GPU Computing for Computational Science

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State of Computational Science

Legacy codes in wide use

Computational science community is cautiously exploring GPUs

Major issue: How to handle legacy code?

- Accelerate? Rewrite?
- Is it worth it? (lots of ink spilled about this…)

Wildcard: What about radically different approaches?

Conceptual Roadmap

- Option 1: Accelerate
- Option 2: Rewrite
- Option 3: Rethink

- “But my code already runs on dual core. Why can’t I just recompile?”

Why a GPU isn’t just a CPU with 100x more cores

How do you measure speed?

“How fast can you do one thing?”

(latency)

vs.

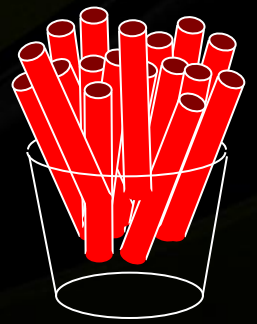
“How much can you do per second?”

(throughput)

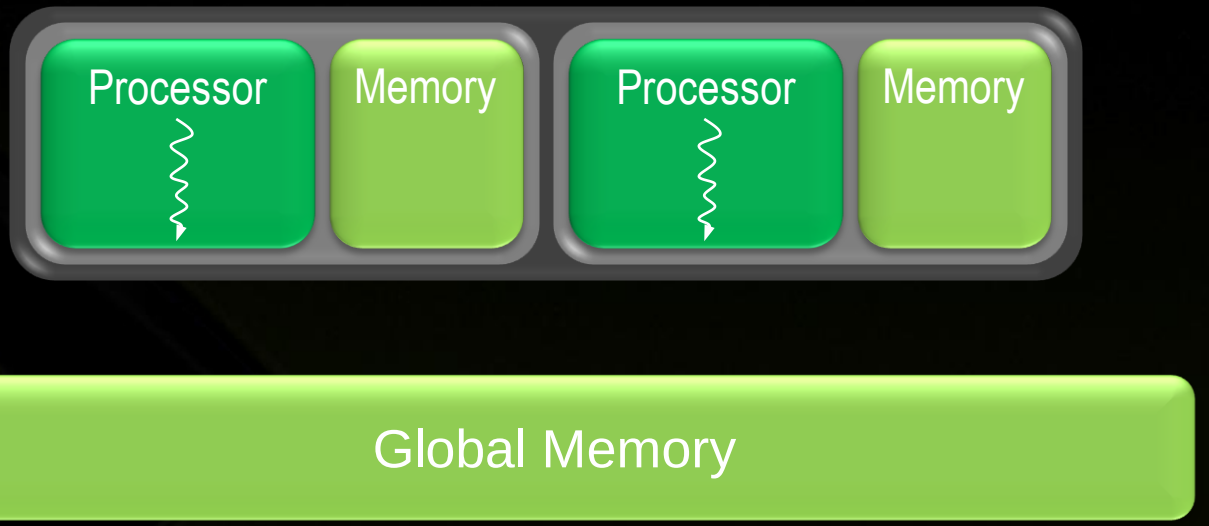
Throughput = Parallelism

Latency: sip through a really big straw

Throughput: Use 100 small straws

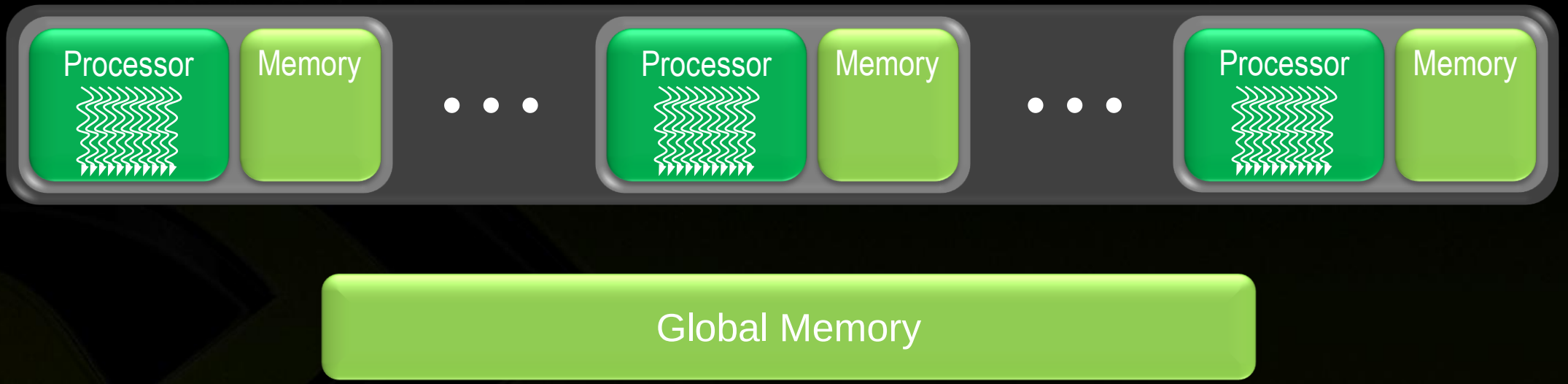


Multicore CPU: Run ~10 Threads Fast



- **Few processors, each supporting 1–2 hardware threads**
- **On-chip memory/cache near processors**
- **Shared global memory space (external DRAM)**

