IMPLEMENTATION OF THE DEFLATED PRE-CONDITIONED CONJUGATE GRADIENT METHOD APPLIED TO THE POISSON EQUATION RELATED TO BUBBLY FLOW ON THE GPU

LITERATURE STUDY

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OUTLINE

- Discretization of Bubbly Flow Problem
- Basic Iterative Methods
- Conjugate Gradients
  - Preconditioning
  - Deflation
- Parallelization Techniques
- The Graphical Processing Unit
  - Parallelization of Iterative Methods on the GPU
- Research Questions

PROBLEM STATEMENT

- Two Phase Flow – Navier Stokes Equation
- Linear System Ax=b
- Finite Difference Disrcetization – Neumann Boundary Conditions
- Preconditioning of the Sparse Matrix
- Deflation Techniques (second Level of Preconditioning)
- Optimization of DPCG on the GPU

DISCRETIZATION TECHNIQUES

- Finite Differences
  - Centered, Backward and Forward
  - 1-D and 2-D discretization
- Finite Element
  - Weak Formulation
- Finite Volume
  - Green's Theorem

BASIC ITERATIVE METHODS

$$x_{k+1} = Gx_k + f$$

- Jacobi

  G = $I - D^{-1}A$

- Gauss Seidel

  G = $I - (D - E)^{-1}A$

- Successive Over- Relaxation

  G = $(D - \omega C_1)^{-1}((1 - \omega)D + \omega C_2)$

CONJUGATE GRADIENT

- Projection method on Krylov Subspace

- Coefficient matrix A has to be Symmetric Positive Definite

- Much better than Jacobi and Gauss Siedel in terms of speed of convergence

CONJUGATE GRADIENT ALGORITHM

- Arnoldi Orthogonalization
- Lanczos Method
- Conjugate Gradient Iteration

PRECONDITIONING

Improving the Condition Number K(A)

- Diagonal Preconditioning
- Incomplete Cholesky
- Other Forms (ILU(0), ILU(p), ILUT)

DOMAIN DECOMPOSITION

- Divide the Problem into Smaller domains.
- Solve the Linear System for each domain separately.
- Represent mesh points as a graph then build the matrix.
- Vertex, Edge or Element based Partitioning.
- Block matrix structure emerges.

DEFLATION

- Attempt to treat bad eigenvalues of Preconditioned Matrix

- A different splitting of **A.** PAx=Pb (new system to be solved)

- The deflection vectors approximate the eigenspace of **A**

PARALLELIZATION TECHNIQUES

- Preconditioner setup (internal loop within outer iteration)
- Matrix vector multiplications (storage formats)
- Preconditioning operations (multi-coloring, block-ILU)
- Using BLAS libraries

