FEM Techniques for in Flow Simulation

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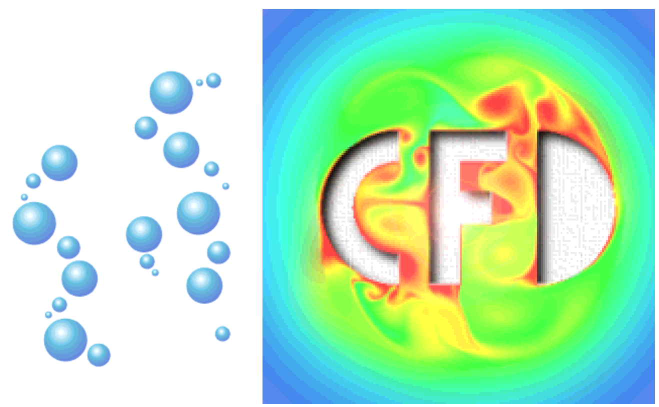
`http://www.mathematik.uni-dortmund.de/LS3`

`http://www.featflow.de`

- Examples for complex flow models
- Aspects of (FEM) discretizations
- Aspects of fast (Multigrid) solvers
- Aspects of (CFD) software



Computational Fluid Dynamics

‘Preserve the <u>high efficiency</u> of special PDE solvers for complex flow problems’

Computational Fluid Dynamics

‘Preserve the high efficiency of special PDE solvers for complex flow problems’

$\longrightarrow$ **High (guaranteed) accuracy for user-specific quantities !**

$\longrightarrow$ **With minimal #d.o.f.s !**

$\longrightarrow$ **Via robust solvers with ‘optimal’ numerical complexity !**

$\longrightarrow$ **Exploiting the huge sequential/parallel GFLOP/s rates !**

$$\Downarrow$$

Realization for incompressible CFD ?

Incompressible Flow Models

$$\rho(\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u}) = \mathbf{f} + \mu\Delta\mathbf{u} - \nabla p \quad , \quad \nabla\cdot\mathbf{u} = 0$$

+

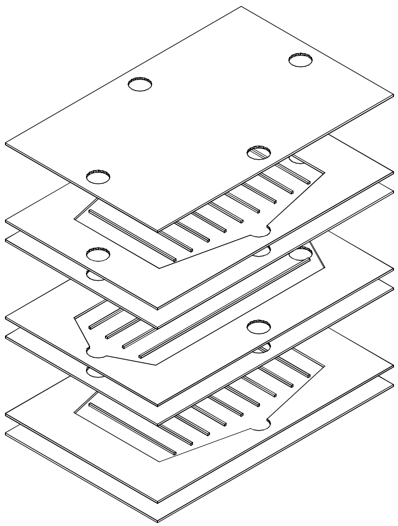
‘Complex’ extensions

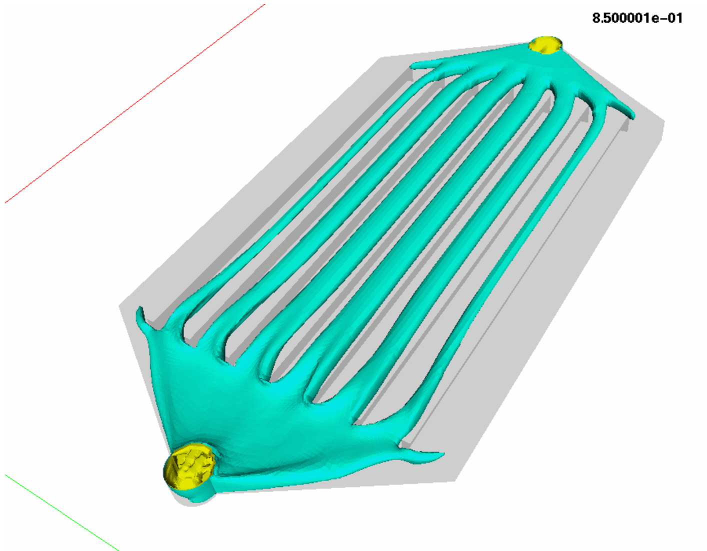
1. ‘Optimization’ of complex geometrical configurations
   $\longrightarrow$ *Ceramic plate heat exchanger*
2. Multiphase flow with chemical reaction
   $\longrightarrow$ *Gas-liquid reactors*
3. Granular flow/Powders
   $\longrightarrow$ *Fluids with pressure-dependent viscosity: Sand in silos*
4. Fluid-Structure interaction
   $\longrightarrow$ *Particulate flow*
   $\longrightarrow$ *Flow around elastic structures*

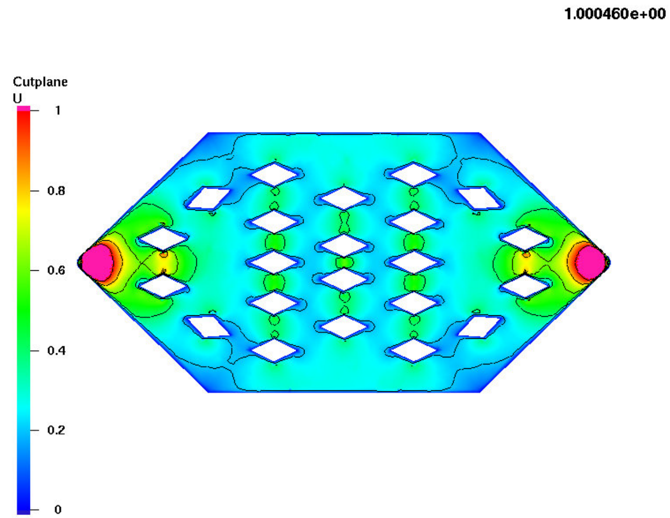
I: Plate Heat Exchanger (OMG+HITK)

Development of optimization tools for the understanding of:

1. The internal flow characteristics ($\rightarrow$ coating ?)
2. The heat transfer characteristics (ceramic material ? coupled stacks ?)







- Robust and flexible tools for small-scale details ! Optimization !
- Fluid-Heat transfer (‘stacks’) ? Chemical reaction ? Tracer/RTD ?

II: Multiphase Flow in Gas-Liquid Reactors

Drift-Flux model with mass transfer and chemical reaction

(Gas holdup ϵ, Number density n, Mass flux N, Interfacial area a_S)

$$\frac{\partial \mathbf{v}_L}{\partial t} + \mathbf{v}_L \cdot \nabla \mathbf{v}_L = -\nabla P + \nu \Delta \mathbf{v}_L - \epsilon \mathbf{g} \, , \; \nabla \cdot \mathbf{v}_L = 0 \quad , \quad \mathbf{v}_G = \mathbf{v}_L + \mathbf{v}_{\mathrm{slip}} + \mathbf{v}_{\mathrm{drift}}$$

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$$\frac{\partial \tilde{\rho}_G}{\partial t} + \nabla \cdot (\tilde{\rho}_G \mathbf{v}_G) = -a_S m_\mu N \quad , \quad N = E k_L^0 (p/H - c_A)$$

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{v}_G) = 0 \quad , \quad \epsilon = \frac{\tilde{\rho}_G RT}{p m_\mu} \quad , \quad a_S = (4\pi n)^{1/3} (3\epsilon)^{2/3}$$

