Towards Efficient Two-Level Preconditioned Conjugate Gradient on the GPU

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- GPU Computing
- Solver Overview
- Preconditioning
- Deflation
- Results
- Conclusions

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Bird's Eye View

Comparison of CPU optimized code with respect to GPU code



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Bird's Eye View

Comparison of CPU optimized code with respect to GPU code



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Problem Description

Mass-Conserving Level Set Method to Solve the Navier Stokes Equation.



Air bubbles rising in Water.



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Computational Model

Computational Hotspot - Solution of the Pressure Correction equation in 2D



$$-\nabla \cdot \left(\frac{1}{\rho(x)}\nabla p(x)\right) = f(x), \ x \in \Omega \tag{0}$$

$$\frac{\partial}{\partial n}p(x) = g(x), \ x \in \partial\Omega \tag{0}$$

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Nature of the Coefficient Matrix

$$Ax = b$$
, where $x^T Ax > 0$ (0)

A is a sparse matrix with a 5-point stencil. It has a very large condition number due to a huge jump in the density.

- Condition Number $\rightarrow \kappa(A) := \frac{\lambda_n}{\lambda_1}$
- Stopping criterion $\rightarrow \frac{\|b Ax_k\|_2}{\|r_0\|} \le 10^{-6}$

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Nature of the Coefficient Matrix



Huge jump at the interface due to contrast in densities.



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A Brief Introduction to the GPU

- SIMD Architecture
- Large Memory Bandwidth
- User Managed Caches



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- Basic Unit of Execution Thread
- Each Thread Executes a Kernel
- Aggregates of Threads = Blocks
- Shared Memory within a block



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Architecture	TeslaC1060	TeslaC2070(Fermi)		
Number of Compute Cores	240 cores	448 cores		
Memory Bandwidth	102Gb/s	144 Gb/s		
Double Precision Throughput(Peak)	78 Gflops/s	515 Gflops/s		
Memory	4GB	6GB		
Shared Memory / L1cache				
configurability	No	Yes		

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Most Important Optimizations for GPU Code

- Reduce Host-GPU Transfers
- Maximize use of Memory Bandwidth
- Minimize Thread Divergence
- Utilize Shared Memory/ L1 cache based on kernel



Control Flow in the Algorithm



Conjugate Gradient with Two Level Preconditioning



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- Diagonal Preconditioning
- Block Incomplete Cholesky
- Incomplete Poisson(IP)
- Modifications based on IP



Block Incomplete Cholesky Preconditioning ^{a b}



Within blocks the computation is sequential

^aAn Iterative Solution Method for Linear Systems of Which the Coefficient Matrix is a Symmetric M-

Matrix. J.A. Meijerink, H.A.van der Vorst (1977). Math. Comp. (American Mathematical Society)

^bIterative methods for sparse linear systems. 2nd ed., Society for Industrial and Applied Mathematics,

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Incomplete Poisson

$$M = K * K^T$$
, where $K = (I - L * D)$. (0)

$$Stencilfor A = (-1, -1, 4, -1, -1).$$
 (0)

$$CorrespondingStencilfor M^{-1} = (\frac{1}{4}, \frac{1}{16}, \frac{1}{4}, \frac{9}{8}, \frac{1}{4}, \frac{1}{16}, \frac{1}{4})$$
(0)

Drop the lowest terms (i.e. $\frac{1}{16}$). M^{-1} has the same sparsity pattern as A. Degree of Parallelism for $M^{-1} * r$ is N.



A Parallel Preconditioned Conjugate Gradient Solver for the Poisson Problem on a Multi-GPU Platform, M. Ament. PDP 2010

Incomplete Poisson Variants ^a Scaling of *A* matrix. $\hat{A} = D^{-\frac{1}{2}} * A * D^{-\frac{1}{2}}$ As parallel as IP and as effective as Block-IC Slightly more computations compared to IP.



^aA vectorizable variant of some ICCG methods. Henk A. van der Vorst, SIAM Journal of Scientific Computing. Vol. 3 No. 3 September 1982.

Operations involved in deflation ^{a b}

•
$$b = Z^T * x$$

- $m = E^{-1}b$
- w = A * Z * m
- w = x w

where, E is the Galerkin Matrix and Z is the matrix of deflation vectors.

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^aEfficient deflation methods applied to 3-D bubbly flow problems. J.M. Tang, C. Vuik Elec. Trans. Numer. Anal. 2007.

^bAn efficient preconditioned CG method for the solution of a class of layered problems with extreme contrasts in the coefficients. C. Vuik, A. Segal, J.A. Meijerink J. Comput. Phys. 1999.

Stripe-Wise Domains

57	58	59	60	61	62	63	64
49							56
41							48
33							40
25							32
17							24
9							16
1	2	3	4	5	6	7	8

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Efficient Data Structures

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Efficient Data Structures

This data Structure has the advantages of the DIA Storage format^a.



^aEfficient Sparse Matrix-Vector Multiplication on CUDA. N. Bell and M. Garland, 2008, NVIDIA Corporation, NVR-2008-04

- Breaking Up of Operations
- Stripe-Wise Domains
- Efficient Data Structures



Single Precision Experiments

SpeedUp and Convergence across GridSizes - Poisson Type Problem



Deflation Vectors are of size 8n. Precision Criteria is 10^{-5} till 260k and for 1m it is 10^{-4}

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Single Precision Experiments Wall Clock Times across GridSizes - Poisson Type Problem

Wall Clock Times across Grid Sizes

Deflated Preconditioned CG.



Deflation Vectors are of size 8n. Precision Criteria is 10^{-5} till 260k and for 1m it is 10^{-4}

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Single Precision Experiments Accuracy across GridSizes - Poisson Type Problem



Deflation Vectors are of size 8n. Precision Criteria is 10^{-5} till 260k and for 1m it is 10^{-4}

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IP Variants For two Phase Problem - Double Precision



Deflation Vectors are of size 2n. Precision Criteria is 10^{-6} . Block size is 2n for $n \times n$ grid where $N = n \times n$ and N is the number of unknowns

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IP Variants For two Phase Problem - Double Precision



Improvement in Error Norm of the Solution

Deflation Vectors are of size 2n. Precision Criteria is 10^{-6} .

Block size is 2n for $n \times n$ grid where $N = n \times n$ and N is the number of unknowns



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Double Precision Experiments

SpeedUp and Convergence across GridSizes - Two-Phase Problem



Deflation Vectors are 8n. Density Contrast (1000 : 1). Precision Criteria is 10^{-6} .

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Double Precision Experiments Wall Clock Times across GridSizes - Two-Phase Problem

Wall Clock Times across Grid Sizes

Deflated Preconditioned CG.



Deflation Vectors are 8n. Density Contrast (1000 : 1). Precision Criteria is 10^{-6} .



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Double Precision Experiments Accuracy across GridSizes - Two-Phase Problem



Deflation Vectors are 8n. Density Contrast (1000:1). Precision Criteria is 10^{-6} .



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Conclusions

- Deflation is highly parallelizable.
- Suitable Preconditioning for GPU must be used.
- More optimizations in order for Double Precision results.



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Further Information

• Masters Thesis of Rohit Gupta

http://ta.twi.tudelft.nl/users/vuik/numanal/gupta_eng.html

• GPU page

http://ta.twi.tudelft.nl/users/vuik/gpu.html

• Open Source GPU software

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http://ta.twi.tudelft.nl/users/vuik/gpu.html#software



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