

Efficient Tridiagonal Solvers for ADI methods and Fluid Simulation

Nikolai Sakharnykh - NVIDIA San Jose Convention Center, San Jose, CA | September 21, 2010

Introduction

 Tridiagonal solvers - very popular technique in both compute and graphics applications

Application in Alternating Direction Implicit (ADI) methods

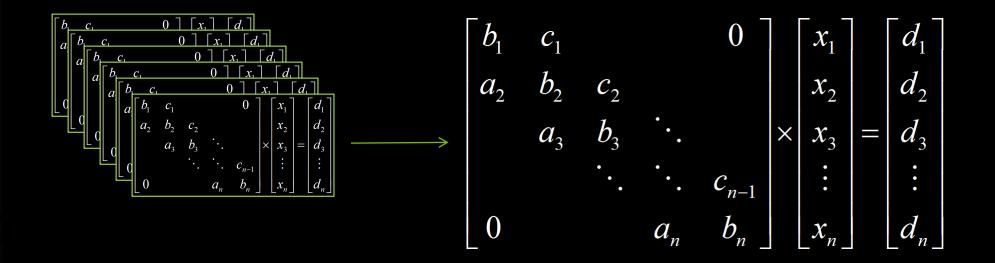
- 2 different examples will be covered in this talk:
 - 3D Fluid Simulation for research and science
 - 2D Depth-of-Field Effect for graphics and games



Outline

- Tridiagonal Solvers Overview
 - Introduction
 - Gauss Elimination
 - Cyclic Reduction
- Fluid Simulation in 3D domain
- Depth-of-Field Effect in 2D domain

Tridiagonal Solvers



- Need to solve many independent tridiagonal systems
 - Matrix sizes configurations are problem specific



Gauss Elimination (Sweep)

$$c_i = \frac{c_i}{b_i - c_{i-1}a_i}$$

■ Forward sweep:
$$c_i = \frac{c_i}{b_i - c_{i-1}a_i}$$
 $d_i = \frac{d_i - d_{i-1}a_i}{b_i - c_{i-1}a_i}$ $i = 1, 2, ..., n$

$$i = 1, 2, ..., n$$

■ Backward substitution:
$$x_n = d_n$$
 $x_i = d_i - c_i x_{i+1}$ $i = n-1,...,1$

$$x_n = d_n$$

$$x_i = d_i - c_i x_{i+1}$$

$$i=n-1,\ldots,1$$

- The fastest serial approach
 - O(N) complexity
 - Optimal number of operations

Cyclic Reduction

• Eliminate unknowns using linear combination of equations:

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = y_i \longrightarrow \overline{a}_i x_{i-2} + \overline{b}_i x_i + \overline{c}_i x_{i+2} = \overline{y}_i$$

• After one reduction step a system is decomposed into 2:

$$\begin{bmatrix} b_1 & c_1 & & & & \\ a_2 & b_2 & c_2 & & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & a_{n-1} & b_{n-1} & c_{n-1} \\ & & & a_n & b_n \end{bmatrix} \longrightarrow \begin{bmatrix} \overline{b_1} & 0 & \overline{c_1} & & & \\ 0 & \overline{b_2} & 0 & \overline{c_2} & & & \\ \overline{a_3} & 0 & \overline{b_3} & 0 & \overline{c_3} & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \overline{a_{n-2}} & 0 & \overline{b_{n-2}} & 0 & \overline{c_{n-2}} \\ & & \overline{a_n} & 0 & \overline{b_n} \end{bmatrix} \longrightarrow \begin{bmatrix} \overline{b_1} & \overline{c_1} \\ \overline{a_3} & \overline{b_3} & \ddots & & \\ & \ddots & \ddots & \overline{c_{n-3}} \\ \overline{a_4} & \overline{b_4} & \ddots & & \\ & & \overline{a_n} & \overline{b_n} \end{bmatrix}$$