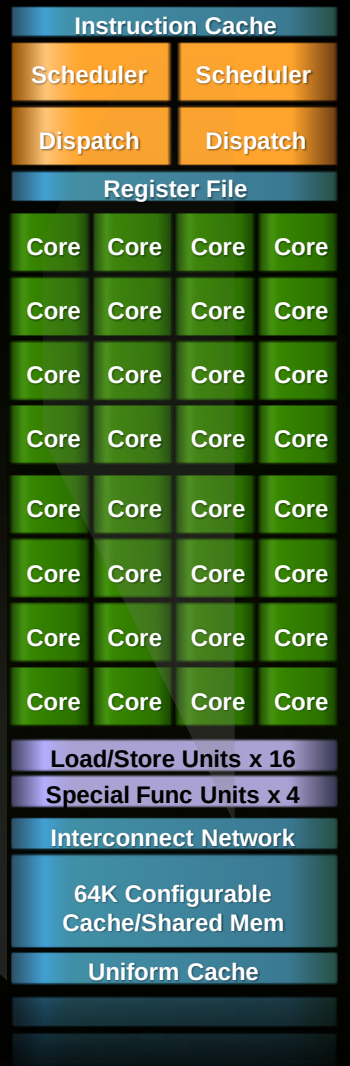
Manycore GPU: Run ~10,000 Threads Fast



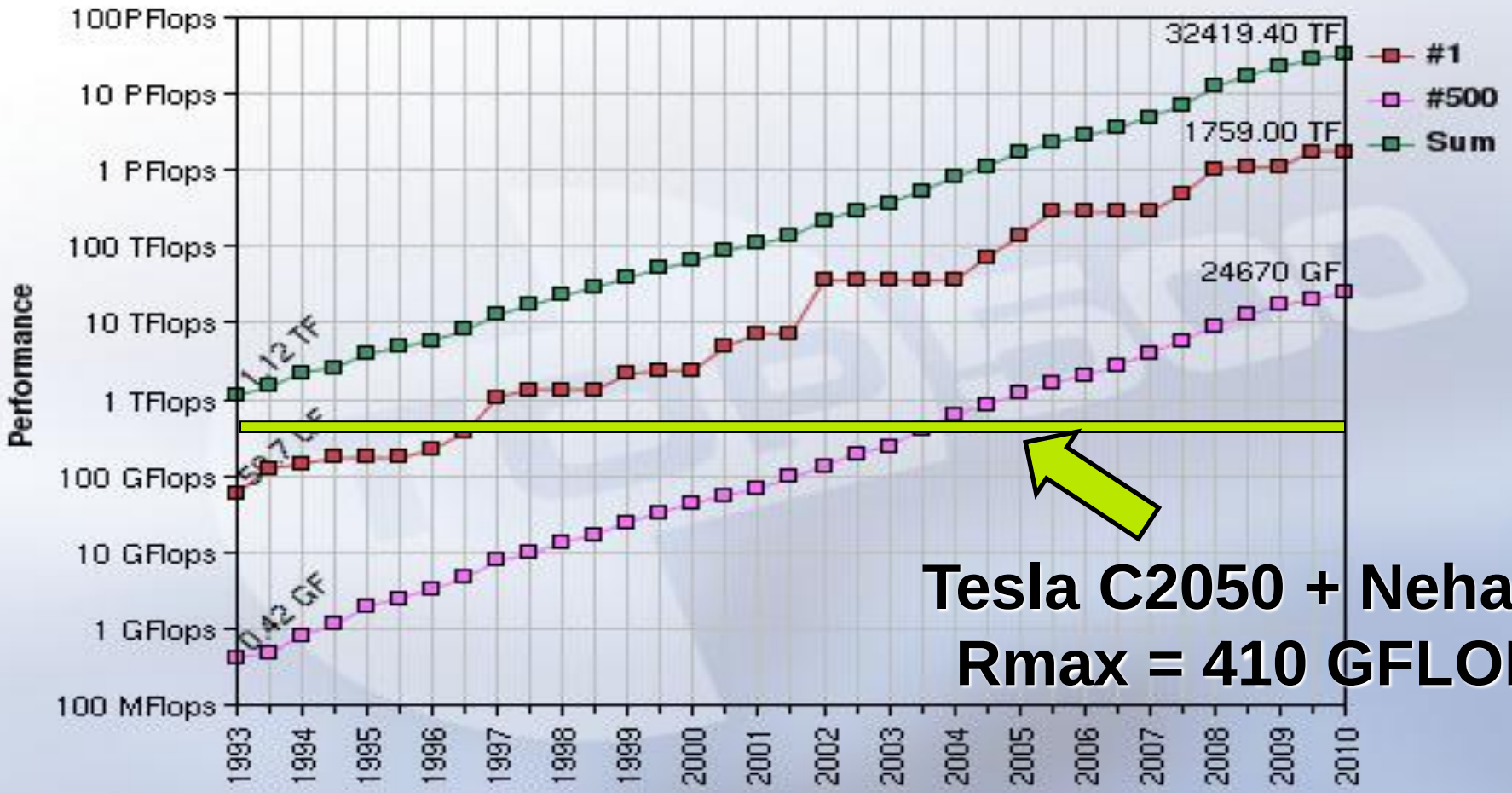
- **Hundreds of processors, each supporting hundreds of hardware threads**
- **On-chip memory/cache near processors**
- **Shared global memory space (external DRAM)**

NVIDIA “Fermi” Parallel Computing Architecture

- Designed for throughput
- Up to 512 Cores
- Singe Precision: >1 TFLOPS
- Double Precision: ~0.5 TFLOPS



Performance Development



Tesla C2050 + Nehalem
Rmax = 410 GFLOPS

What Computational Science Breakthroughs Happened in 2003?

