Sparse Matrix Algorithms on GPUs and their Integration into SCIRun

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• NSF CenSSIS - The Center for Subsurface Sensing and Imaging

• BIAT – A Biomedical Imaging Acceleration Testbed: NSF Award Number 0946463

• CIBC, the Center for Integrative Biomedical Computing, which develops and maintains SCIRun
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   iii. GPU Architecture
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Goals

- Accelerate SCIRun Problem Solving
  - To create an implementation of double precision sparse linear solvers in a problem solving environment for the GPU including:
    - Conjugate Gradient Method (CG)
    - Minimal Residual Method (MinRes)
    - Jacobi Method
  - To provide a mechanism to accelerate many SCIRun algorithms while remaining transparent to the scientist
    - Retaining in-progress algorithm visualizations
    - Allowing for future GPU algorithm development within the environment
University of Utah’s SCIRun

- SCIRun is a biomedical problem solving environment (BioPSE)
- Center for Integrative Biomedical Computing (CIBC)
- Designed to be **extensible and scalable**.
- Supports interaction among the modeling, computation and visualization phases of biomedical imaging
- Uses include:
  - Cardiac electro-mechanical simulation
  - ECG & EEG forward and inverse calculations
  - Deep brain stimulation modeling
- Available for Windows, Mac/OSX and Linux
University of Utah’s SCIRun

- Allows scientists to create a network of mathematical functions
- The network visualizes a simulation from start to finish
- Many of these algorithms are time consuming

... and display parallelism!
Heart Ischemia Model

- **Ischemia:** Tissue damaged by a lack of blood flow
- The model is a 3D interactive model based on a scan of an ischemic dog heart
  - For measuring and predicting extracellular cardiac potentials
- The network on the previous slide generates this image
- The sparse data in this model is 107,000 x 107,000 with 1.2 million nonzeros
  - Compressed Row Storage Format
SolveLinearSystem Module

- Solves sparse linear systems with a variety of algorithms
- Allows the user to modify parameters such as preconditioners, target error, and iteration limit
- Displays current error, iteration count and convergence graph
  - This helps the scientist visualize results
GPU Architecture – NVIDIA GeForce GTX 280

- Graphics processing units are Single Instruction Multiple Data (SIMD)
- 240 cores (32 multiprocessors with 8 processors in each)
- Multi-tiered memory layout
  - 1GB global memory
  - 16kB per-core shared memory
  - 64kB total read-only constant memory
  - 16384 registers per multiprocessor
- 32 warp threads perform the same instruction on a set of data
- Programmable using NVIDIA CUDA C or OpenCL

Images from NVIDIA and Geeks3D.com
Conjugate Gradient Method

- The most commonly used iterative solver of linear systems, \( Ax=b \)
- Matrix \( A \) must be square, symmetric and positive definite
- Benefits include:
  - Ease of use
  - Minimal storage requirement
  - Good convergence rate if there is sufficient numerical precision

Iterate:

\[
\alpha(i) = \frac{r^T(i) r(i)}{d^T(i) A d(i)}
\]

\[
x(i+1) = x(i) + \alpha(i) d(i),
\]

\[
r(i+1) = r(i) - \alpha(i) A d(i),
\]

\[
\beta(i+1) = \frac{r^T(i+1) r(i+1)}{r^T(i) r(i)},
\]

\[
d(i+1) = r(i+1) + \beta(i+1) d(i).
\]
Other Methods

• **Jacobi**
  • Simplest algorithm for linear solvers
  • Matrix $A$ must be diagonal – the absolute value of each diagonal element must be:
    • Non-zero
    • Greater than the absolute value of each element in that row.

  ![Diagram](Ax = b, (Diag + Rem)x = b, Diag * x_1 = b - Rem * x_{i-1})

  Solve for $x_i$
  Use previous iteration $x$ as $x_{i-1}$

• **Minimal Residual**
  • More complicated than CG
  • Can also solve symmetric indefinite systems
  • Stronger convergence behavior with infinite precision
  • Guaranteed to have non-decreasing residual errors each iteration

Algorithm descriptions from Wolfram MathWorld
All algorithms exist at SCIRun’s module level - SolveLinearSystem