Reduction step can be done by N threads in parallel



Cyclic Reduction

- Parallel Cyclic Reduction (PCR)
 - Apply reduction to new systems and repeat O(log N)
 - For some special cases can use fewer steps

- Cyclic Reduction (CR)
 - Forward reduction, backward substitution
 - Complexity O(N), but requires more operations than Sweep



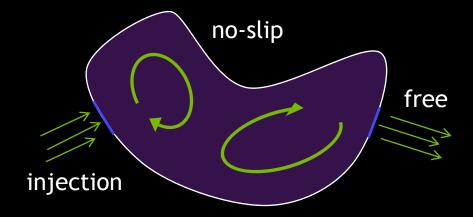
Outline

- Tridiagonal Solvers Overview
- Fluid Simulation in 3D domain
 - Problem statement, applications
 - ADI numerical method
 - GPU implementation details, optimizations
 - Performance analysis and results comparisons
- Depth-of-Field Effect in 2D domain



Problem Statement

- Viscid incompressible fluid in 3D domain
- New challenge: complex dynamic boundaries

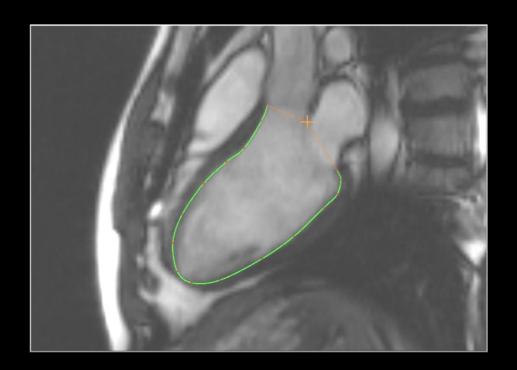


• Euler coordinates: velocity and temperature



Applications

Blood flow simulation in heart



Capture boundaries movement from MR or US

Simulate blood flow inside heart volume



Applications

Sea and ocean simulations



Static boundaries

Additional simulation parameters: salinity, etc.



Definitions

Density	$\rho = const = 1$
Velocity	$\mathbf{u} = (u, v, w)$
Temperature	T
Pressure	p

Equation of state

- Describe relation between p and T
- Example: $p = \rho RT = RT$

R - gas constant for air

Governing equations

- Continuity equation
 - For incompressible fluids: $\operatorname{div} \mathbf{u} = 0$
- Navier-Stokes equations:
 - Dimensionless form, use equation of state

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla T + \frac{1}{\mathrm{Re}} \nabla^2 \mathbf{u}$$

Re - Reynolds number (= inertia/viscosity ratio)



Governing equations

- Energy equation:
 - Dimensionless form, use equation of state

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = -\nabla T + \frac{1}{\text{Pr} \cdot \text{Re}} \Delta T + \frac{\gamma - 1}{\gamma \cdot \text{Re}} \Phi$$

 γ - heat capacity ratio

Pr - Prandtl number

 Φ - dissipative function

ADI numerical method

• Alternating Direction Implicit

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{\partial T}{\partial x} + \frac{1}{\text{Re}} \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$



$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{\partial T}{\partial x} + \frac{1}{\text{Re}} \left(\frac{\partial^2 u}{\partial x^2} \right) \qquad \frac{\partial u}{\partial t} + v \frac{\partial u}{\partial y} = \frac{1}{\text{Re}} \left(\frac{\partial^2 u}{\partial y^2} \right) \qquad \frac{\partial u}{\partial t} + w \frac{\partial u}{\partial z} = \frac{1}{\text{Re}} \left(\frac{\partial^2 u}{\partial z^2} \right)$$

