

Turbomachinery CFD on many-core platforms – experiences and strategies

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MUSAF Colloquium, CERFACS, Toulouse September 27-29 2010



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Overview

- The future (the present) is "many-core"
- GPU hardware
- A strategy for programming GPUs for CFD
- Turbostream a many-core CFD solver for Turbomachinery
- Example simulations
- Conclusions

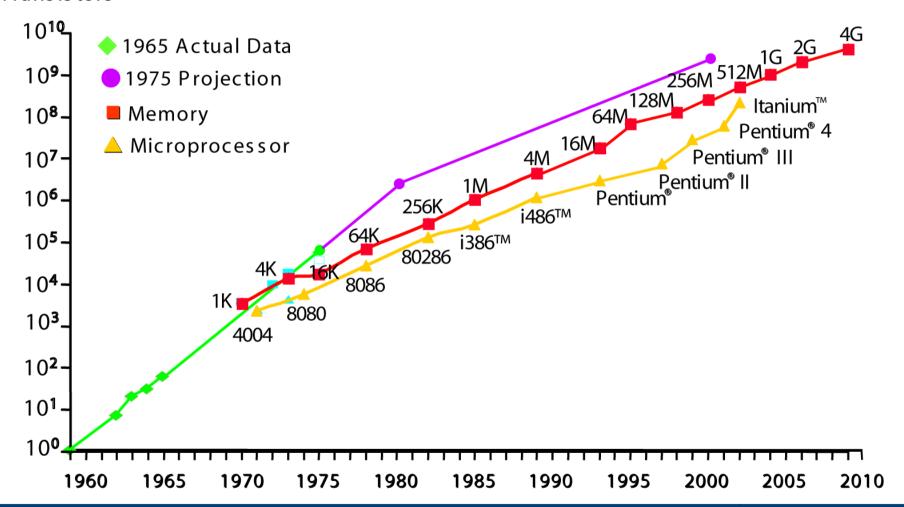




Many-core

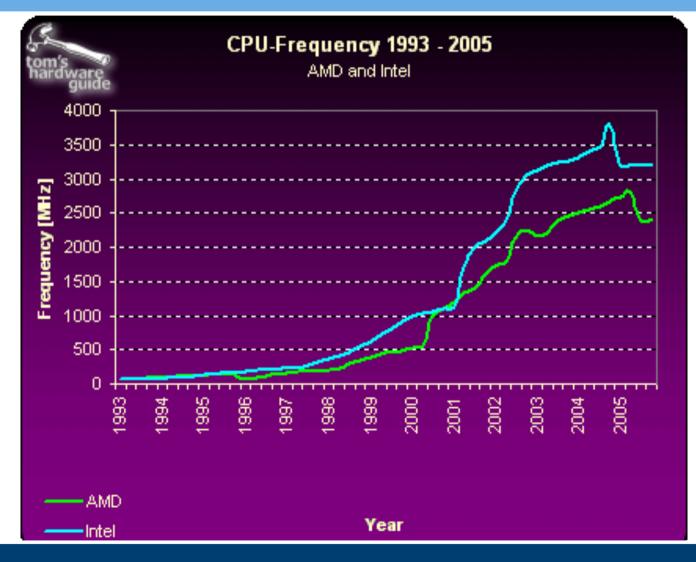
Moore's "Law"

Transistors



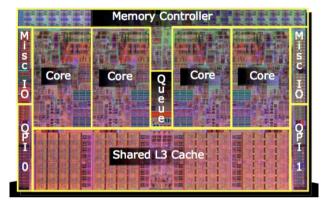
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Clock speed – the "power wall"

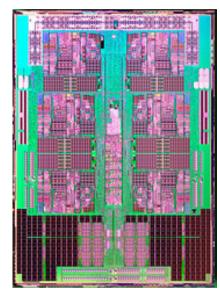




Today's many-core chips



Intel 4 core CPU



AMD 6 core CPU

| Processor Cores Brown Frederic Processor Cores Brown Frederic Brown Frederic Brow | ROP | Texture | Processor Cores |
|--|-----|-----------------|--------------------|
| Frame Buffer | | Frame Buffer | |
| Processor Cores | ROP | Texture | Processor Cores |

NVIDIA 240 cores GPU



NVIDIA Tesla GPUs

 C2050 card for desktop PC; 448 cores, 3GB; peak 515 GFLOP/s (DP)

 S2050 1U rack mount; 4 x C2050 cards; requires connection to CPU host – typical average density is 2 GPUs per 1U





Many-core summary

- Many-core computing is here today and the trend is for greater and greater core count in future
- The run-time of a scalar (non-parallel) code is no longer guaranteed to reduce with each new computer (it may even increase)
- Codes need to be parallel to take advantage of new hardware
- The current distributed parallel computing model (MPI) will not work well here (for many-core CPUs), and may not work at all (for GPUs)

