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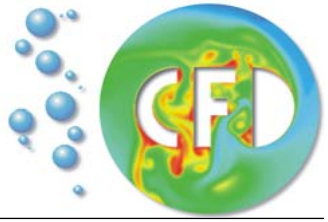
fakultät für mathematik
LS III (IAM)



UnConventional High Performance Computing (UCHPC) for Finite Element Simulations

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http://www.mathematik.tu-dortmund.de/LS3
http://www.featflow.de
http://www.feast.tu-dortmund.de

3 Observations

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- The ‘free ride’ is over, paradigm shift in HPC:
  - physical barriers (heat, power consumption, leaking voltage)
  - memory wall (in particular for sparse Linear Algebra problems)
  - applications no longer run faster automatically on newer hardware
- Heterogeneous hardware: commodity CPUs plus co-processors
  - graphics cards (GPU)
  - CELL BE processor
  - HPC accelerators (e.g. ClearSpeed)
  - reconfigurable hardware (FPGA)
- Finite Element Methods (FEM) and Multigrid solvers: most flexible, efficient and accurate simulation tools for PDEs nowadays.

Aim of this Talk

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High Performance Computing

meets

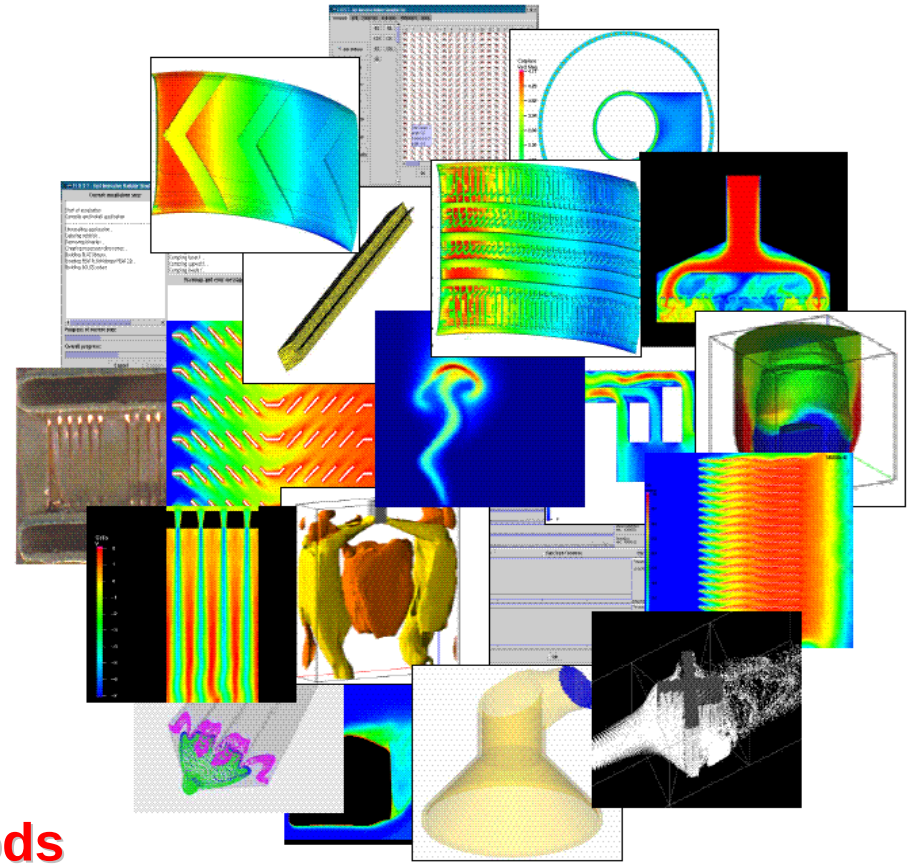
Hardware-oriented Numerics

on

Unconventional Hardware

for

Finite Element Multigrid Methods



Hardware-Oriented Numerics

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What is **'Hardware-Oriented Numerics'**?

- It is more than '*good Numerics*' and '*good Implementation'* on High Performance Computers
- Critical quantity: **'Total Numerical Efficiency'**

Vision: Total Numerical Efficiency

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- '**High** (guaranteed) **accuracy** for user-specific quantities with minimal #d.o.f. (~ *N*) via **fast and robust solvers** – for a wide class of parameter variations – with **optimal numerical complexity** (~ *O*(*N*)) while exploiting a significant percentage of the **available huge sequential/ parallel GFLOP/s rates** at the same time'

- Is it easy to achieve high **'Total Numerical Efficiency'**?

- **FEM Multigrid solvers** with **a posteriori error control** for **adaptive meshing** are a candidate

Example: Fast Poisson Solvers

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- 'Optimized' **Multigrid** methods for **scalar PDE** problems (≈Poisson problems) on **general meshes** should require ca. **1000 FLOPs** per unknown (in contrast to LAPACK for dense matrices with ***O(N³)* FLOPs**)

- Problem size 10^6 : Much less than 1 sec on PC (???)
- Problem size 10^{12}: Less than 1 sec on PFLOP/s computer

➔ **More realistic (and much harder) 'Criterion' for Petascale Computing in Technical Simulations**

Main Component: ‘Sparse’ MV

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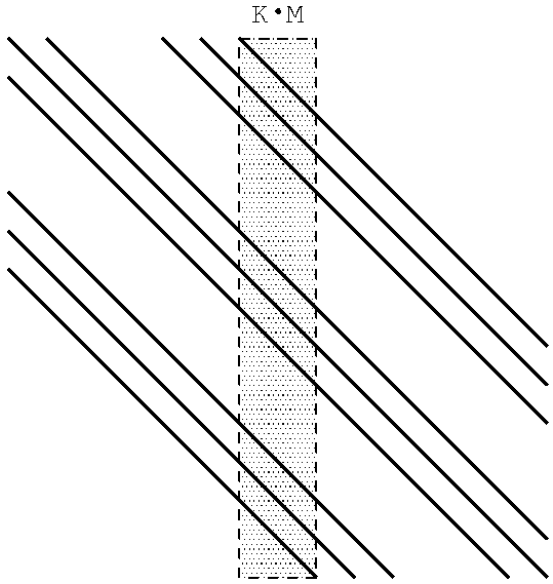
- Sparse **Matrix-Vector techniques** (‘indexed DAXPY’) on **general unstructured grids**

```
   DO 10 IROW=1,N
      DO 10 ICOL=KLD(IROW),KLD(IROW+1)-1
10      Y(IROW)=DA(ICOL)*X(KCOL(ICOL))+Y(IROW)
```

- Sparse Banded **MV techniques** on **generalized TP grids**



Grid Structures

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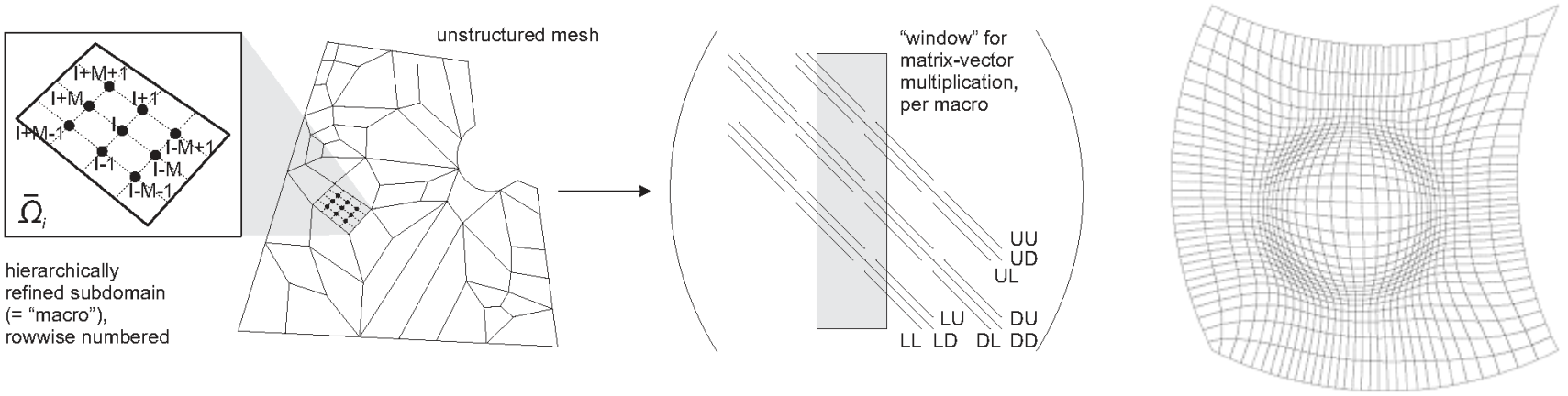
Fully adaptive grids

Maximum flexibility
‚Stochastic' numbering
Unstructured sparse matrices
Indirect addressing (very slow)

Locally structured grids

Logical tensor product
Fixed banded matrix structure
Direct addressing (fast)
r-adaptivity