Fixed Y, Z

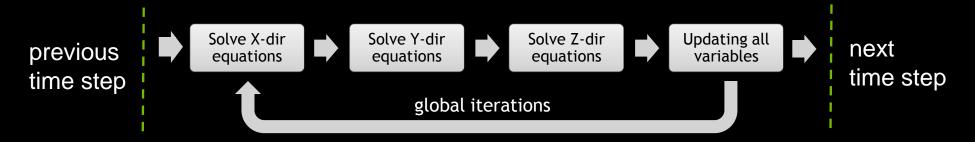
Fixed X, Z

Fixed X, Y



ADI method - iterations

Use global iterations for the whole system of equations



Some equations are not linear:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{\partial T}{\partial x} + \frac{1}{\text{Re}} \left(\frac{\partial^2 u}{\partial x^2} \right)$$

— Use local iterations to approximate the non-linear term



Discretization

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{\partial T}{\partial x} + \frac{1}{\text{Re}} \left(\frac{\partial^2 u}{\partial x^2} \right)$$

Use regular grid, implicit finite difference scheme:

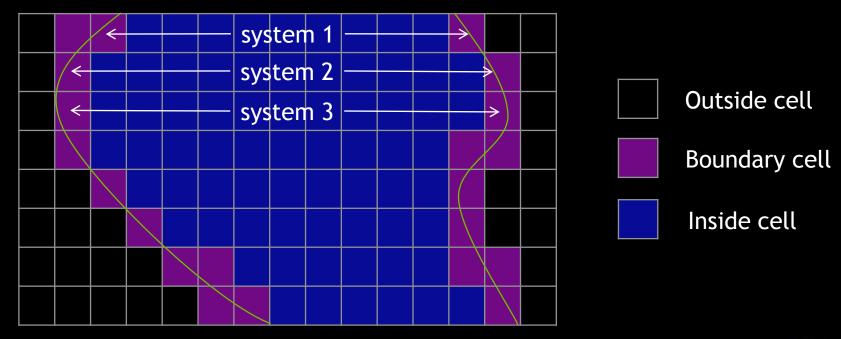
$$\underbrace{\frac{\mathbf{i}}{u_{i,j,k}^{n+1}} - u_{i,j,k}^{n}}_{\Delta t} + u_{i,j,k}^{n} + u_{i,j,k}^{n} - \underbrace{\frac{\mathbf{i}+1}{u_{i-1,j,k}} - u_{i-1,j,k}^{n+1}}_{\Delta x} = -\underbrace{\frac{T_{i+1,j,k}^{n} - T_{i-1,j,k}^{n}}{\Delta x}}_{\mathbf{i}} + \underbrace{\frac{\mathbf{i}+1}{\mathbf{i}}}_{\mathbf{Re}} + \underbrace{\frac{\mathbf{i}+1}{u_{i+1,j,k}^{n+1}} - \underbrace{\frac{\mathbf{i}+1}{u_{i+1,j,k}^{n+1}} - \underbrace{\frac{\mathbf{i}+1}{u_{i-1,j,k}^{n+1}}}_{\Delta x^{2}} + \underbrace{\frac{\mathbf{i}+1}{\mathbf{i}}}_{\mathbf{Re}} + \underbrace{\frac{\mathbf{i}+1}{u_{i+1,j,k}^{n+1}} - \underbrace{\frac{\mathbf{i}+1}{u_{i+1,j,k}^{n+1}} - \underbrace{\frac{\mathbf{i}+1}{u_{i-1,j,k}^{n+1}}}_{\Delta x^{2}} + \underbrace{\frac{\mathbf{i}+1}{u_{i+1,j,k}^{n+1}} - \underbrace{\frac{\mathbf{i}+1}{u_{i+1,j,$$

- Got a tridiagonal system for $u_{i,j,k}^{n+1}$ $i=1,...,N_x$
 - Independent system for each fixed pair (j, k)



Tridiagonal systems

- Need to solve lots of tridiagonal systems
- Sizes of systems may vary across the grid



Implementation details

```
<for each direction X, Y, Z>
    <for each local iteration>
        <for each equation u, v, w, T>
             build tridiagonal matrices and rhs
             solve tridiagonal systems
        update non-linear terms
```