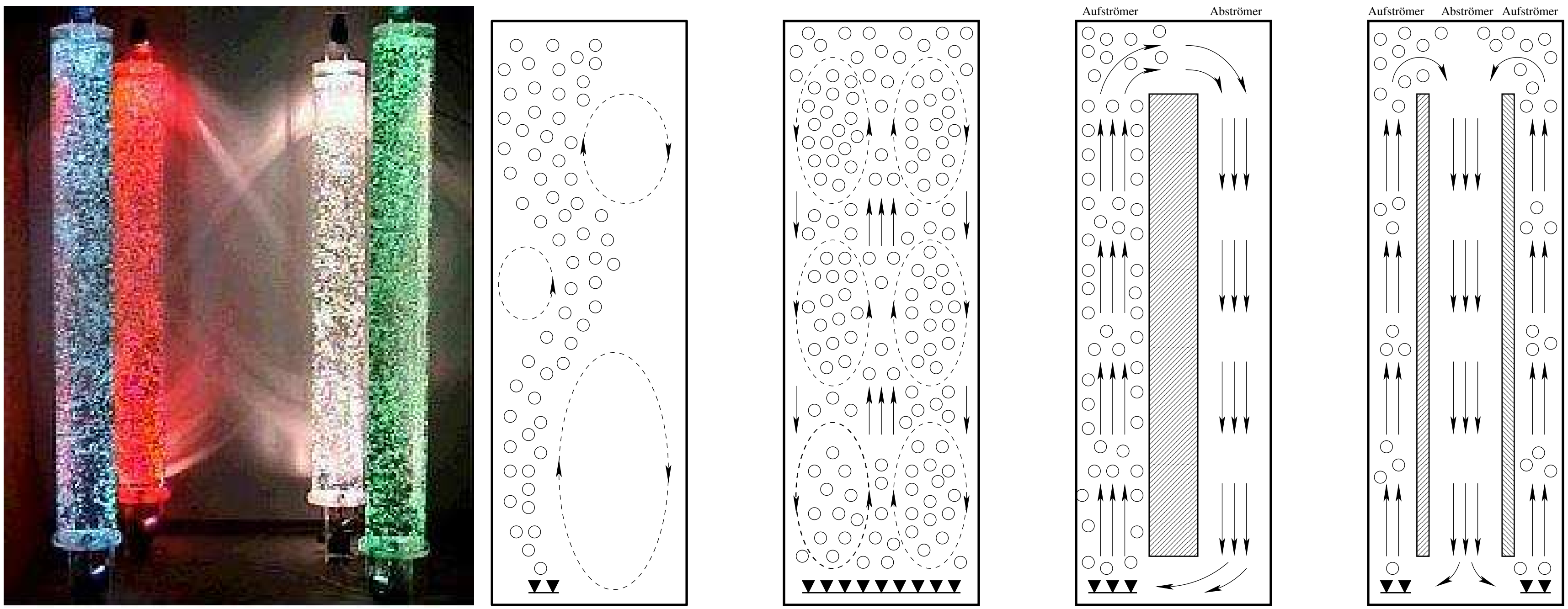
$$\frac{\partial \tilde{c}_A}{\partial t} + \nabla \cdot (\tilde{c}_A \mathbf{v}_L) = \nabla \cdot (\tilde{D}_A \nabla c_A) - \tilde{k}_2 c_A c_B + a_S N$$

$$\frac{\partial \tilde{c}_B}{\partial t} + \nabla \cdot (\tilde{c}_B \mathbf{v}_L) = \nabla \cdot (\tilde{D}_B \nabla c_B) - \nu_B \tilde{k}_2 c_A c_B$$

$$\frac{\partial \tilde{c}_P}{\partial t} + \nabla \cdot (\tilde{c}_P \mathbf{v}_L) = \nabla \cdot (\tilde{D}_P \nabla c_P) + \nu_P \tilde{k}_2 c_A c_B$$

Properties of Drift-Flux simulations

No explicit tracking of bubbles via Euler-Euler formulation



- Modelling of 'small-scale' effects (single bubbles) !
- Two-Phase turbulence ? Population Balance models ?

Extension I: Two-Phase Turbulence

'Effective' viscosity ($k - \varepsilon$ model)

$$\nu_{\text{eff}} = \nu + \nu_T, \qquad \nu_T = C_\mu \frac{k^2}{\varepsilon} + \underbrace{C_g \epsilon |\mathbf{u}_{\text{slip}}| r}_{BIT}$$

with

$k = \frac{1}{2}\langle|\mathbf{u}'|^2\rangle$ turbulent kinetic energy

$\varepsilon = \frac{\nu}{2}\langle|\nabla\mathbf{u}' + (\nabla\mathbf{u}')^T|^2\rangle$ dissipation rate

$$\frac{\partial k}{\partial t} + \nabla \cdot \left(k\mathbf{u} - \frac{\nu_T}{\sigma_k}\nabla k \right) = P_k + S_k - \varepsilon$$

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot \left(\varepsilon\mathbf{u} - \frac{\nu_T}{\sigma_\varepsilon}\nabla \varepsilon \right) = \frac{\varepsilon}{k}(C_1 P_k + C_\varepsilon S_k - C_2 \varepsilon)$$

Modelling of production terms

$P_k = \frac{\nu_T}{2}|\nabla\mathbf{u} + \nabla\mathbf{u}^T|^2$ shear induced turbulence

$S_k = -C_k \epsilon \nabla p \cdot \mathbf{u}_{\text{slip}}$ bubble induced turbulence

Extension II: Population Balance Models

$$\frac{\partial f}{\partial t} + \nabla \cdot (f\,\mathbf{u}_G) + \frac{\partial}{\partial m}(f\,\dot{m}) = Q - S$$

$f = f(\mathbf{x}, m, t)$	Bubble size distribution
$\mathbf{u}_G = \mathbf{u} + \mathbf{u}_{\text{slip}}(m)$	Gas velocity
$\dot{m} = E k_L^0 \left(c_A - \frac{p}{H}\right) \eta a_B$	Mass transfer rate
$Q - S$	Coalescence and breakup rates

Calculation of the local gas holdup

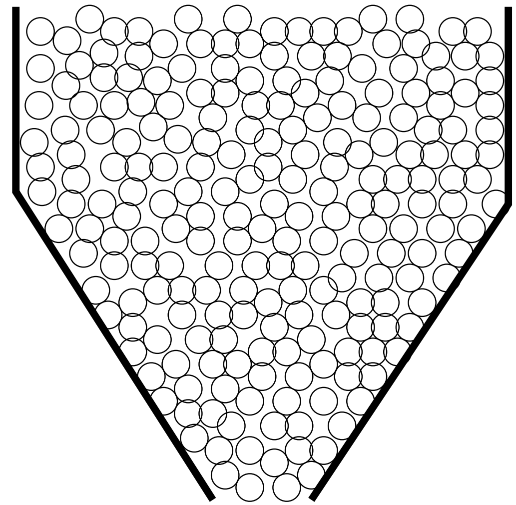
$$\epsilon(\mathbf{x}, t) = \frac{RT}{p\eta} \int_0^\infty m\, f(\mathbf{x}, m, t)\, dm$$

Treatment of Integro-Differential equation ???