Unstructured macro mesh of tensorproduct subdomains



Generalized Tensorproduct Grids

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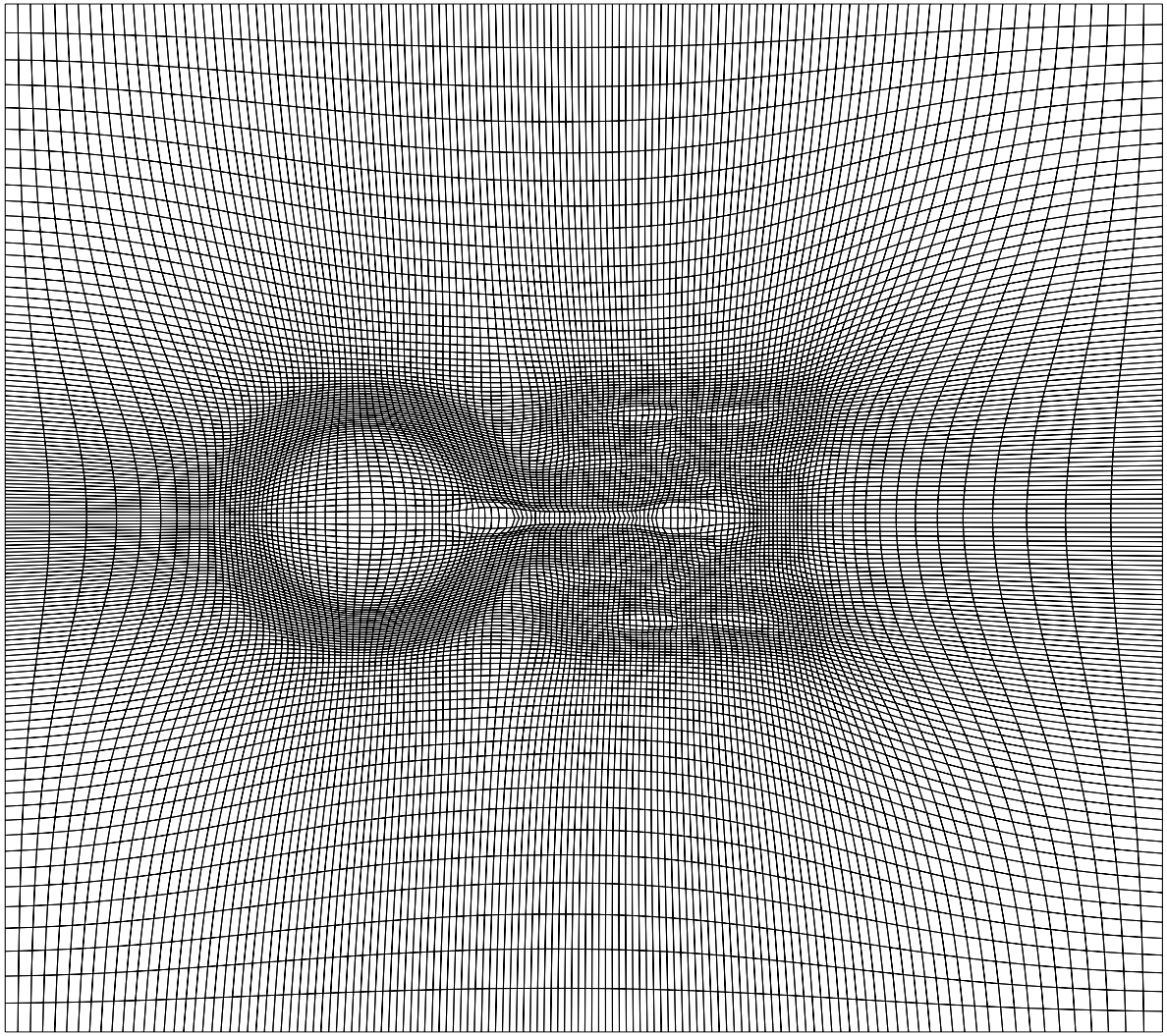

Generalized Tensorproduct Grids

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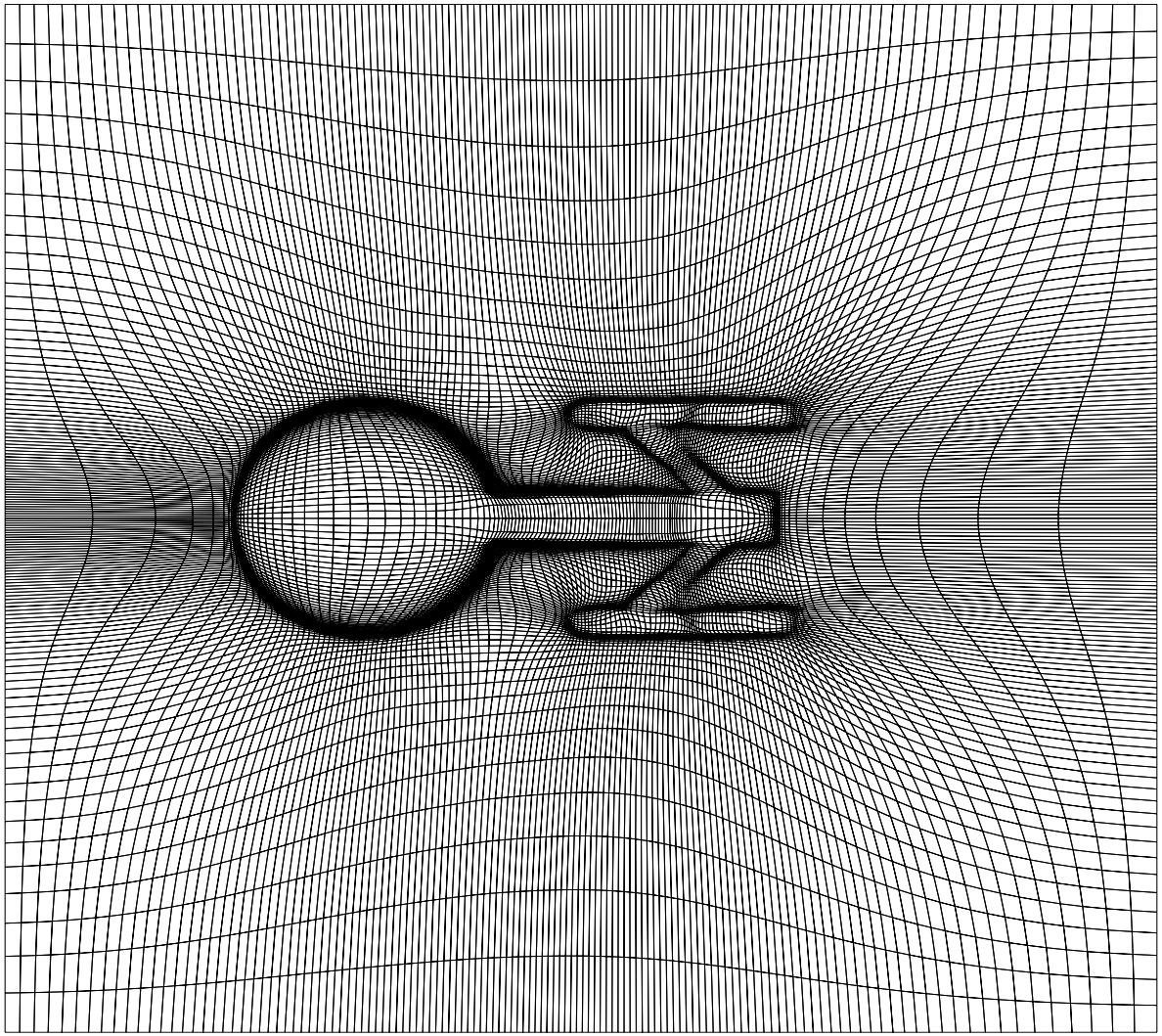

Generalized Tensorproduct Grids

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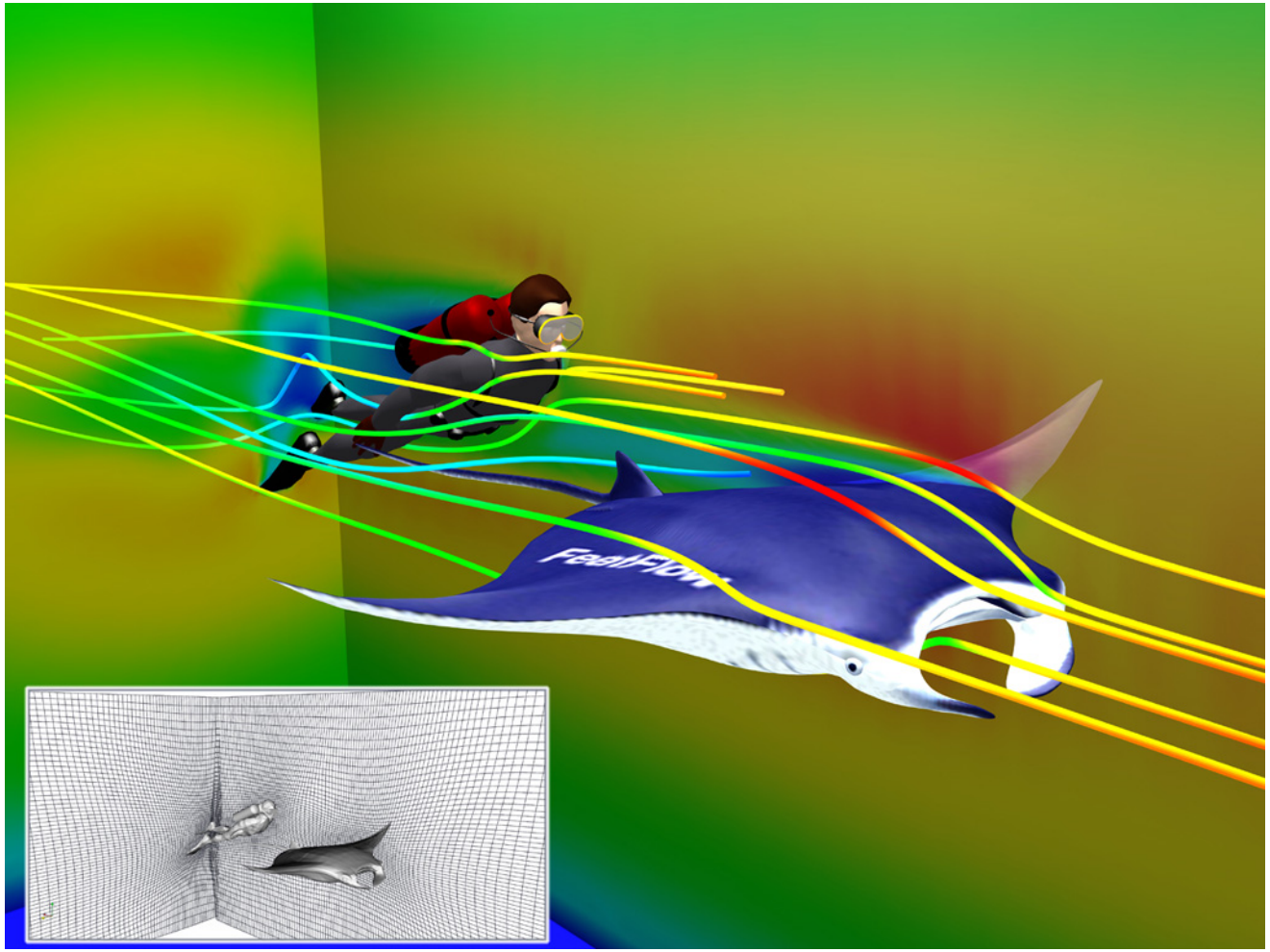

…with appropriate Fictitious Boundary techniques in FEATFLOW…..