GPU implementation

- Store all data arrays entirely on GPU in linear memory
 - Reduce amount of memory transfers to minimum
 - Map 3D arrays to linear memory
- Main tasks
 - Build matrices
 - Solve systems

$$(X, Y, Z)$$

$$\downarrow$$

$$Z + Y * dimZ + X * dimY * dimZ$$

Z - fastest-changing dimension

- Additional routines for non-linear updates
 - Merge, copy 3D arrays with masks

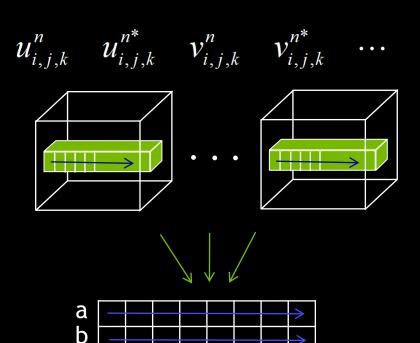


Building matrices

- Input data:
 - Previous/non-linear 3D layers

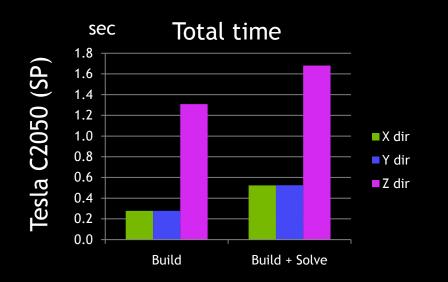


- Coefficients of a tridiagonal matrix
- Right-hand side vector



Use C++ templates for direction and equation

Building matrices - performance



Build kernels

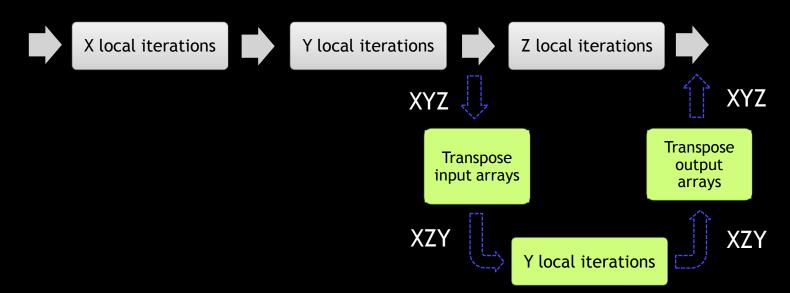
Dir	Requests per load	L1 global load hit %	IPC
Χ	2 - 3	25 - 45	1.4
Υ	2 - 3	33 - 44	1.4
Z	32	0 - 15	0.2

- Poor Z direction performance compared to X/Y
 - Threads access contiguous memory region
 - Memory access is uncoalesced, lots of cache misses



Building matrices - optimization

- Run Z phase in transposed XZY space
 - Better locality for memory accesses
 - Additional overhead on transpose





Building matrices - optimization



Duita Kernets						
Z dir	Requests per load	sts L1 global ad load hit %				
Original	32	0 - 15	0.2			
Transposed	2 - 3	30 - 38	1.3			

Ruild karnals

- Tridiagonal solver time dominates over transpose
 - Transpose will takes less % with more local iterations



Problem analysis

- Big number of tridiagonal systems
 - Grid size squared on each step: 16K for 128^3

- Relatively small system sizes
 - Max of grid size: 128 for 128³

- 1 thread per system is a suitable approach for this case
 - Enough systems to utilize GPU