Coupling with CFD ???

III: Granular Flow

Pharmaceutical Industry, Food Processing, Soil Mechanics



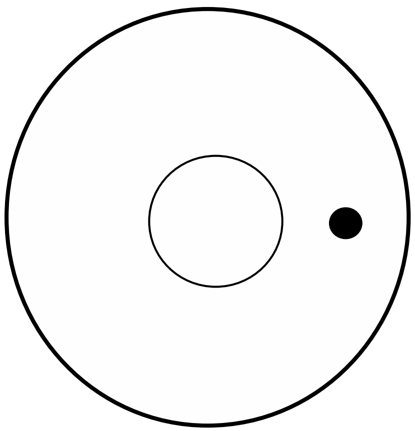
The behaviour of **granular flow** *is different from that of fluids since it does not exhibit* **viscosity** *and the dominant interaction between particles is* **friction**.

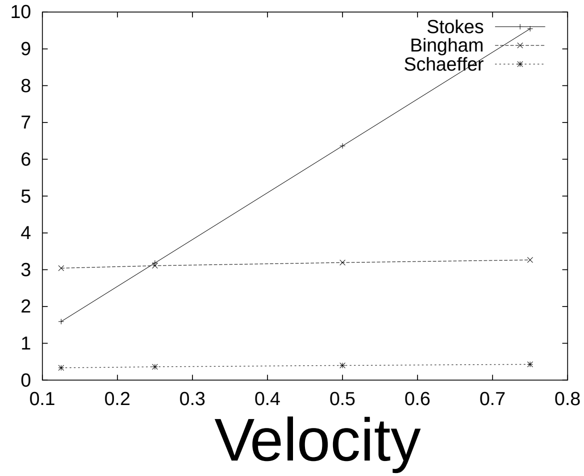
We do not examine flow of large grains but **slow smaller-sized bulk powders** *where a* **continuum approach** *may be more advantageous*.

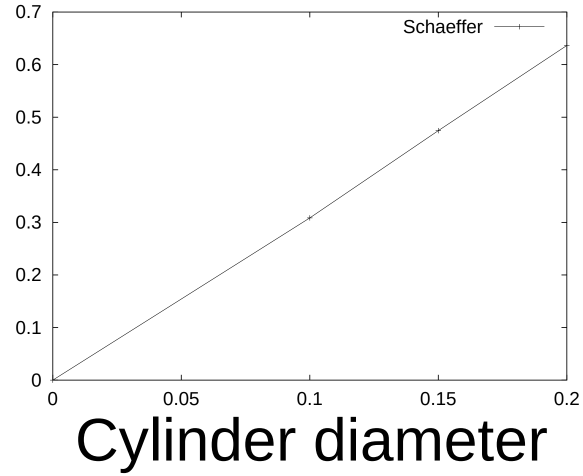
Characteristics of Slow Granular Flow

- Open a silo hopper and.....???

- The **drag force** for Schaeffer and Bingham flow acting on a cylinder is **independent** of the grain **velocity**, contrary to Stokes flow







‘When mechanical ploughs replaced draught animals, it was observed that ploughing at greater speeds does not require greater forces!’

Compressible Powder Models (cf. Tardos)

- **General equation of motion for a powder**

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \left[\frac{q(p,\rho)}{\|\mathbf{D} - \frac{1}{n}\nabla \cdot \mathbf{u} I\|} \left(\mathbf{D} - \frac{1}{n}\nabla \cdot \mathbf{u} I\right)\right] + \rho g, \text{ with}$$

- **Continuity equation**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \text{ and}$$

- **Normality condition**

$$\nabla \cdot \mathbf{u} = \frac{\partial q(p,\rho)}{\partial p} \|\mathbf{D} - \frac{1}{n}\nabla \cdot \mathbf{u} I\|$$

- **Yield condition $q(p,\rho)$ is given by:**

Powder properties	Non-cohesive	Cohesive
Incompressible	$p \sin \phi$	$p \sin \phi + c \cos \phi$
Compressible	$p \sin \phi \left[2 - \frac{p}{\rho^{\frac{1}{\beta}}}\right]$	$p \sin \phi \rho^{\frac{1}{\beta}} - C \frac{(p - \rho^{\frac{1}{\beta}})^2}{\rho^{\frac{1}{\beta}}}$

Hypoplastic Model by Kolymbas

$$\text{Re}\ [\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}] = -\nabla p + \nabla\cdot\mathbf{S} + \mathbf{f} \quad , \quad \nabla\cdot\mathbf{u} = 0$$

$$\mathbf{S} = \frac{Q(p)}{|\mathbf{D}(\mathbf{u})|}\mathbf{D}(\mathbf{u}) \text{ (Schaeffer/Power Law/etc.) } + \mathbf{T} \text{ (Kolymbas)}$$

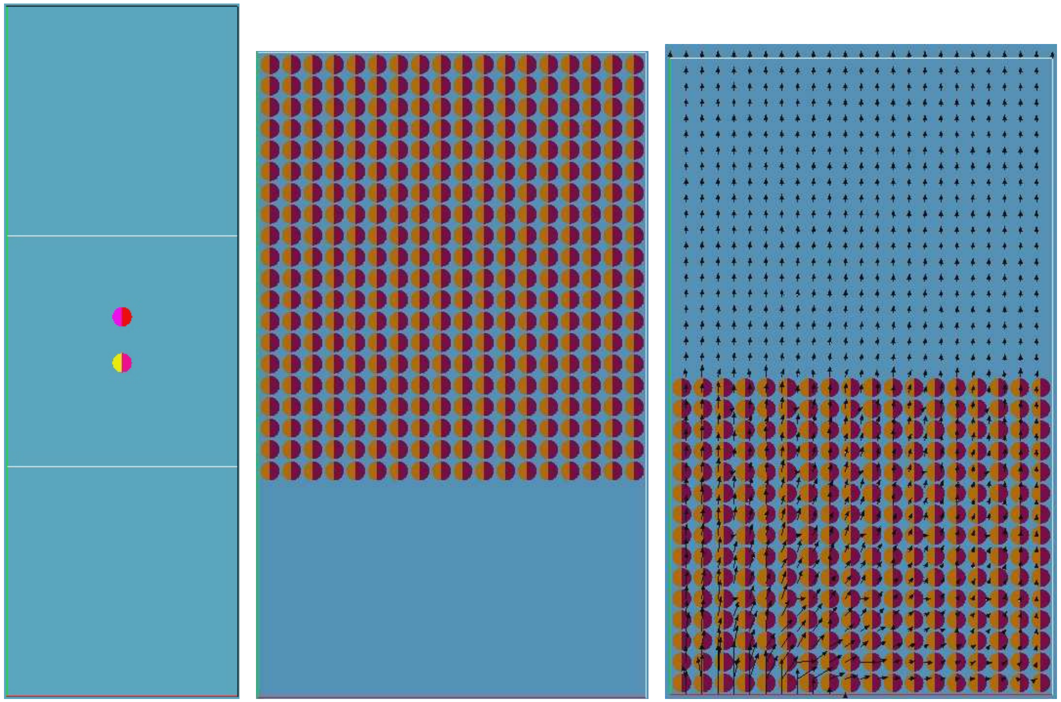
$$\begin{aligned}\frac{\partial \mathbf{T}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{T} \quad &= \quad -[\mathbf{TW} - \mathbf{WT}] + C_1\frac{1}{2}(\mathbf{TD} - \mathbf{DT}) \\ &+C_2 tr(\mathbf{TD})\cdot\mathbf{I} + C_3\sqrt{tr\mathbf{D}^2}\mathbf{T} + C_4\frac{\sqrt{tr\mathbf{D}^2}}{tr\mathbf{T}}\mathbf{T}^2 \\ &+\nu(\mathbf{D})[\frac{\partial \mathbf{D}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{D} + \mathbf{DW} - \mathbf{WD}]\end{aligned}$$

1. FEM discretization and solver ?
2. Free boundary ? Fluid-Structure interaction ?
3. Numerical ‘falsification’ of material/flow models !?