- Universe of protein structures mapped
- Discovery that 80% of tropopause height increase due to human activity – global warming “fingerprint”
- First comprehensive analysis of Y chromosome
- Analysis of WMAP data establishes age of universe, curvature, Hubble’s constant
- High resolution simulations of 1994 Northridge Quake
- Human Genome Project published first complete version

This was not the stone ages!

What does this mean for computational science?

Option 1: Accelerate

Case Study: FEAST from TU Dortmund

Finite Element Analysis and Solution Tools

Complex FE code for CFD and Structural Mechanics

Dominik Göddeke et al. accelerated using GPUs

FEAST-GPU Approach: High level of abstraction

- Minimally invasive co-processor integration
- Identify and isolate "accelerable" parts of a computation
- Chunks must be large enough to amortize co-processor drawbacks (PCIE, change of data layout, etc.)

Portions of this slide courtesy Dominik Göddeke

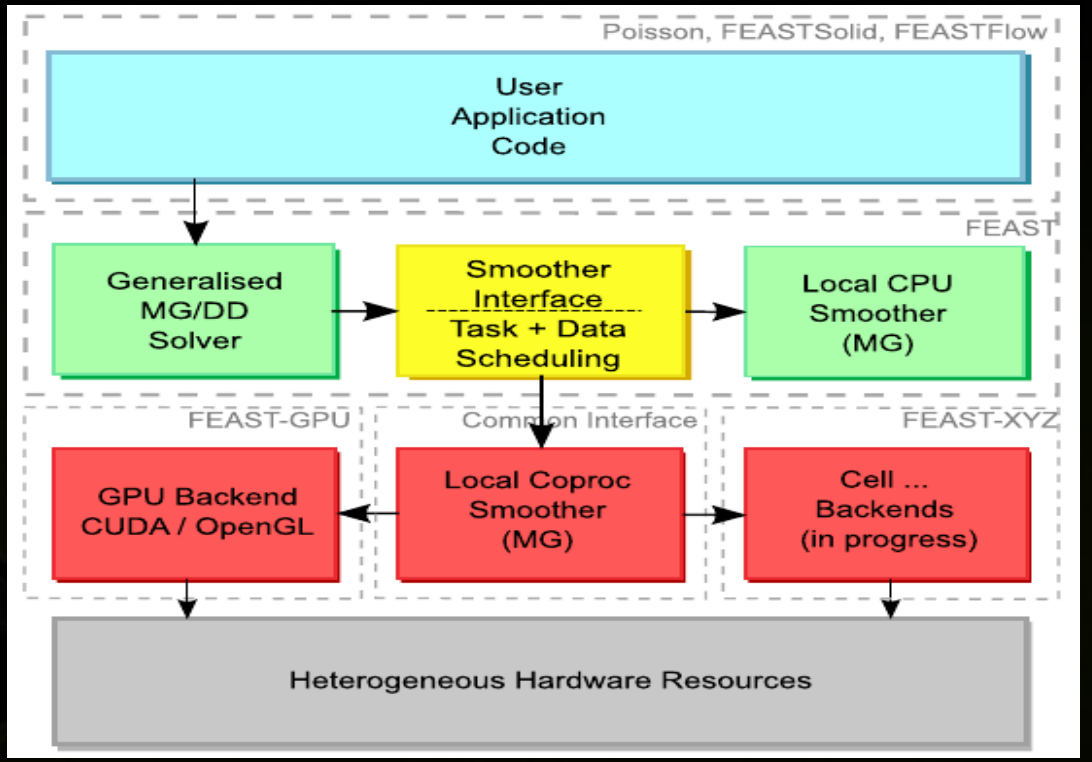
FEAST-GPU Design Philosophy

FEAST-GPU Goal:

- Integrate several co-processors into existing large-scale software package...
- *...without modifying application code*

- NOT mapping single application to GPU / GPU Cluster

Balance acceleration potential and acceleration effort



Portions of this slide courtesy Dominik Göddeke

FEAST-GPU Integration Results

Opteron 2214, 4 nodes

GeForce 8800 GTX

CUDA backend

18.8 M DOF

$$\begin{pmatrix} A_{11} & A_{12} & B_1 \\ A_{21} & A_{22} & B_2 \\ B_1^T & B_2^T & C \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ p \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ g \end{pmatrix}$$

