H L R S

High Performance Computing in Science and Engineering

The 6th Results & Review Workshop
of the HPC Center Stuttgart (HLRS)

parpp3d++ – a Parallel HPC Research Code for CFD

Block smoothers in parallel multigrid methods; Hitachi SR8000 vs. Linuxcluster

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- Presentation of a portable research code for the simulation of 3-D incompressible nonstationary flows.

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- Use of block smoothers in parallel multigrid methods
  $\hookrightarrow$ (numerical) consequences for parallel efficiencies
- Some current and recent applications of the code

The underlying problem

- Incompressible nonstationary Navier–Stokes equations

$$\mathbf{u}_t - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \mathbf{f}, \qquad \nabla\cdot\mathbf{u} = 0$$

  have to be solved

- Finite element discretisation of this system of PDEs leads to huge systems of (non-)linear equations ($\geqslant 10^7$ unknowns per timestep)

- Solving with parallel multigrid methods (chosen for their optimal numerical complexity for ill-conditioned PDE problems)

Mathematical background (1)

Numerics applied to solve the Navier–Stokes equations:

- (implicit) 2nd order discretisation in time
  (both Fractional-Step-Θ- and Crank-Nicolson-scheme
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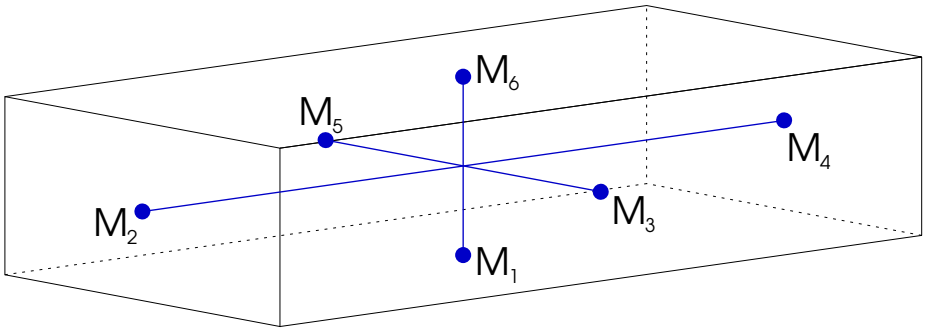

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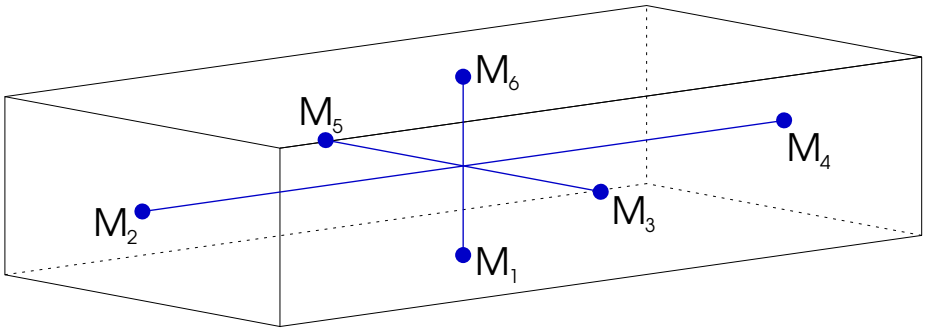

  $\hookrightarrow$ hexahedral grids
- Stabilisation of convective term with (Samarskij)
  Upwind scheme

Mathematical background (2)

Numerics applied to solve the Navier–Stokes equations (cont.):

- Within each time step:
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- Within each time step:
  - Discrete Projection method to decouple velocity-pressure problem
  - The resulting nonlinear Burgers equation in $\mathbf{u}$ is solved by fixed point defect correction method (outer loop) and multigrid (inner loop)
  - Remaining linear problem in p (Pressure Poisson problem, ill-conditioned!) is solved with multigrid preconditioned conjugate gradient method

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Parallelisation strategy

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- block smoothing

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Idea of block smoothing:

- Avoid direct parallelisation of global smoother (significant amount of communication!)
- Instead: Apply the same smoothing algorithm within each parallel block only
  (parallel block = one patch of elements from the partitioning algorithm)

Mathematical background (6)

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With increasing number of parallel processes:

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  – for Burgers equation: probably not, good conditioned (scaling with time step k)

  – **for discrete Pressure Poisson equation: probably, problem with condition of** $\mathrm{O}(h^{-2})$

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  ↪ does not incorporate explicit vector processing routines
- has a well-tested sequential (F77) counterpart from the FEATFLOW package (author: Turek et al., since 1985)

Numerical section

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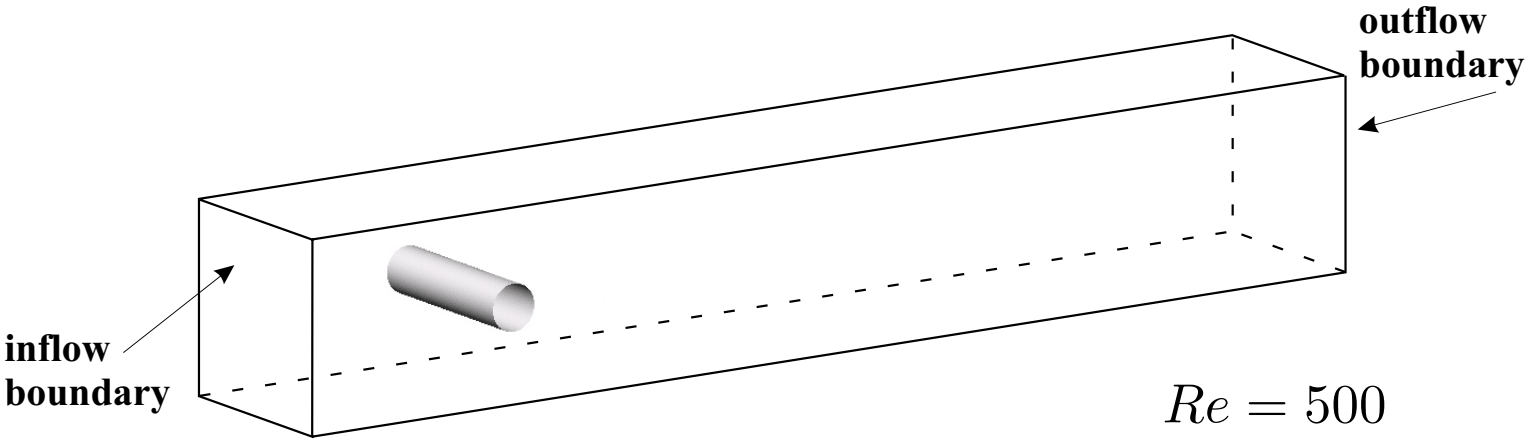
- Pars pro toto, the typical effects that can be observed will be illustrated on the basis of the DFG benchmark 3D-2Z from 1995 ("channel flow around a cylinder")

Numerical section

DFG benchmark 3D-2Z from 1995:

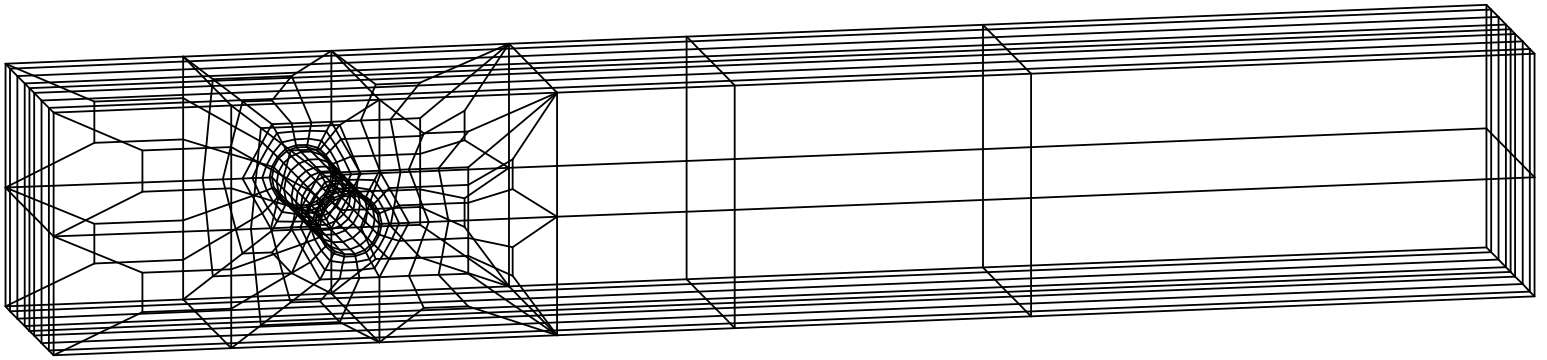


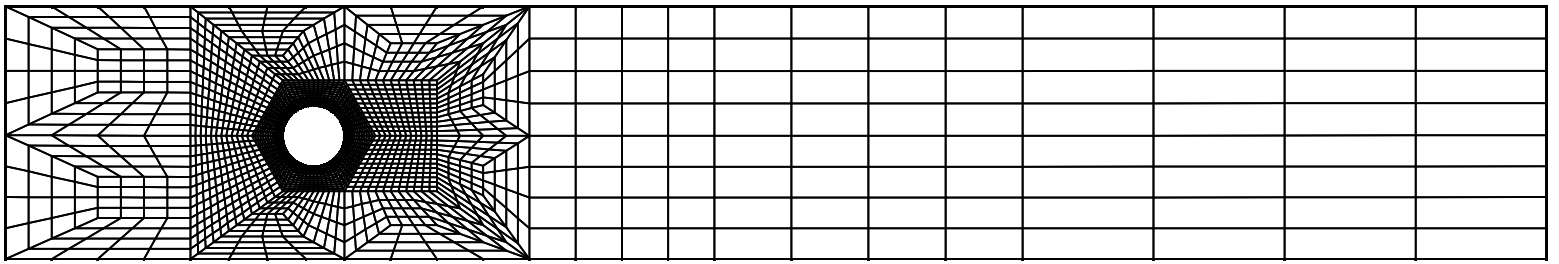
$Re = 500$

aspect ratio ≈ 20

Numerical section

Grids:





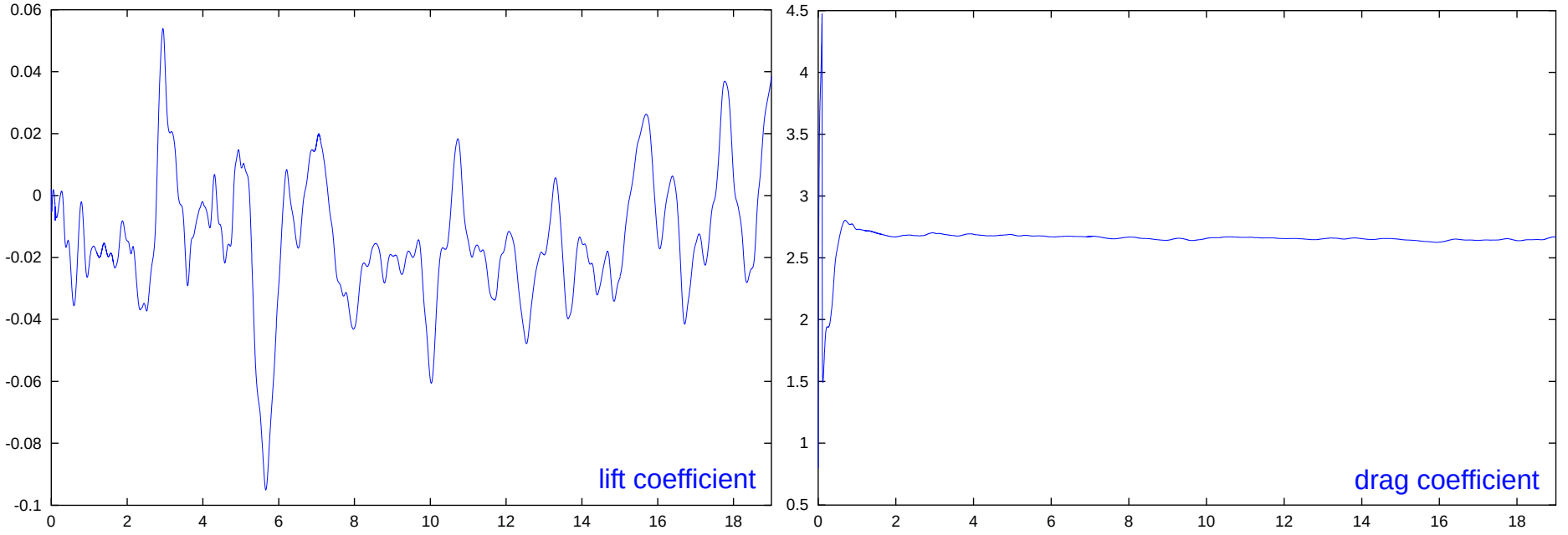
2x refined grid, side view

Numerical section

We did some long term simulation ($T_{End} = 20s$) ...

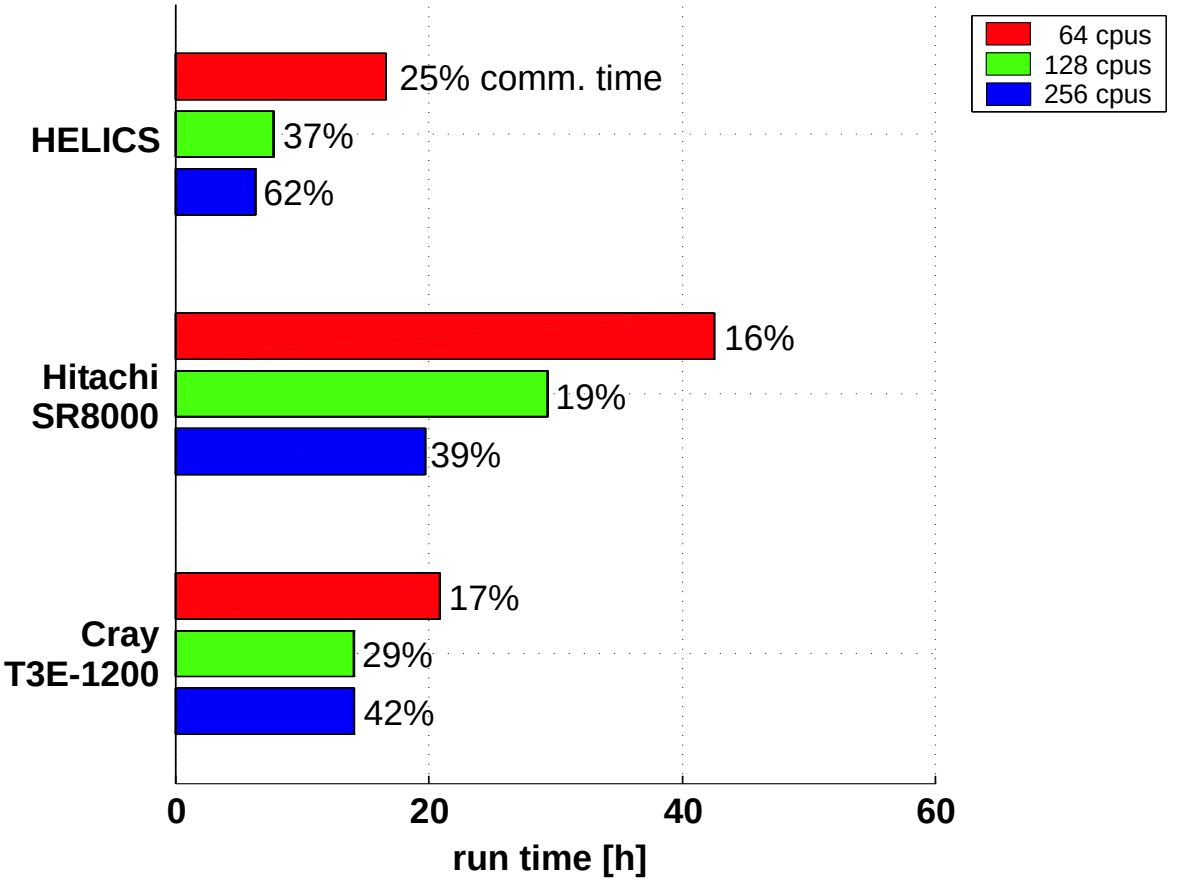
- degrees of freedom: 32 million (9 GByte RAM)
- #time steps: 6.500