Generalized Tensorproduct Grids

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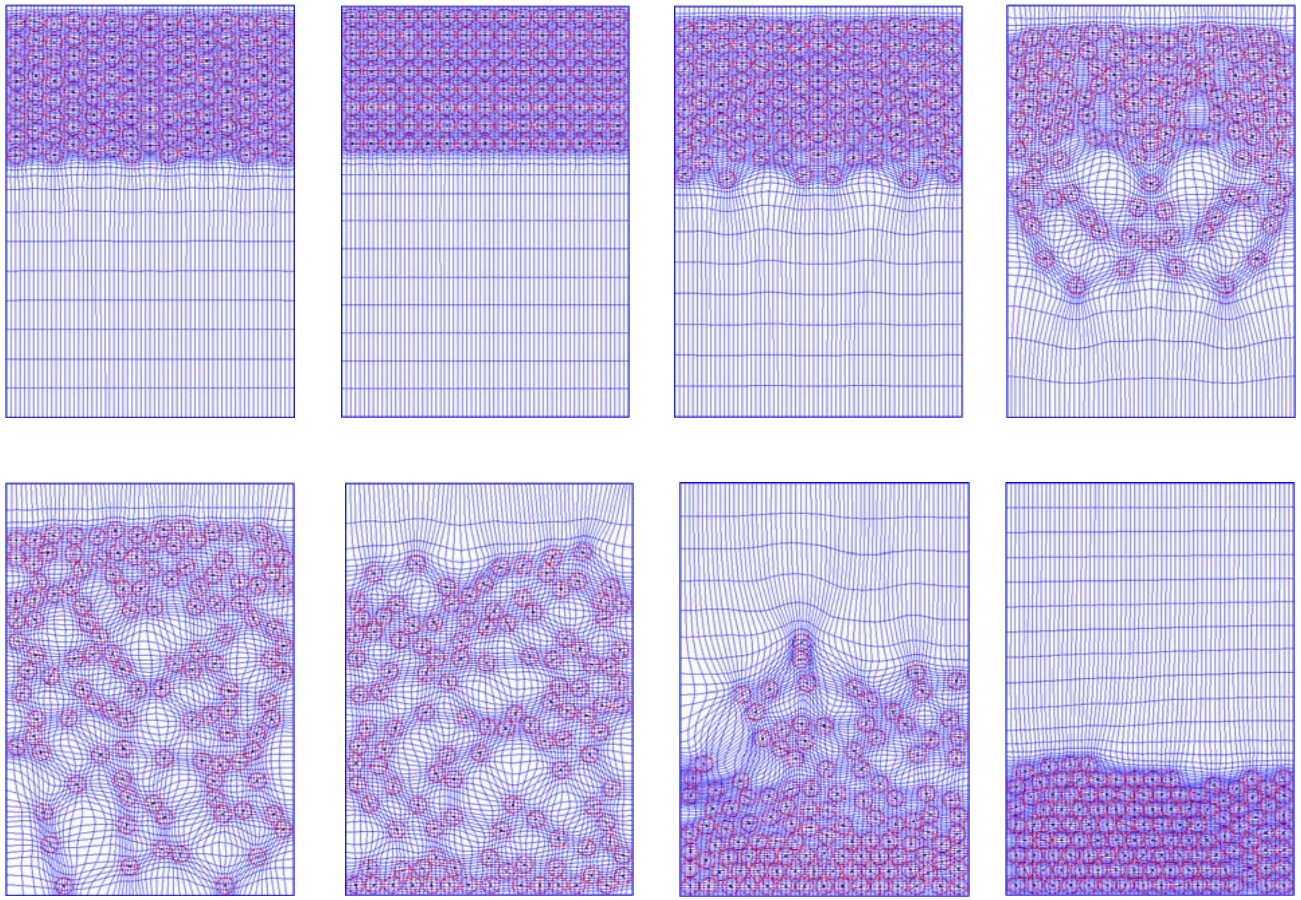
….dynamic CFD problems…..



Observation I: Sparse MV on TP Grid

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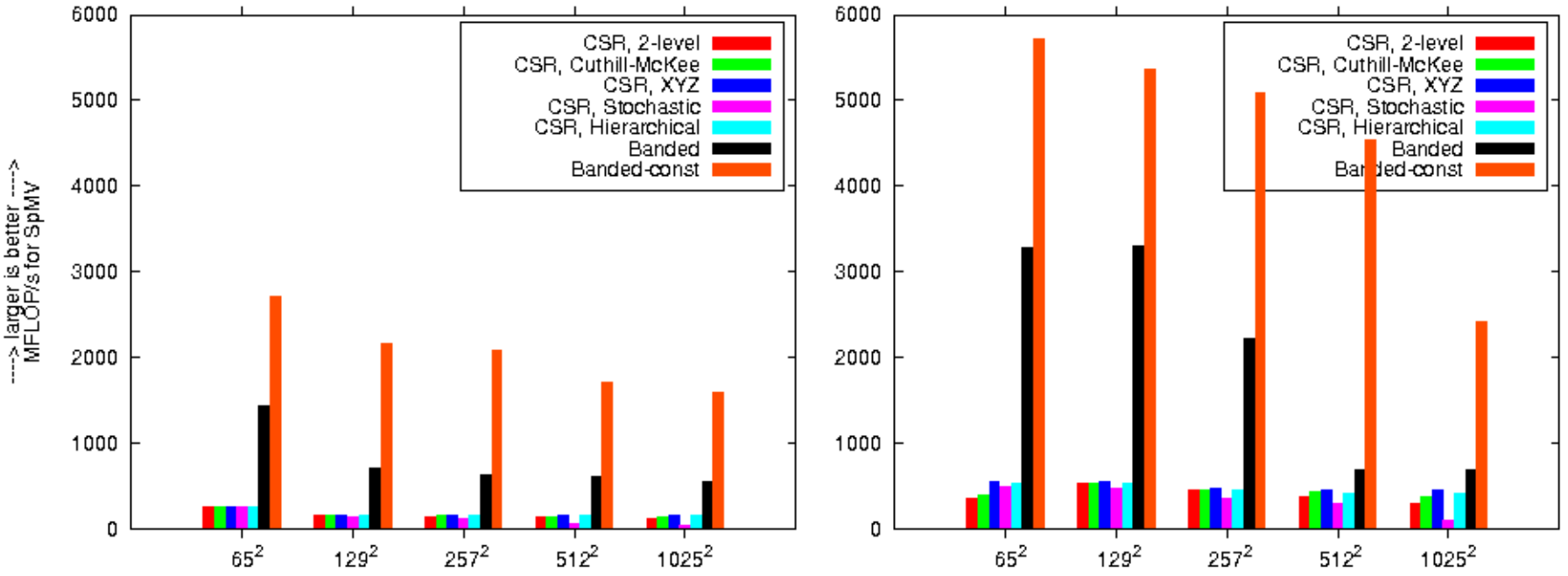

- Opteron X2 2214 (1MB C$, 2.2 GHz)
  vs.
- Xeon E5450 (6MB C$, 3 GHz, LiDO2)
- One thread, 3 cores idle („best case“ test for memory bound FEM)
- Production runs expected to be much slower, but not asymptotically
- Banded-const: constant coefficients (stencil), fully in-cache

Observation II: Sparse MV (again)

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LiDO 2			
Numbering	**4K DOF**	**66K DOF**	**1M DOF**
Stochastic	500	364	**95**
Hierarchical	536	445	**418**
Banded	3285	2219	**687**
Stencil (const)	5720	5094	**2415**

In realistic scenarios, MFLOP/s rates are

- often poor, and
- problem size dependent

Observation III: (Sparse) CFD

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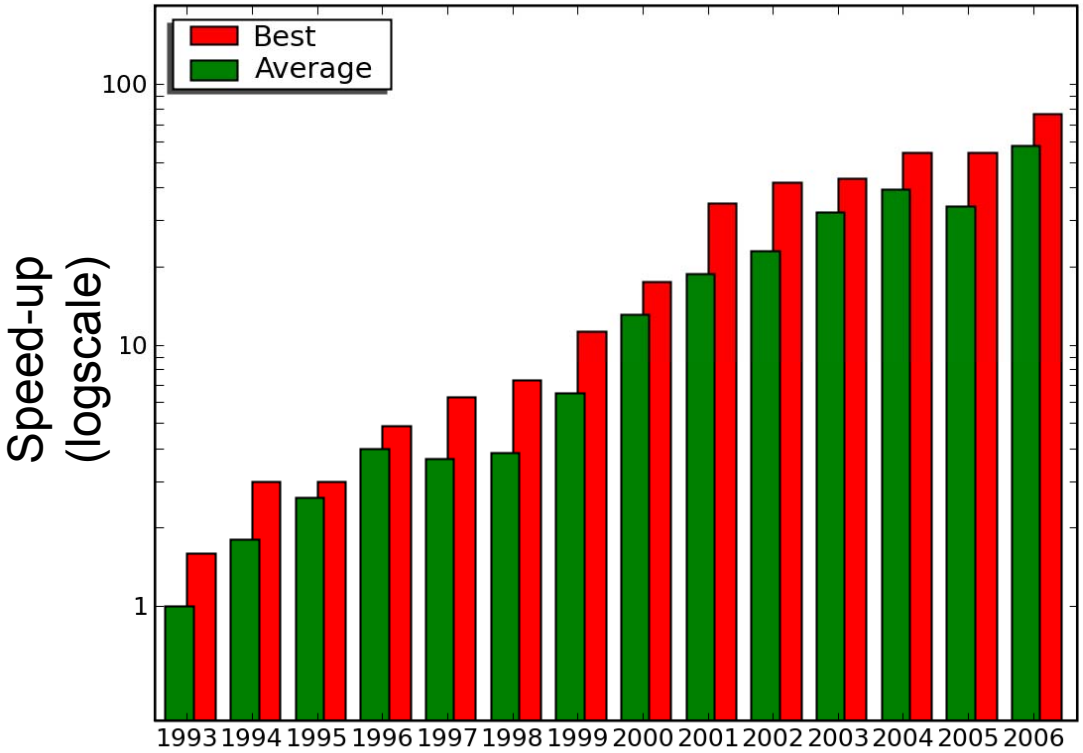