Accel. fraction R_{acc}: 75%
Local speedup S_{local}: 11.5x
Theoretical limit S_{max}: 4x
Global speedup S_{total}: 3.8x

fixed point iteration
solving linearised subproblems with
global BiCGStab (reduce initial residual by 1 digit)
Block-Schurcomplement preconditioner
1) approx. solve for velocities with
global MG (V 1+0), additively smoothed by
for all Ω_i: solve for $\mathbf{u_1}$ with **local MG**
for all Ω_i: solve for $\mathbf{u_2}$ with **local MG**
2) update RHS: $\mathbf{d_3} = -\mathbf{d_3} + \mathbf{B^T}(\mathbf{c_1}, \mathbf{c_2})^T$
3) scale $\mathbf{c_3} = (\mathbf{M_p^L})^{-1}\mathbf{d_3}$

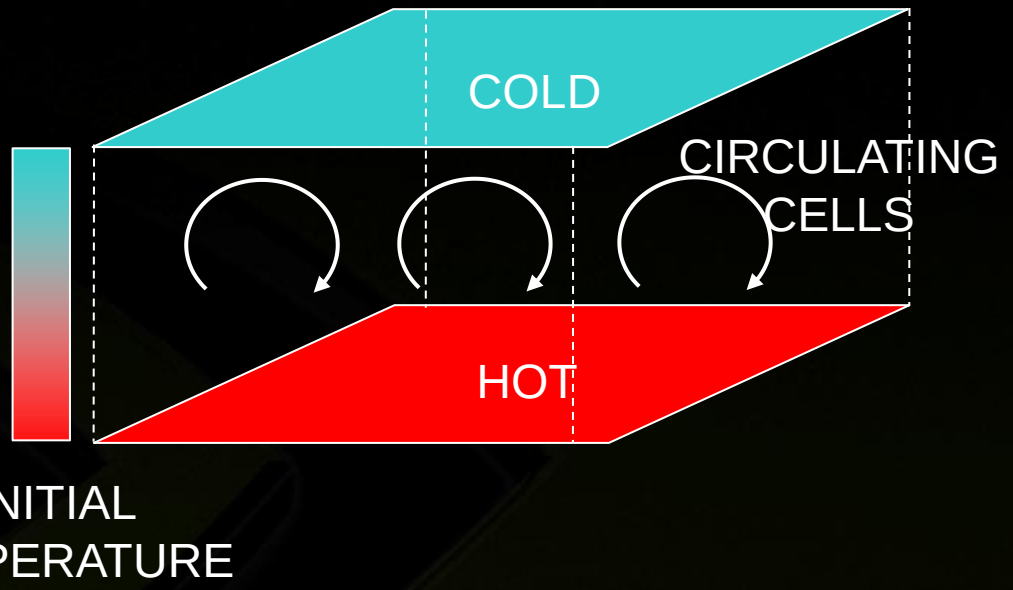
Portions of this slide courtesy Dominik Göddeke

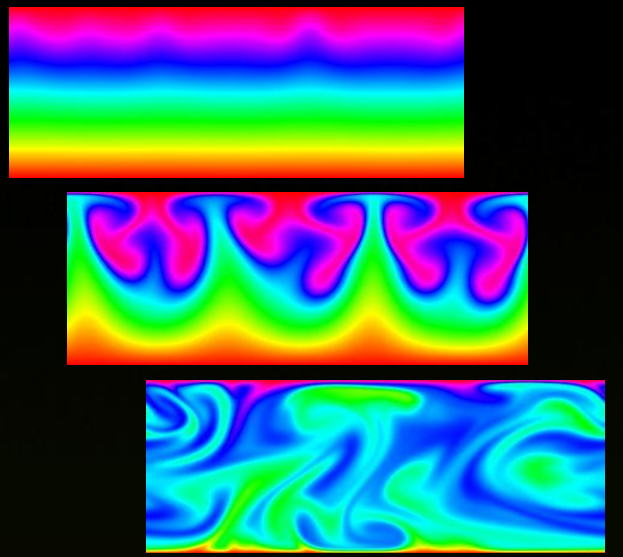
Option 2: Rewrite

- If you were to attempt a rewrite:
  - Good overall design?
  - What data structures / algorithms to use?
  - Is it worth the effort – does 10x improvement on bottlenecks translate into 10x improvement for entire system?
- Major Take-away: Avoid All Serial Bottlenecks
- In particular: Avoid All PCIE Transfers

  => Move Everything to GPU

Rayleigh-Bénard Benchmark





- "OpenCurrent": 2nd order Finite Volume Cartesian fp64 CUDA code - entire code runs on GPU
- Transition from stratified (top) to turbulent (bottom)
- Validated / benchmarked non-linear problems against published results & existing Fortran code

Benchmark Methodology

- Fortran code
  - Written by Jeroen Molemaker @ UCLA
  - 8 Threads (via MPI and OpenMP) on 8-core 2.5 GHz Xeon
  - Several oceanography pubs using this code, ~10 years of code optimizations. Code is small & fast.
- Per-step calculation time varies due to convergence rate of pressure solver
- Record time once # of v-cycles stabilizes
  - Point relaxer on GPU – 1 FMG + 7 v-cycles
  - Line relaxer on CPU – 1 FMG + 13 v-cycles
- See Cohen & Molemaker, ParCFD 2009