IV: Particulate Flow

Development of simulation tools for the understanding of:

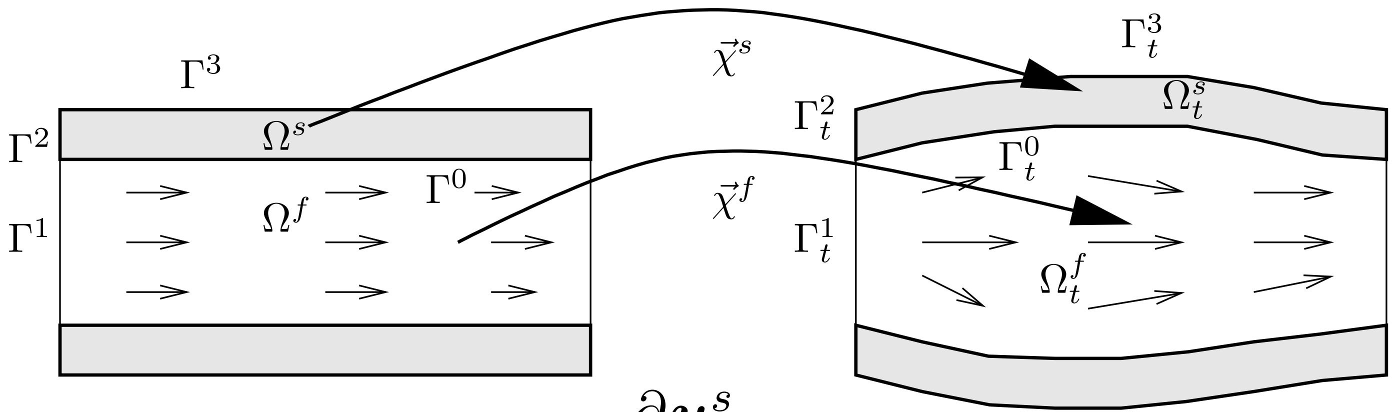
1. Interaction of solid particles with flow ($\rightarrow$ many complex objects ?)
2. Behaviour of non-newtonian fluids



- 'Fictitious Boundary Method' on fixed meshes + Operator-Splitting !
- 'Many' particles ? Nonlinear fluids ? Wide range of applications !

V: Fluid-Structure Interaction

Efficient numerical simulation of dynamic fluid-structure interaction
of incompressible fluids (newtonian) and solids (elastic)



$$\boldsymbol{u}^s = \boldsymbol{\chi}^s(X,t) - X \quad , \quad \boldsymbol{v}^s = \frac{\partial \boldsymbol{u}^s}{\partial t} \quad , \quad \boldsymbol{F} = \boldsymbol{I} + \nabla \boldsymbol{u}^s \, , \; J = \det \boldsymbol{F}$$

$$\varrho^f \frac{\partial \boldsymbol{v}^f}{\partial t} + \varrho^f (\nabla \boldsymbol{v}^f)\boldsymbol{v}^f = -\nabla p^f + \nabla \cdot (\boldsymbol{\sigma}^f[\boldsymbol{D}]) \quad , \quad \nabla \cdot \boldsymbol{v}^f = 0 \qquad \text{in } \Omega_t^f$$

$$\varrho^s \frac{\partial \boldsymbol{v}^s}{\partial t} + \varrho^s (\nabla \boldsymbol{v}^s)\boldsymbol{v}^s = -\nabla p^s + \nabla \cdot (\boldsymbol{\sigma}^s[\boldsymbol{F}]) \quad , \quad \nabla \cdot \boldsymbol{v}^s = 0 \qquad \text{in } \Omega_t^s$$

$$-p^f \boldsymbol{n} + \boldsymbol{\sigma}^f \boldsymbol{n} = -p^s \boldsymbol{n} + \boldsymbol{\sigma}^s \boldsymbol{n} \quad , \quad \boldsymbol{v}^f = \boldsymbol{v}^s \qquad \text{on } \Gamma_t^0$$

$$\boldsymbol{\sigma}^f[\boldsymbol{D}] = 2\mu \boldsymbol{D}(\boldsymbol{v}^f) \quad , \quad \boldsymbol{\sigma}^s[\boldsymbol{F}] = 2\boldsymbol{C}(\boldsymbol{F}\boldsymbol{F}^T - \boldsymbol{I})$$

Fully coupled FSI formulation

$$\frac{\partial \boldsymbol{u}}{\partial t} = \begin{cases} \boldsymbol{v} & \text{in } \Omega^s \\ \Delta \boldsymbol{u} \text{ “mesh deformation operator”} & \text{in } \Omega^f \end{cases} \tag{0}$$

$$\frac{\partial \boldsymbol{v}}{\partial t} = \begin{cases} -(\nabla \boldsymbol{v})\boldsymbol{F}^{-1}(\boldsymbol{v} - \frac{\partial \boldsymbol{u}}{\partial t}) + \frac{1}{J}\nabla\cdot(-Jp^f\boldsymbol{F}^{-T} + J\boldsymbol{\sigma}^f\boldsymbol{F}^{-T}) & \text{in } \Omega^f \\ \frac{1}{J\beta}\nabla\cdot(-Jp^s\boldsymbol{F}^{-T} + J\boldsymbol{\sigma}^s\boldsymbol{F}^{-T}) & \text{in } \Omega^s \end{cases} \tag{1}$$

$$0 = \begin{cases} \nabla\cdot(J\boldsymbol{v}\boldsymbol{F}^{-T}) & \text{in } \Omega^f \\ J - 1 & \text{in } \Omega^s \end{cases} \tag{2}$$

$$\Downarrow$$

Sequence of discrete Saddlepoint problems

$$\begin{pmatrix} M - \frac{k}{2}L^f & \frac{k}{2}M^s & 0 \\ \frac{1}{2}\frac{\partial N_2}{\partial u_h} + \frac{k}{2}\frac{\partial(N_1+S^s+S^f)}{\partial u_h} + k\frac{\partial B}{\partial u_h}p_h & M^s + \beta M^f + \frac{1}{2}\frac{\partial N_2}{\partial v_h} + \frac{k}{2}\frac{\partial(N_1+S_f^2)}{\partial v_h} & kB \\ B^{sT} + \frac{\partial B^{f\,T}}{\partial u_h}v_h & B^{f\,T} & 0 \end{pmatrix}$$

