific Software



What is Missing from this Scheme?

- Unstructured graph traversal
  - Iteration over cells in FEM
    - Use a copy via numpy, use a kernel via Queue
  - (Transitive) Closure of a vertex
    - Use a visitor and copy via numpy
  - Depth First Search
    - Hell if I know
- Logic in computation
  - Limiters in FV methods
    - Can sometimes use tricks for branchless logic
  - Flux Corrected Transport for shock capturing
    - Maybe use WENO schemes which can be branchless
  - Boundary conditions
    - Restrict branching to PETSc C numbering and assembly calls
- **Audience???**

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2 Tools
- numpy
- petsc4py
- PyCUDA
- FEniCS

3 FEM on the GPU

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2 Tools

- numpy
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numpy

numpy is ideal for building Python data structures

- Supports multidimensional arrays
- Easily interfaces with C/C++ and Fortran
- High performance BLAS/LAPACK and functional operations
- Python 2 and 3 compatible
- Used by petsc4py to talk to PETSc

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petsc4py

petcs4py provides Python bindings for PETSc

- Provides ALL PETSc functionality in a Pythonic way
  - Logging using the Python `with` statement
- Can use Python callback functions
  - SNESSetFunction(), SNESSetJacobian()
- Manages all memory (creation/destruction)
- Visualization with matplotlib

petsc4py Installation

- Automatic
  - `pip install -install-options=-user petscp4y`
  - Uses `$PETSC_DIR` and `$PETSC_ARCH`
  - Installed into `$HOME/.local`
  - No additions to **PYTHONPATH**
- From Source
  - `virtualenv python-env`
  - `source ./python-env/bin/activate`
  - Now everything installs into your proxy Python environment
  - `hg clone https://petsc4py.googlecode.com/hg petsc4py-dev`
  - `ARCHFLAGS="-arch x86_64" python setup.py sdist`
  - `ARCHFLAGS="-arch x86_64" pip install dist/petsc4py-1.1.2.tar.gz`
  - **ARCHFLAGS** only necessary on Mac OSX

petsc4py Examples

- `externalpackages/petsc4py-1.1/demo/bratu2d/bratu2d.py`
  - Solves Bratu equation (SNES ex5) in 2D
  - Visualizes solution with matplotlib
- `src/ts/examples/tutorials/ex8.py`
  - Solves a 1D ODE for a diffusive process
  - Visualize solution using `-vec_view_draw`
  - Control timesteps with `-ts_max_steps`

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2 Tools

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PyCUDA and PyOpenCL

Python packages by Andreas Klöckner

for embedded GPU programming

- Handles unimportant details automatically
  - CUDA compile and caching of objects
  - Device initialization
  - Loading modules onto card
- Excellent Documentation & Tutorial
- Excellent platform for Metaprogramming
  - Only way to get portable performance
  - Road to FLAME-type reasoning about algorithms

Code Template

```
<%namespace name="pb" module="performanceBenchmarks"/>
${pb.globalMod(isGPU)} void kernel(${pb.gridSize(isGPU)} float *output) {
  ${pb.gridLoopStart(isGPU, load, store)}
  ${pb.threadLoopStart(isGPU, blockDimX)}
  float G[${dim*dim}] = {${','.join(['3.0']*(dim*dim))}};
  float K[${dim*dim}] = {${','.join(['3.0']*(dim*dim))}};
  float product       = 0.0;
  const int Ooffset   = gridIdx*${numThreads};

  // Contract G and K
% for n in range(numLocalElements):
%   for alpha in range(dim):
%     for beta in range(dim):
<%      gIdx = (n*dim + alpha)*dim + beta %>
<%      kIdx = alpha*dim + beta %>
  product += G[${gIdx}] * K[${kIdx}];
%     endfor
%   endfor
% endfor
  output[Ooffset+idx] = product;
  ${pb.threadLoopEnd(isGPU)}
  ${pb.gridLoopEnd(isGPU)}
  return;
```

Rendering a Template

We render code template into strings using a dictionary of inputs.

```
args = {'dim':              self.dim,
        'numLocalElements': 1,
        'numThreads':       self.threadBlockSize}
kernelTemplate = self.getKernelTemplate()
gpuCode = kernelTemplate.render(isGPU = True, **args)
cpuCode = kernelTemplate.render(isGPU = False, **args)
```

GPU Source Code

```
__global__ void kernel(float *output) {
  const int        gridIdx = blockIdx.x + blockIdx.y*gridDim.x;
  const int        idx     = threadIdx.x + threadIdx.y*1; // This is (i,j)
  float G[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float K[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float product       = 0.0;
  const int Ooffset   = gridIdx*1;

  // Contract G and K
  product += G[0] * K[0];
  product += G[1] * K[1];
  product += G[2] * K[2];
  product += G[3] * K[3];
  product += G[4] * K[4];
  product += G[5] * K[5];
  product += G[6] * K[6];
  product += G[7] * K[7];
  product += G[8] * K[8];
  output[Ooffset+idx] = product;
  return;
}
```

CPU Source Code

```
void kernel(int numInvocations, float *output) {
  for(int gridIdx = 0; gridIdx < numInvocations; ++gridIdx) {
    for(int i = 0; i < 1; ++i) {
      for(int j = 0; j < 1; ++j) {
        const int  idx = i + j*1; // This is (i,j)
  float G[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float K[9] = {3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0,3.0};
  float product       = 0.0;
  const int Ooffset   = gridIdx*1;

  // Contract G and K
  product += G[0] * K[0];
  product += G[1] * K[1];
  product += G[2] * K[2];
  product += G[3] * K[3];
  product += G[4] * K[4];
  product += G[5] * K[5];
  product += G[6] * K[6];
  product += G[7] * K[7];
  product += G[8] * K[8];
  output[Ooffset+idx] = product;
      }
    }
```

Creating a Module

CPU:

```
# Output kernel and C support code
self.outputKernelC(cpuCode)
self.writeMakefile()
out, err, status = self.executeShellCommand('make')
\end{minted}

\bigskip

GPU:
\begin{minted}{python}
from pycuda.compiler import SourceModule

mod = SourceModule(gpuCode)
self.kernel = mod.get_function('kernel')
self.kernelReport(self.kernel, 'kernel')
```

