A new fast and accurate grid deformation method for adaptivity on locally structured grids

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Overview

Overview

FEAST Finite Element Analysis and Solution Tools

- under development at TU Dortmund in Stefan Turek's group
- http://www.feast.tu-dortmund.de

Core features

- separation of unstructured and structured data for optimised linear algebra components
- Finite Element discretisations (Q_1)
- parallel generalised domain decomposition multigrid solvers
- usage of GPUs as coprocessors
- grid adaptivity and error control
- scalar and vector-valued problems
- applications in CFD and CSM

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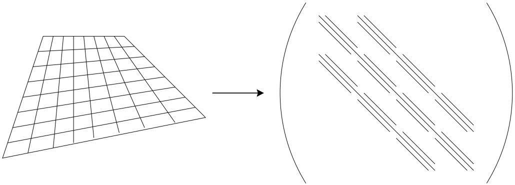
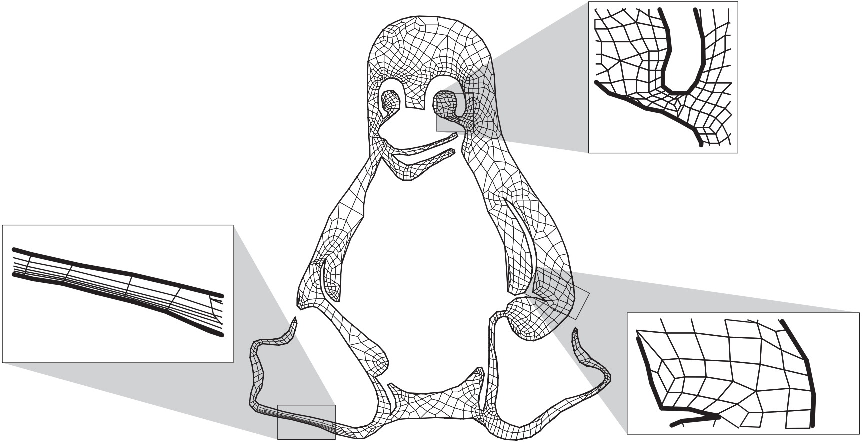
local band matrices

- Poisson equation
- generalised tensor product mesh
- conforming bilinear Finite Elements Q_1
- matrix consists of 9 bands



FEAST grids



data structures

Cover domain by unstructured collection of subdomains

- resolve complex geometries, boundary layers in fluid dynamics, etc.

Refine each subdomain independently and discretise using FEs

- generalised tensorproduct fashion
- isotropic and anisotropic refinement combined with r/h/rh adaptivity

Performance

- clear separation of globally unstructured and locally structured parts
- nonzero pattern of local FE matrices known a priori
- exploit spatial and temporal locality for tuned LA building blocks (Sparse Banded BLAS)

ScaRC solver

Contradictory properties

- numerical vs. computational efficiency
- weak and strong scalability vs. numerical scalability

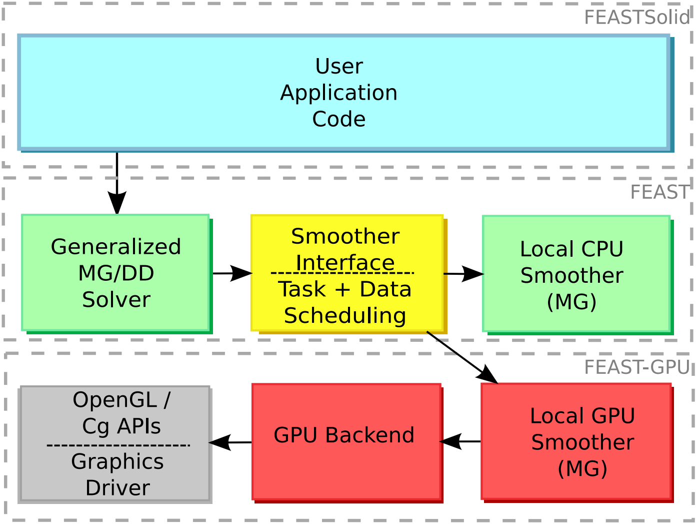
Parallel multigrid

- strong recursive coupling optimal in serial codes
- usually relaxed to block-Jacobi due to high comm requirements
- degrades convergence rates in the presence of local anisotropies

Generalised DD/MG approach (ScaRC)

- global MG, block-smoothed by local MGs (optimal asymptotic complexity)
- hide anisotropies locally
- good scalability by design
- global operations realised via special local BCs and syncronisation across subdomain boundaries (no overlap!)

Overview of GPU integration



Overview

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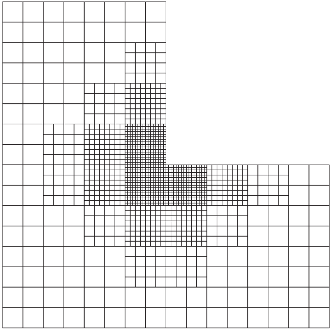
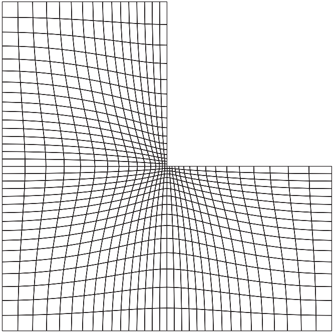
h-adaptivity
(h: mesh width)