Solving tridiagonal systems

Matrix layout is crucial for performance

Sequential layout

system 1

system 2

a0 a1 a2 a3 a0 a1 a2 a3

PCR and CR friendly

Interleaved layout

a0 a0 a0 a0 a0 a1 a1 a1 a1 a1

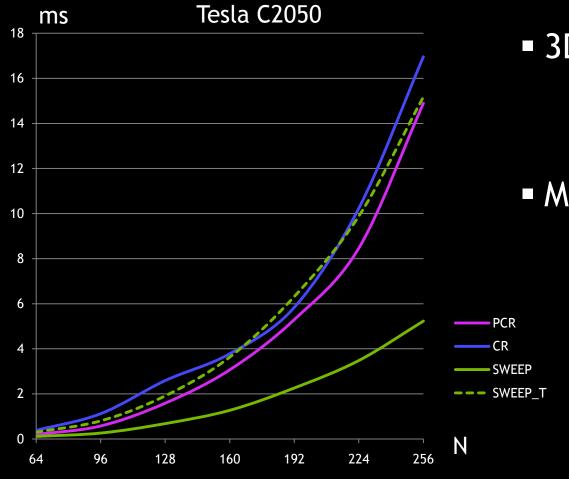
The part of th

ADI - Z direction

ADI - X, Y directions



Tridiagonal solvers performance



- 3D ADI test setup
 - Systems size = N
 - Number of systems = N^2
- Matrix layout
 - *CR, SWEEP_T: sequential
 - SWEEP: interleaved

PCR/CR implementations from: "Fast tridiagonal solvers on the GPU" by Y. Zhang, J. Cohen, J. Owens, 2010



Choosing tridiagonal solver

- Application for 3D ADI method
 - For X, Y directions matrices are interleaved by default
 - Z is interleaved as well if doing in transposed space

- Sweep solver seems like the best choice
 - Although can experiment with PCR for Z direction



Performance analysis - Fermi

- L1/L2 effect on performance
 - Using 48K L1 instead of 16K gives 10-15% speed-up.
 - Turning L1 off reduces performance by 10%
 - Really help on misaligned accesses and spatial reuse

- Sweep effective bandwidth on Tesla C2050
 - Single Precision = 119 GB/s, 82% of peak
 - Double Precision = 135 GB/s, 93% of peak



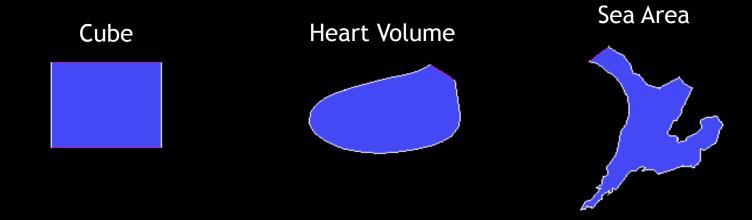
Performance benchmark

- CPU configuration:
 - Intel Core i7 4 cores @ 2.8 GHz
 - Use all 4 cores through OpenMP (3-4x speed-up vs 1 core)
- GPU configurations:
 - NVIDIA Tesla C1060
 - NVIDIA Tesla C2050

Measure Build + Solve time for all iterations



Test cases

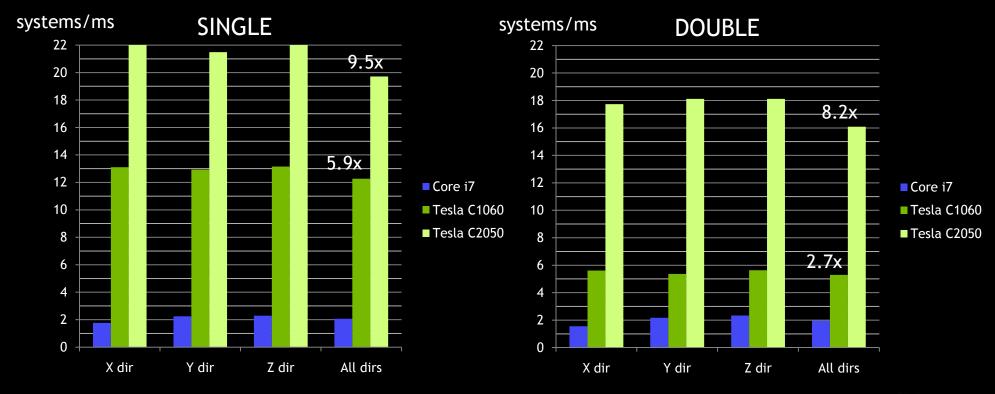


Test	Grid size	X dir	Y dir	Z dir
Cube	128 x 128 x 128	10K	10K	10K
Heart Volume	96 x 160 x 128	13K	8K	8K
Sea Area	160 x 128 x 128	18K	20K	6K