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$$\begin{bmatrix} S_{\mathbf{uu}} & S_{\mathbf{uv}} & 0 \\ S_{\mathbf{vu}} & S_{\mathbf{vv}} & kB \\ c_{\mathbf{u}}B_s^T & c_{\mathbf{v}}B_f^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f_u} \\ \mathbf{f_v} \\ f_p \end{bmatrix}$$

Challenges and Problems

- Coupled ('monolithic') + fully implicit FEM discretization
- Efficient coupling/decoupling strategies for solver
- Adaptive meshing/Error control of user-specific quantities

$\rightarrow$ **Prototypical for many (multiphase) flow problems ?**

Challenges and Problems

- Coupled (‘monolithic’) + fully implicit FEM discretization
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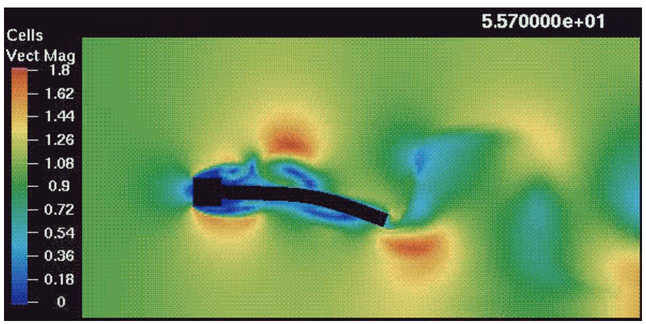
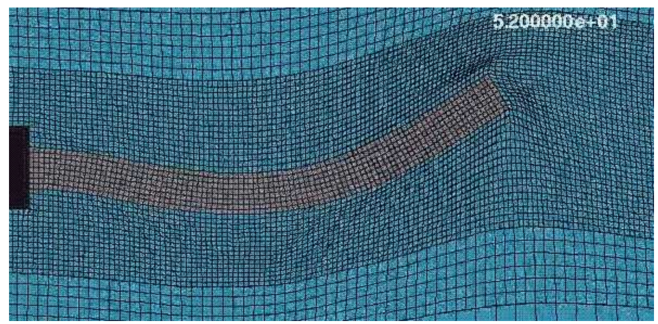
→ Prototypical for many (multiphase) flow problems ?

But: Problems with large deformations ? Remeshing of solid interfaces ?





Similar techniques (implicit reconstruction, accurate and oscillation-free transport solvers) as for multiphase flow ?

Summary

⇒ **Modelling:** '$\mathbf{u}_t - \nu\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{f}\,,\ \nabla\cdot\mathbf{u} = 0$'

⇒ **Discretization:** 'Find $\mathbf{u}_h \in \mathbf{V}_h$: $a_h(\mathbf{u}_h, \mathbf{v}_h) = (\mathbf{f}, \mathbf{v}_h)\,\forall\mathbf{v}_h \in \mathbf{V}_h$'

⇒ **Solver:** 'Solve (nonlinear) System $A \cdot X = F$'

Software: FEATFLOW/FEASTFLOW

Mathematical, algorithmic and software tools for research and industrial CFD applications

Aspects of FEM Discretization

1) BB Condition: $$\min_{q_h \in L_h} \max_{\mathbf{v}_h \in \mathbf{V}_h} \frac{(q_h, \nabla \cdot \mathbf{v}_h)}{\|\mathbf{v}_h\|_{1,h} \|q_h\|_0} \geq \alpha > 0$$

$\longrightarrow$ Deformations of the mesh w.r.t. highly stretched elements !
$\longrightarrow$ Quantitative (nonlinear) stabilization strategies ?

2) Korn's Inequality: $$\|D(\mathbf{v}_h)\|_0 \geq \beta \|\mathbf{v}_h\|_{1,h}$$

$\longrightarrow$ For 'discontinuous' FEM ?

3) Stabilization of the convective term '$\mathbf{u}_h \cdot \nabla \mathbf{u}_h$'

$\longrightarrow$ Upwind/Streamline-Diffusion for 'diffusion-dominated' case !
$\longrightarrow$ FEM-Stabilization for pure 'transport-dominated' case ?

$\Rightarrow$ *Accurate, monotone and oscillation-free !*

Why nonconforming FEM?

1) BB Condition for highly deformed elements

2) Korn's Inequality: $$[E_h]_{i,j} = h^{-1} \sum_{\text{Edges}} \int_{\text{Edge}} [\phi_i][\phi_j]ds$$

3) Stabilization of convective terms via FCT/TVD-FEM techniques

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And: **Very efficient multigrid solvers are available !!!**

Aspects of Discretization (in time)

1) (Semi) Implicit + (Strongly) A-Stable

$\longrightarrow$ Allowing huge time steps for (quasi-) stationary flow !
$\longrightarrow$ No CFL-type restrictions !

2) Second Order Accurate

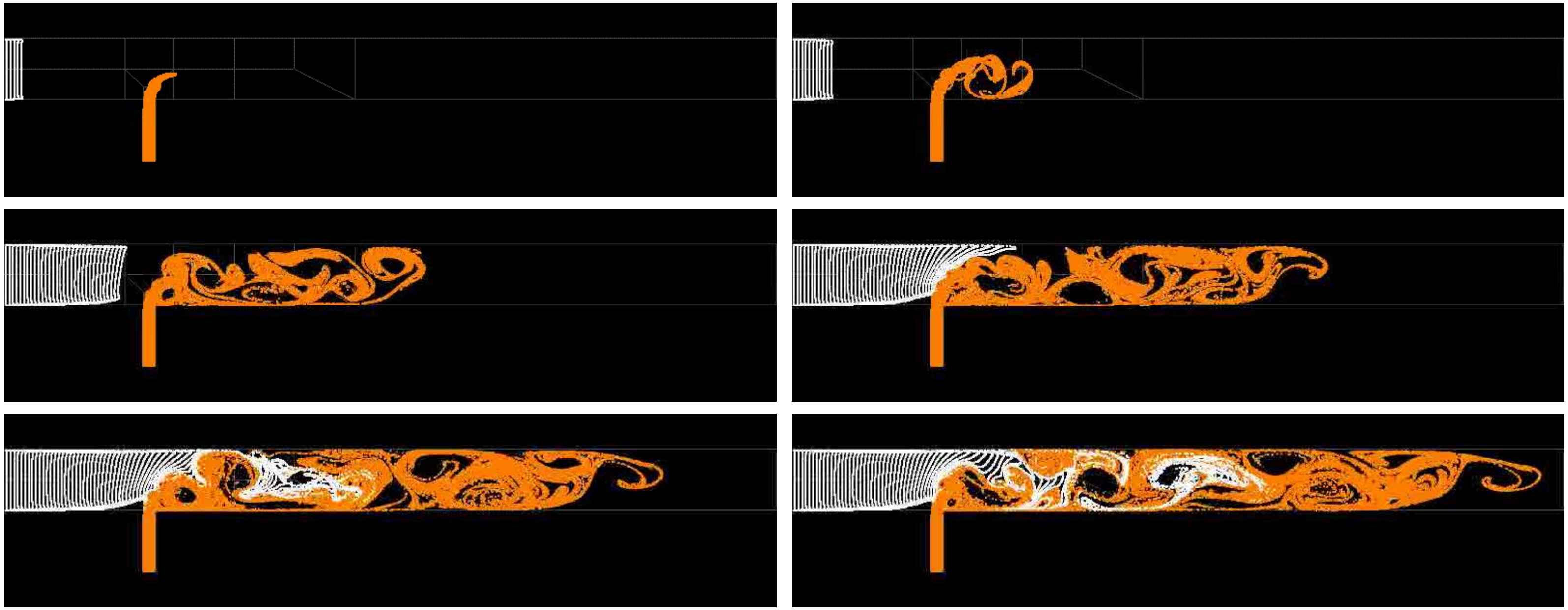
3) Accuracy-Based (Implicit) Error Indicator

