Implementing Fast Parallel Linear System Solvers In OpenFOAM based on CUDA

Daniel P. Combest and Dr. P.A. Ramachandran and Dr. M.P. Dudukovic

Chemical Reaction Engineering Laboratory (CREL) Department of Energy, Environmental, and Chemical Engineering. Washington University, St. Louis, MO.

Optimization, HPC, and Pre- and Post-Processing I Session. 6th OpenFOAM Workshop Penn State University. June 15th 2011

Objectives

Objective

 To introduce a tool to integrate linear system solvers on the GPU into OpenFOAM

Topics

- Introduction to the GPU and CUDA
- Integrating CUSP into OpenFOAM
- Some preliminary results
- Important considerations when using this tool
- Next steps
- Take home messages

What exactly is CUDA?

Defined as: Compute Unified Device Architecture. I.e. a parallel computing architecture used in graphics processing units (GPU), developed by Nvidia.

What exactly is CUDA?

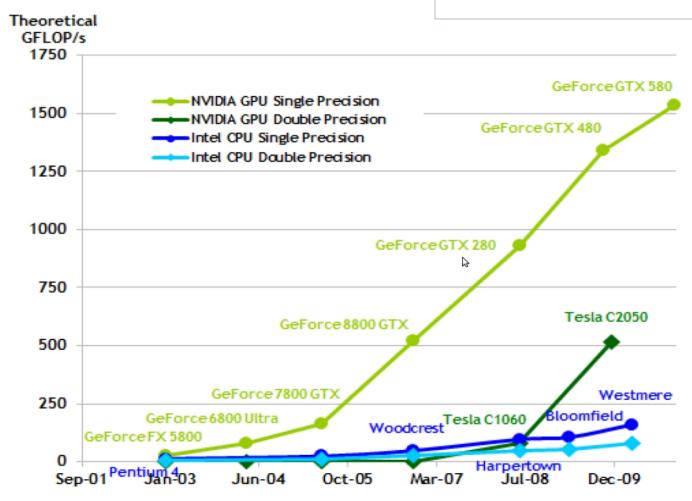
Defined as: Compute Unified Device Architecture. I.e. a parallel computing architecture used in graphics processing units (GPU), developed by Nvidia.

What is CUDA C/C++?

A language that provides an interface so that parallel algorithms can be run on CUDA enabled Nvidia GPUs



GPU v.s CPU Calculations



CPU-GPU Comparison of Floating-point operations per second [1]

Why are we interested?

Larger problems require more computing resources (LES, coupled physics)

GPUs are <u>fast</u> when used properly

They are relatively cheap

Why are we interested?

Larger problems require more computing resources (LES, coupled physics)

GPUs are <u>fast</u> when used properly

They are relatively cheap

Where can GPUs be applied?

Where parallel algorithms live

Linear algebra i.e. sparse matrix math

Why are we interested?

Larger problems require more computing resources (LES, coupled physics)

GPUs are <u>fast</u> when used properly

They are relatively cheap

Where can GPUs be applied?

Where parallel algorithms live

Linear algebra i.e. sparse matrix math

Why don't we compile everything to work on the GPU?

Only programs written in CUDA language can be parallelized on GPU. So we cannot just recompile OF.



cusp-Library http://code.google.com/p/cusp-library/

"Cusp is a library for **sparse linear algebra** and **graph** computations on CUDA. Cusp provides a flexible, **high-level** interface for manipulating sparse matrices and solving sparse linear systems."[2]

Provided Template Solvers:

- · (Bi-) Conjugate Gradient (-Stabilized)
- · GMRES

Matrix Storage

· CSR, COO, HYB, DIA

Provided Preconditioners

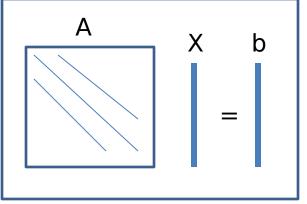
- · Jacobi (diagonal) preconditioners
- · Sparse Approximate inverse preconditioner
- · Smoothed-Aggregation Algebraic Multigrid preconditioner