Benchmark Results – early 2009

- CUDA (1 Tesla C1060) vs. Fortran (8-core 2.5 GHz Xeon)
- As "apples-to-apples" as possible ($ and manpower)
  - Equal price nodes (in 2009: ~$3k)
  - Skilled programmers in each paradigm

Resolution	CUDA time/step	Fortran time/step	Speedup
64 x 64 x 32	24 ms	47 ms	2.0x
128 x 128 x 64	79 ms	327 ms	4.1x
256 x 256 x 128	498 ms	4070 ms	8.2x
384 x 384 x 192	1616 ms	13670 ms	8.5x

HOOMD blue

NVIDIA

- **MD Code from Joshua Anderson *et al.***
- **Designed to run on GPU(s) or CPU(s)**

Integration
- NVT (Nosé-Hoover)
- NPT
- Langevin Dynamics
- NVE

Bond forces
- harmonic
- FENE

Angle forces
- harmonic
- CGCMM

Dihedral/Improper forces
- harmonic

Simulation types
- 2D and 3D
- Replica exchange

Snapshot formats
- MOL2
- DCD
- PDB
- XML

Pair forces
- Lennard Jones
- Gaussian
- CGCMM
- Morse
- Table (arbitrary)
- Yukawa

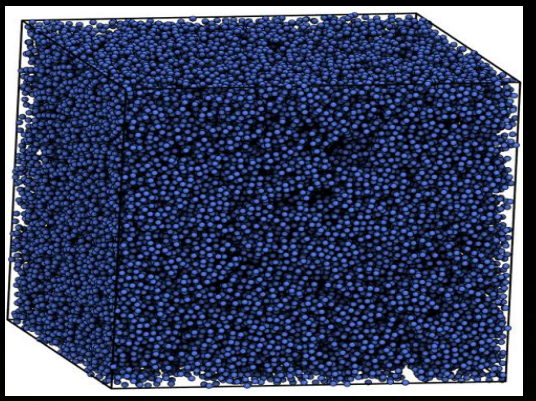
Many-body forces
- EAM (*coming soon*)

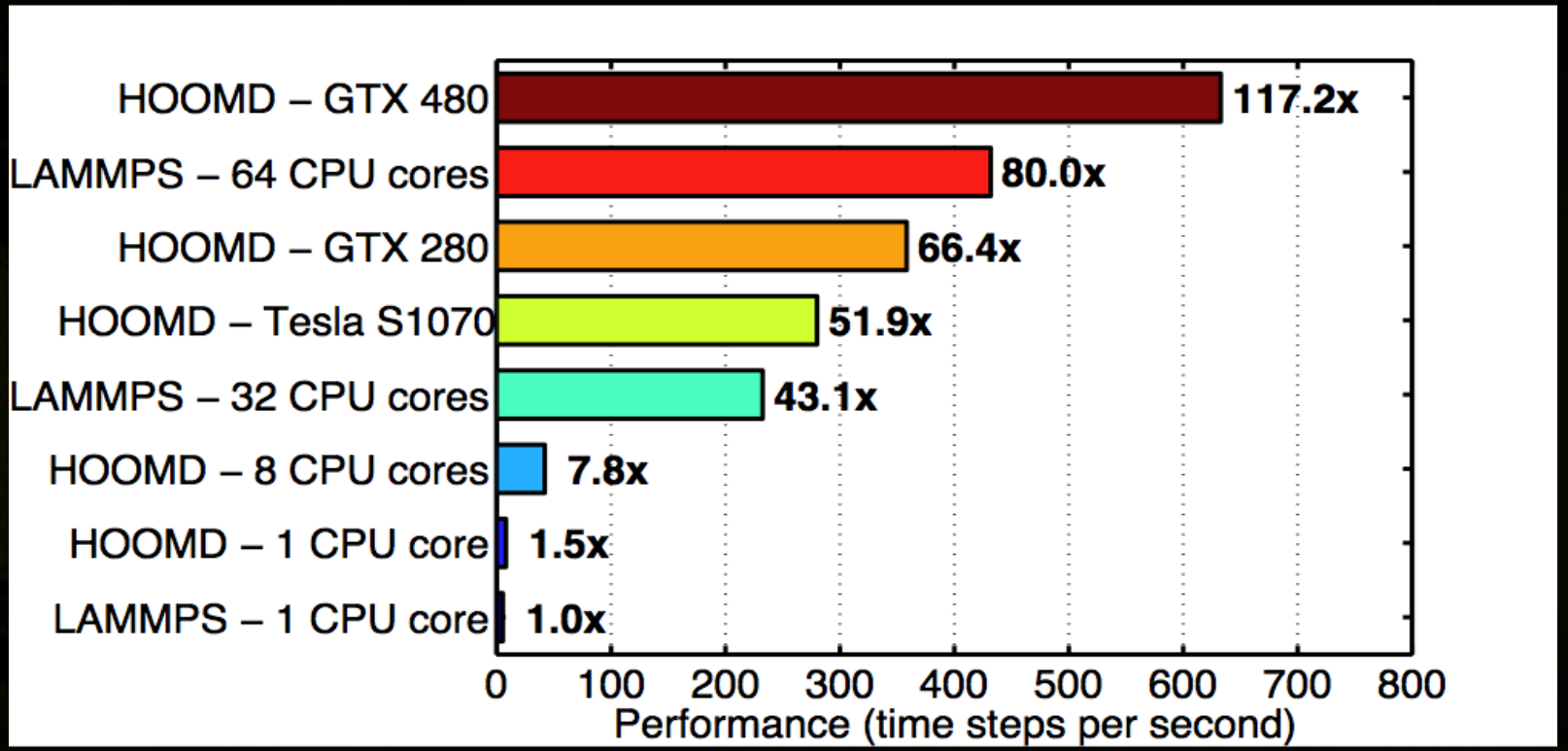
Hardware support
- All recent NVIDIA GPUs
- Multi-core CPUs via OpenMP