Speed-up of 100x for free in 10 years

Stagnation for standard simulation tools on conventional hardware

Observation IV: Parallel Performance

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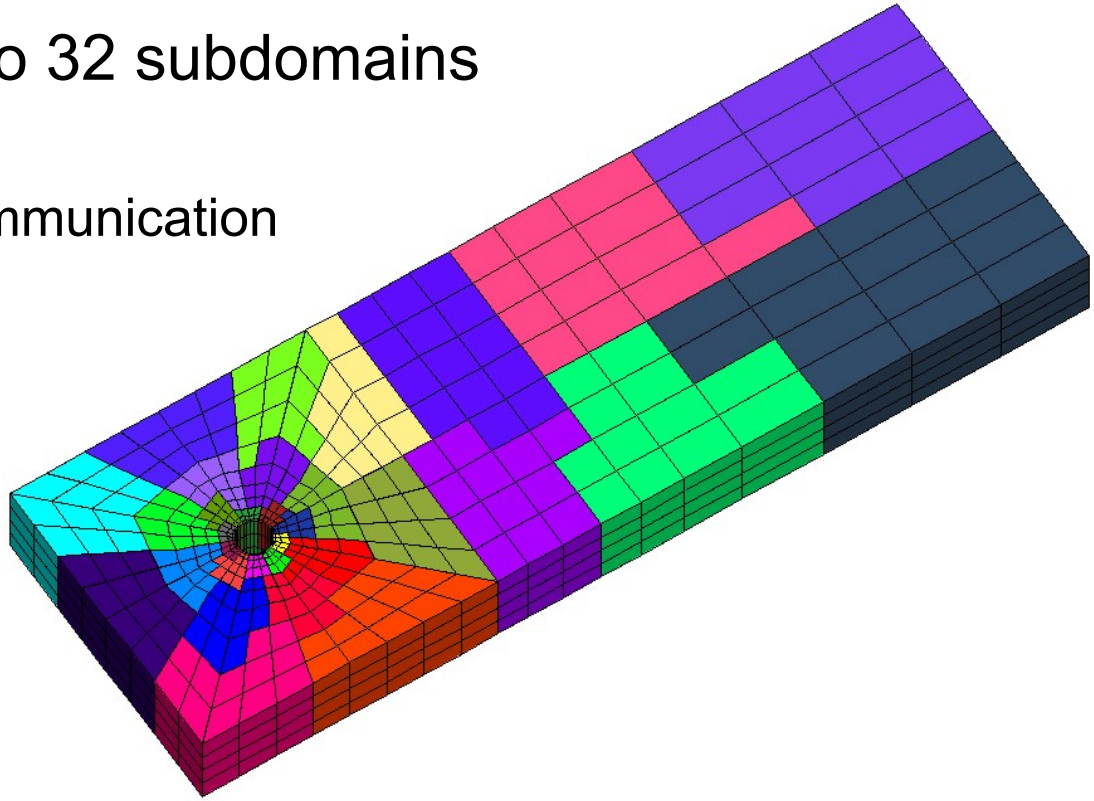
- Mesh partitioned into 32 subdomains
  - Problems due to communication
  - Numerical behavior vs. anisotropic meshes



	1 P.	2 P.	4 P.	8 P.	16 P.	32 P.	64 P.
%Comm.	10%	24%	36%	45%	47%	55%	56%
# PPP-IT	2.2	3.0	3.9	4.9	5.2	5.7	6.2

First Summary

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- It is (almost) impossible to come close to **Single Processor Peak Performance** with modern (**= high numerical efficiency**) simulation tools

- **Parallel Peak Performance** with modern Numerics even harder, already for moderate processor numbers

Hardware-oriented Numerics (HwoN)

Example for HwoN

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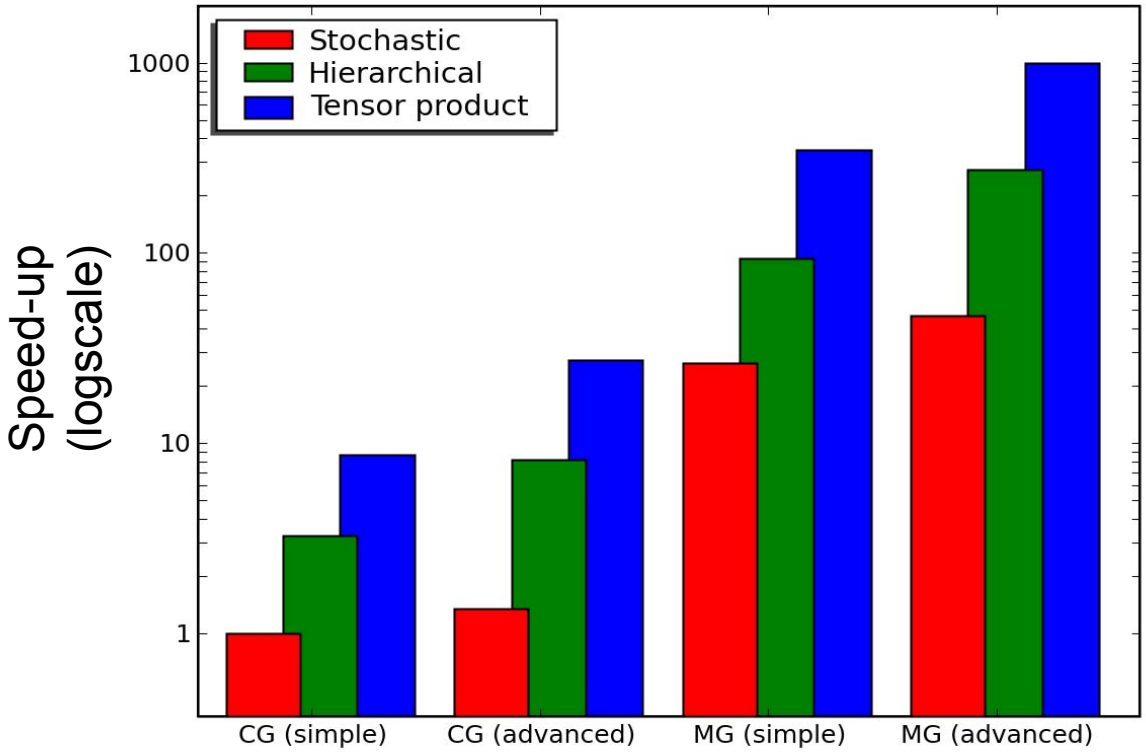
FEM for 8 Mill. unknowns on general domain, 1 CPU, Poisson Problem in 2D



Dramatic improvement (factor 1000) due to **better Numerics** AND **better data structures/ algorithms** on 1 CPU

FEAST – Realization of HwoN

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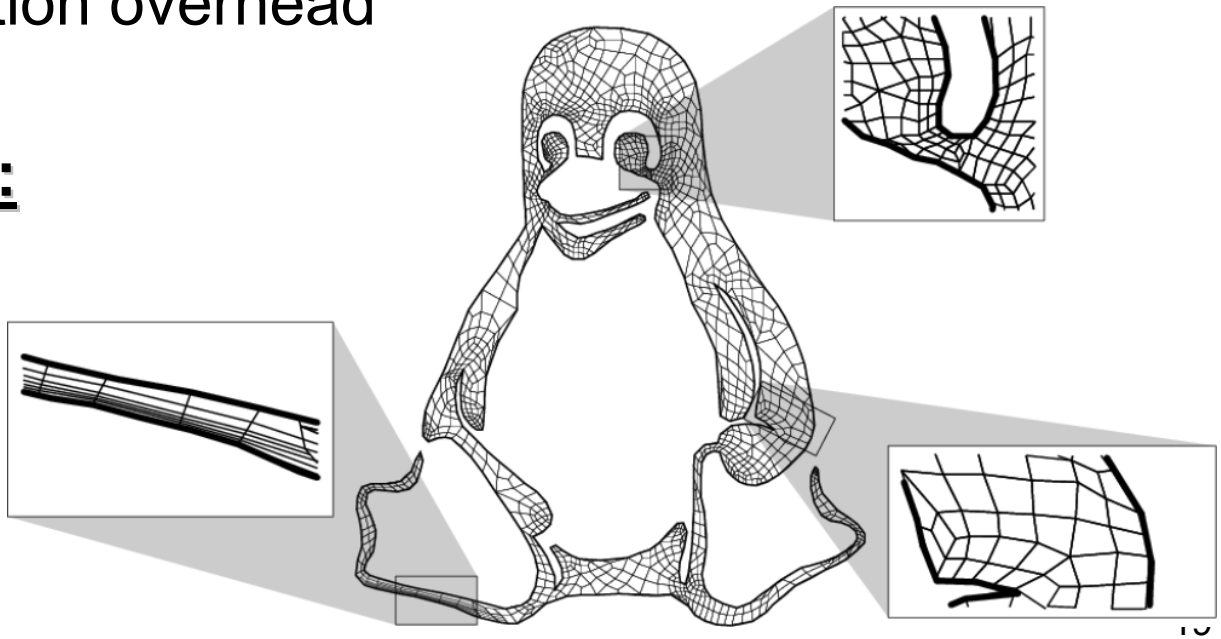
- **ScaRC** solver: Combine advantages of (parallel) domain decomposition and multigrid methods
- Cascaded multigrid scheme
- Hide anisotropies locally to increase robustness
- Globally unstructured – locally structured
- Low communication overhead

FEAST applications:

FEASTFLOW (CFD)
FEASTSOLID (CSM)
FEASTLBM (CFD)
→ SkaLB Project



SkaLB Project

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- BMBF-Initiative “HPC-Software für skalierbare Parallelrechner”
- **“SkaLB - Lattice-Boltzmann-Methoden für skalierbare Multi-Physik-Anwendungen”**
- Partners: Braunschweig, Erlangen, Stuttgart, Dortmund (1.8 MEuro)
  - Lehrstuhl für Angewandte Mathematik und Numerik (LS3)
  - ITMC
  - IANUS
- Industry: Intel, Cray, IBM, BASF, Sulzer, hhpberlin, HP

Bundesministerium für Bildung und Forschung

des Bundesministeriums für Bildung und Forschung von Richtlinien zur Förderung von Forschungsvorhaben auf dem Gebiet "HPC-Software für skalierbare Parallelrechner" im Rahmen des Förderprogramms "IKT 2020 - Forschung für Innovationen"

(Preliminary) State-of-the-Art

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- **Numerical efficiency?**
  → OK
- **Parallel efficiency?**
  → OK (tested up to 256 CPUs on NEC and commodity clusters)
  → More than 10.000 CPUs???
- **Single processor efficiency?**
  → OK (for CPU)
- **'Peak' efficiency?**
  → NO
  → Special ***unconventional*** FEM Co-Processors

UnConventional HPC

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- CELL multicore processor (PS3),
  7 synergistic processing units
  @ 3.2 GHz, 218 GFLOP/s,
  Memory @ 3.2 GHz

- GPU (NVIDIA GTX 285):
  240 cores @ 1.476 GHz,
  1.242 GHz memory bus (160 GB/s)
  ≈ 1.06 TFLOP/s

UnConventional High Performance Computing (UCHPC)

Why are GPUs and CELLs so fast?