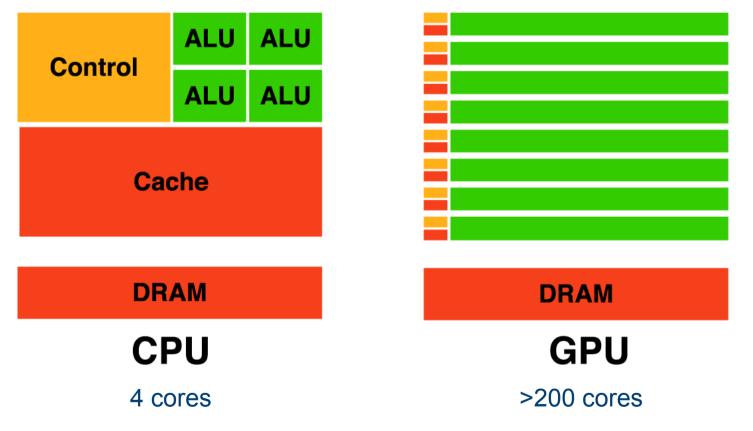




GPUs – what do we get from all those cores?

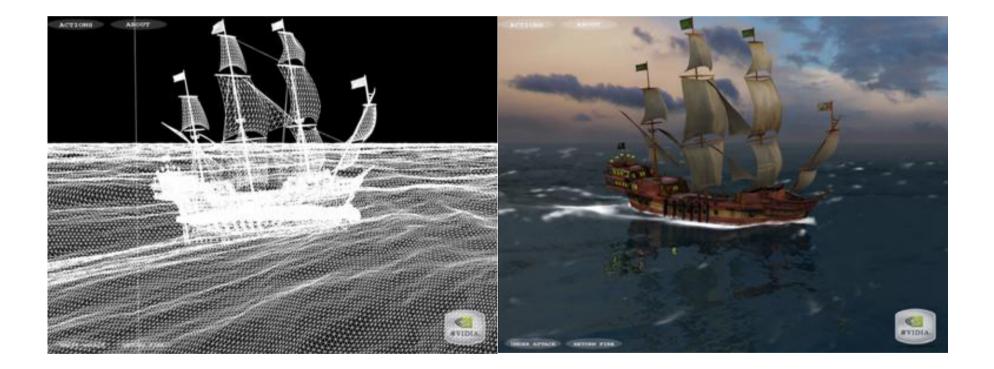
How so many cores on a GPU?

Transistor usage:





Why so many cores on a GPU?





GPUs and scientific computing

GPUs are designed to apply the

same shading function

to many *pixels* simultaneously



GPUs and scientific computing

GPUs are designed to apply the

same *function*

to many *data* simultaneously

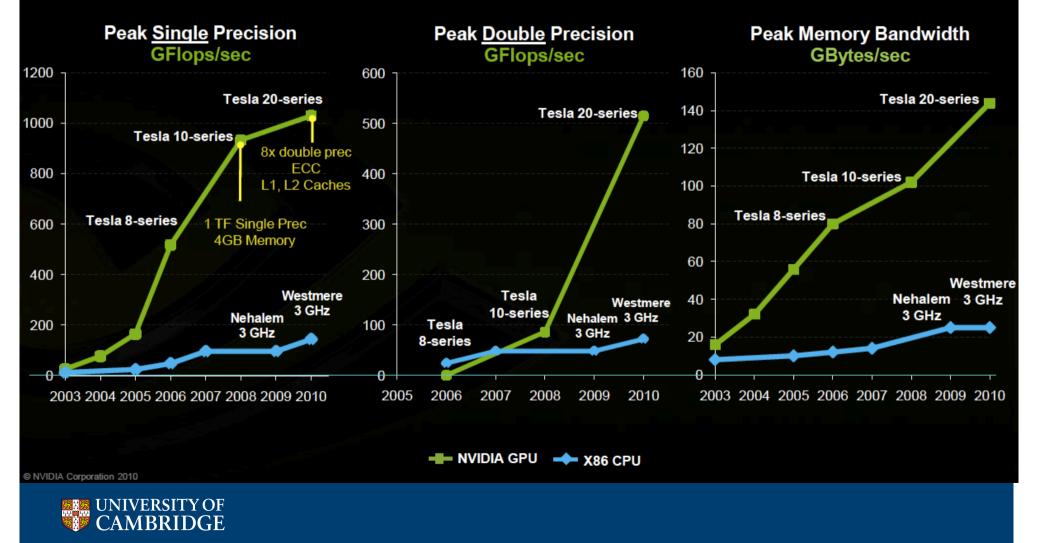
This is what CFD needs!