Executing a Module

```
import pycuda.driver as cuda
import pycuda.autoinit

blockDim = (self.dim, self.dim, 1)
start    = cuda.Event()
end      = cuda.Event()
grid     = self.calculateGrid(N, numLocalElements)
start.record()
for i in range(iters):
  self.kernel(cuda.Out(output),
              block = blockDim, grid = grid)
end.record()
end.synchronize()
gpuTimes.append(start.time_till(end)*1e-3/iters)
```

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Weak Form Definition

Laplacian

```python
# $P^k$ element
element = FiniteElement("Lagrange", domains[self.dim], k)
v = TestFunction(element)
u = TrialFunction(element)
f = Coefficient(element)

a = inner(grad(v), grad(u))*dx
L = v*f*dx
```

Form Decomposition

Element integrals are decomposed into analytic and geometric parts:

$$
\begin{aligned}
& \int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) d\mathbf{x} && (1)\\
= & \int_{\mathcal{T}} \frac{\partial\phi_i(\mathbf{x})}{\partial x_\alpha} \frac{\partial\phi_j(\mathbf{x})}{\partial x_\alpha} d\mathbf{x} && (2)\\
= & \int_{\mathcal{T}_{\mathrm{ref}}} \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\xi_\gamma}{\partial x_\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} |J| d\mathbf{x} && (3)\\
= & \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\mathrm{ref}}} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} d\mathbf{x} && (4)\\
= & G^{\beta\gamma}(\mathcal{T}) K^{ij}_{\beta\gamma} && (5)
\end{aligned}
$$

Coefficients are also put into the geometric part.

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
```

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Element integrals are decomposed into analytic and geometric parts:

$$
\begin{aligned}
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= & \int_{\mathcal{T}} \frac{\partial\phi_i(\mathbf{x})}{\partial x_\alpha} \frac{\partial\phi_j(\mathbf{x})}{\partial x_\alpha} d\mathbf{x} && (7)\\
= & \int_{\mathcal{T}_{\mathrm{ref}}} \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\xi_\gamma}{\partial x_\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} |J| d\mathbf{x} && (8)\\
= & \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\mathrm{ref}}} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} d\mathbf{x} && (9)\\
= & G^{\beta\gamma}(\mathcal{T}) K^{ij}_{\beta\gamma} && (10)
\end{aligned}
$$

Coefficients are also put into the geometric part.

Form Decomposition

Additional fields give rise to multilinear forms.

$$\begin{aligned}
& \int_{\mathcal{T}} \phi_i(\mathbf{x}) \cdot \left(\phi_k(\mathbf{x}) \nabla \phi_j(\mathbf{x})\right) dA && (11)\\
= \quad & \int_{\mathcal{T}} \phi_i^\beta(\mathbf{x}) \left(\phi_k^\alpha(\mathbf{x}) \frac{\partial \phi_j^\beta(\mathbf{x})}{\partial x_\alpha}\right) dA && (12)\\
= \quad & \int_{\mathcal{T}_{\mathrm{ref}}} \phi_i^\beta(\xi) \phi_k^\alpha(\xi) \frac{\partial \xi_\gamma}{\partial x_\alpha} \frac{\partial \phi_j^\beta(\xi)}{\partial \xi_\gamma} |J| dA && (13)\\
= \quad & \frac{\partial \xi_\gamma}{\partial x_\alpha} |J| \int_{\mathcal{T}_{\mathrm{ref}}} \phi_i^\beta(\xi) \phi_k^\alpha(\xi) \frac{\partial \phi_j^\beta(\xi)}{\partial \xi_\gamma} dA && (14)\\
= \quad & G^{\alpha\gamma}(\mathcal{T}) K^{ijk}_{\alpha\gamma} && (15)
\end{aligned}$$

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

$$
\begin{aligned}
& \int_{\mathcal{T}} \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x}) dA && (16)\\
= & \int_{\mathcal{T}} \frac{\partial\phi_i(\mathbf{x})}{\partial x_\alpha} \frac{\partial\phi_j(\mathbf{x})}{\partial x_\alpha} dA && (17)\\
= & \int_{\mathcal{T}_{\mathrm{ref}}} \frac{\partial\xi_\beta}{\partial x_\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \frac{\partial\xi_\gamma}{\partial x_\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} |J| dA && (18)\\
= & |J| \int_{\mathcal{T}_{\mathrm{ref}}} \phi_k J_k^{\beta\alpha} \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \phi_l J_l^{\gamma\alpha} \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} dA && (19)\\
= & J_k^{\beta\alpha} J_l^{\gamma\alpha} |J| \int_{\mathcal{T}_{\mathrm{ref}}} \phi_k \frac{\partial\phi_i(\xi)}{\partial\xi_\beta} \phi_l \frac{\partial\phi_j(\xi)}{\partial\xi_\gamma} dA && (20)\\
= & G_{kl}^{\beta\gamma}(\mathcal{T}) K_{\beta\gamma}^{ijkl} && (21)
\end{aligned}
$$

A different space could also be used for Jacobians

Element Matrix Formation

- Element matrix K is now made up of small tensors
- Contract all tensor elements with each the geometry tensor $G(\mathcal{T})$

3 0 0 0	0 -1 0 0	1 1 0 0	-4 -4 0 0	0 4 0 0	0 0 0 0
0 0 -1 0	0 0 0 3	0 0 1 1	0 0 0 0	0 0 4 0	0 0 -4 -4
1 0 1 0	0 1 0 1	3 3 3 3	-4 0 -4 0	0 0 0 0	0 -4 0 -4
-4 0 -4 0	0 0 0 0	-4 -4 0 0	8 4 4 8	0 -4 -4 -8	0 4 4 0
0 0 4 0	0 4 0 0	0 0 0 0	0 -4 -4 -8	8 4 4 8	-8 -4 -4 0
0 0 0 0	0 -4 0 -4	0 0 -4 -4	0 4 4 0	-8 -4 -4 0	8 4 4 8

Mapping $G^{\alpha\beta} K^{ij}_{\alpha\beta}$ to the GPU

Problem Division

For N elements, map blocks of N_L elements to each Thread Block (TB)

- Launch `grid` must be $g_x \times g_y = {}^{N}/_{N_L}$
- TB grid will depend on the specific algorithm
- Output is size $N_{\mathrm{basis}} \times N_{\mathrm{basis}} \times N_L$

We can split a TB to work on multiple, N_B, elements at a time

- Note that each TB always gets N_L elements, so N_B must divide N_L

Mapping $G^{\alpha\beta}K^{ij}_{\alpha\beta}$ to the GPU

Kernel Arguments