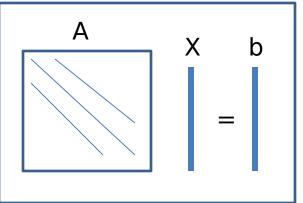
http://code.google.com/p/thrust/

"Thrust is a CUDA library of parallel algorithms with an interface resembling the C++ Standard Template Library (STL). Thrust provides a flexible **high-level**interface for GPU programming that greatly enhances developer **productivity**. "[3]

OpenFOAM solve(...);

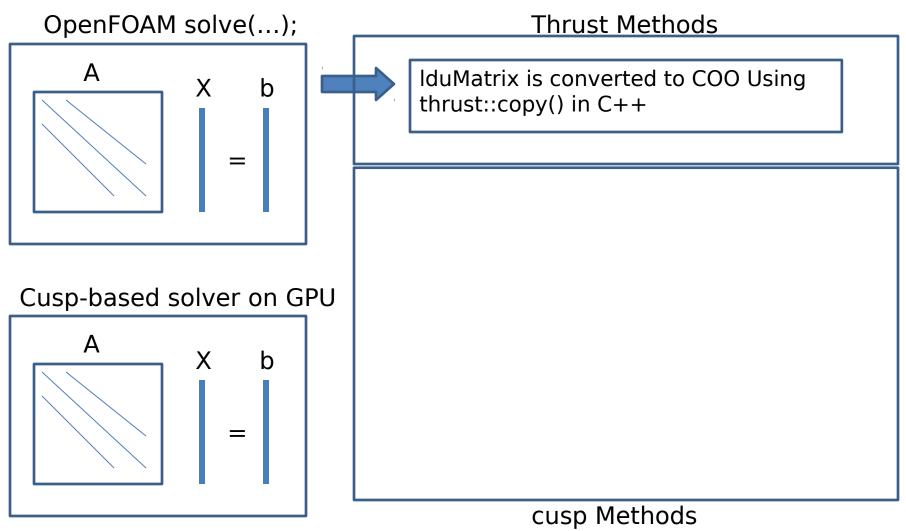


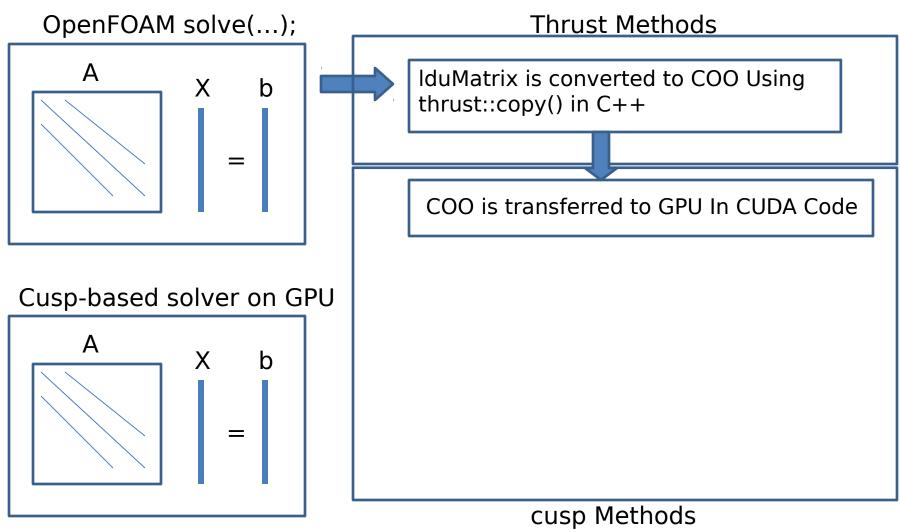
Cusp-based solver on GPU

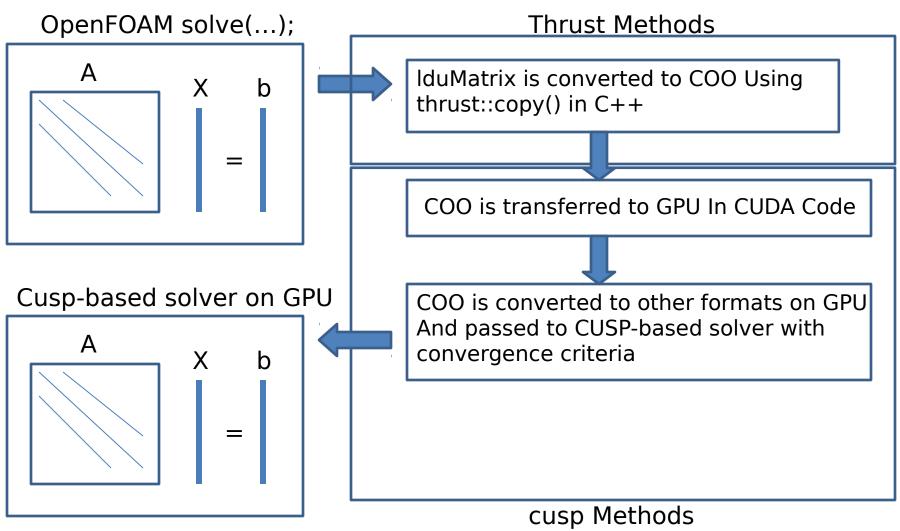