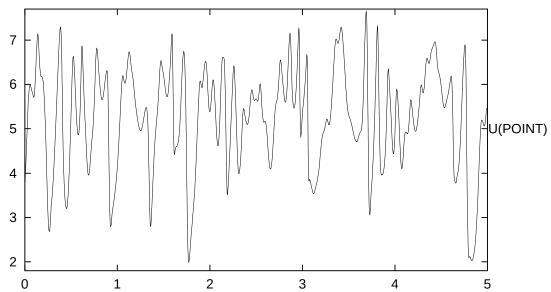
$\longrightarrow$ Based on local truncation error for pressure <u>and</u> velocity !

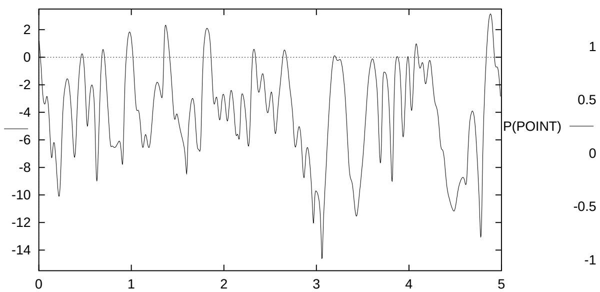
4) Rigorous Error Control

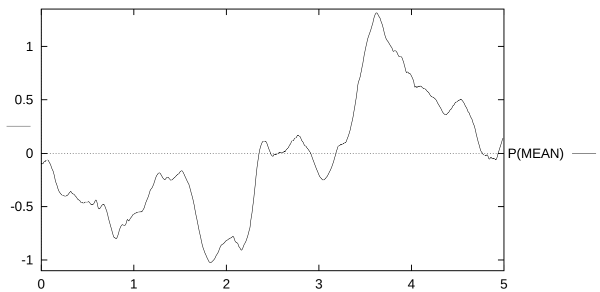
$\longrightarrow$ Residual-based a posteriori error control via dual problem ?
$\longrightarrow$ For user-defined time-averaged quantities ?

Merger of Perpendicular Pipe Flow









RIGOROUS **Adaptive Error Control** OF
Mean Values (‘WALL PRESSURE’) IN **Space/Time** ?!?

Aspects of 'Fast Solvers'

1) Newton Schemes: $U^{n+1} = U^n - \tilde{F}_\delta(U^n)^{-1} F(U^n)$

$\longrightarrow$ Dependence on Re ? Frechet derivative $F_\delta(U^n)$?

$\longrightarrow$ Complex non-newtonian behaviour ? Simplifications $\tilde{F}_\delta(U^n)$?

2) Linear Multigrid/DD Schemes: $A_{lev} U_{lev} = F_{lev}$

$\longrightarrow$ Re ? Mesh size/deformations ? FEM types ? Time step ?

$\longrightarrow$ Robustness ! Efficiency ! **Parallelism !**

3) (De)Coupling: $U^{n+1} = f(P^n), P^{n+1} = g(U^{n+1})$

$\longrightarrow$ Coupling of NSE with other components ?

$\longrightarrow$ Decoupling of pressure from velocity/temperature/etc. ?

$\Longrightarrow$ *Pressure Schur Complement (PSC) solvers !*

Key Ideas of MPSC Approaches

‘Re-interpretation of Navier-Stokes solvers (Chorin, Van Kan, Uzawa, etc.) as "incomplete solvers" for discrete saddle-point problems’

LOCAL MPSC (‘MULTILEVEL PRESSURE SCHUR COMPLEMENT’):

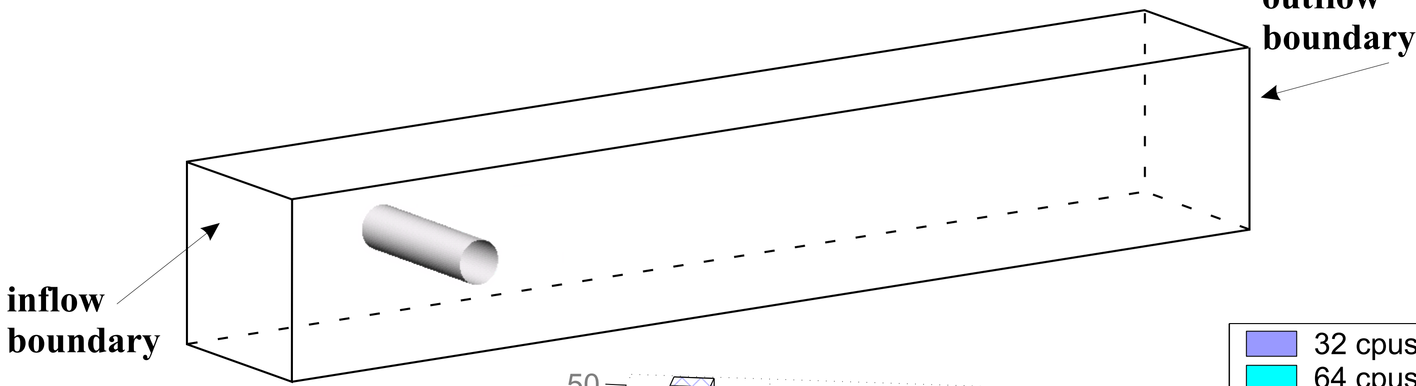
‘*Fully coupled Newton-like solver as outer nonlinear procedure*’
‘*Solve "exactly" on "subsets/patches" and perform an outer Block–Gauß-Seidel/Jacobi iteration as smoother*’

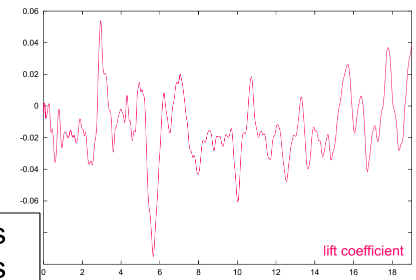
GLOBAL MPSC (‘MULTILEVEL PRESSURE SCHUR COMPLEMENT’):