Performance results - Cube

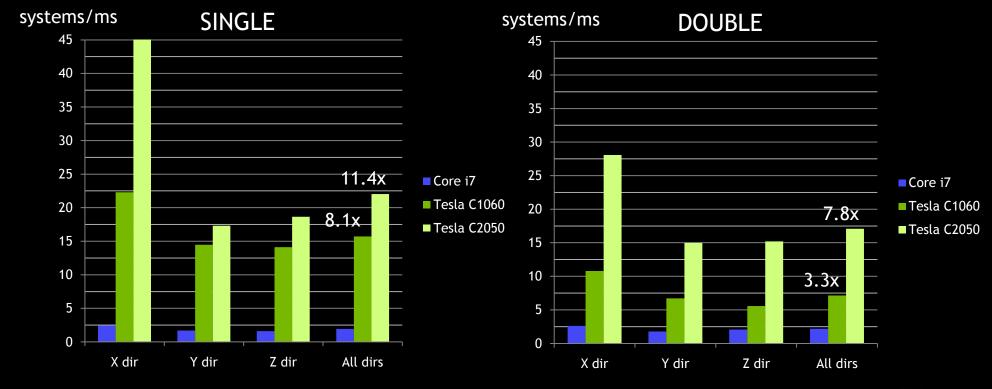
Same number of systems for X/Y/Z, all sizes are equal





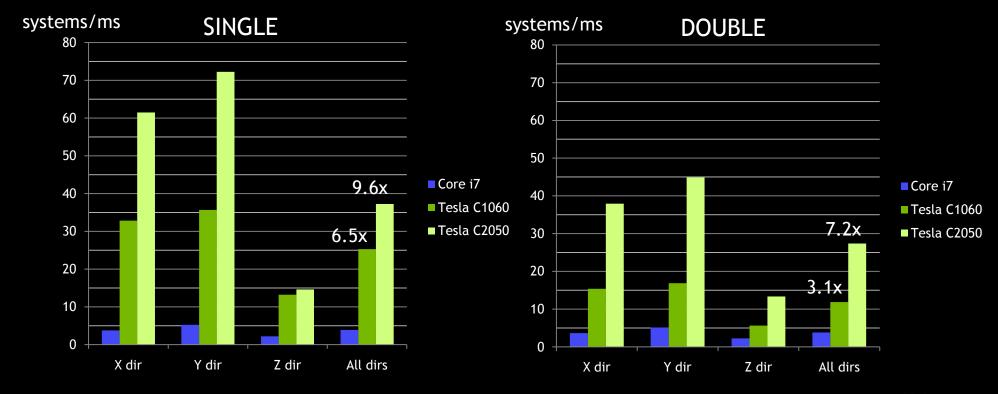
Performance results - Heart Volume

More systems for X, sizes vary smoothly



Performance results - Sea Area

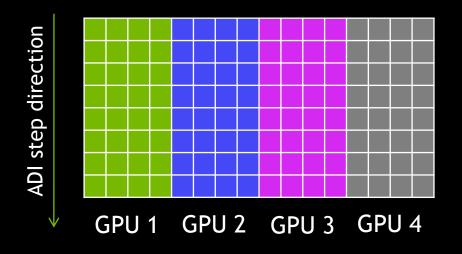
Lots of small systems of different size for X/Y



Future work

- Current main limitation is memory capacity
 - Lots of 3D arrays: grid data, time layers, tridiagonal matrices