```
__global__
void integrateJacobian(float *elemMat,
                       float *geometry,
                       float *analytic)
```

- **geometry**: Array of G tensors for each element
- **analytic**: K tensor
- **elemMat**: Array of $E = G : K$ tensors for each element

Mapping $G^{\alpha\beta} K^{ij}_{\alpha\beta}$ to the GPU

Memory Movement

We can interleave stores with computation, or wait until the end

- Waiting could improve coalescing of writes
- Interleaving could allow overlap of writes with computation

Also need to

- Coalesce accesses between global and local/shared memory (use `moveArray()`)
- Limit use of shared and local memory

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

Mapping $G^{\alpha\beta} K^{ij}_{\alpha\beta}$ to the GPU

Reduction

Choose strategies to minimize reductions

- Only reductions occur in summation for contractions
  - Similar to the reduction in a quadrature loop
- **Strategy #1**: Each thread uses all of K
- **Strategy #2**: Do each contraction in a separate thread

Strategy #1
TB Division

Each thread computes an entire element matrix, so that

$$\mathrm{blockDim} = \left({}^{N_L}\!/_{N_B}, 1, 1\right)$$

We will see that there is little opportunity to overlap computation and memory access

Strategy #1

Analytic Part

Read *K* into shared memory (need to synchronize before access)

```
__shared__ float K[${dim*dim*numBasisFuncs*numBasisFuncs}];

${fm.moveArray('K', 'analytic',
               dim*dim*numBasisFuncs*numBasisFuncs, '', numThreads)}
__syncthreads();
```

Strategy #1

Geometry

- Each thread handles N_B elements
- Read G into local memory (not coalesced)
- Interleaving means writing after each thread does a single element matrix calculation

```
float      G[${dim*dim*numBlockElements}];

if (interleaved) {
  const int Goffset = (gridIdx*${numLocalElements} + idx)*${dim*dim};
  for n in range(numBlockElements):
    ${fm.moveArray('G', 'geometry', dim*dim, 'Goffset',
                   blockNumber = n*numLocalElements/numBlockElements,
                   localBlockNumber = n, isCoalesced = False)}
  endfor
} else {
  const int Goffset = (gridIdx*${numLocalElements/numBlockElements} + idx)
                      *${dim*dim*numBlockElements};
  ${fm.moveArray('G', 'geometry', dim*dim*numBlockElements, 'Goffset',
                 isCoalesced = False)}
}
```

Strategy #1
Output

We write element matrices out contiguously by TB

```
const int matSize = numBasisFuncs*numBasisFuncs;
const int Eoffset = gridIdx*matSize*numLocalElements;

if (interleaved) {
  const int        elemOff = idx*matSize;
  __shared__ float E[matSize*numLocalElements/numBlockElements];
} else {
  const int        elemOff = idx*matSize*numBlockElements;
  __shared__ float E[matSize*numLocalElements];
}
```

Strategy #1
Contraction

```
matSize = numBasisFuncs*numBasisFuncs
if interleaveStores:
  for b in range(numBlockElements):
    # Do 1 contraction for each thread
    __syncthreads();
    fm.moveArray('E', 'elemMat',
                 matSize*numLocalElements/numBlockElements,
                 'Eoffset', numThreads, blockNumber = n, isLoad = 0)
else:
  # Do numBlockElements contractions for each thread
  __syncthreads();
  fm.moveArray('E', 'elemMat',
               matSize*numLocalElements,
               'Eoffset', numThreads, isLoad = 0)
```

Strategy #2
TB Division

Each thread computes a single element of an element matrix, so that

$$\mathrm{blockDim} = (N_{\mathrm{basis}}, N_{\mathrm{basis}}, N_B)$$

This allows us to overlap computation of another element in the TB with writes for the first.

Strategy #2
Analytic Part

- Assign an (i,j) block of K to local memory
- N_B threads will simultaneously calculate a contraction

```
const int Kidx    = threadIdx.x + threadIdx.y*${numBasisFuncs}; // This is
const int idx     = Kidx + threadIdx.z*${numBasisFuncs*numBasisFuncs};
const int Koffset = Kidx*${dim*dim};
float     K[${dim*dim}];

% for alpha in range(dim):
%   for beta in range(dim):
<%     kIdx = alpha*dim + beta %>
K[${kIdx}] = analytic[Koffset+${kIdx}];
%   endfor
% endfor
```

Strategy #2

Geometry

- Store N_L G tensors into shared memory
- Interleaving means writing after each thread does a single element calculation

```
const int          Goffset = gridIdx*${dim*dim*numLocalElements};
__shared__ float G[${dim*dim*numLocalElements}];

${fm.moveArray('G', 'geometry', dim*dim*numLocalElements,
               'Goffset', numThreads)}
__syncthreads();
```

Strategy #2

Output

- We write element matrices out contiguously by TB
- If interleaving stores, only need a single product
- Otherwise, need ${}^{N_L}/_{N_B}$, one per element processed by a thread

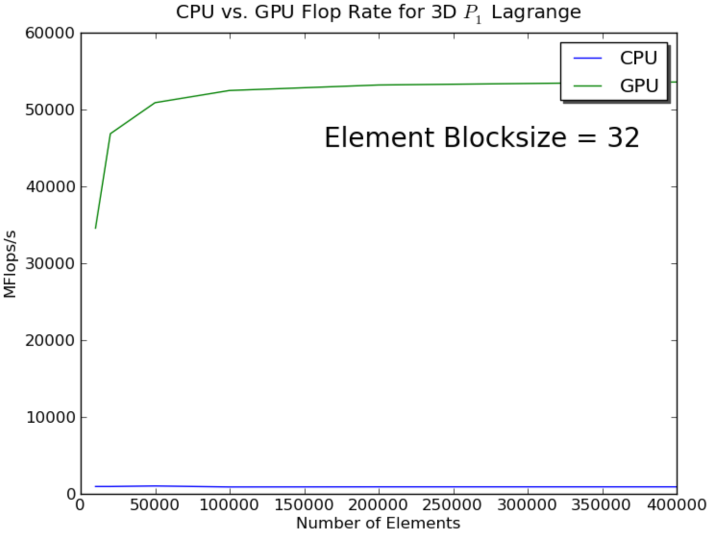
```
const int matSize = numBasisFuncs*numBasisFuncs;
const int Eoffset = gridIdx*matSize*numLocalElements;