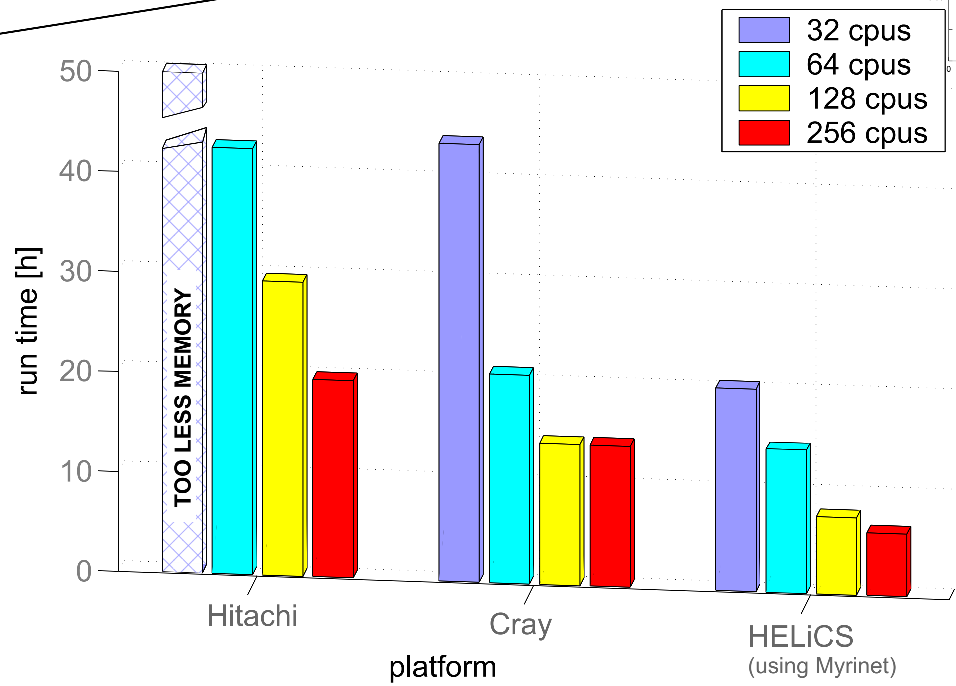
‘Outer (multigrid) coupling of velocity and pressure’
‘Newton/Multigrid solver for all scalar subproblems’

Parallel realization of GLOBAL MPSC

Dynamic simulations for ‘Channel Flow around Cylinder’ with 32 Mill. d.o.f.s for 6.500 implicit time steps (20 sec real time)

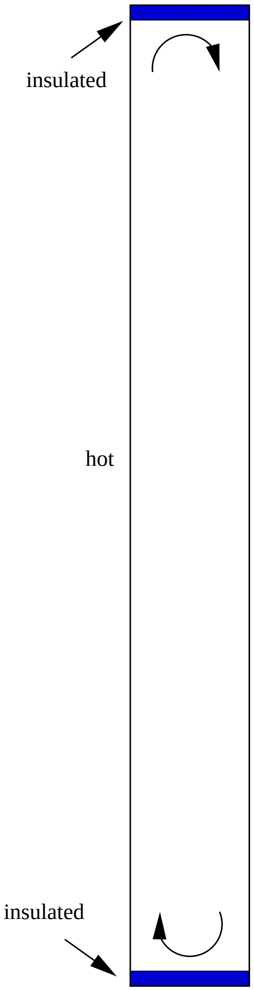


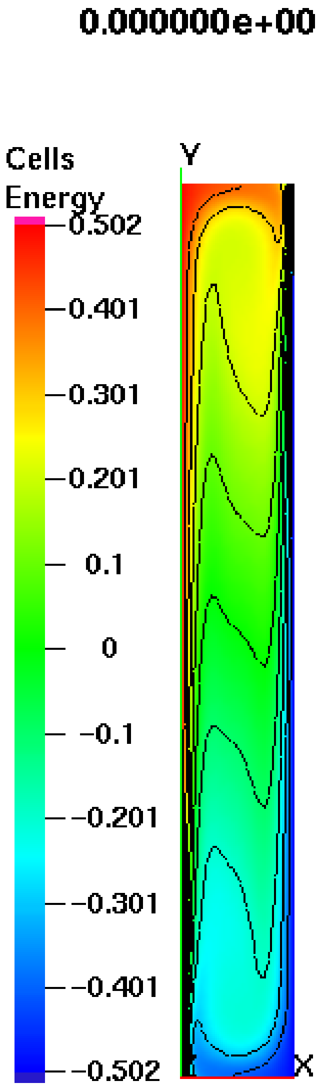




250 Mill. d.o.f.s are possible on HELICS LINUX cluster !

LOCAL MPSC: Natural Convection (MIT/01)





$$\mathbf{Ra} = 3.0 \cdot 10^5 \quad , \quad \mathbf{Pr} = 0.71$$

$$\nu_u = \sqrt{Pr/Ra} \approx 1.5 \cdot 10^{-3}$$

$$\nu_T = \sqrt{1/PrRa} \approx 2.1 \cdot 10^{-3}$$

(max. patchsize 64 elements,
SD-stabilization)

	Nonlinear Solver (γ)	
#NEL/#NEQ	Fixed Point	Newton
1.408/10.000	55/2.1	11/2.5
5.632/40.000	70/1.9	8/2.4
22.528/160.000	54/1.8	5/2.0

Mathematical Design Aspects for CFD

Combination of high accuracy of **Galerkin-type methods** *with high efficiency of* **operator splitting-type solvers** *via* **multigrid coupling** *is possible !*

Robust *solvers for NS-like subproblems are available !*

Residual-based *a posteriori error control in space/time with dual solutions based on* **meanvalue** *functionals in* **space/time** *is aimed ?*

$$\Downarrow$$

Future CFD Software !

Future CFD Software

Implicit FEM schemes in space/time, adaptivity, FCT/TVD, Newton/multigrid, operator splitting...

+

1 PC in 10 years $\approx$ 1 CRAY T3E today !!!

???

Typical Performance Measurements

‘Generalized Tensorproduct’ meshes

2D case	NEQ	MV-STO(ROW)	MV-SBB-V	MV-SBB-C
DEC 21264	65^2	178 (205)	538	795
(667 MHz)	257^2	110 (224)	358	1010
‘ES40’	1025^2	11 (78)	158	813

SPARSE **MV techniques** (STO/ROW)

MFLOP/s rates vs. ‘Peak Performance’ on **unstructured** meshes ???

SPARSE BANDED **MV techniques** (SBB)

‘Supercomputing’ (up to 1 GFLOP/s) vs. FEM for complex domains ???

Consequences

‘Special requirements for numerical

and algorithmic approaches in

correspondance to existing hardware !!!’

$$\Downarrow$$

‘Hardware-Oriented Numerics for PDEs (?)’

'Hardware-Oriented Numerics

I) *Patch-oriented adaptivity*

'Many' tensorproduct grids (SBB)
'Few' unstructured grids (SPARSE)

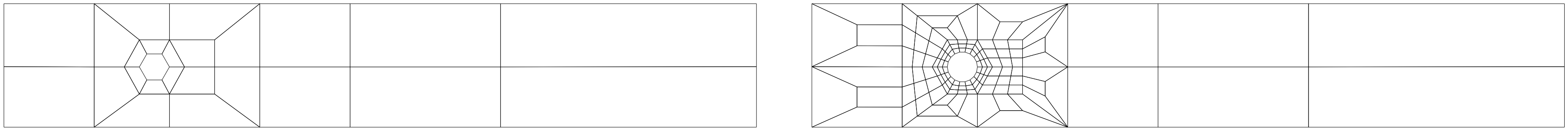
II) *Generalized MG-DD solver:* SCARC

Exploit locally 'regular' structures **(efficiency)**
Recursive 'clustering' of anisotropies **(robustness)**
'Strong local solvers improve global convergence !'