GPU performance

The Performance Gap





GPUs and CFD

Good speedups (> 10x) can be expected for:

- Codes that apply the same function to lots of data
- Codes where amount communication to/from card is small (compared to the time to compute the data on the card – up to 4GB)



GPUs and CFD

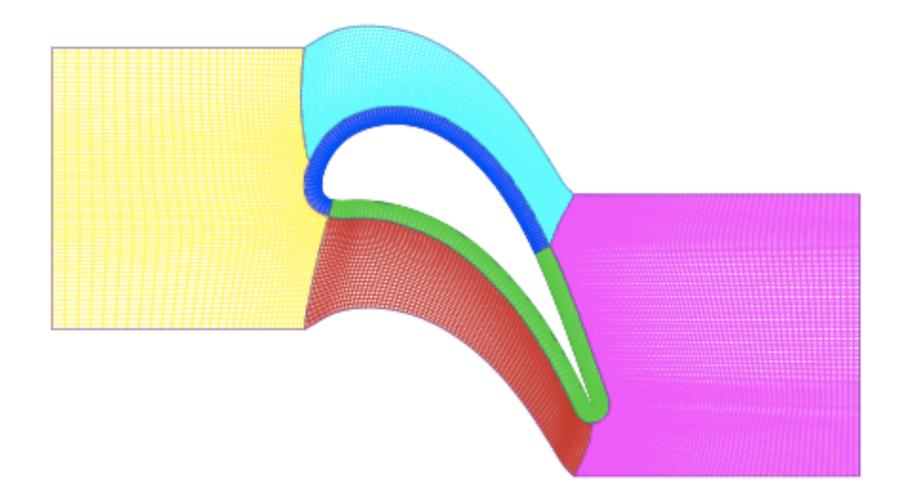
Good speedups (> 10x) can be expected for:

- Codes that apply the same function to lots of data
- Codes where amount communication to/from card is small (compared to the time to compute the data on the card – up to 4GB)
- Turbomachinery CFD is an excellent fit!





Programming GPUs for CFD





Navier-Stokes



Navier-Stokes

Finite volume, explicit time stepping



Navier-Stokes

Finite volume, explicit time stepping

Second order central differences, Scree scheme



Navier-Stokes

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Set flux, Sum flux, Shear Stress ...



Navier-Stokes

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Second order central differences, Scree scheme

Set flux, Sum flux, Shear Stress ...

Multigrid, Mixing plane, Sliding plane ...



Navier-Stokes

Finite volume, explicit time stepping

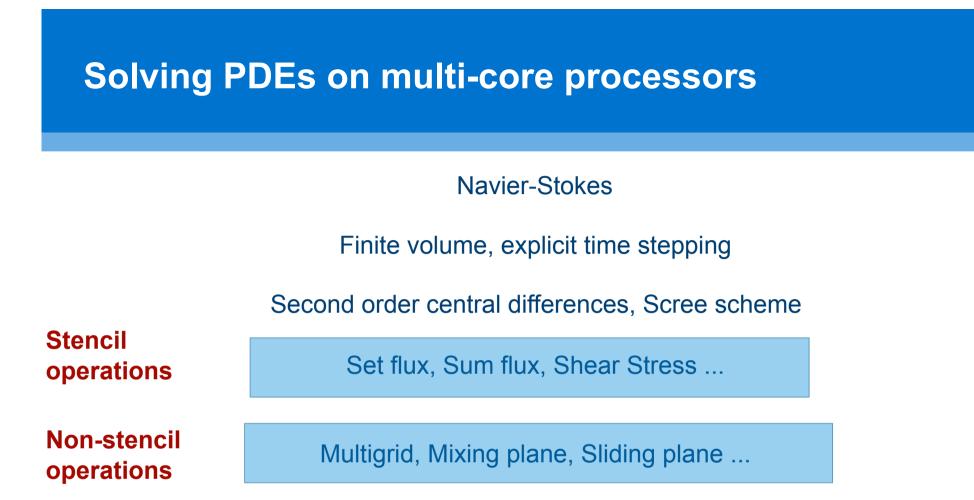
Second order central differences, Scree scheme