if (interleaved) {
  float                product = 0.0;
  const int            elemOff = idx*matSize;
} else {
  float                product[numLocalElements/numBlockElements];
  const int            elemOff = idx*matSize*numBlockElements;
}
```

Strategy #2

Contraction

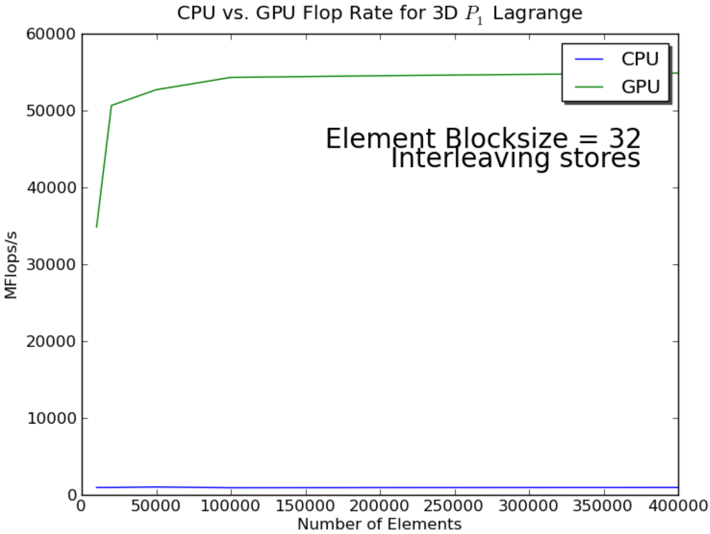
```
if interleaveStores:
  for n in range(numLocalElements/numBlockElements):
    # Do 1 contraction for each thread
    __syncthreads()
    # Do coalesced write of element matrix
    elemMat[Eoffset+idx + n*numThreads] = product
else:
  # Do numLocalElements/numBlockElements contractions
  #   save results in product[]
  for n in range(numLocalElements/numBlockElements):
    elemMat[Eoffset+idx + n*numThreads] = product[n]
```

Results
GTX 285



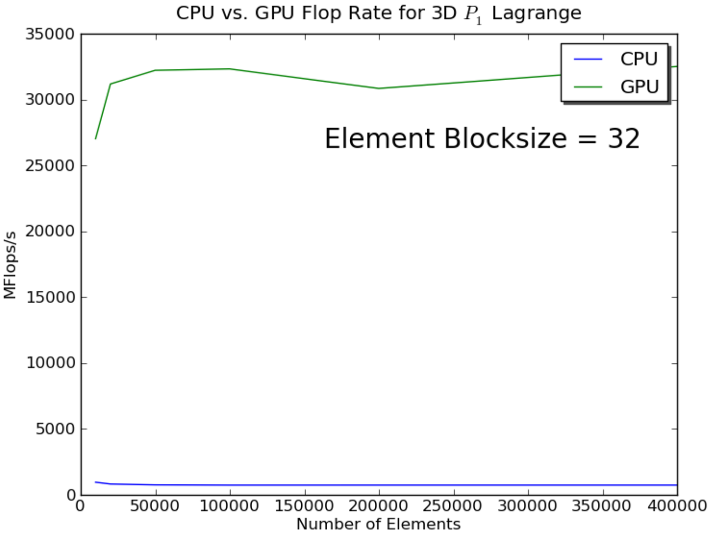
Results

GTX 285



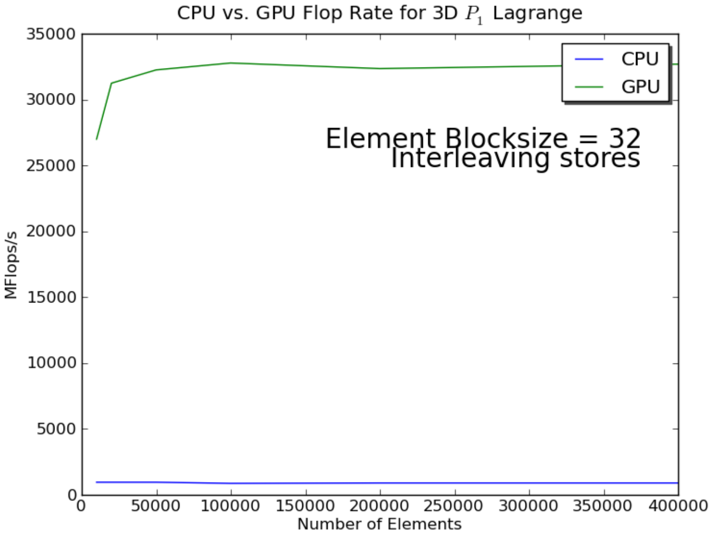
Results

GTX 285, 2 Simultaneous Elements



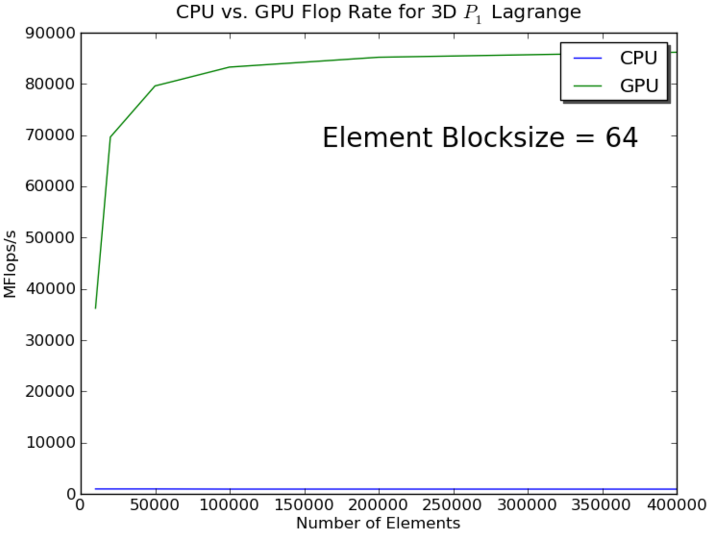
Results

GTX 285, 2 Simultaneous Elements

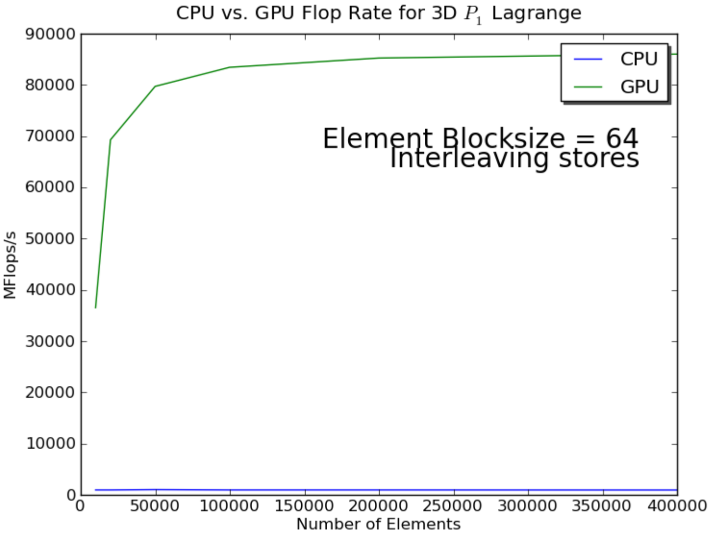


Results

GTX 285

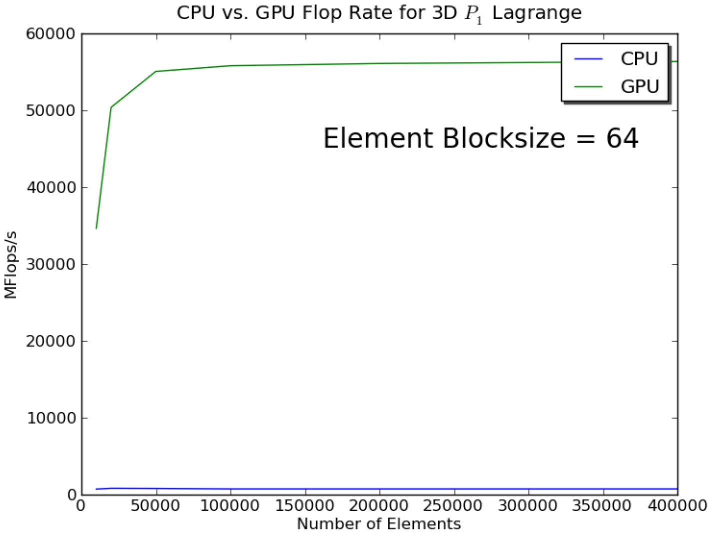


Results