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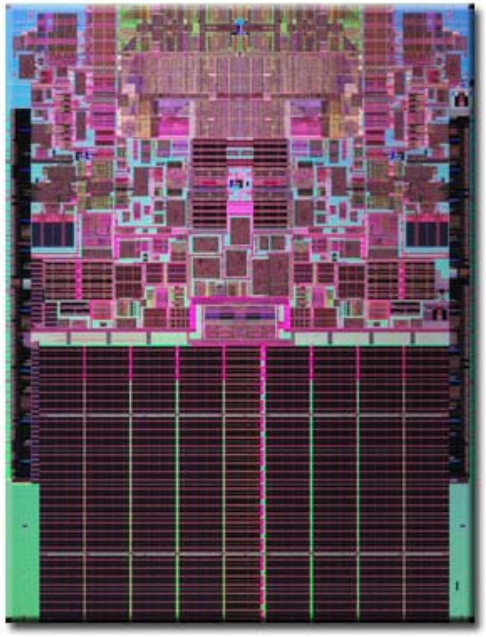
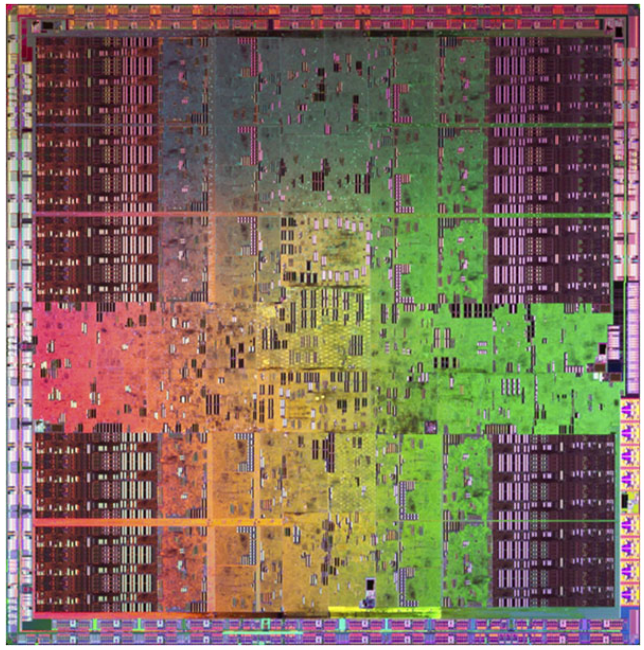


CPUs minimise latency of individual operations (cache hierarchy to combat memory wall problem)



GPUs and **CELLs** maximise throughput over latency and exploit data-parallelism (more “ALU-efficient“ and parallel memory system)

Bandwidth in a CPU/GPU Node

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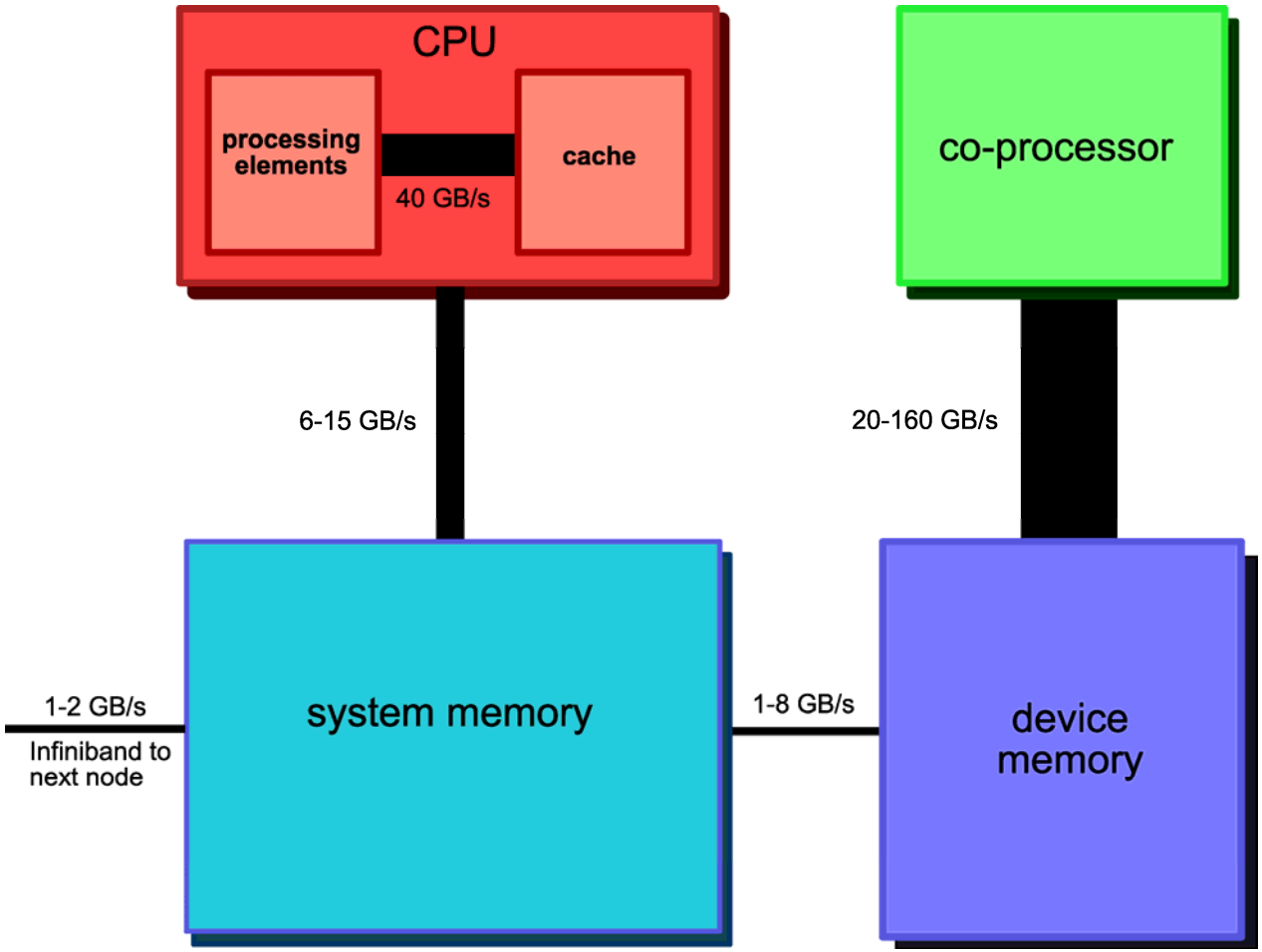

Example: Sparse MV on TP Grid

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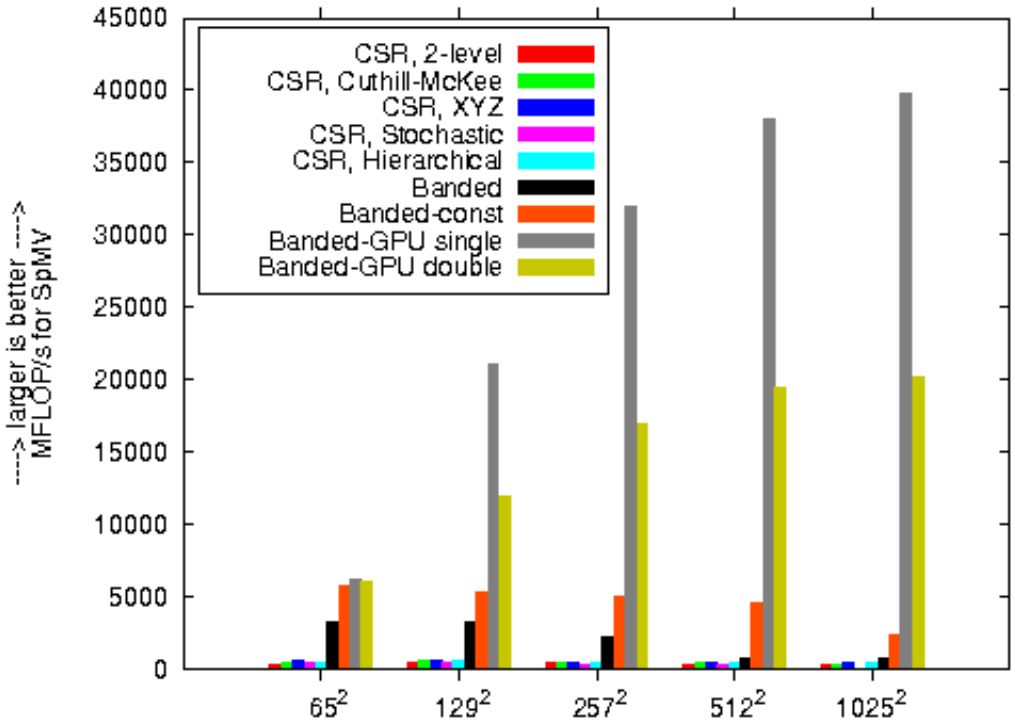