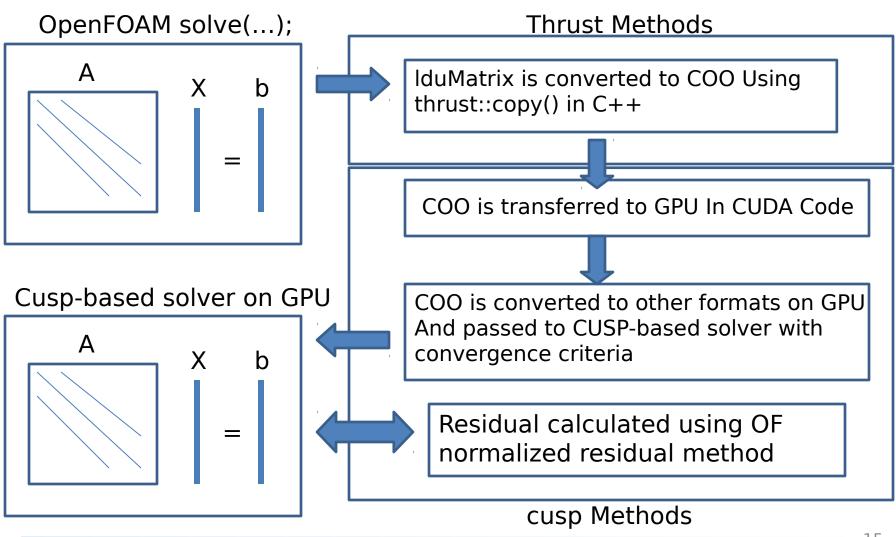
Thrust Methods

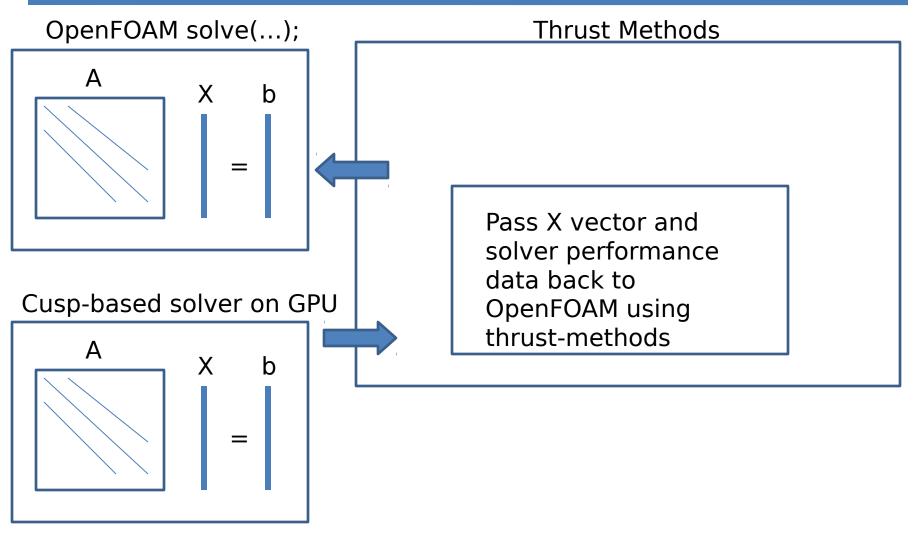
cusp Methods









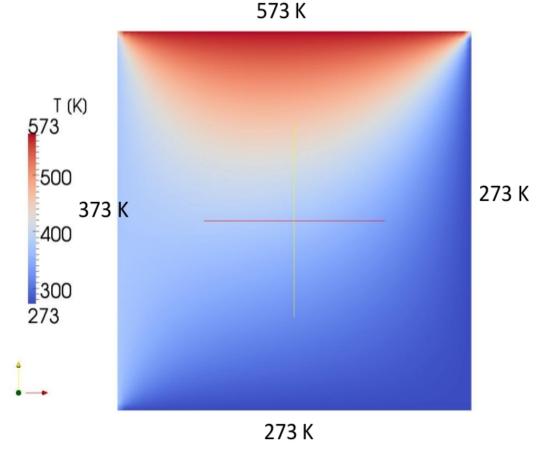


A test Problem.

2D Heat Equation

$$\nabla^2 T = 0$$

Vary N from 10-2000 where $N^2 = nCells$



Solver Settings

All CG solvers

Tolerance = 1e-10; MaxIter 1000; solver GAMG;
tolerance 1e-10;
smoother GaussSeidel;
nPreSweeps 0;
nPostSweeps 2;
cacheAgglomeration true;
nCellsInCoarsestLevel sqrt(nCells);
agglomerator faceAreaPair;
mergeLevels 1;