GTX 285



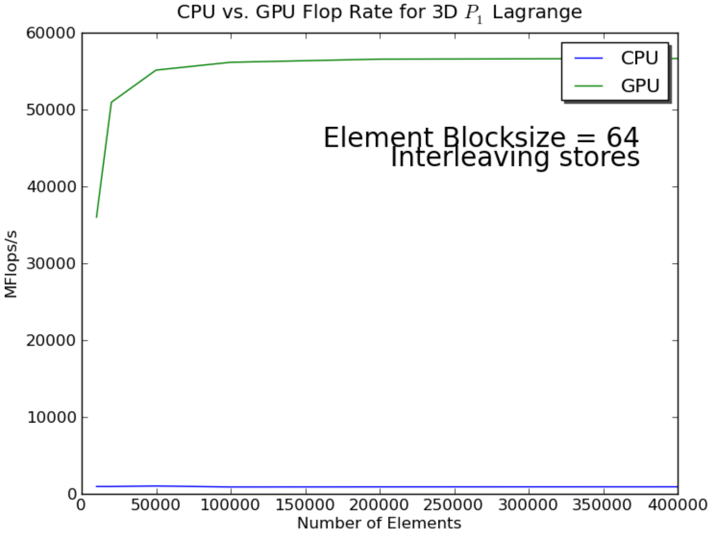
Results

GTX 285, 2 Simultaneous Elements



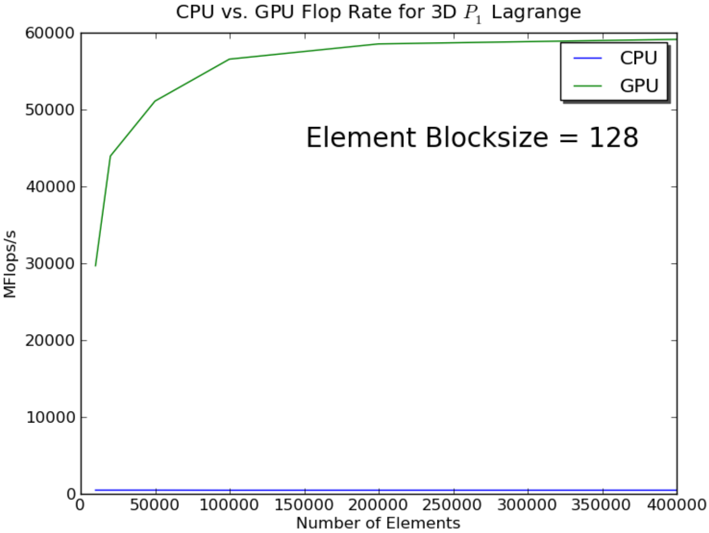
Results

GTX 285, 2 Simultaneous Elements



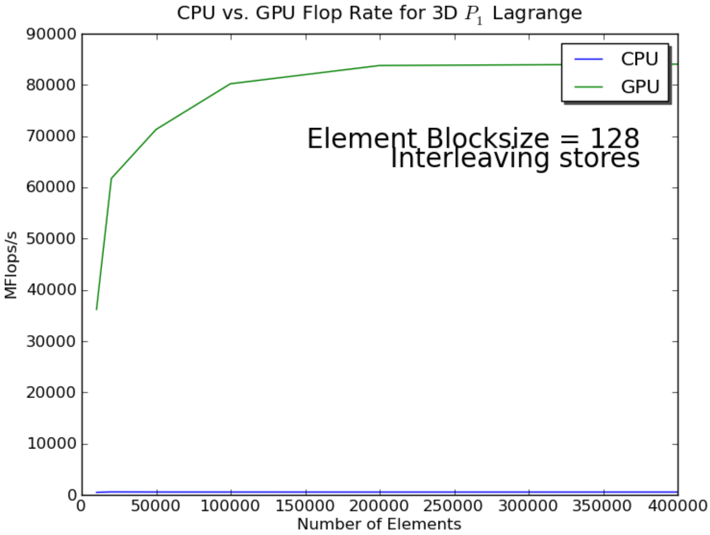
Results

GTX 285



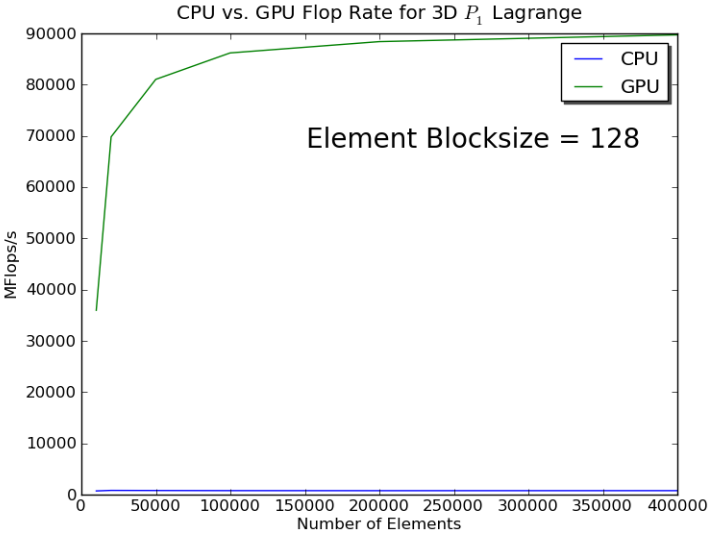
Results

GTX 285



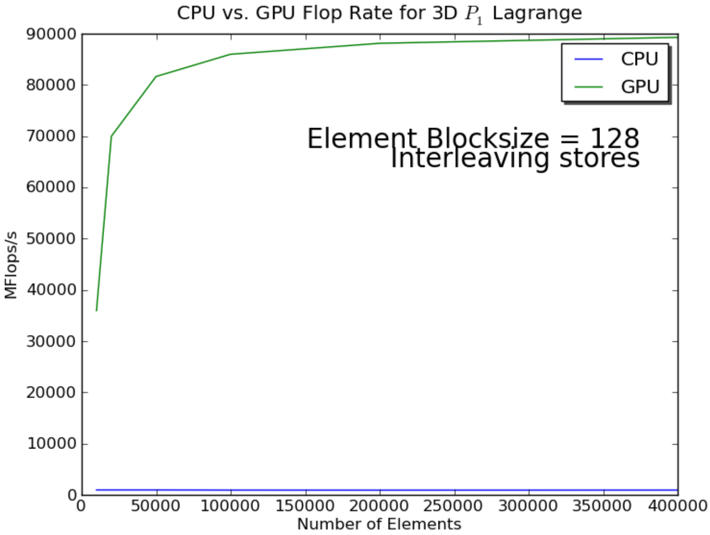
Results

GTX 285, 2 Simultaneous Elements



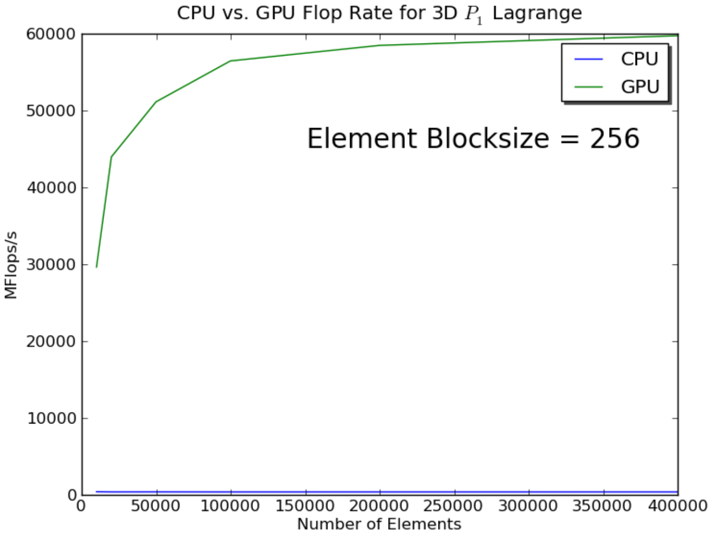
Results

GTX 285, 2 Simultaneous Elements



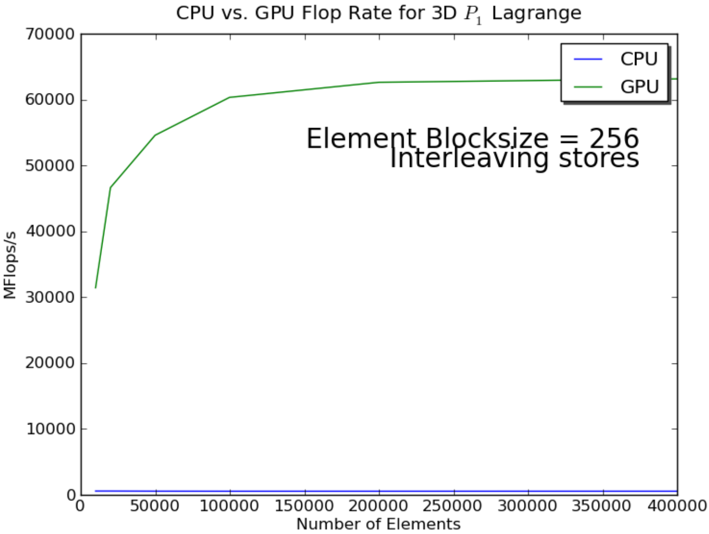
Results

GTX 285, 2 Simultaneous Elements