Portions of this slide courtesy Joshua Anderson

HOOMD-blue Benchmark

- 64,000 particle Lennard-Jones fluid simulation
- representative of typical performance gains





*CPU: Intel Xeon E5540 @ 2.53GHz

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Option 3: Rethink the Numerics

- Numerical methods + programming languages + compilers + architectures + programming paradigms = co-evolution
  - Popular methods are easy to express in popular languages, run well on popular hardware
  - Not a coincidence!
- New architectures = opportunity for new numerics
- We overlooked approaches because they were impractical … maybe no longer true
- Paradigm shifts upend conventional wisdom

Example:
Nodal Discontinuous Galerkin Methods

Work from Tim Warburton & Andreas Klöckner *et al.* @ Brown & Rice

Solve conservation laws over unstructured grids

$$u_t + \nabla \cdot F(u) = 0$$

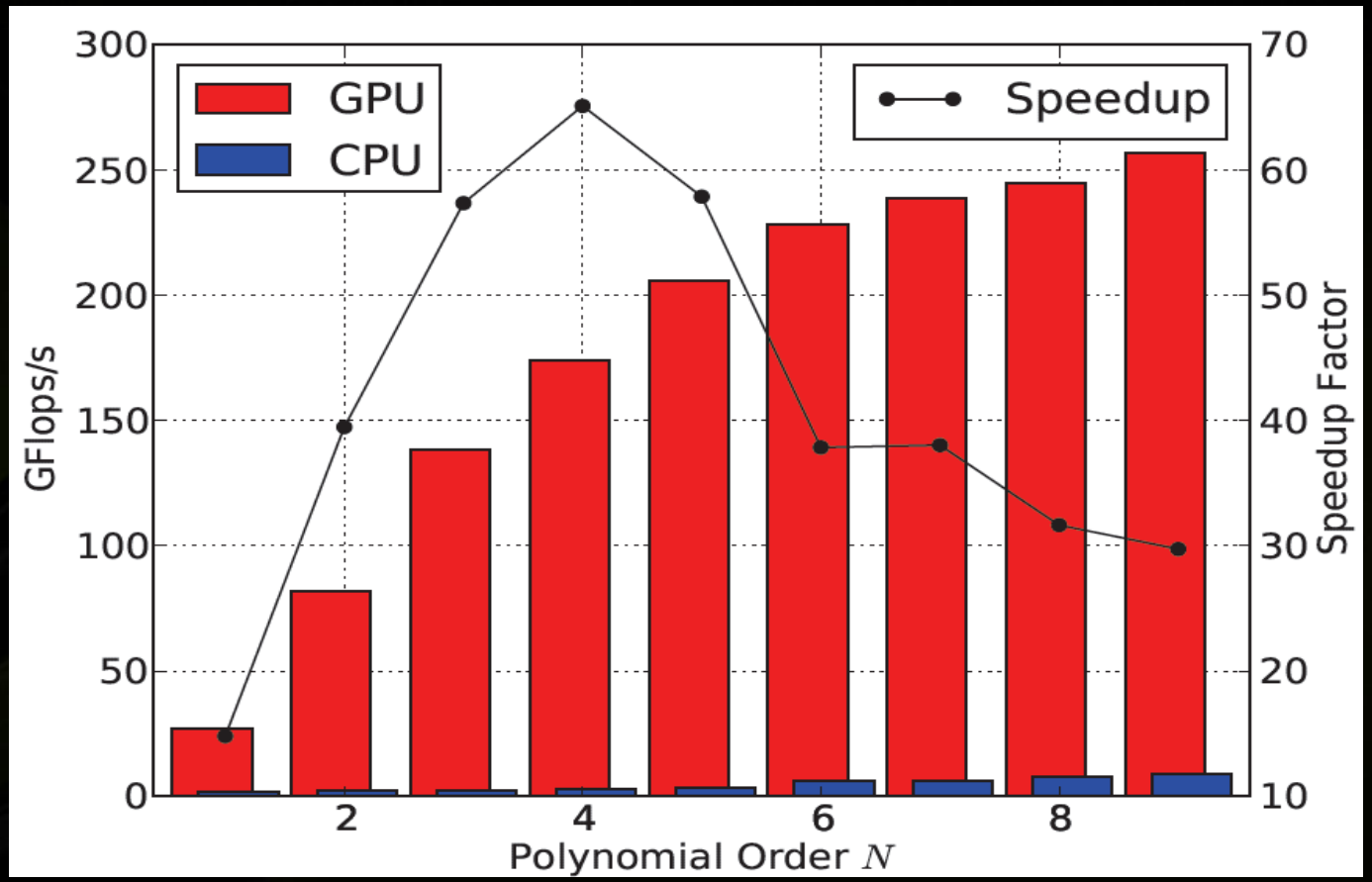
DG on GPUs: Why?