Setup

CUDA version 4.0 CUSP version 0.2

Thrust version 1.4 Ubuntu 10.04

CPU: Dual Intel Xeon Quad Core E5430 2.66GHz

Motherboard: Tyan S5396

RAM: 24 gig

GPU: Tesla C2050 3GB DDR5

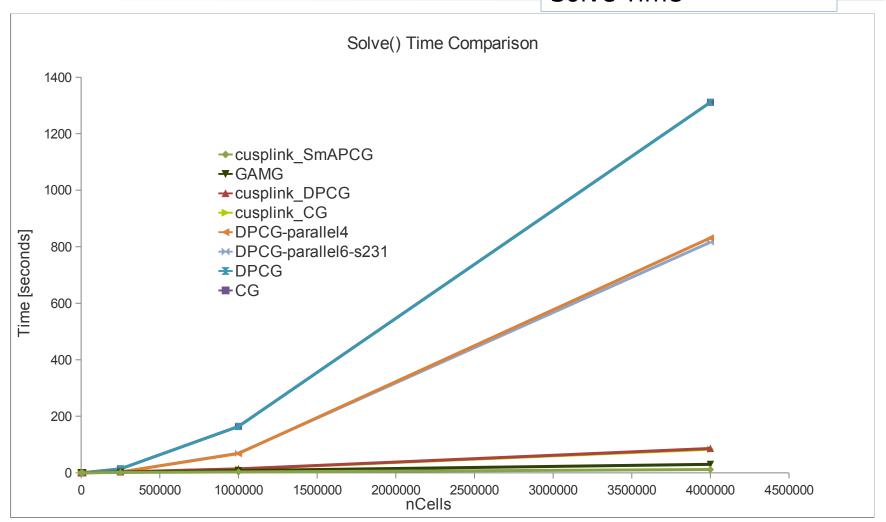
515 Gflops peak double precision

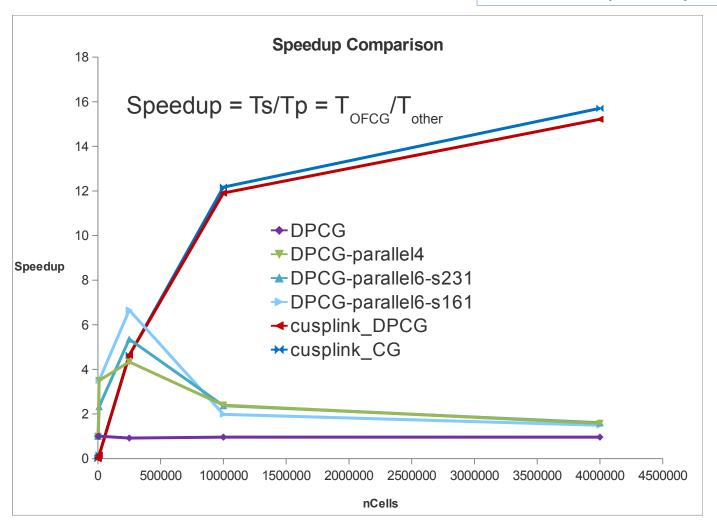
1.03 Tflops Peak single precision

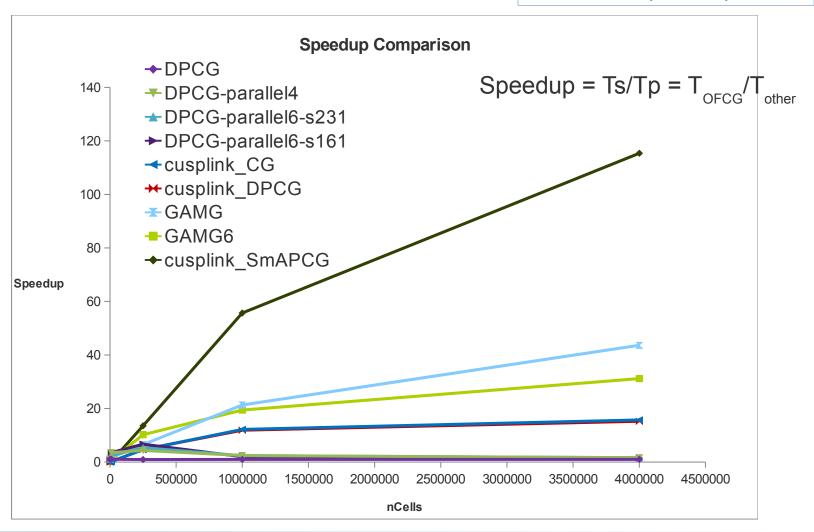
14 MP * 32 cores/MP = 448 cores

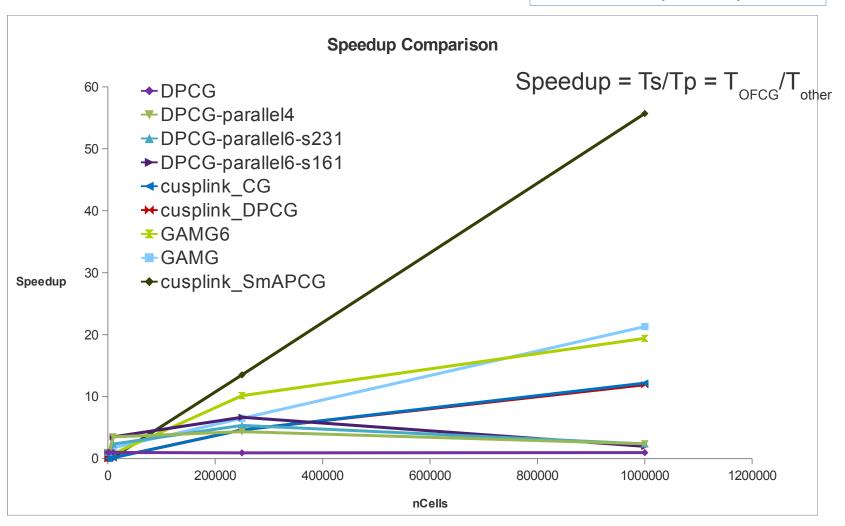
Host-device memory bw = 1566 MB/sec (Motherboard specific)

Solve Time









Notes on Comparison

- GPU Tesla C2050
- All are double precision results in CSR
- Low precision timers used
- Parallel CPU results a little skewed, i.e. other processes occurring on cpu
- Residuals are scaled in the same manner as OF
- GPU Results include data transfer time
- The GPU smoothed aggregate preconditioner was 115x faster than CG

Important Considerations

Before you jump....