40 GFLOP/s, 140 GB/s on GeForce GTX 280

0.7 (1.4) GFLOP/s on 1 core of LiDO2

Example: Multigrid on TP Grid

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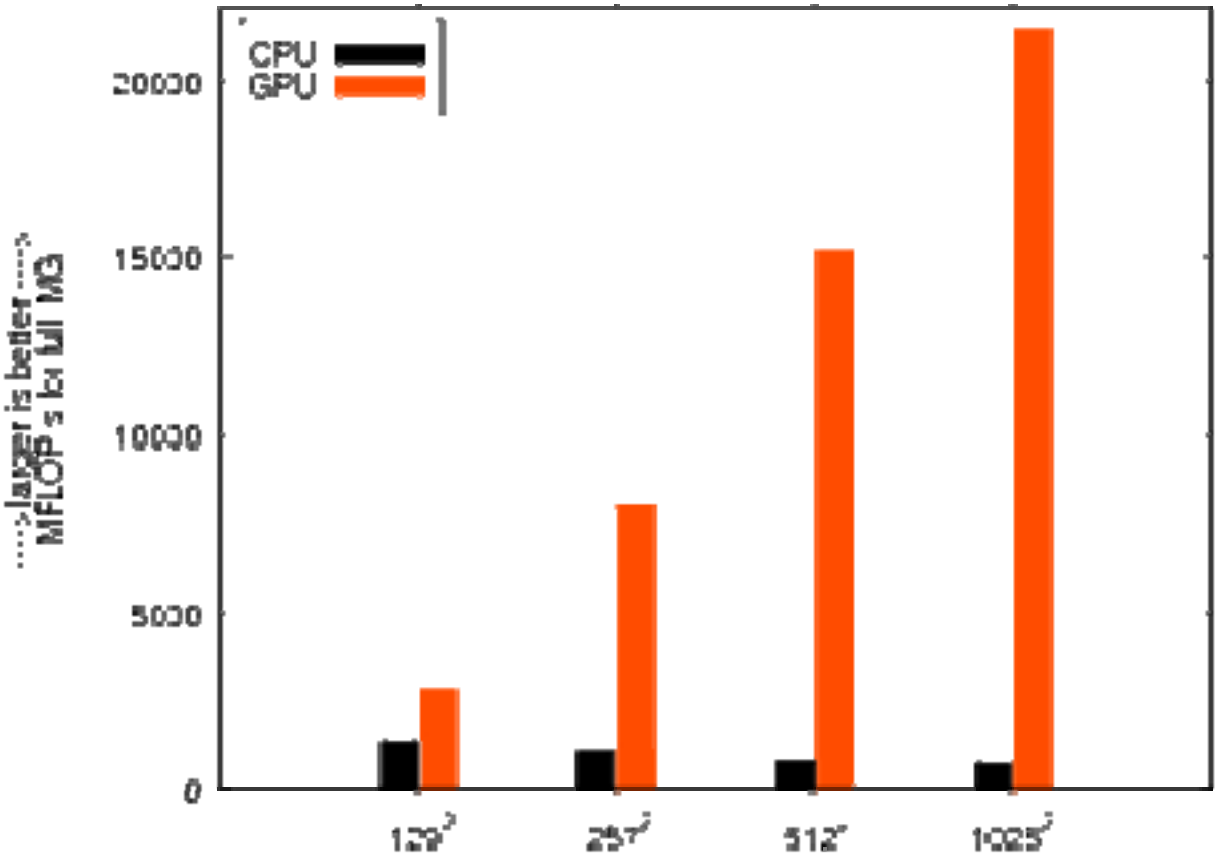

Example: Multigrid on TP Grid

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	LiDO2 (double)		GTX 280 (mixed)		
Level	time(s)	MFLOP/s	time(s)	MFLOP/s	speedup
7	0.021	1405	0.009	2788	2.3x
8	0.094	1114	0.012	8086	7.8x
9	0.453	886	0.026	15179	17.4x
10	1.962	805	0.073	21406	26.9x

- 1M unknowns in less than 0.1 seconds!
- 27x faster than CPU

Promising results,
attempt to integrate GPUs as FEM Co-Processors

Design Goals

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Include GPUs into FEAST

- without
  - changes to application codes FEASTFLOW / FEASTSOLID
  - fundamental re-design of FEAST
  - sacrificing either functionality or accuracy

- but with
  - noteworthy speedups
  - a reasonable amount of generality w.r.t. other co-processors
  - and additional benefits in terms of space/power/etc.

But: no --march=gpu/cell compiler switch

Integration Principles

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- **Isolate suitable parts**
  - Balance acceleration potential and acceleration effort
- **Diverge code paths as late as possible**
  - Local MG solver
  - Same interface for several co-processors
- **Important benefit of minimally invasive approach: No changes to application code**
  - Co-processor code can be developed and tuned on a single node
  - Entire MPI communication infrastructure remains unchanged

Minimally invasive integration

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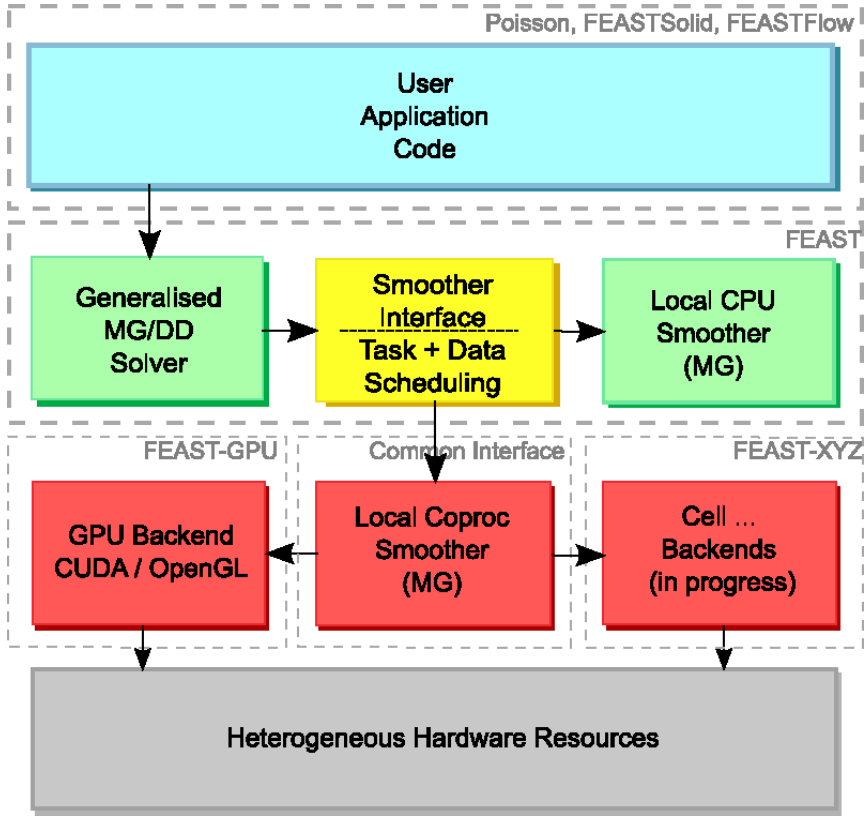
global BiCGStab
preconditioned by
global multilevel (V 1+1)
additively smoothed by
for all Ω_i: **local multigrid**
coarse grid solver: UMFPACK



- All outer work: CPU, double
- Local MGs: GPU, single
- GPU is preconditioner
- Applicable to many co-processors

Show-Case: FEASTSolid

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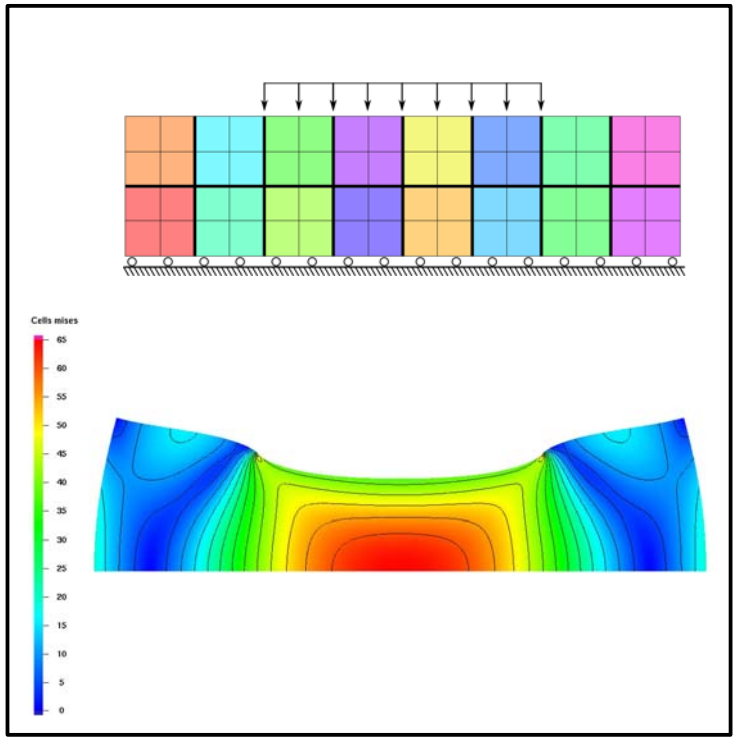
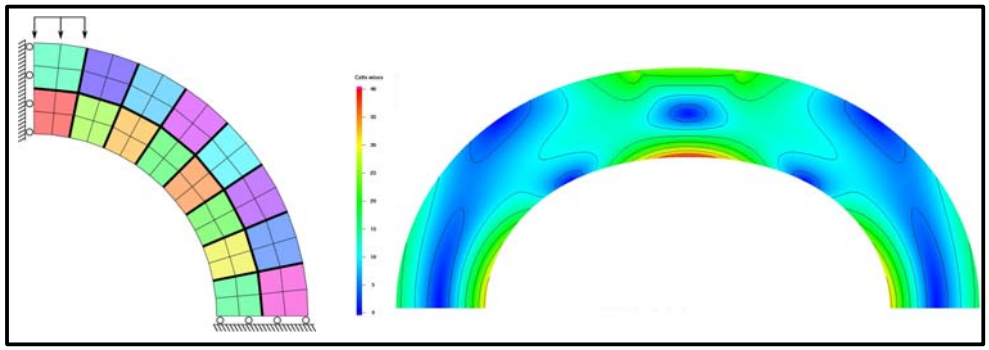
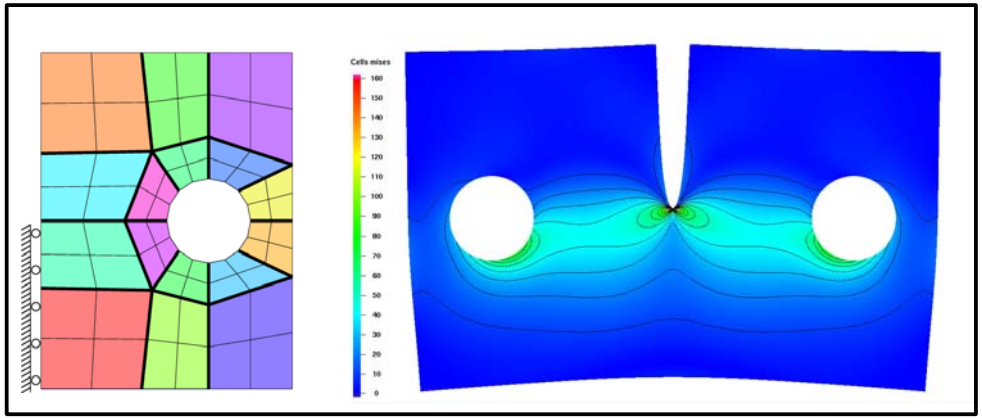
- Fundamental model problem:
  - solid body of elastic, compressible material (e.g. steel)
  - exposed to some external load