Stencil operations

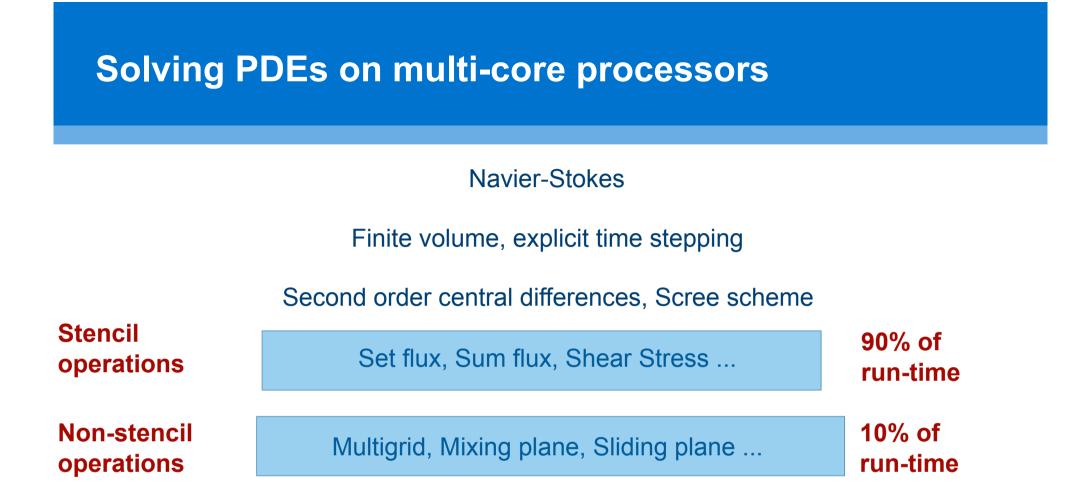
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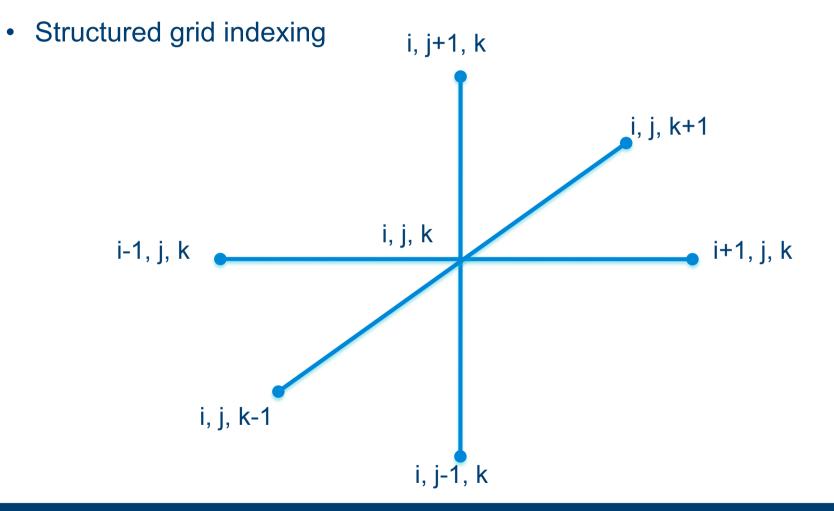
Stencil operations on multi-core processors

- Single implementation? e.g. OpenCL but need to optimize for hardware
- Multiple implementations? e.g. C with SSE for CPU, CUDA for NVIDIA GPUs, …
- Alternative:
 - High level language for stencil operations a DSL
 - Source-to-source compilation

Brandvik, T. and Pullan, G. (2010) "SBLOCK: A Framework for Efficient Stencil-Based PDE Solvers on Multi-Core Platforms" 1st International Workshop on the Frontier of GPU Computing, Bradford, July 2010



Stencil example





Stencil example

•
$$\frac{\partial^2 u}{\partial x^2}$$
 in Fortran
DO K=2,NK-1
DO J=2,NJ-1
DO I=2,NI-1
D2UDX2(I,J,K) = (U(I+1,J,K) - 2.0*U(I,J,K) +
& U(I-1,J,K))/(DX*DX)
END DO
END DO
END DO



Stencil example

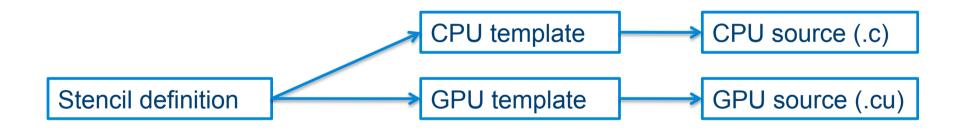
• Stencil definition:

```
input_scalars = ["dx"]
input_arrays = ["u"]
output_arrays = ["d2udx2"]
```



Source-to-source compilation

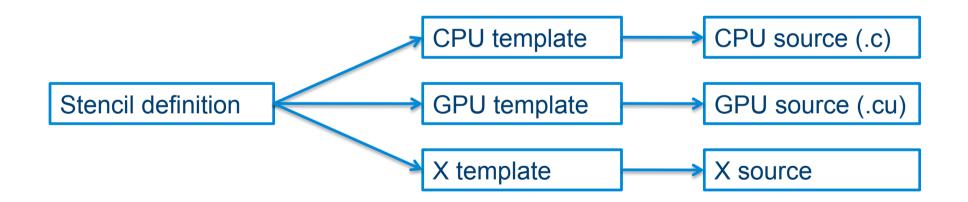
- The stencil definition is transformed at compile-time into code that can run on the chosen processor
- The transformation is performed by filling in a pre-defined template using the stencil definition





Source-to-source compilation

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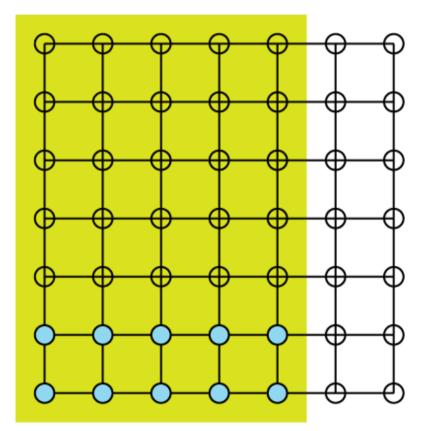