GRAPHICAL PROCESSING UNIT

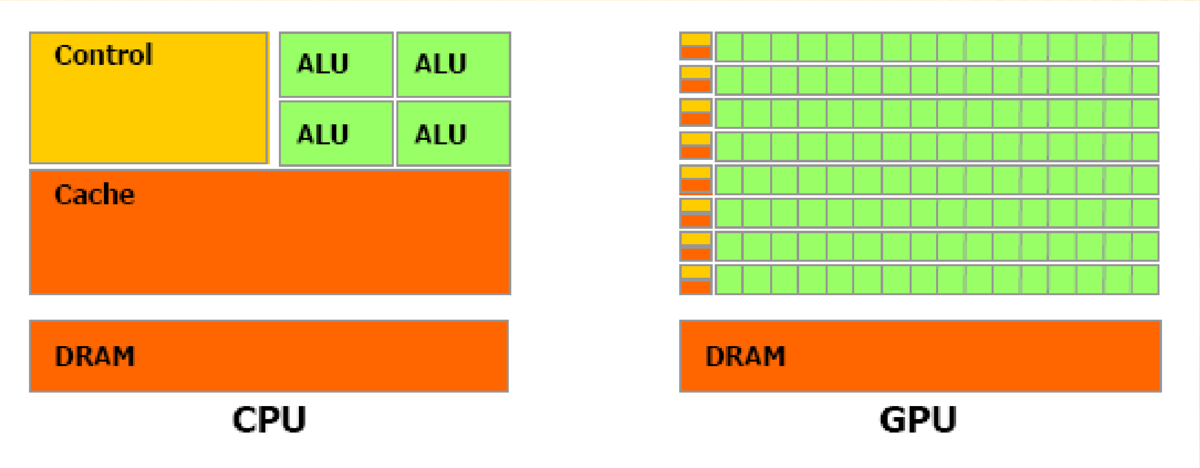
- SIMD Processor

- Hierarchy of Memories

- Capable of delivering hundreds of GFLOPS*

*Conditions Apply

GPU ORIENTATION



More transistors for Data Processing

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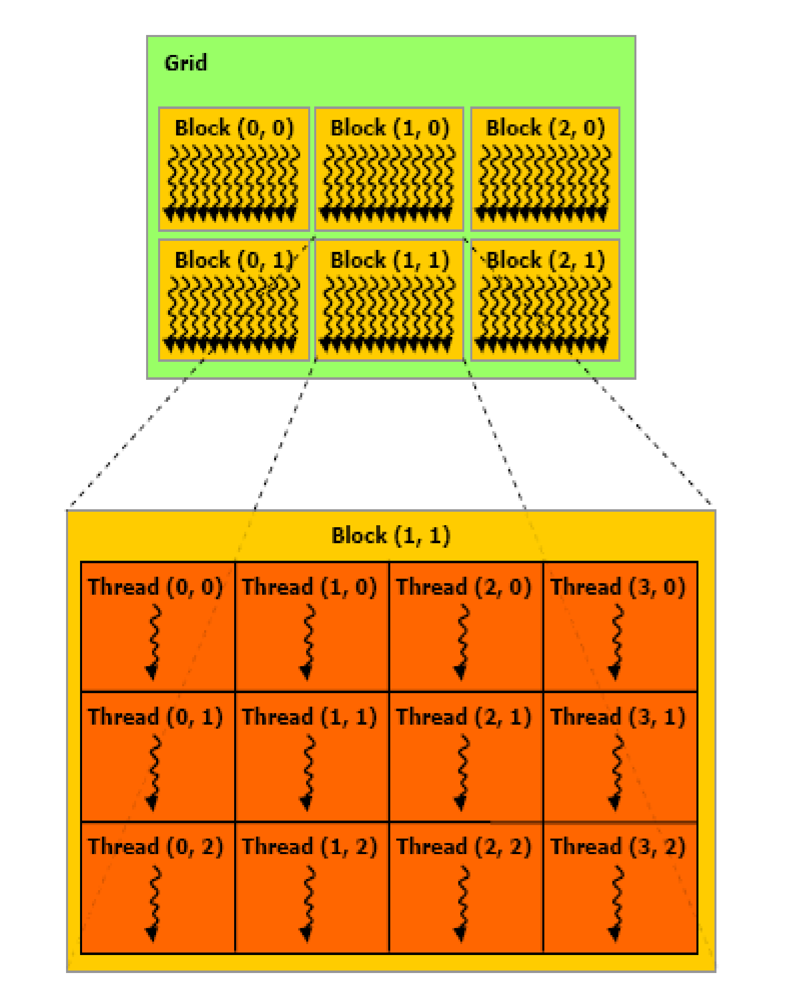
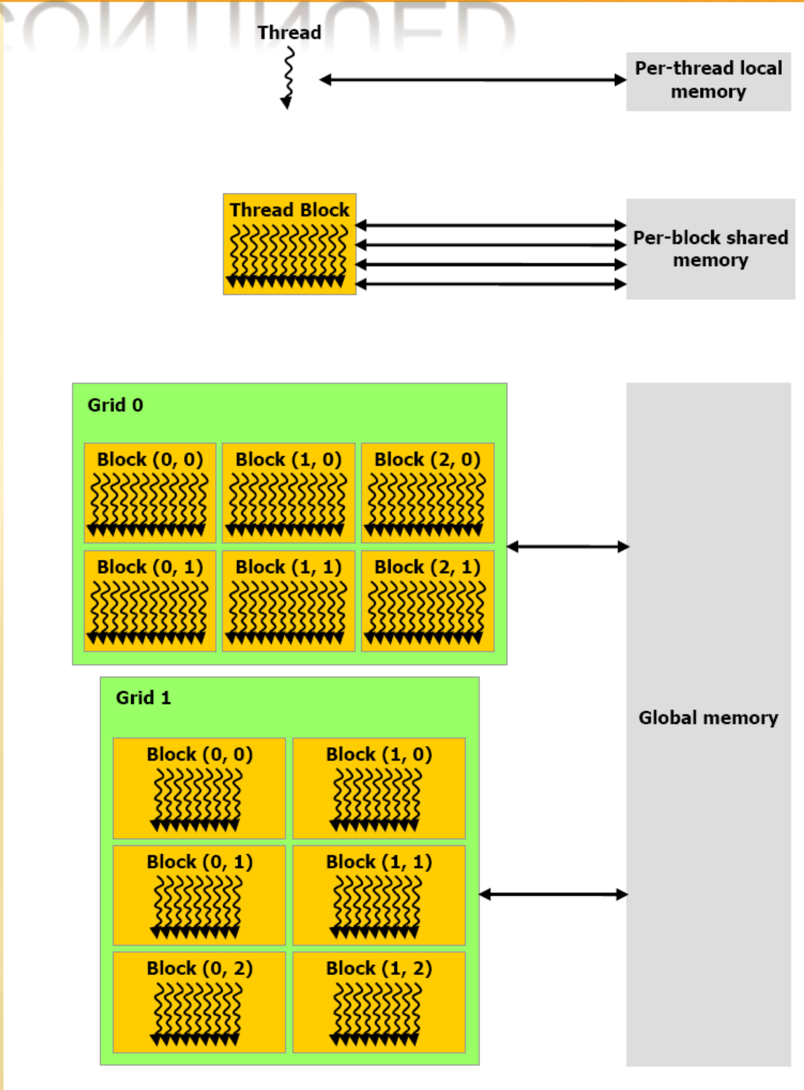
GPU ORIENTATION CONTINUED