Mixed Precision Approach

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	single precision		double precision	
Level	Error	Reduction	Error	Reduction
2	2.391E-3		2.391E-3	
3	5.950E-4	4.02	5.950E-4	4.02
4	1.493E-4	3.98	1.493E-4	3.99
5	3.750E-5	3.98	3.728E-5	4.00
6	1.021E-5	3.67	9.304E-6	4.01
7	6.691E-6	1.53	2.323E-6	4.01
8	2.012E-5	0.33	5.801E-7	4.00
9	7.904E-5	0.25	1.449E-7	4.00
10	3.593E-4	0.22	3.626E-8	4.00

- Poisson problem with bilinear Finite Elements (Q1)
- Mixed precision solver: double precision Richardson, preconditioned with single precision MG („gain one digit“)
- Same results as entirely in double precision

Resulting Accuracy

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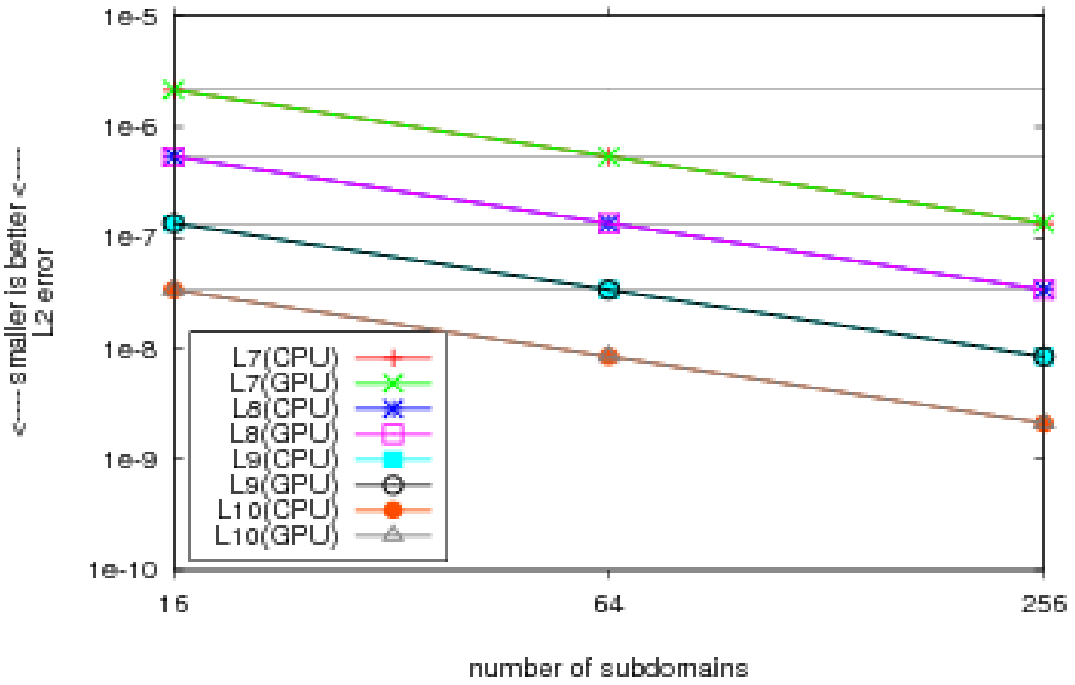
- L_2 error against reference solution



- Same results for CPU and GPU
  - expected error reduction independent of refinement and subdomain distribution

(Weak) Scalability

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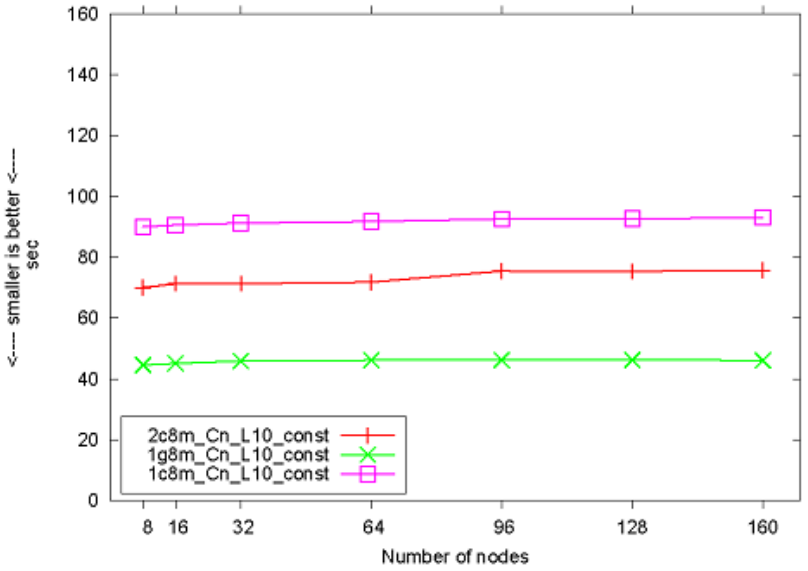

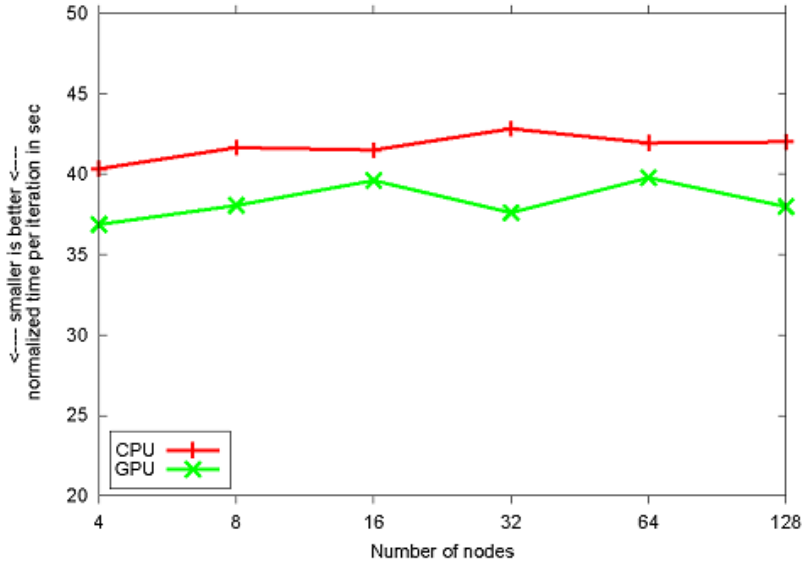

- Outdated cluster, dual Xeon EM64T
- 1 NVIDIA Quadro FX 1400 per node
- (one generation behind the Xeons, 20 GB/s BW)
- Poisson problem (left): up to 1.3B DOF, 160 nodes
- Elasticity (right): up to 1B DOF, 128 nodes

Realistic Absolute Speedup

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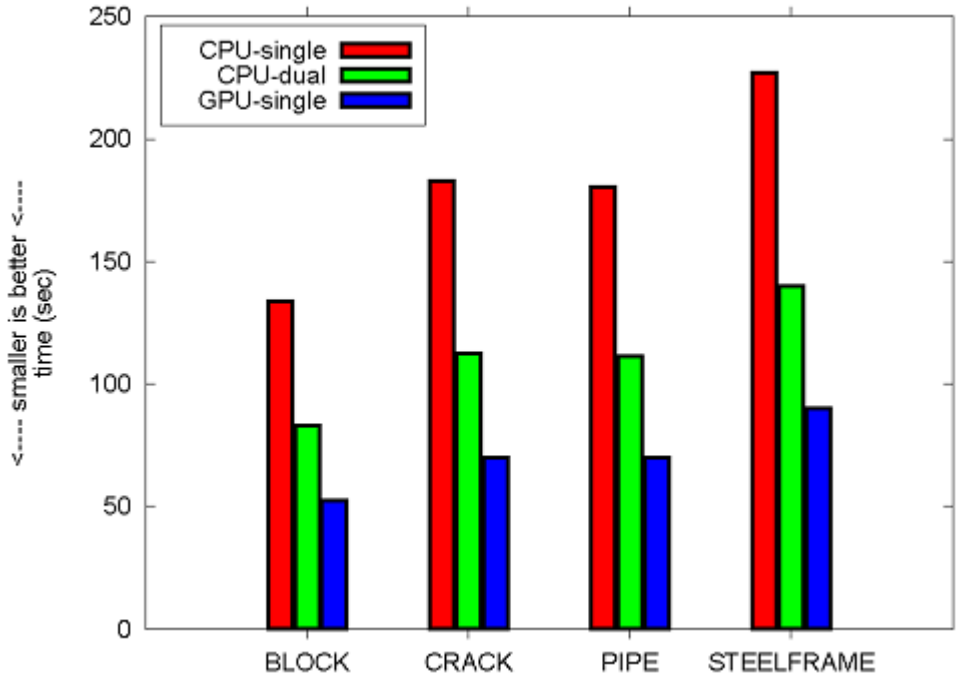

- 16 nodes, Opteron X2 2214
- NVIDIA Quadro FX 5600 (76 GB/s BW), OpenGL
- Problem size 128 M DOF
- Dualcore 1.6x faster than singlecore
- GPU 2.6x faster than singlecore, 1.6x than dual