Multi-GPU and clusters enable high-resolution grids



Split grid along current direction (X, Y or Z)

Assign each partition to one GPU

Solve systems and update common 3D layers



References

- http://code.google.com/p/cmc-fluid-solver/
- "Tridiagonal Solvers on the GPU and Applications to Fluid Simulation", GPU Technology Conference, 2009, Nikolai Sakharnykh
- "A dynamic visualization system for multiprocessor computers with common memory and its application for numerical modeling of the turbulent flows of viscous fluids", Moscow University Computational Mathematics and Cybernetics, 2007, Paskonov V.M., Berezin S.B., Korukhova E.S.

Outline

- Tridiagonal Solvers Overview
- Fluid Simulation in 3D domain
- Depth-of-Field Effect in 2D domain
 - Problem statement
 - ADI numerical method
 - Analysis and hybrid approach
 - Shared memory optimization
 - Visual results



Problem statement

ADI method application for 2D problems

- Real-time Depth-Of-Field simulation
 - Using diffusion equation to blur the image

$$\frac{\partial u}{\partial t} = \nabla \cdot (\beta \cdot \nabla u)$$

- Now need to solve tridiagonal systems in 2D domain
 - Different setup, different methods for GPU



Numerical method

• Alternating Direction Implicit method

$$\frac{\partial u}{\partial t} = \nabla \cdot (\beta \cdot \nabla u)$$

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(\beta(x, y_j) \frac{\partial u}{\partial x} \right) \qquad \frac{\partial u}{\partial t} = \frac{\partial}{\partial y} \left(\beta(x_i, y) \frac{\partial u}{\partial y} \right)$$

for all fixed
$$y_j = 0, \dots, H-1$$

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial y} \left(\beta(x_i, y) \frac{\partial u}{\partial y} \right)$$

for all fixed
$$x_i = 0, \dots, W-1$$

Implementing ADI method

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(\beta(x, y_j) \frac{\partial u}{\partial x} \right)$$

- Implicit scheme is always stable
- After discretization on a regular grid with dx = dt = 1:

$$\underbrace{u_{i,j}^{n+1}}_{i} - u_{i,j}^{n} = \underbrace{u_{i-1,j}^{n+1}}_{i-1,j} \beta_{i-1,j} - \underbrace{u_{i,j}^{n+1}}_{i,j} (\beta_{i-1,j} + \beta_{i,j}) + \underbrace{u_{i+1,j}^{n+1}}_{i+1,j} \beta_{i,j}$$

Got a tridiagonal system for each fixed j

Problem analysis

- Small number of systems
 - Max 2K for high resolutions

- Large matrix dimensions
 - Up to 2K for high resolutions

- Using 1 thread per system wouldn't be so efficient
 - Low GPU utilization



GPU implementation

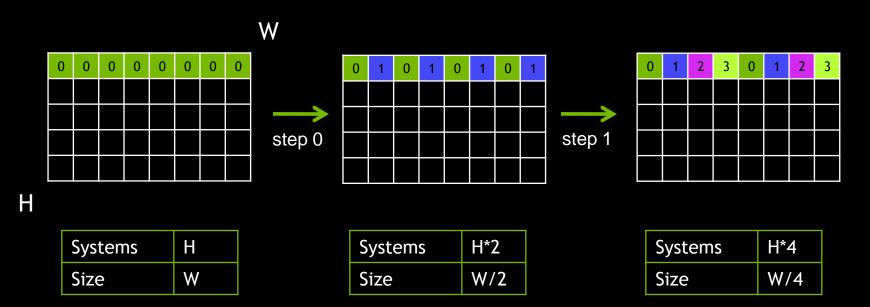
- Matrix layout
 - Sequential for X direction
 - Interleaved for Y direction

- Use hybrid algorithm
 - Start with Parallel Cyclic Reduction (PCR)
 - Subdivide our systems into smaller ones
 - Finish with Gauss Elimination (Sweep)
 - Solve each new system by 1 thread