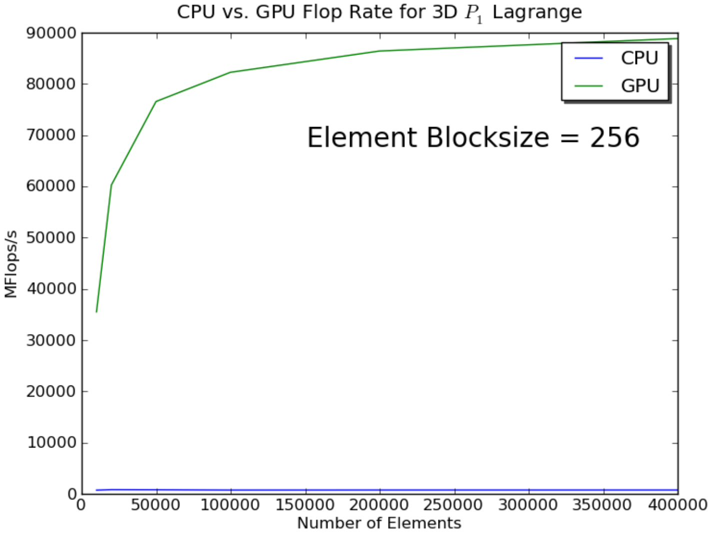
Results

GTX 285, 2 Simultaneous Elements



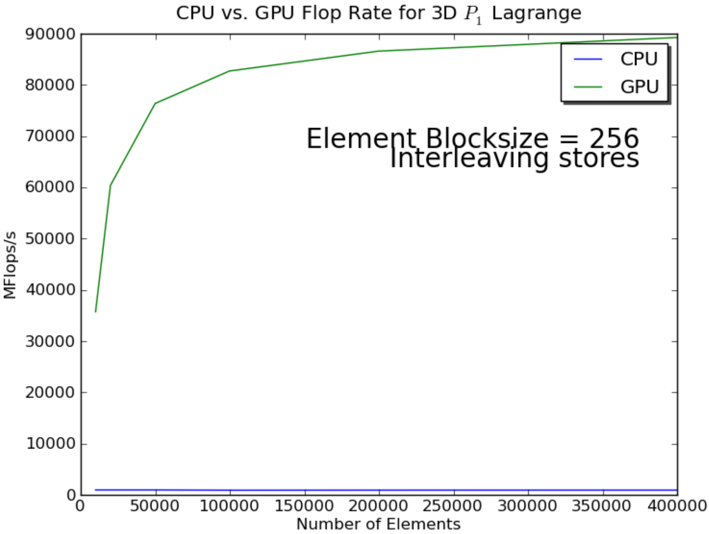
Results

GTX 285, 4 Simultaneous Elements



Results

GTX 285, 4 Simultaneous Elements



Outline

1 Introduction

2 Tools

3 FEM on the GPU

4 PETSc-GPU

5 Conclusions

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

1 Introduction

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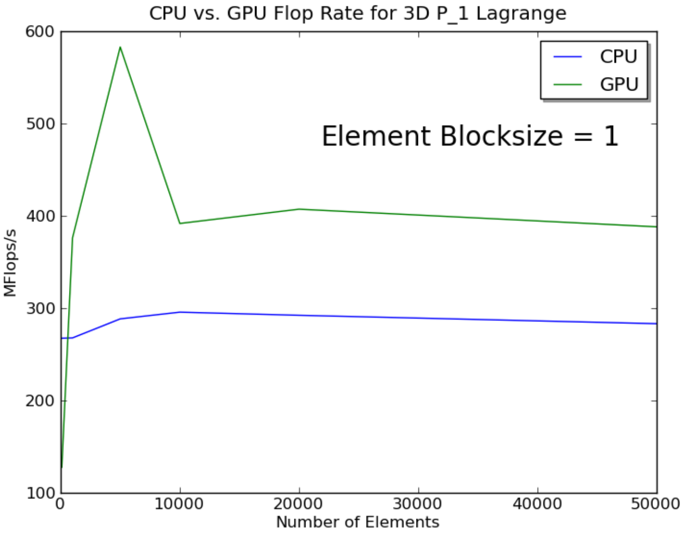
How Will Algorithms Change?

- 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