Stationary Navier-Stokes

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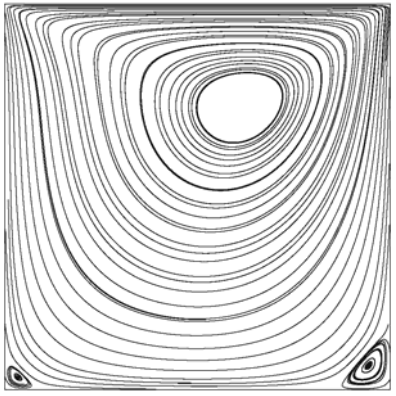
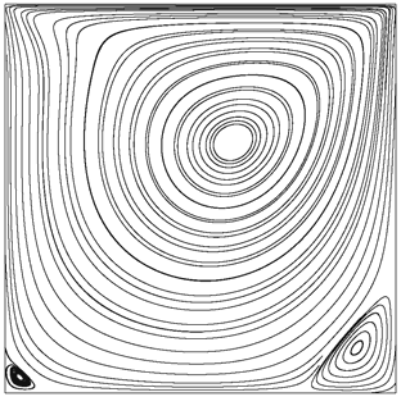
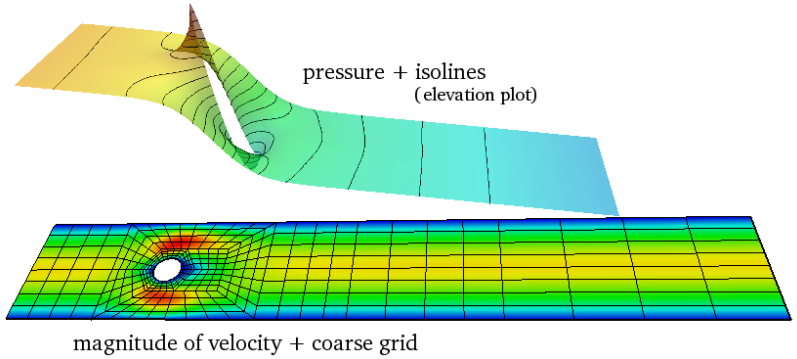
$$\begin{pmatrix} A_{11} & A_{12} & B_1 \\ A_{21} & A_{22} & B_2 \\ B_1 & B_2 & C \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ p \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ g \end{pmatrix}$$

- ★ 4-node cluster
- ★ Opteron X2 2214
- ★ GeForce 8800 GTX (90 GB/s BW), CUDA
- ★ Driven cavity and channel flow around a cylinder

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 u_1 with
local MG
for all Ω_i: solve for u_2 with
local MG
2) update RHS: $d_3 = -d_3 + B(c_1, c_2)$
3) scale $c_3 = (M_p^{\mathrm{L}})d_3$







Navier-Stokes results

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Speedup analysis

	R_{acc}		S_{local}		S_{total}	
	L9	L10	L9	L10	L9	L10
DC Re100	41%	46%	6x	12x	1.4x	1.8x
DC Re250	56%	58%	5.5x	11.5x	1.9x	2.1x
Channel flow	60%	–	6x	–	1.9x	–

Important consequence:

Ratio between assembly and linear solve changes significantly

DC Re100		DC Re250		Channel flow	
plain	accel.	plain	accel.	plain	accel.
29:71	50:48	11:89	25:75	13:87	26:74

Acceleration analysis

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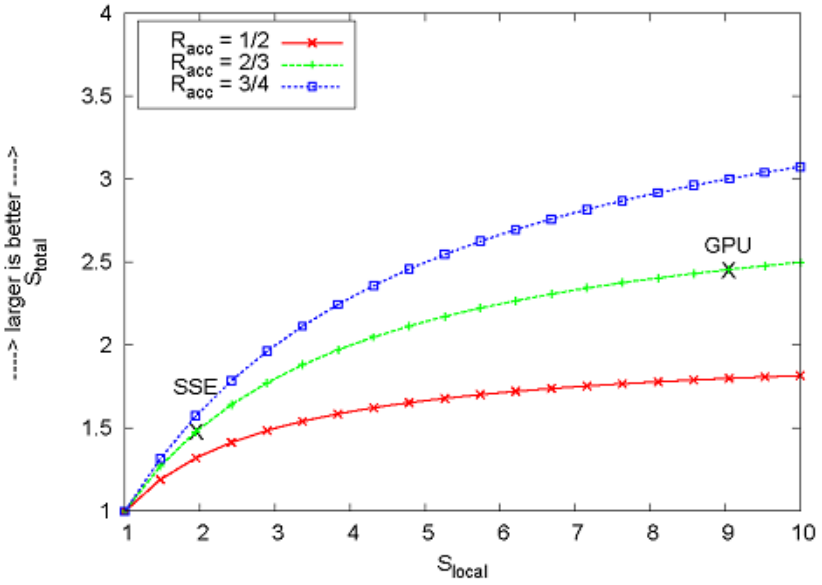
Speedup analysis

- ★ Addition of GPUs increases resources
- ★ ⇒ Correct model: strong scalability inside each node
- ★ Accelerable fraction of the elasticity solver: 2/3
- ★ Remaining time spent in MPI and the outer solver

Accelerable fraction R_{acc}: 66%
Local speedup S_{local}: 9x
Total speedup S_{total}: 2.6x
Theoretical limit S_{max}: 3x



Speedup Analysis

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- Speedups in 'time to solution' for one GPU:
  2.6x vs. Singlecore, 1.6x vs. Dualcore

- Amdahl's Law is lurking
  - Local speedup of 9x and 5.5x by the GPU
  - 2/3 of the solver accelerable => theoretical upper bound 3x

- Future work
  - Three-way parallelism in our system:
    - coarse-grained (MPI)
    - medium-grained (heterogeneous resources within the node)
    - fine-grained (compute cores in the GPU)
  - Better interplay of resources within the node
  - Adapt **Hardware-oriented Numerics** to increase accelerable part

There is a Huge Potential for the Future …

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However:

- **High Performance Computing** has to consider recent and future hardware trends, particularly for heterogeneous multicore architectures and massively parallel systems!
- The combination of **'Hardware-oriented Numerics'** and special **'Data Structures/Algorithms'** and **'Unconventional Hardware'** has to be used!

…or most of existing (academic/commercial) FEM software will be 'worthless' in a few years!

Acknowledgements

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- FEAST Group + LIDO Team
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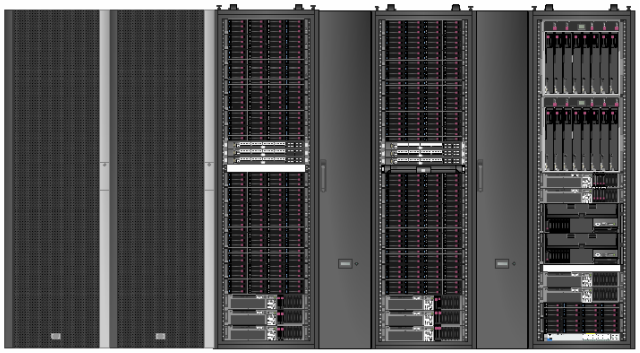

- Robert Strzodka
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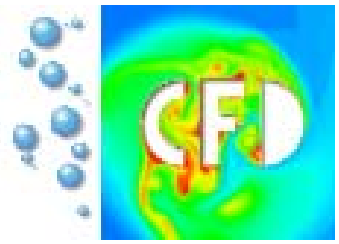
  (Los Alamos National Laboratories)



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Show-Case: FEASTSOLID

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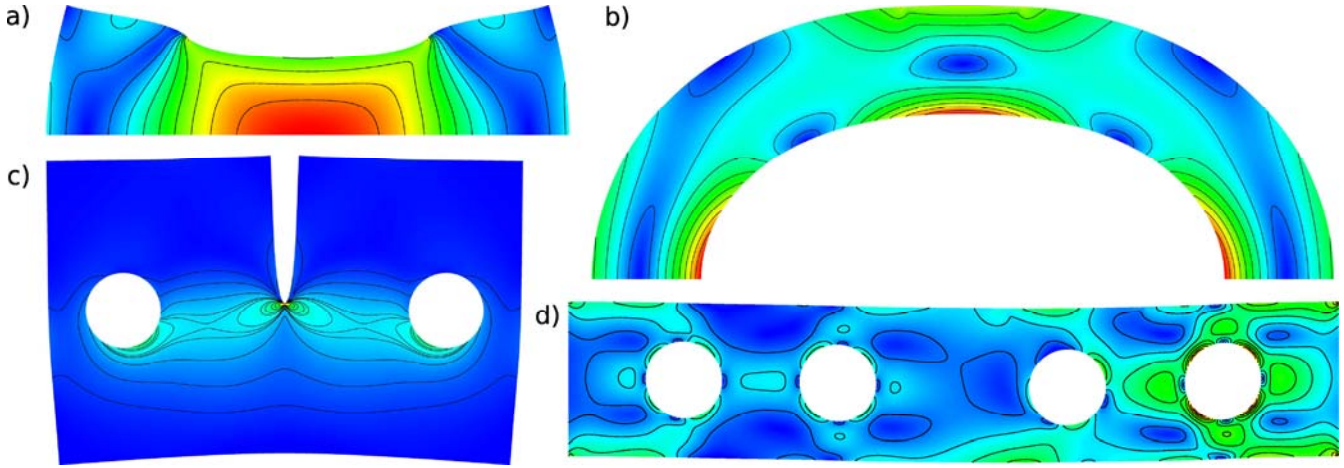
$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = f$$

$$\begin{pmatrix} (2\mu+\lambda)\partial_{xx} + \mu\partial_{yy} & (\mu+\lambda)\partial_{xy} \\ (\mu+\lambda)\partial_{yx} & \mu\partial_{xx} + (2\mu+\lambda)\partial_{yy} \end{pmatrix}$$



Solver Structure

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ScaRC -- Scalable Recursive Clustering

- Minimal overlap by extended Dirichlet BCs
- Hybrid multilevel domain decomposition method
- Inspired by parallel MG ("best of both worlds")
  - Multiplicative vertically (between levels), global coarse grid problem (MG-like)
  - Additive horizontally: block-Jacobi / Schwarz smoother (DD-like)
- Hide local irregularities by MGs within the Schwarz smoother
- Embed in Krylov to alleviate Block-Jacobi character