PCR step

Doubles number of systems, halves systems size



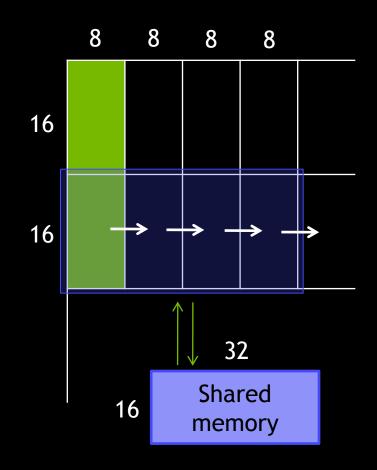
Hybrid approach

- Benefits of each additional PCR step
 - Improves memory layout for Sweep in X direction
 - Subdivides systems for more efficient Sweep
- But additional overhead for each step
 - Increasing total number of operations for solving a system
- Need to choose an optimal number of PCR steps
 - For DOF effect in high-res: 3 steps for X direction



Shared memory optimization

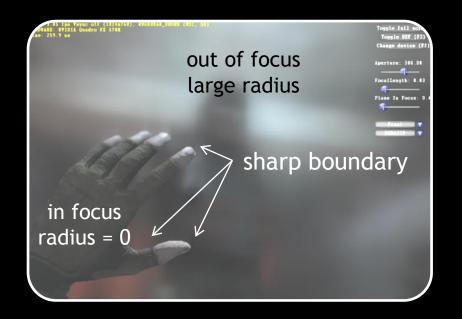
- Shared memory is used as a temporary transpose buffer
 - Load 32x16 area into shared memory
 - Compute 4 iterations inside shared memory
 - Store 32x16 back to global memory
- Gives 20% speed-up



Diffusion simulation idea

Diffuse temperature series (= color) on 2D plate (= image)
 with non-uniform heat conductivity (= circles of confusion)

- Key features:
 - No color bleeding
 - Support for spatially varying arbitrary circles of confusion



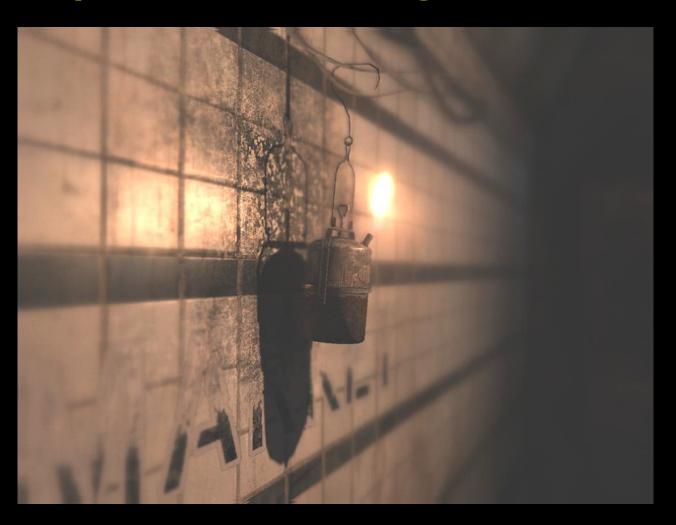
Depth-of-Field in games



From Metro2033, © THQ and 4A Games



Depth-of-Field in games



From Metro2033, © THQ and 4A Games



References

Pixar article about Diffusion DOF:

http://graphics.pixar.com/library/DepthOfField/paper.pdf

Cyclic reduction methods on CUDA:

http://www.idav.ucdavis.edu/func/return_pdf?pub_id=978

Upcoming sample in NVIDIA SDK



Summary

- 10x speed-ups for 3D ADI methods in complex areas
 - Great Fermi performance in double precision

- Achieve real-time performance in graphics and games
 - Realistic depth-of-field effect

Tridiagonal solvers performance is problem specific



Questions?