Execution Model



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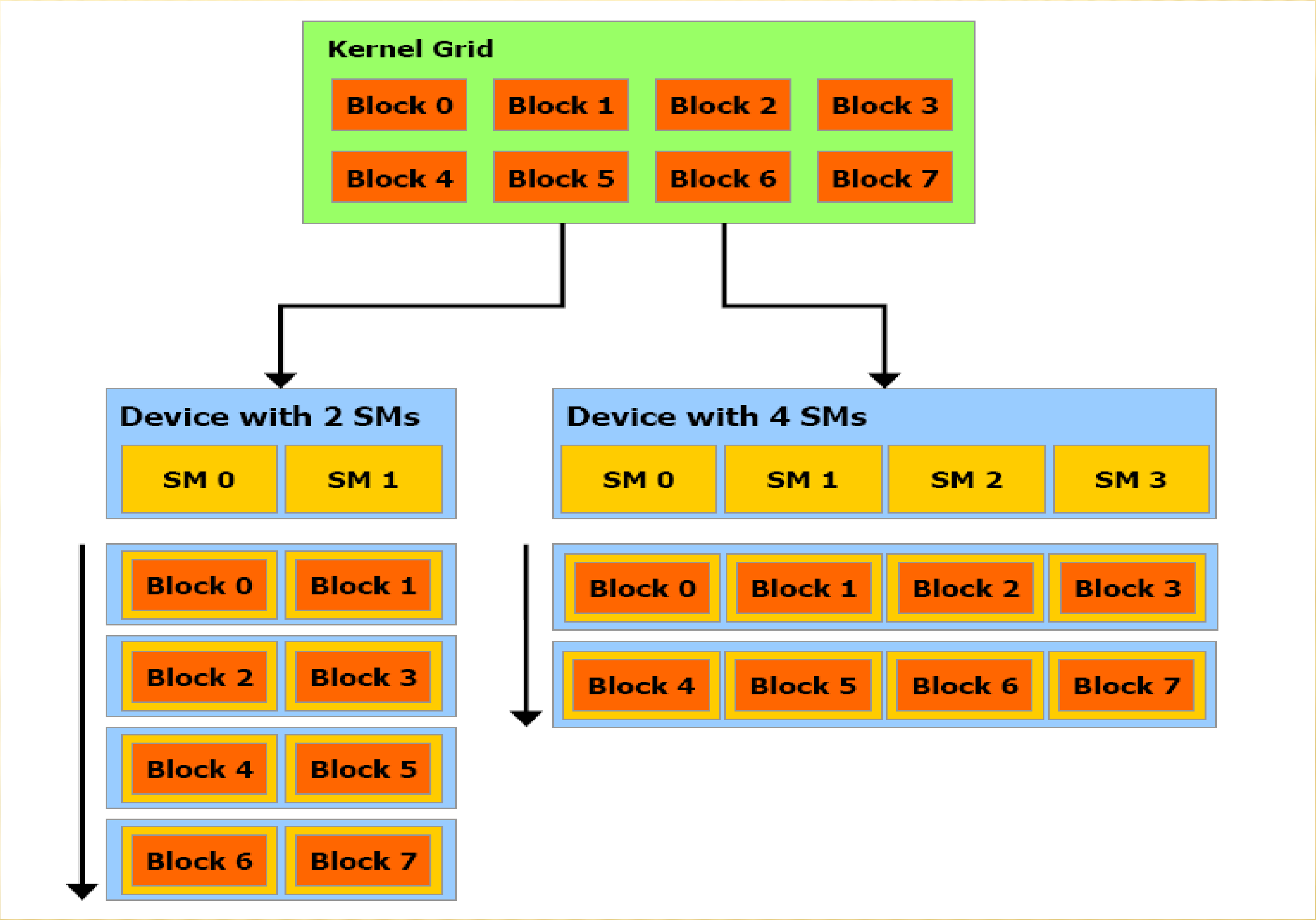
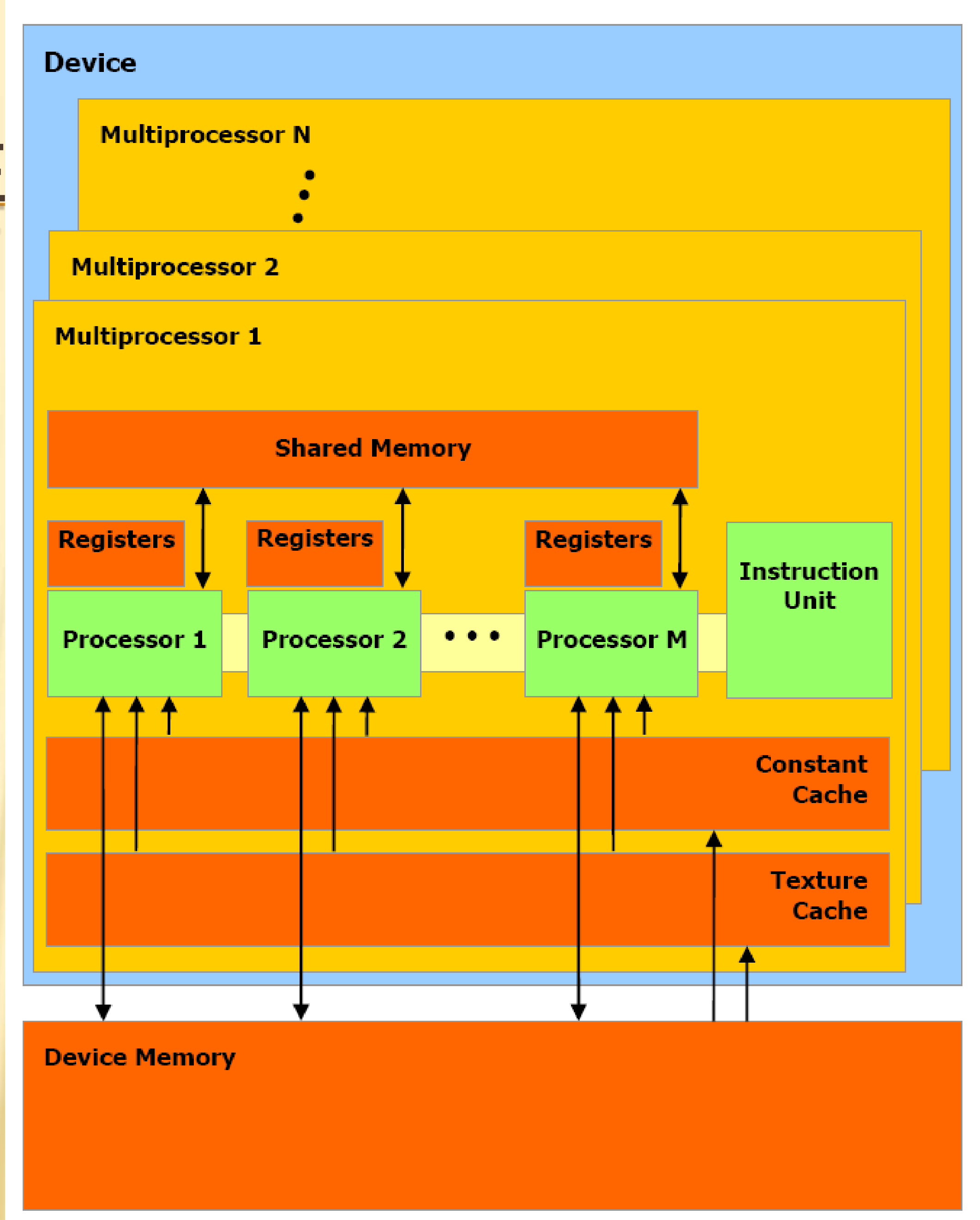
PERFORMANCE SCALING