... computed lift and drag coefficients ...



Numerical section

... and studied the scaling of the program on different platforms for this problem (64, 128, 256 cpus) ($T = [0, 1]$)



(HELICS = Linuxcluster at IWR Heidelberg, 512 Athlons 1.4 GHz, Myrinet, www.helics.de)

Observations (1)

- Hitachi SR8000 is conspicuously in last position
  - sCC compiler (latest release) used
  - run times with g++ worse
  - code does not compile with KCC
    (although it does on Cray T3E-1200)
- The fact that Hitachi is outperformed by a (much cheaper) Linux cluster (factor 2–3 in average) has been perceived for different problem sizes, degrees of parallelism and geometries.
  That's the price for just using MPI and not incorporating vector processing techniques directly into the code.

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- But:
  How many of the codes being granted access to SR8000 are especially designed for this architecture?
  Percentage?
- I bet: a significant percentage uses SR8000 as one MPP unit among others, too.
  (relying on MPI and compiler optimisations of the code)

Observations (3)

Things are not merely bad at SR8000!

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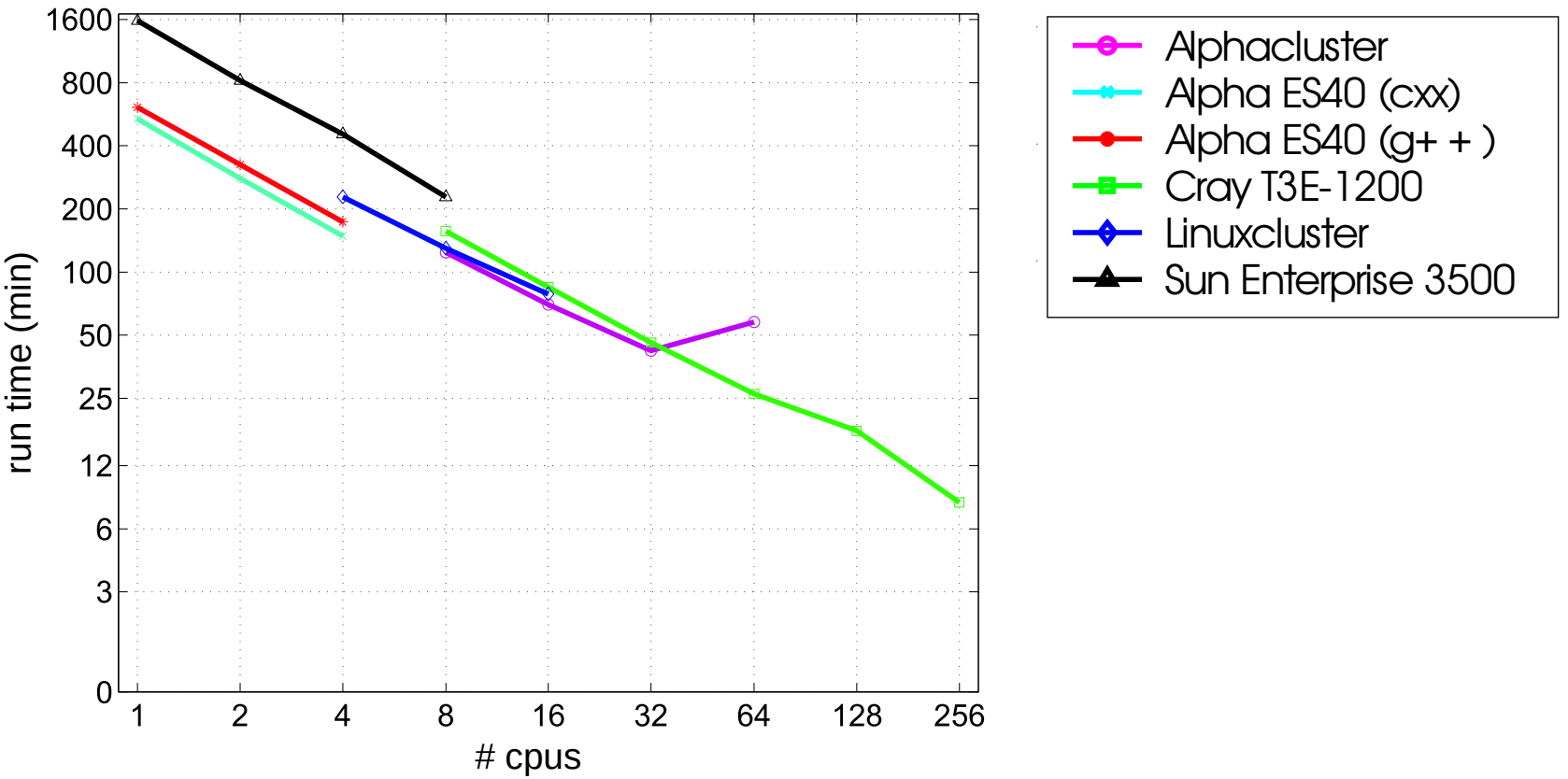
- best communication network, least time spent in communication routines
- hence, scaling is best of all tested platforms yet