All low-level parallel computations exist at SCIRun’s algebra level – ParallelLinearAlgebra
  - CPU matrix and vector computations with optimizations
  - Algorithms call these low level math functions as an abstraction
    - This structure lends itself to a convenient GPULinearAlgebra sibling
• Operations Accelerated:
  • GPULinearAlgebra now contains accelerated versions of all functions in the ParallelLinearAlgebra CPU library provided with SCIRun
  • Sparse Matrix-Vector multiplication (SpMV)
  • Vector addition, simultaneously adding and scaling, subtraction, copy, dot product, normalization, maximum, and minimum, threshold invert and more…
  • Operations implemented using NVIDIA CUBLAS libraries and direct coding in CUDA
    • CUBLAS does not handle sparse data
Computation Details

- **Numerical Precision**
  - Double precision floating point is necessary for accurate convergence of these algorithms
  - The GPU version is performed in double precision in order to achieve convergence in all examples, as in SCIRun’s double precision CPU implementation

- **Data Storage**
  - The problems are large in size, with sparsely populated matrices
  - Sparse data formats are required, adding complexity and decreasing parallelism
### Compressed Sparse Row Storage

- **Non-zero Values**: 1 2 7 3 9 1 8 3 4 1 1 1 2 2
- **Column Index**: 0 2 4 1 7 2 3 4 6 0 3 7 6 7
- **Row Pointer**: 0 1 3 4 5 8 9 12 14

14 Non-zeros requires 59 memory fetches in one SpMV
Filling ratio in memory = 100%

- Rows may have few nonzero entries
  - Lots of wasted memory and calculations if stored in a dense format
- Instead, store only relevant points \( A[i] \) and two location vectors
  - Location vectors
    - Column index \( C[i] \) gives column number of element \( A[i] \)
    - Row pointer \( R[i]=j \) gives location \( A[j] \) of a row change

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Experiment Details

• Test Machine
  • CPU – Intel Core 2 E6300 1.86GHz, 2Mb L2 cache, 1066MHz FSB
  • GPU - NVIDIA GeForce 280 GTX 1GB RAM PCIe card

• Test conditions
  • Tests were run >10 times each to assure accurate results
  • Test time is end to end – includes all data transfer and setup overheads involved in GPU version

• Test data
  • Heart Ischemia Model
  • University of Florida’s Sparse Matrix Collection
• The sparse matrices vary in size from 6.3K to 3.5M rows

• Nonzeros vary from 42K to 14.8M
Conjugate Gradient

GPU/CPU End to End Speedup – Nearly identical performance in each of 10 runs

CPU: Intel Core 2 1.86GHz
GPU: NVIDIA GeForce GTX 280
Double Precision is used in all examples
Jacobi and Minimal Residual

CPU: Intel Core 2 1.86GHz
GPU: NVIDIA GeForce GTX 280
Double Precision is used in all examples

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time (seconds)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CPU</td>
<td>GPU</td>
</tr>
<tr>
<td>CG</td>
<td>164.57</td>
<td>31.05</td>
</tr>
<tr>
<td>Jacobi</td>
<td>7.42</td>
<td>1.46</td>
</tr>
<tr>
<td>MinRes</td>
<td>81.96</td>
<td>11.80</td>
</tr>
</tbody>
</table>

107K x 107K Heart Ischemia Model
Third Party Implementations

- Many third party packages are available as open source
- They may perform better but are more difficult or impossible to incorporate into the user experience of SCIRun
- CNC Number Cruncher (CG implementation)
  - Gocad Research Group – Nancy University, France

### 107K x 107K Heart Ischemia Model

<table>
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<tr>
<th>Algorithm</th>
<th>Time (seconds)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>CG</td>
<td>164.57</td>
<td>31.05</td>
</tr>
<tr>
<td>3rd Party CG</td>
<td>164.57</td>
<td>27.98</td>
</tr>
</tbody>
</table>

Validation of Results

- Different orders of operations still affect the iterations necessary to achieve desired error
  - Double precision is necessary to limit this
  - The CPU and GPU differ in the number of iterations needed to converge by less than 1%
Discussion