Implementation details

- There are many optimisation strategies for stencil operations (see paper from Supercomputing 2008 by Datta et al.)
- CPUs:
 - Parallelise with pthreads
 - SSE vectorisation
- GPUs:
 - Cyclic queues



CUDA strategy

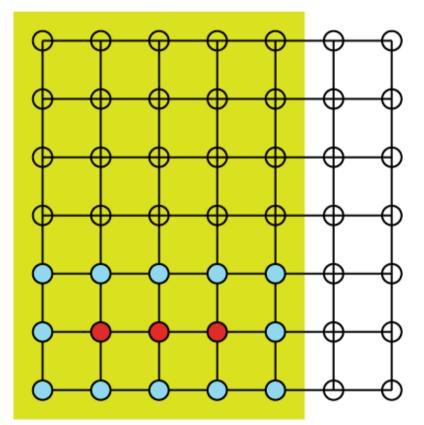


1. Load 2 rows into shared mem 🔘

Zone solved by Block 1



CUDA strategy

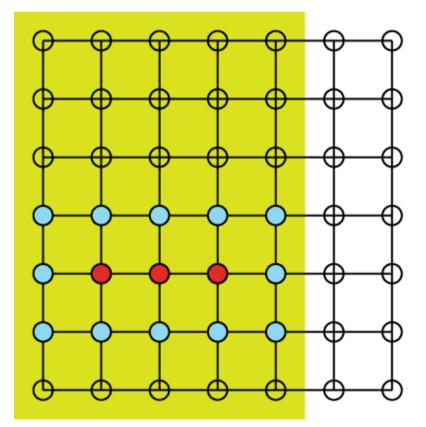


Zone solved by Block 1

1. Load 2 rows into shared mem O

2. To compute **O** points, load next row into shared mem

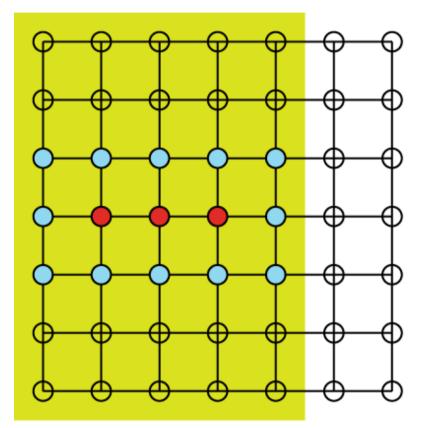




Zone solved by Block 1

- 1. Load 2 rows into shared mem 🔘
- 2. To compute \bigcirc points, load next row into shared mem
- Move up domain, row by row (load new row into shared mem, drop lowest row out of shared mem)

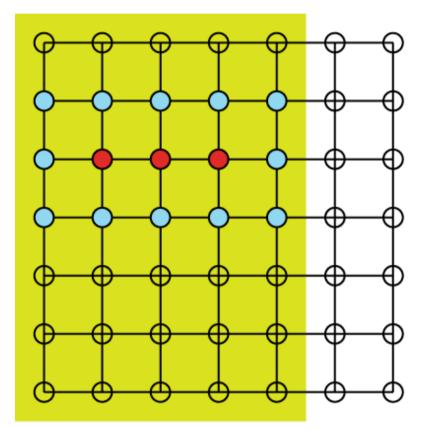




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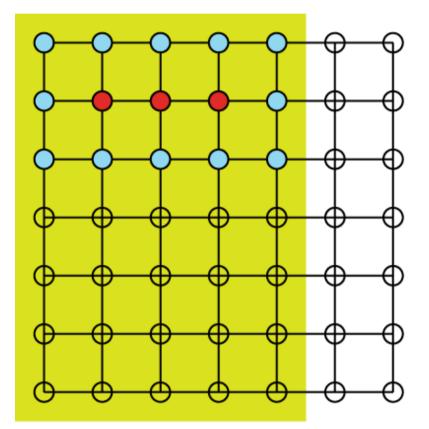




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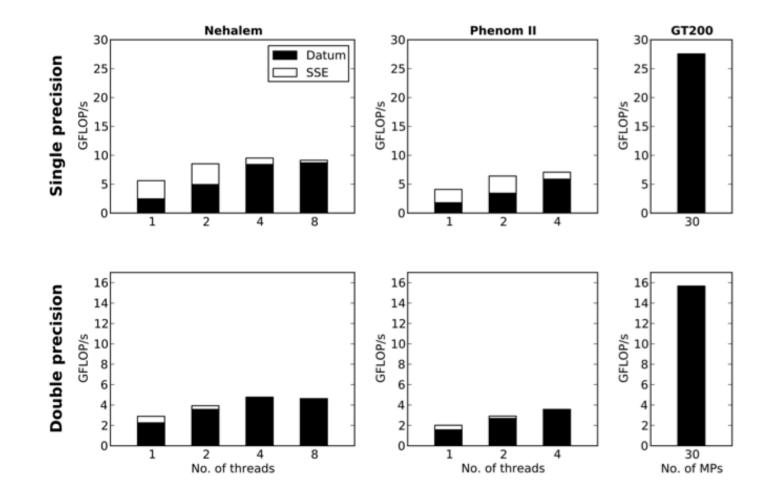