- GPUs have deep memory hierarchy
  - The majority of DG is local (matrix structure)
- Compute Bandwidth >> Memory Bandwidth
  - DG is arithmetically intense.
  - Adopt "FLOPS are free" philosophy

Portions of this slide courtesy Andreas Klöckner

Early DG Results

Nvidia GTX280 vs. single core of Intel E8400 - Maxwell's Equations



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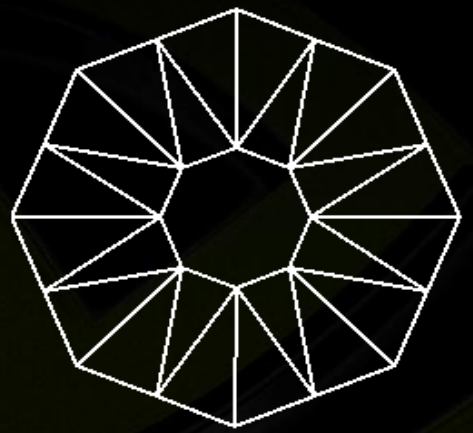
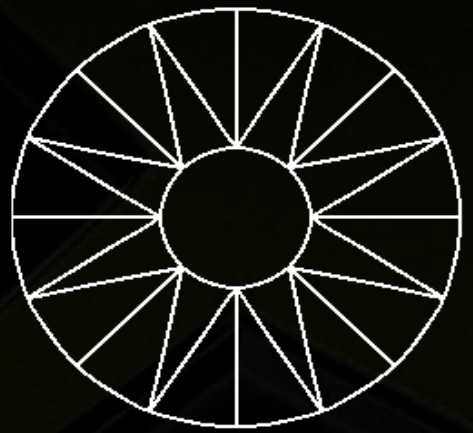
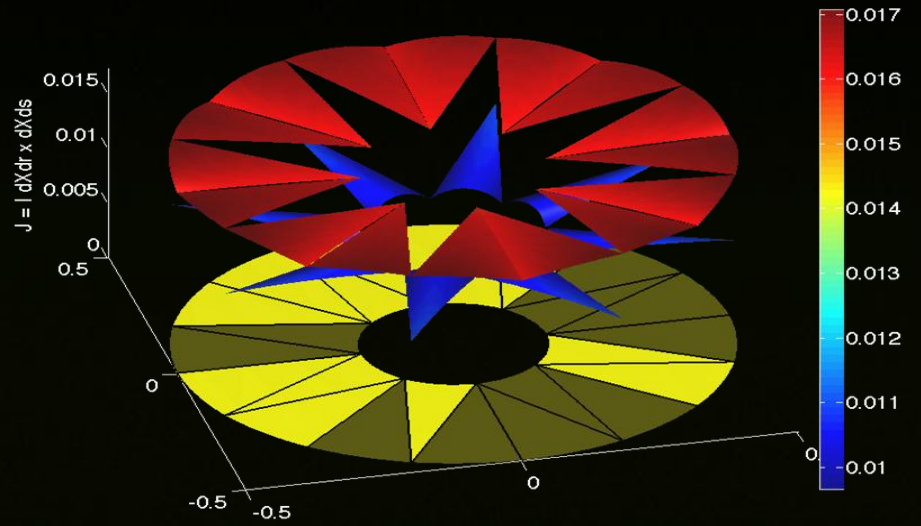
Curvilinear DG: Needs Jacobians

$$J = \left| \frac{\partial \mathbf{x}}{\partial r} \times \frac{\partial \mathbf{x}}{\partial s} \right| \text{ appears in inner products: } (u,v)_T = \iint_{\hat{T}} u(r,s)v(r,s)J(r,s)\,dr\,ds$$