Reduction in run time for different problem



(Lid-Driven Cavity, 11 million d.o.f., 100 time steps)

Parallel efficiencies

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- communication time increases at half the speed the parallel efficiencies drop
  $\hookrightarrow$ there must be a different effect!

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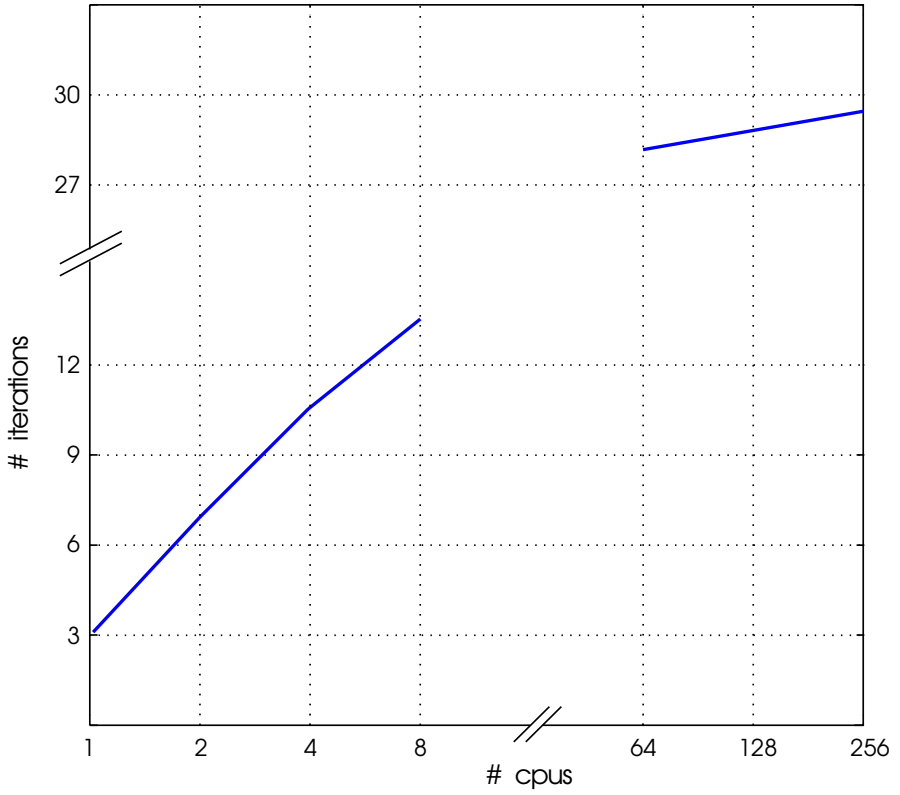