Testbed

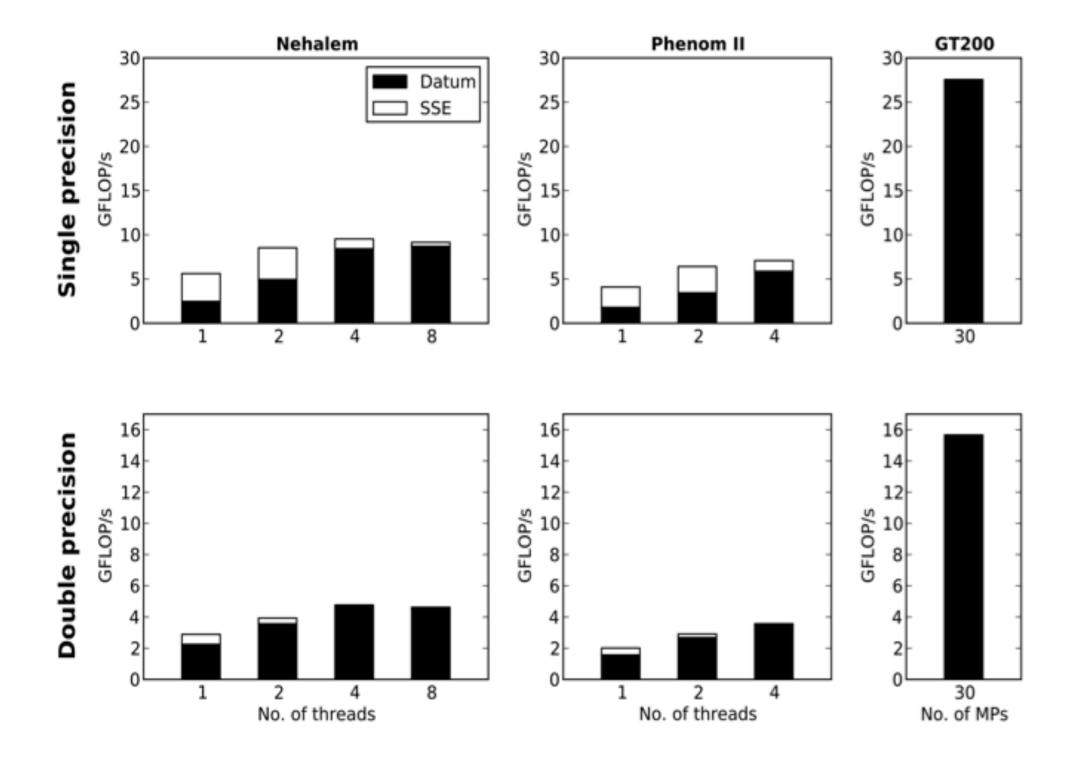
- CPU 1: Intel Core i7 920 (2.66 GHZ)
- CPU 2: AMD Phenom II X4 940 (3.0 GHz)
- GPU: NVIDIA GTX 280



Stencil benchmark









Turbostream

Turbostream

- We have implemented a new solver that can run on both CPUs and GPUs
- The starting point was an existing solver (Fortran, MPI) called TBLOCK
- The new solver is called Turbostream

Brandvik, T. and Pullan, G. (2009) *"An Accelerated 3D Navier-Stokes Solver for Flows in Turbomachines"* ASME IGTI Turbo Expo, Orlando, June 2009





- Developed by John Denton
- Blocks with arbitrary patch interfaces
- Simple and fast algorithm
- 20,000 lines of Fortran 77
- Main solver routines are only 10,000 lines



Turbostream

- 3000 lines of stencil definitions (~15 different stencil kernels)
- Code generated from stencil definitions is 15,000 lines
- Additional 5000 lines of C for boundary conditions, file I/O etc.
- Source code is very similar to TBLOCK every subroutine has an equivalent stencil definition



Turbostream performance

| Processor | TBLOCK | Turbostream |
|---------------|--------|-------------|
| Intel Nehalem | 1.21 | 1.48 |
| AMD Phenom II | 1 | 0.89 |
| NVIDIA GT200 | - | 10.2 |

- TBLOCK runs in parallel on all four CPU cores using MPI
- Initial results from latest NVIDIA Fermi GPU show an further 2x seedup