THE BIG PICTURE



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COMMUNICATION VS COMPUTATION

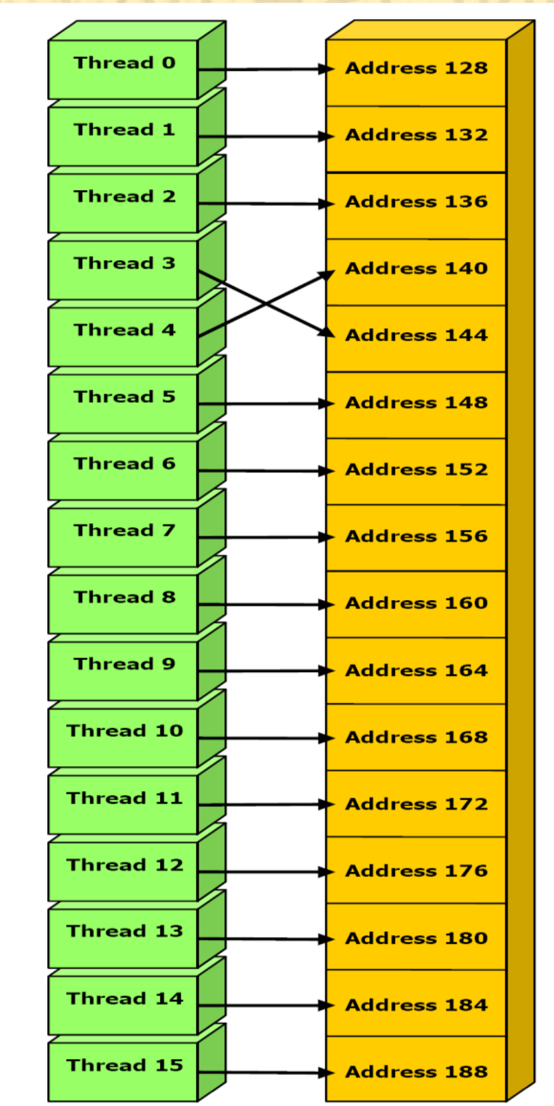
•Parallel Computation Time = T(Execution) + T (Memory Transfers).