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- Speedup is not that bad if comparing e.g. 16 vs. 128 cpus
- But:
  The performance of the code is not yet satisfying enough to kick off incorporating more features like
  - heat transfer (Boussinesq)
  - $k - \epsilon$–model
  - free surface
  - multiphase flow (bubble colon reactors)

  which already exist in sequential.

Remarks

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- And we have found a candidate. The implementation is done in the context of the projects ScaRC and FEAST.

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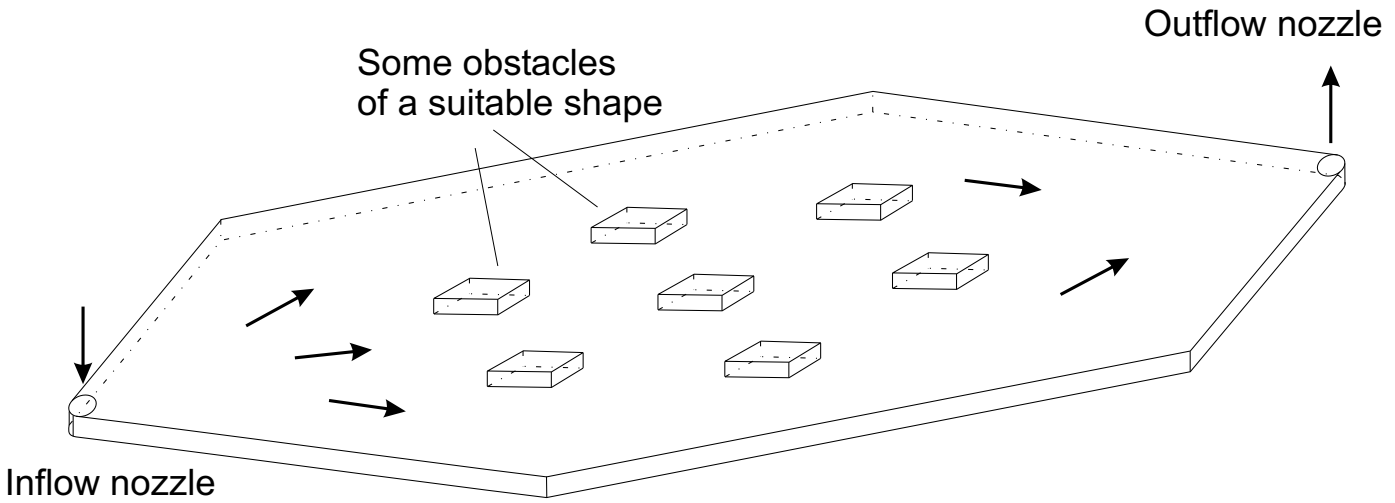
- Main aim: increasing performance of reactor by optimising its geometry to gain a equally distributed velocity field.
- Given this, the partners (Institute of Chemical Engineering, University of Dortmund) and Hermsdorfer Institute for Technical Ceramics) will try to calibrate catalytic activity, diffusive mass transport and heat removal to attain an optimal temperature distribution.