"Darwin" GPU cluster

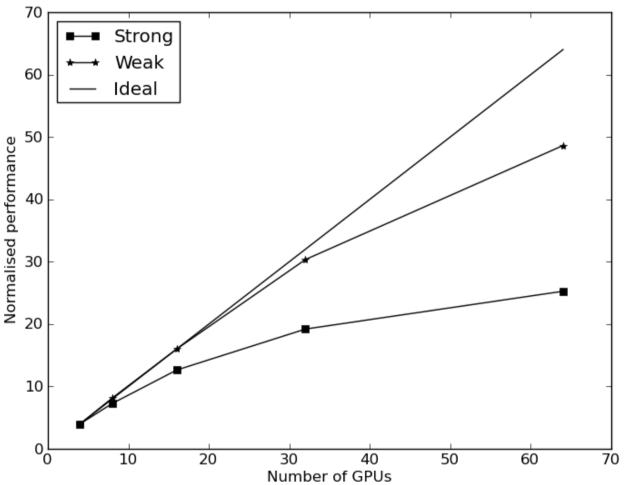
- Darwin is the central Cambridge cluster
- In 2008, NVIDIA made Cambridge a CUDA Centre of Excellence, donating 128 GPUs to Darwin





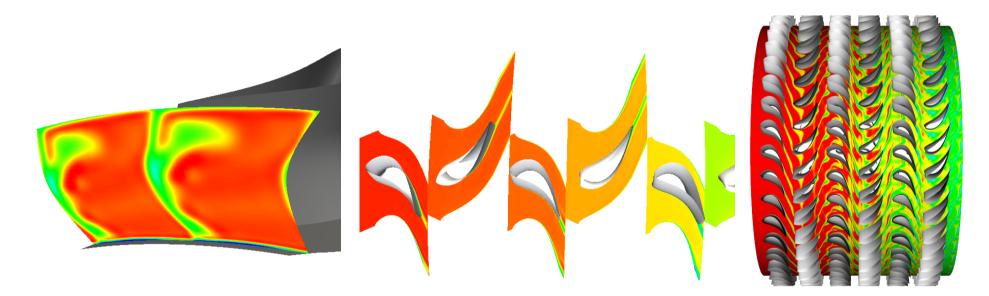
Scaling results

- Unsteady multi-stage turbine
- Baseline: 27 E6 nodes
- Largest: 432 E6 nodes
- Weak scaling: Increase grid size with # GPUs
- Strong scaling: Constan grid size (27 E6 nodes)





What can this be used for?



Steady, single passage: 0.5 million nodes 40s (1 GPU) Steady, 3 stage:3 million nodes7.5 mins (1 GPU)

Unsteady, 3 stage: 120 million nodes 4 hours (16 GPUs) per rev





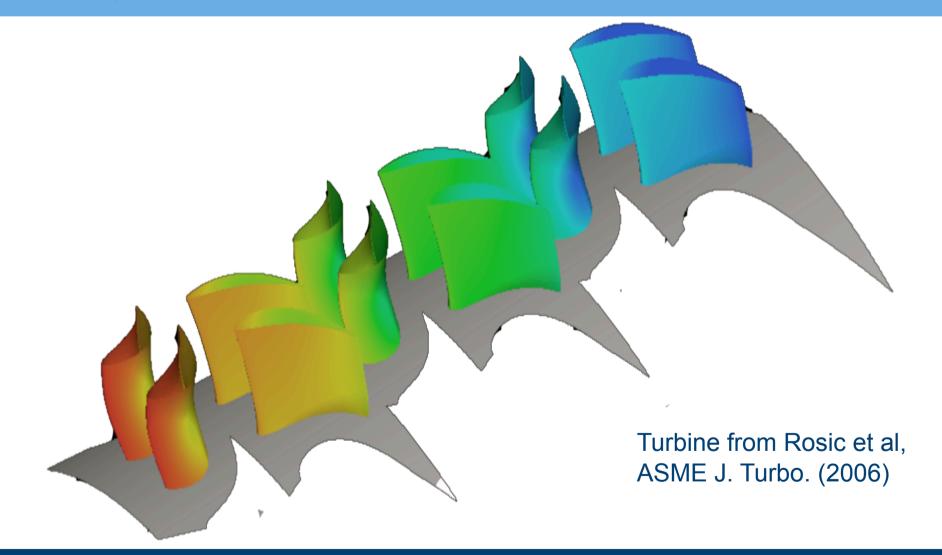
Example simulations

Example simulations

- Three-stage steady turbine simulation (mixing planes)
- Three-stage unsteady compressor simulation (sliding planes)