- Tool is <u>not</u> multi GPU yet.
- Proper motherboard and power source
- CUDA Enabled hardware
- Amount of System Ram >= GPU RAM
- Working install of CUDA, CUSP, and OFext

Next Steps

Where to Start?

- Finish asymmetric solvers
- Clean up current version and release code

- Multi GPU support
- Improve the solvers as CUSP improves

Take Home Messages

- The GPU only solves the Ax=b system
- We have double precision
- GPUs have been integrated into OpenFOAM using Thrust and CUSP
- As cusp and thrust improve, nothing needs to be changed in this code,
 only to update cusp and thrust.
- They have been shown to be faster in the cases provided, because it is mostly solving Ax = b.
- Residuals are calculated the same as in OpenFOAM
- Multi-GPU still needs attention.
- The results show that memory bandwidth still is an issue with this particular setup and results could be faster with other setup.

Acknowledgements

Funding and Support

Nvidia Professor Partnership Program

Chemical Reaction Engineering Laboratory (CREL) MRE Fund (http://crelonweb.eec.wustl.edu/)

OpenFOAM Developers Community

Advisors

Dr. Ramachandran

Dr. Dudukovic

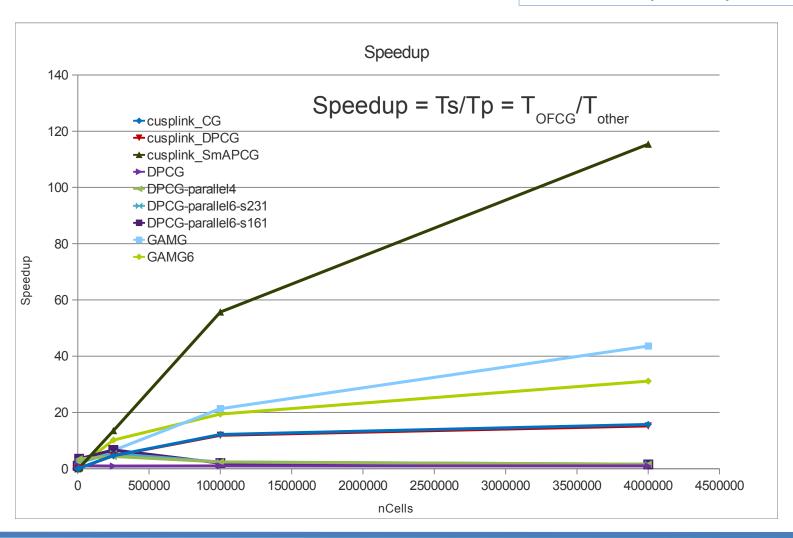
Sources

- Nvidia CUDA Programming Guide, Version 4.0, 2011. Nvidia Corporation.
- Nathan Bell and Michael Garland, Cusp: Generic Parallel Algorithms for Sparse Matrix and Graph Computations, 2010, http://cusp-library.googlecode.com, Version 0.1.0
- Jared Hoberock and Nathan Bell, Thrust: A Parallel Template Library, 2010, http://www.meganewtons.com/,Version 1.3.0

Thanks for your attention!

Questions?

Contact Info: Dan Combest dcombest@seas.wustl.edu



Residual Scaling

```
For matrix A x = b,
residual is defined as
res = b - Ax
We then apply residual scaling with the following normalisation factor procedure:
Type xRef = gAverage(x);
wA = Ax;
pA = A \times Ref;
NormFactor = gSum(cmptMag(wA - pA) + cmptMag(source - pA)) + matrix.small;
and the scaled residual is:
residual = gSum(cmptMag(source - wA))/normFactor;
I will save you from complications with vectors and tensors in my block solver. :-)
Enjoy,
Hrv
Source: http://www.cfd-online.com/Forums/openfoam-solving/57903-residuals-convergence-segregated-
solvers.html
```