A current application:

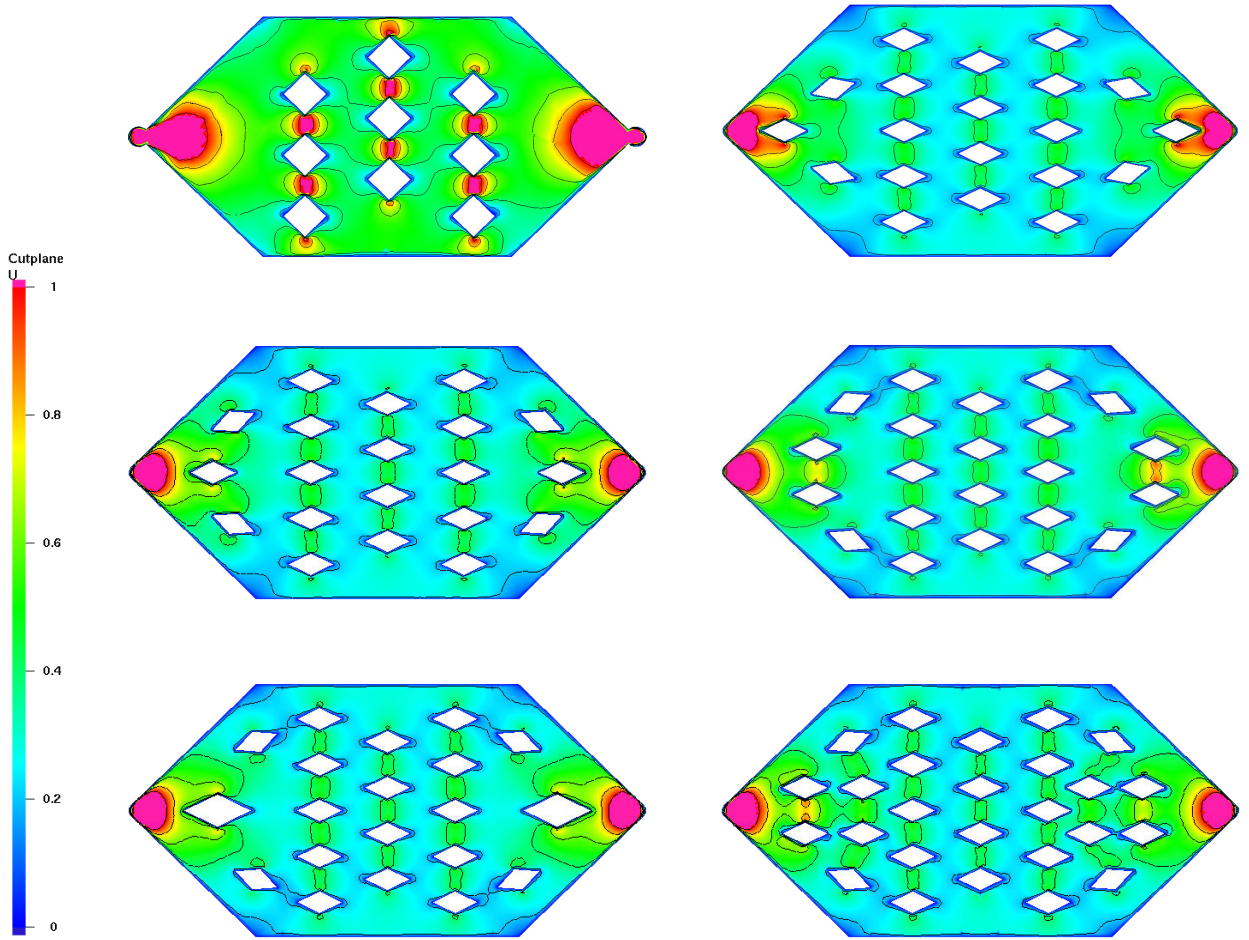
Sketch of overall geometry of ceramic wall reactor and flow directions



- 2 dozen different geometries so far
- average problem size: 60 million d.o.f., 100 time steps to stationary limit case
- 12h with 16 cpus on SR8000 per simulation

A current application:

Velocity field for some geometries



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- Exploitation of performance of computers like Cray T3E1200 and SR8000 is still too poor (due to implementation and numerics)
- But hopefully, my access to SR8000 will not be discarded within the next days!
- A new package is currently written which incorporates both better numerics (hardly any deterioration) and hardware-oriented implementation techniques (vectorisation, better cache exploitation).
  First tests show that we can get nearly 30-50% of machine's peak performance.