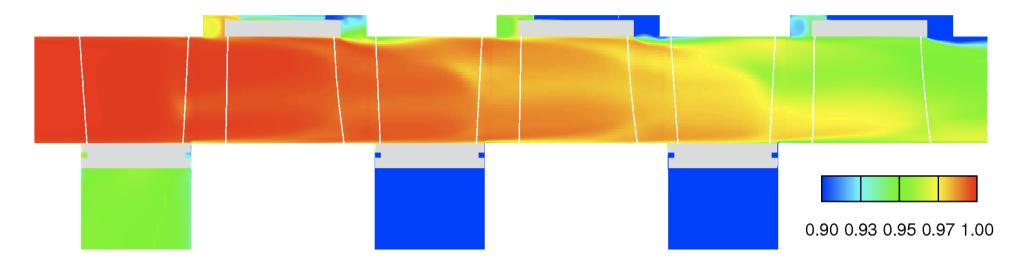


Three-stage turbine





Entropy function through machine

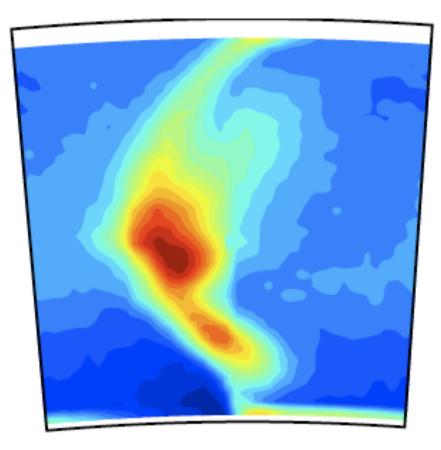


- 10 hours on a single CPU
- 8 minutes on four GPUs

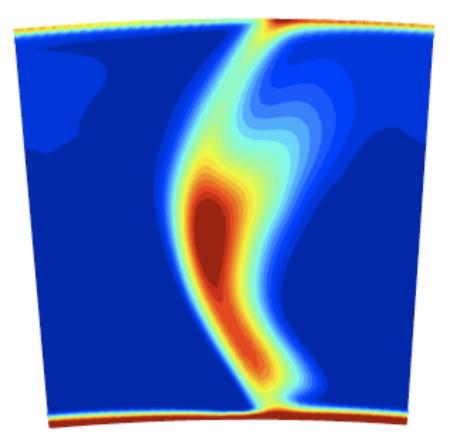


Total pressure loss, Stator 3 exit

Experiment



Turbostream



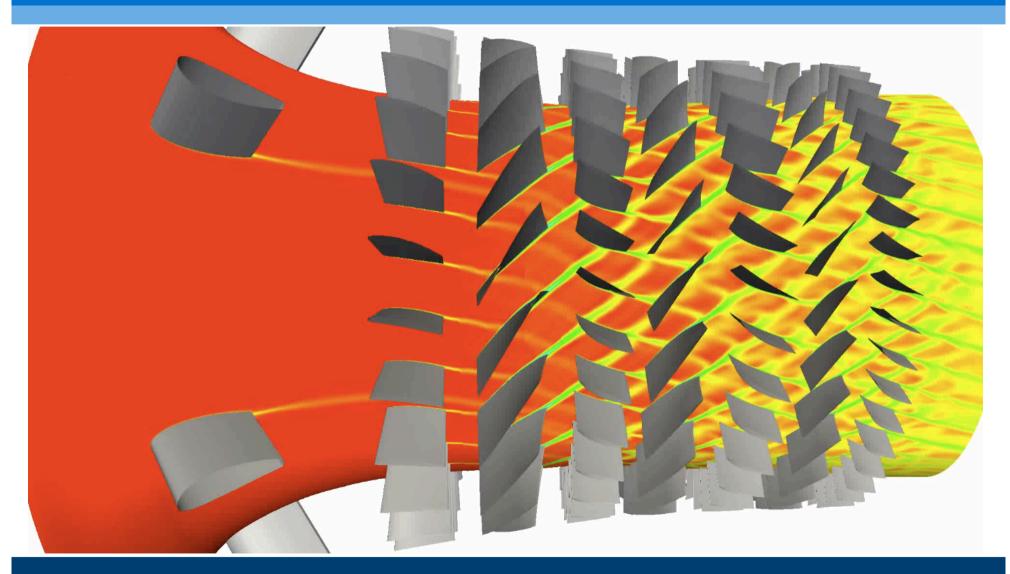


Compressor simulation

- Three-stage compressor test rig at Siemens, UK
- 160 million grid nodes
- 5 revolutions needed to obtain a periodic solution (22500 time steps)
- On 32 NVIDIA GT200 GPUs, each revolution takes 24 hours



Entropy function contours at mid-span







Conclusions



- The switch to multi-core processors enables a step change in performance, but existing codes have to be rewritten
- The differences between processors make it difficult to hand-code a solver that will run on all of them
- We suggest a high level abstraction coupled with source-to-source compilation





- A new solver called Turbostream, which is based on Denton's TBLOCK, has been implemented
- Turbostream is ~10 times faster than TBLOCK when running on an NVIDIA GPU as compared to a quad-core Intel or AMD CPUs
- Single blade-row calculations almost interactive on a desktop (10 30 seconds)
- Multi-stage calculations in a few minutes on a small cluster (\$10,000)
- Full annulus unsteady calculations complete overnight on a modest cluster (\$100,000)