• Speedup was achieved using the original CPU algorithm
  • The only added operations are transferring the data to the GPU
  • The algorithms were accelerated by a simple technique that can be applied to algorithms throughout SCIRun

```
PLA.mult(DIAG, Z, Z);
PLA.sub(Z, X, X);
PLA.mult(A, X, Z);
PLA.sub(Z, B, Z);

error = PLA.norm(Z) / bnorm;

if (error < xmin)
{
    PLA.copy(X, XMIN);
xmin = error;
}

if (PLA.first())
    convergence_[niter] = xmin;
niter++;
```

```
GPUPLA.mult(DIAG, Z, Z);
GPUPLA.sub(Z, X, X);
GPUPLA.mult(A, X, Z);
GPUPLA.sub(Z, B, Z);

error = GPUPLA.norm(Z) / bnorm;

if (error < xmin)
{
    GPUPLA.copy(X, XMIN);
xmin = error;
}

if (GPUPLA.first())
    convergence_[niter] = xmin;
niter++;
```
Where the Performance is Realized

- In SpMV, each row is computed by one thread
  - Small number of rows = low utilization of GPU
- The other vector operations (mostly accelerated via the CUBLAS library) are relatively fast but occupy a low % of total time

<table>
<thead>
<tr>
<th>Calculation</th>
<th>CPU (ms)</th>
<th>GPU (ms)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data Copy and Setup</td>
<td>0.08</td>
<td>190.22</td>
<td>-2377.75x</td>
</tr>
<tr>
<td>Preconditioner</td>
<td>145.11</td>
<td>8.26</td>
<td>17.57x</td>
</tr>
<tr>
<td>SpMV</td>
<td>130.68</td>
<td>9.37</td>
<td>13.95x</td>
</tr>
<tr>
<td>Subtract</td>
<td>21.09</td>
<td>0.72</td>
<td>29.29x</td>
</tr>
<tr>
<td>Dot Product (2 per iter)</td>
<td>12.97</td>
<td>0.53</td>
<td>24.47x</td>
</tr>
<tr>
<td>Norm</td>
<td>6.77</td>
<td>0.45</td>
<td>15.04x</td>
</tr>
<tr>
<td>Scale and Add (2 per iter)</td>
<td>19.62</td>
<td>0.72</td>
<td>27.25x</td>
</tr>
<tr>
<td>Total time per iteration</td>
<td>223.72</td>
<td>13.04</td>
<td>17.15x</td>
</tr>
</tbody>
</table>

Time Distribution of Operations

- SpMV
- Subtract
- Dot Product (2)
- Normalize
- Scale and Add (2)
SolveLinearSystem Module Modifications

1. Use GPU
2. Emit partial solutions
3. Use previous solution as initial guess

Introduction Theory Design Results Discussion
Limitations

• Computation boundaries
  • Double precision availability & performance is limited
    • Even in the new Fermi generation of GPUs, double precision is still limited to 1/8 of single precision speed (1 DP unit per MP)
    • This will get better soon!
  • Sparse data
    • Memory coalescing is essential to good GPU performance

• Varying data characteristics
  • The worst possible data scenario could cause poor GPU performance
Successes

• User experience
  - The scientist using SCIRun gets results quicker
  - Transparency – Same user interaction during GPU accelerated functions
• SCIRun development – SCIRun is an open source PSE
  - GPU can be used following pre-existing programming paradigm
• Extensibility to other PSEs
  - Algorithms can be accelerated and still provide adequate interface communication by performing small individual calculations rather than complex kernels
Future Work

- Choose between CPU and GPU algorithms automatically at runtime
- Experiment with new SpMV techniques and newly released libraries for these functions
- Investigate better asynchronous techniques for inter-algorithm visualizations
- Demonstrate acceleration of algorithms outside of the linear solver module
A video recording of the CPU and GPU versions of the Conjugate Gradient Algorithm

**Methods**

- Conjugate Gradient & Precond. (SCI)
- BiConjugate Gradient & Precond. (SCI)
- Jacobi & Precond. (SCI)
- MINRES & Precond. (SCI)

**Convergence**

- Current Target: Blue
- Target Error: Cyan
- Current Error: Red

**CPU**

- **Target error:** 0.0000100
- **Maximum Iterations:** 17172
- **Partial Solution Emitted Every:** 50
- **Use previous solution as initial guess:**

**GPU**

- **Target error:** 0.0000100
- **Maximum Iterations:** 17172
- **Partial Solution Emitted Every:** 50
- **Use previous solution as initial guess:**

**Results**

- **Original Error:** 1.0
- **Current Error:** 6.83975906725293e-6
- **Previous Execution Time (s):** 19

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**Discussion**
Thank You

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