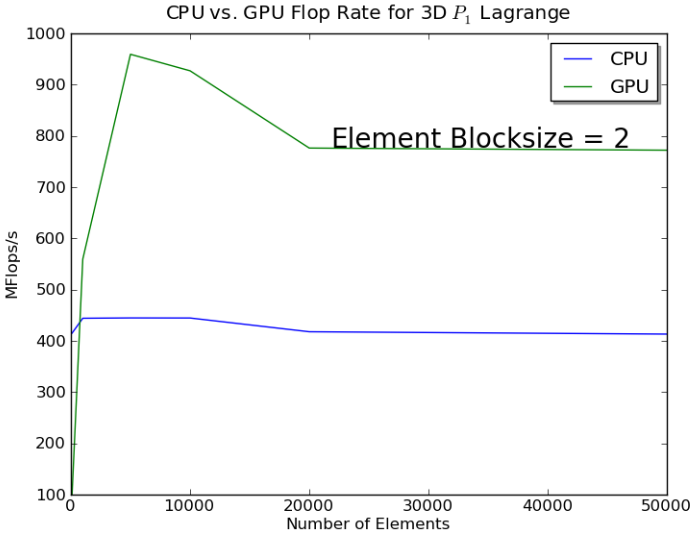
Results

9400M



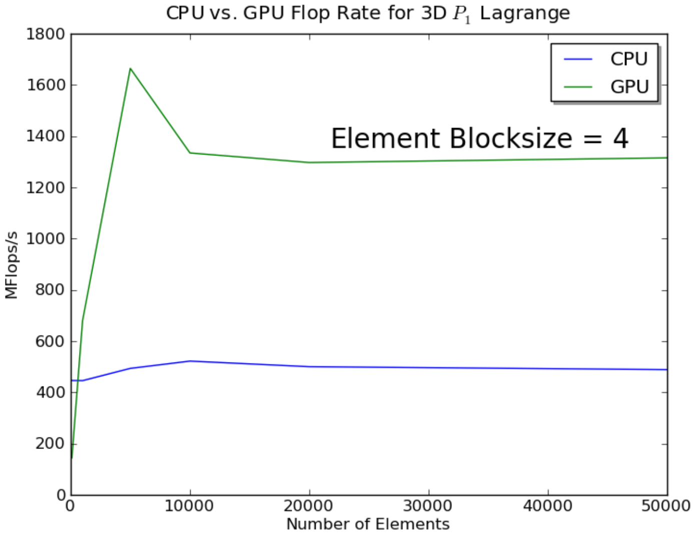
Results

9400M



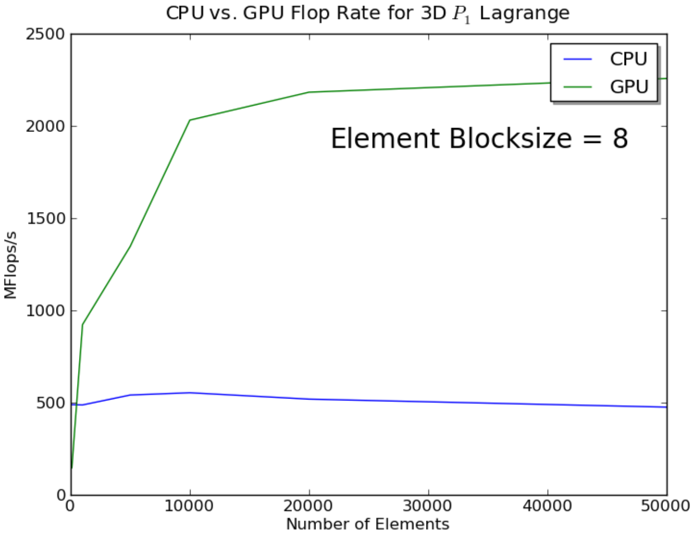
Results

9400M



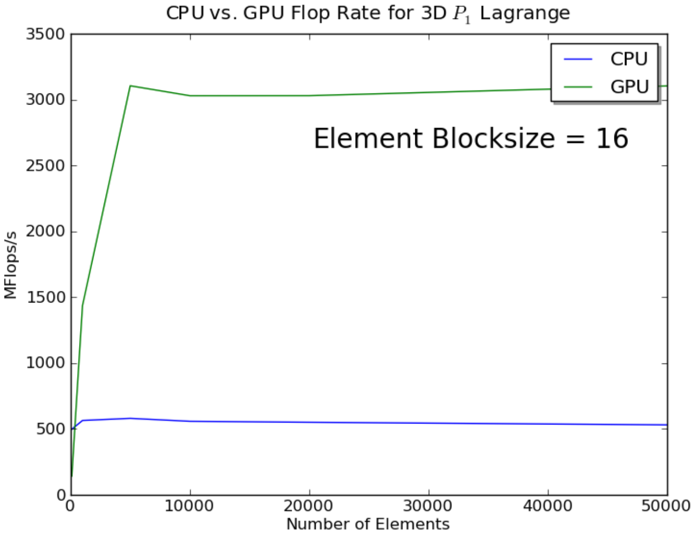
Results

9400M



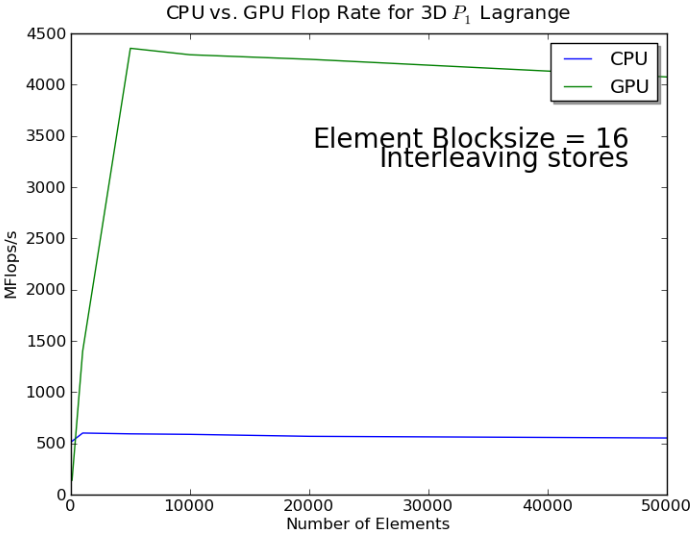
Results

9400M



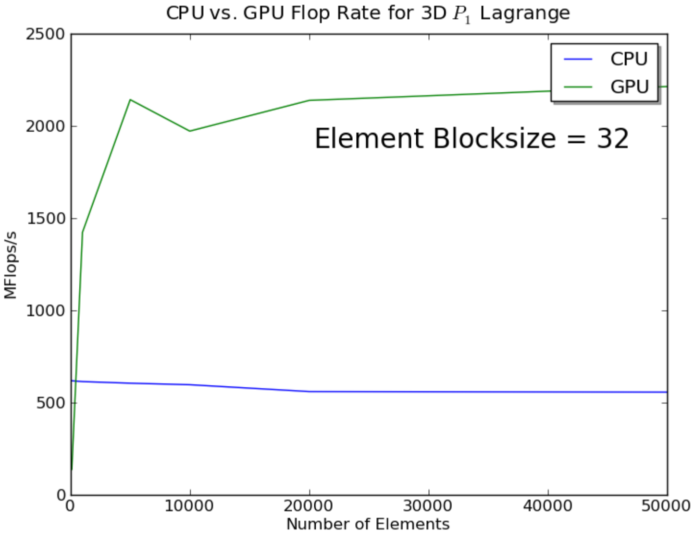
Results

9400M



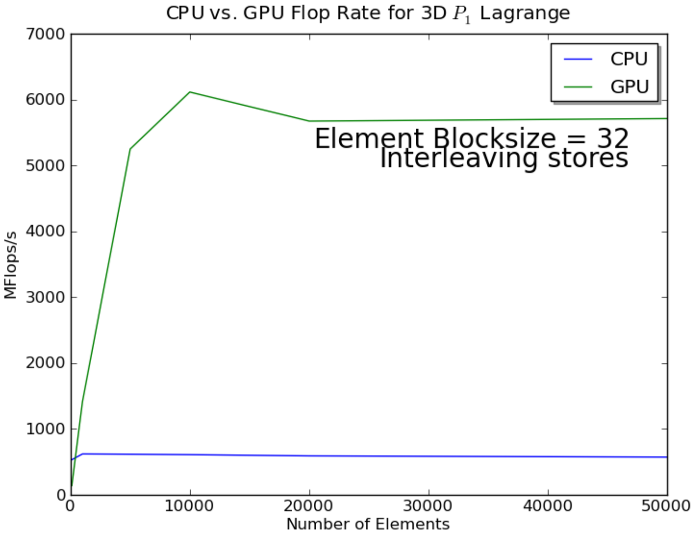
Results

9400M



Results

9400M


CPU vs. GPU Flop Rate for 3D P_1 Lagrange
MFlops/s
Number of Elements
CPU
GPU
Element Blocksize = 32
Interleaving stores