•Computation can be reduced by a factor p, Number of Processors.

•Communication is problem dependent.

•Important to get more flops per byte (or per float).

COALESCING



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Thread 15
Address 128
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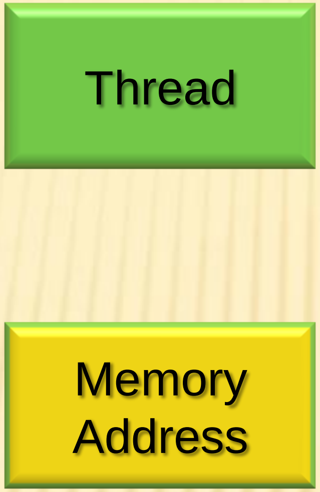
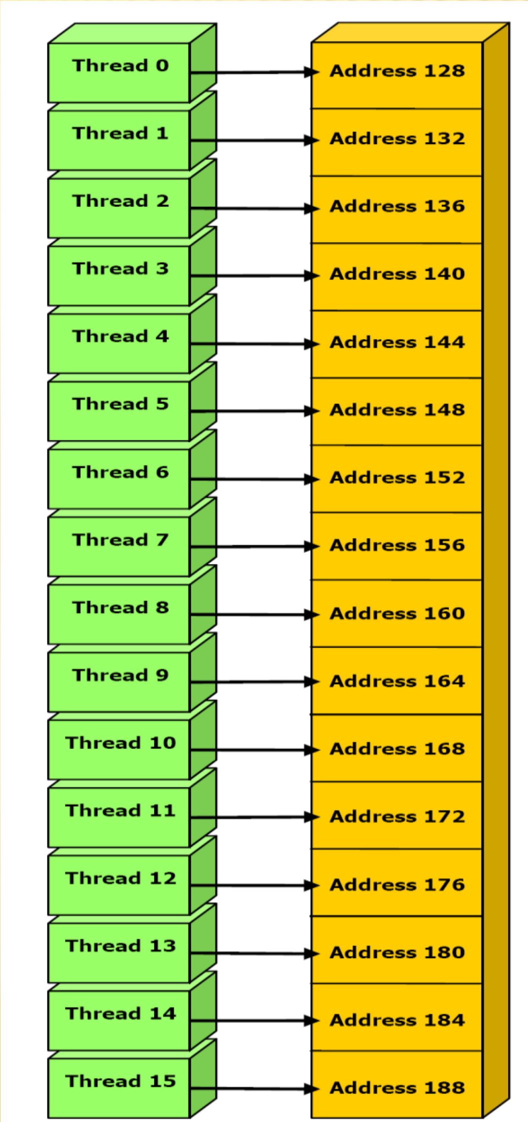
Address 188