FEM Mesh

Curvilinear Mesh

Piecewise polynomial determinant of the Jacobian plotted vertically

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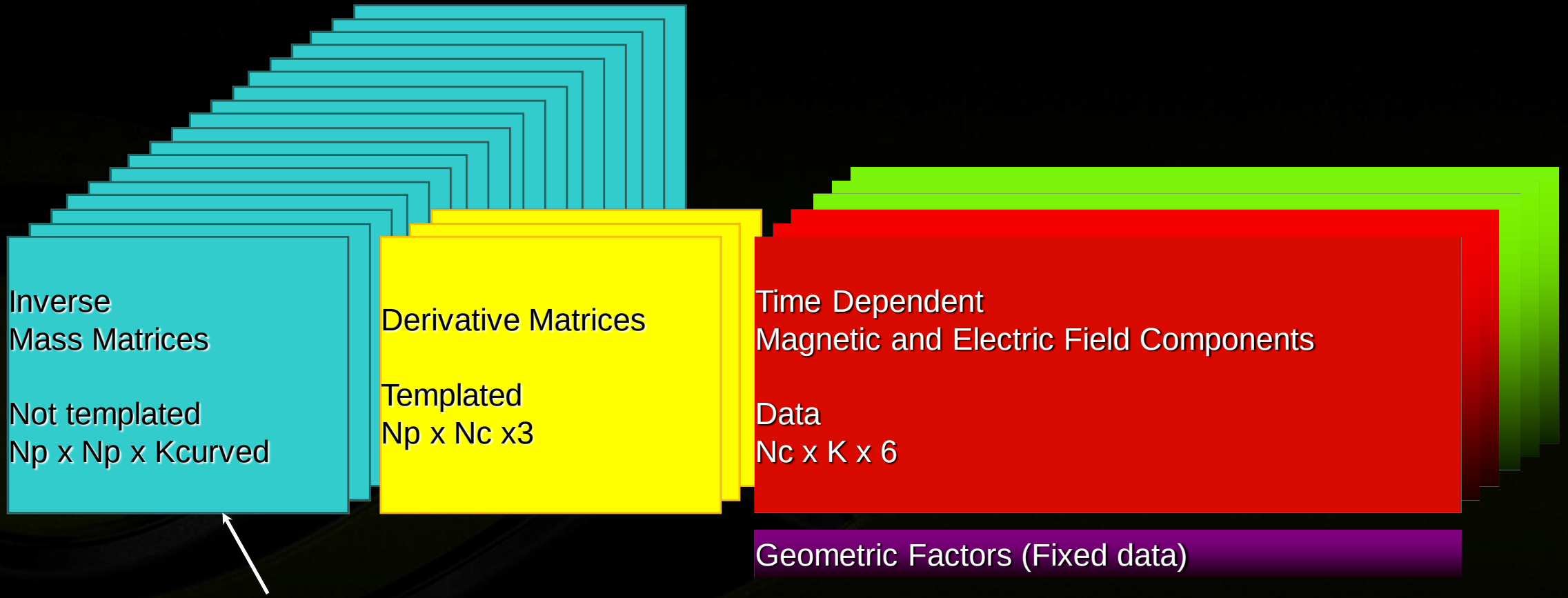
Curvilinear DG Matrix Structures



Each curved element requires its own mass matrix (lots of memory)
Compute on the fly on GPU since FLOPS are free

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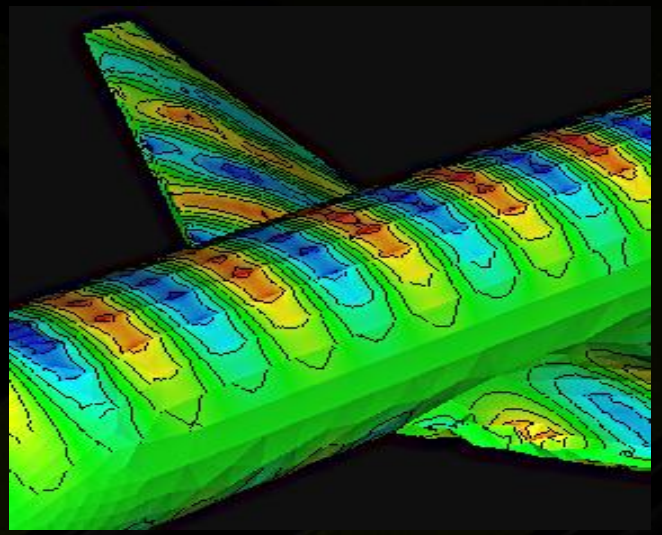
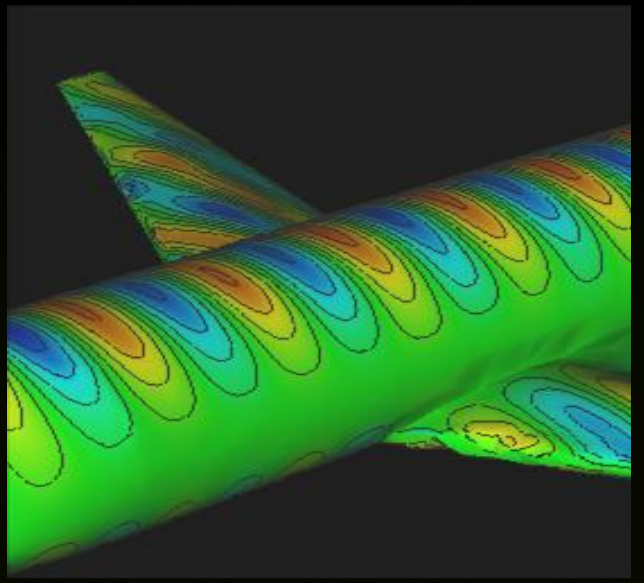
Maxwell Equation Solution with Curvilinear DG



Paneled



Curvilinear

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Accelerate, Rewrite, or Rethink?

- **Accelerate** Legacy Codes
  - Use CUBLAS / CUFFT / thrust / matlab / cusp / PGI-Accelerator / etc.
    => good work for domain scientists (minimal computer science required)
- **Rewrite** New Codes
  - Opportunity for clever algorithmic thinking
    => good work for computer scientists (minimal domain knowledge required)
- **Rethink** Numerical Methods
  - Potential to transform science
    => Interdisciplinary: requires CS *and* domain insight
    => Exciting time to be a computational scientist!

Thanks

- Andreas Klöckner
- Tim Warburton
- Dominik Göddeke
- Joshua Anderson