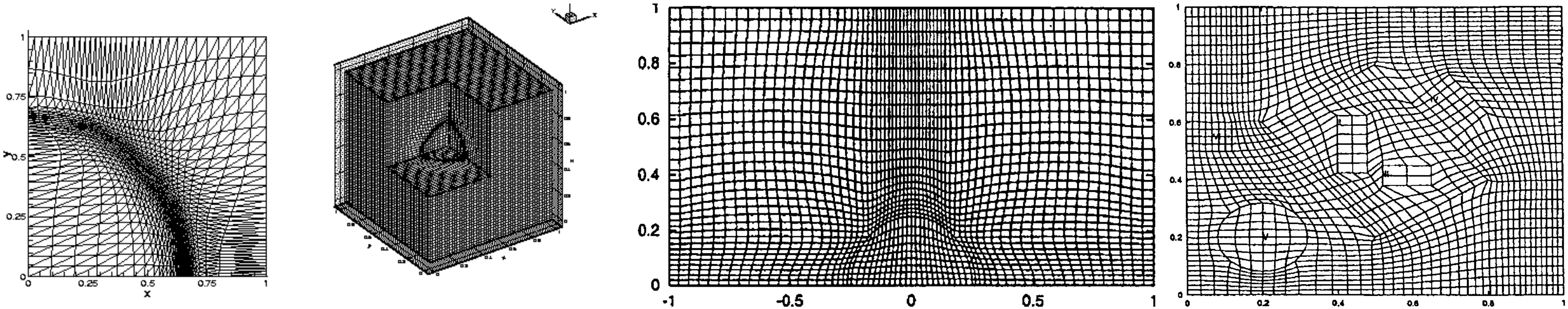
'Exploit locally regular structures !!!'

Concepts for Adaptive Meshing

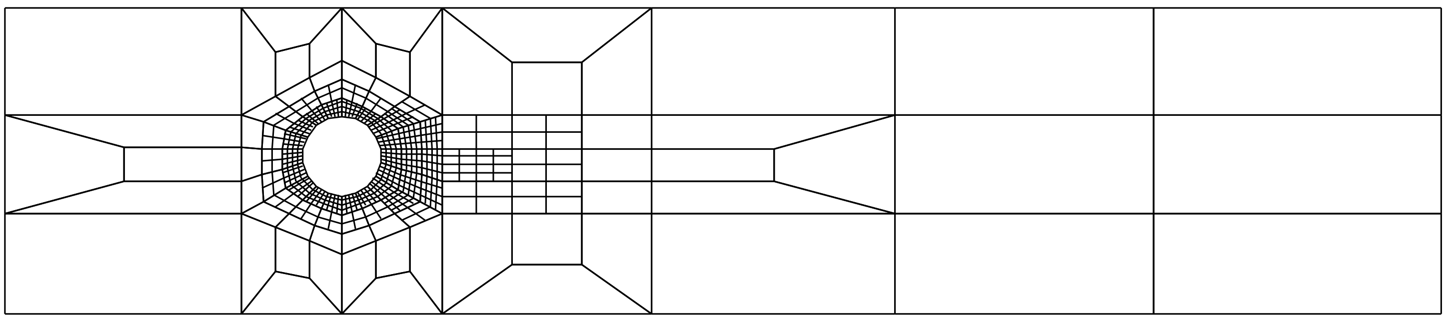
1) macro-oriented adaptivity



2) patchwise ‘deformation’ adaptivity



3) (patchwise) ‘local’ adaptivity



Example for ScaRC

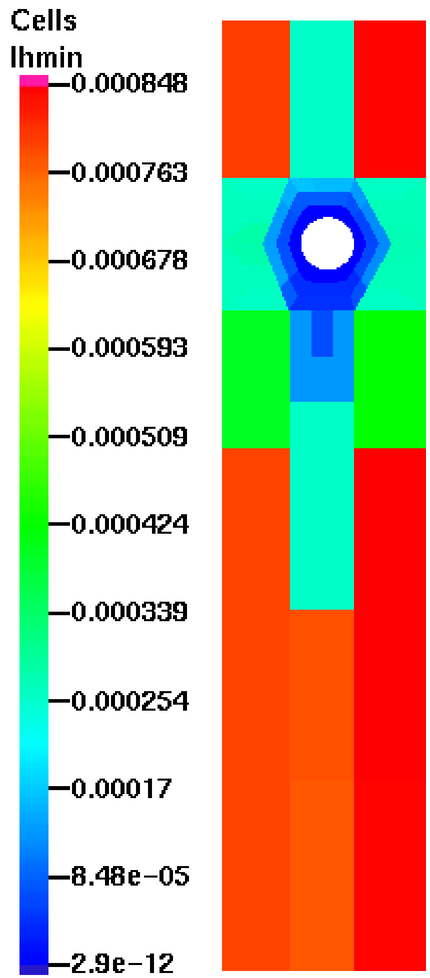
Parallel convergence rates for ScaRC-CG (2 global smoothing, V-cycle; 2 local 'MGTRI', F-cycle) with direct coarse mesh solver

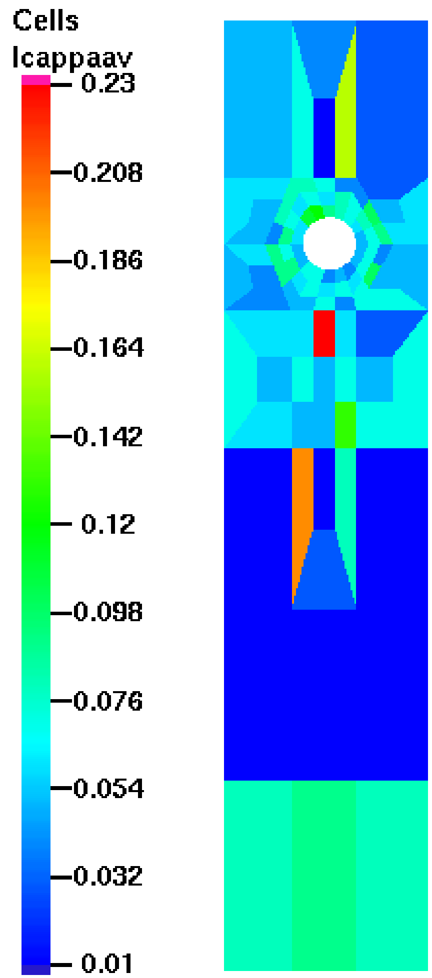
#NEQ-global	AR	$\rho\,(\#IT)$
1,704	3	0.03 (5)
44,544	3	0.03 (5)
431,317	10	0.09 (6)
1,722,773	10	0.08 (6)
9,344,533	10	0.09 (6)
37,366,805	10^7	0.09 (6)

Global (parallel) convergence rates

#NEQ-local	MV-V/C	MGTRI-V/C
65^2	245/1275	299/706
257^2	193/638	173/382
1025^2	168/614	146/288

Local MFLOP/s rates (AMD 'XP 1500+')





Conclusions

There is a huge potential...

There is much to do...:-)