Thread
Memory Address



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Address 128
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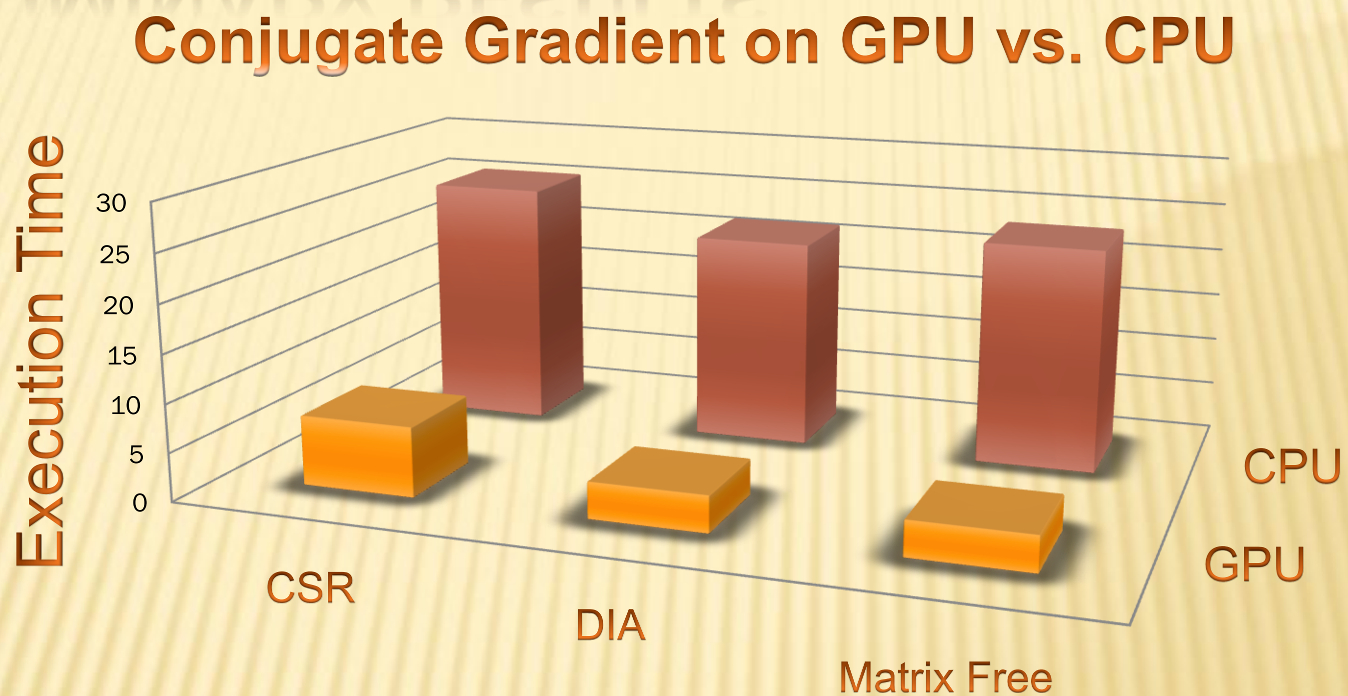
PARALLELIZATION OF ITERATIVE METHODS ON THE GPU

- NVIDIA's SpMV Library
- Work for Dense Matrices (Demmel, Volkov)
- Precision studies (baboulin, et.al)
- Modest Speed-Ups reported with Preconditioned CG

RESEARCH QUESTIONS

- Conjugate Gradient on the GPU
- Preconditioned Conjugate Gradient (different flavors)
- Precision (Mixed and Double)
- Deflation applied on PCG on the GPU
- Multiple GPUs for better performance

PRELIMINARY RESULTS



	CSR	DIA	Matrix Free
GPU	7.286702	3.800385	3.660142
CPU	25.711725	21.787317	23.362423
speedup	3.5x	5.7x	6.4x

Relative Error = 10^{-5} . Iterations on GPU = ~1422. Iterations on CPU=~1250.

Grid Size = 512 X 512

QUESTIONS AND SUGGESTIONS

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EXTRA SLIDES

Operator Splitting
Dy/dt (K) = L(K)

And L(k) can be split up into L(k1) + L(k2)

$$
\begin{array}{ll}
\text{Dirichlet Condition} & u(x) = \phi(x) \\
\text{Neumann Condition} & \dfrac{\partial u}{\partial \vec{n}}(x) = 0 \\
\text{Cauchy Condition} & \dfrac{\partial u}{\partial \vec{n}}(x) + \alpha(x)u(x) = \gamma(x)
\end{array}
$$

The vector $\vec{n}$ refers to a unit vector that is normal to Γ and directed outwards. For a given vector $\vec{v}$, with components $v1$ and $v2$, the directional derivative $\frac{\partial u}{\partial \vec{v}}$ is defined by

$$
\begin{aligned}
\frac{\partial u}{\partial \vec{v}}(x) &= \lim_{h \to 0} \frac{u(x + h\vec{v}) - u(x)}{h} \\
&= \frac{\partial u}{\partial x_1}(x)v_1 + \frac{\partial u}{\partial x_2}(x)v_2 \\
&= \nabla u.\vec{v}
\end{aligned}
$$

EXTRA SLIDES II

ALGORITHM 1.1: Gram-Schmidt

1. Compute $r_{11} := \|x_1\|_2$. If $r_{11} = 0$ Stop, else compute $q_1 := x_1/r_{11}$.
2. For $j = 2, \ldots, r$ Do:
3. Compute $r_{ij} := (x_j, q_i)$, for $i = 1, 2, \ldots, j-1$
4. $\hat{q} := x_j - \sum_{i=1}^{j-1} r_{ij} q_i$
5. $r_{jj} := \|\hat{q}\|_2$,
6. If $r_{jj} = 0$ then Stop, else $q_j := \hat{q}/r_{jj}$
7. EndDo

ARNOLDI

Arnoldi's procedure is an algorithm for building an orthogonal basis of the Krylov subspace $\mathcal{K}_m$. In exact arithmetic, one variant of the algorithm is as follows:

ALGORITHM 6.1: Arnoldi

1. *Choose a vector* v_1 *of norm 1*
2. *For* $j = 1, 2, \ldots, m$ *Do:*
3. Compute $h_{ij} = (Av_j, v_i)$ for $i = 1, 2, \ldots, j$
4. Compute $w_j := Av_j - \sum_{i=1}^{j} h_{ij} v_i$
5. $h_{j+1,j} = \|w_j\|_2$
6. *If* $h_{j+1,j} = 0$ *then Stop*
7. $v_{j+1} = w_j / h_{j+1,j}$
8. *EndDo*

At each step, the algorithm multiplies the previous Arnoldi vector v_j by A and then orthonormalizes the resulting vector w_j against all previous v_i's by a standard Gram-Schmidt procedure. It will stop if the vector w_j computed in line 4 vanishes.

CG Derivation

Gradient algorithm which we now derive. The vector x_{j+1} can be expressed as

$$x_{j+1} = x_j + \alpha_j p_j.$$

Therefore, the residual vectors must satisfy the recurrence

$$r_{j+1} = r_j - \alpha_j A p_j.$$

If the r_j's are to be orthogonal, then it is necessary that $(r_j - \alpha_j A p_j, r_j) = 0$ and as a result

$$\alpha_j = \frac{(r_j, r_j)}{(A p_j, r_j)}.$$

Also, it is known that the next search direction p_{j+1} is a linear combination of r_{j+1} and p_j, and after rescaling the p vectors appropriately, it follows that

$$p_{j+1} = r_{j+1} + \beta_j p_j.$$

Thus, a first consequence of the above relation is that

$$(A p_j, r_j) = (A p_j, p_j - \beta_{j-1} p_{j-1}) = (A p_j, p_j)$$

CG DERIVATION

because Ap_j is orthogonal to p_{j-1}. Then, becomes $\alpha_j = (r_j, r_j)/(Ap_j, p_j)$. In addition, writing that p_{j+1} as defined by ( ) is orthogonal to Ap_j yields

$$\beta_j = -\frac{(r_{j+1}, Ap_j)}{(p_j, Ap_j)}.$$

Note that from

$$Ap_j = -\frac{1}{\alpha_j}(r_{j+1} - r_j)$$

and therefore,

$$\beta_j = \frac{1}{\alpha_j}\frac{(r_{j+1}, (r_{j+1} - r_j))}{(Ap_j, p_j)} = \frac{(r_{j+1}, r_{j+1})}{(r_j, r_j)}.$$

Putting these relations together gives the following algorithm.

DOMAIN DECOMPOSITION