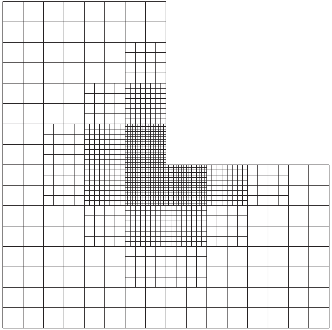
r-adaptivity
(r: "relocate")



grid deformation: building block for *r*-adaptivity

adaptivity concepts in FEM

h-adaptivity
(h: mesh width)



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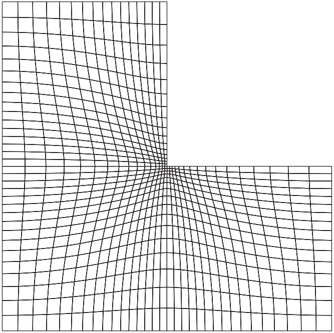
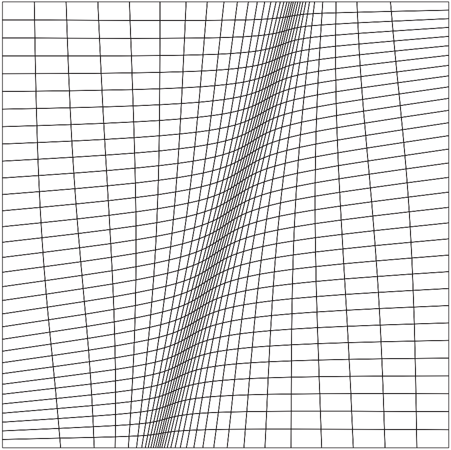


grid deformation: building block for *r*-adaptivity flexibility



observation: MFlop/s-rate ≪ peak performance

example: AMD Opteron 852, peak performance : 4280 MFlop/s

$y = Ax$, Poisson equation, N unknowns, Q_1:

NEQ	SP-MOD	SP-STO	SBB-V (FEAST)
4.225	557	561	1.805
66.049	395	223	660
1.050.625	391	75	591

- SP-STO: ca. 2% of peak performance (worst case)
- FEAST: ca. 15% of peak performance (worst case)

⇒ acceleration by factor 8

FEAST: local logical tensor product grids

goal: adaptivity with local structured grids!

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Overview

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derivation

- domain Ω
- triangulation $\mathcal{T}$, quads T
- "monitor function" $0 < \varepsilon_f < f \in \mathcal{C}^1(\bar{\Omega})$: desired area distribution
- "weighting function" $0 < \varepsilon_g < g \in \mathcal{C}^1(\bar{\Omega})$: current area distribution

goal: mapping $\Phi : \Omega \to \Omega$ with

$$g(x)|J\Phi(x)| = f(\Phi(x)) \quad \forall x \in \Omega$$

and

$$\Phi : \partial\Omega \to \partial\Omega.$$

$$\mathcal{T}^d = \Phi(\mathcal{T}), \quad X := \Phi(x)$$

derivation II

$$m(\Phi(T)) := \int_{\Phi(T)} 1 \, dx = \int_T |J\Phi(x)| dx,$$

1×1 Gauss formula:

$$g(x_c)\frac{m(\Phi(T))}{m(T)} = f(\Phi(x_c)) + \mathcal{O}(h).$$

If

$$g(x) = ch^{-2}\, m(T) + \mathcal{O}(h), x \in T$$

holds, then

$$ch^{-2}\, m(\Phi(T)) = f(\Phi(x_c)) + \mathcal{O}(h)$$

Deformation$(f, \mathcal{T})$

compute $\tilde{f} - \tilde{g}$, $\quad \tilde{f} := c/f, \tilde{g} = C/g, \int \tilde{f} \stackrel{!}{=} \int \tilde{g}$

solve $-\mathrm{div}(v(x)) = \tilde{f}(x) - \tilde{g}(x),\ x \in \Omega, \qquad v(x) \cdot \mathfrak{n} = 0,\ x \in \partial\Omega$

DO FORALL $x \in \mathcal{T}$

solve
$$\partial_t \varphi(x,t) = \frac{v(\varphi(x,t),t)}{t\tilde{f}(\varphi(x,t)) + (1-t)\tilde{g}(\varphi(x,t))}, \quad 0 \le t \le 1,\ \varphi(x,0) = x$$

$\Phi(x) := \varphi(x,1)$

ENDDO

END Deformation

realisation: $v := \nabla w \Rightarrow -\Delta w = \tilde{f} - \tilde{g}, \quad \partial_{\mathfrak{n}} w = 0$ auf $\partial\Omega$

total amount:

1 Poisson problem + $2N$ decoupled IVPs

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assumptions:

Let $(\mathcal{T}_i)_{i\in I}, N_i < N_{i+1}$ with

$$h_i := \max_{e\in\mathcal{E}_i} |e| = \mathcal{O}(N_i^{-1/2}) \quad \forall i \in I \text{(edge-length regularity)}$$

$$\exists 0 < c, C : ch_i^2 \leq m(T) \leq Ch_i^2 \quad \forall T \in \mathcal{T}_i \, \forall i \in I \text{ (size regularity)}$$

$$\exists\, 0 < g_{\min} < g < g_{\max} < \infty:$$

$$\frac{1}{h_i^2} c_i m(T) = g(x) + \mathcal{O}(h_i) \quad \forall x \in T \quad \forall T \in \mathcal{T}_i \forall i \in I, \quad c_s \leq c_i \leq C_s$$

(similarity condition)

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(similarity condition)

1. approach: comparison with "reference deformation": $||\Phi_h - \Phi|| \rightarrow 0$

but:

- Φ unique only by $\mathrm{curl} v \stackrel{!}{=} 0$
- $||\Phi_h - \Phi||$ hard to compute

2. approach: $q(x) = \frac{f(x)}{g(x)} - 1 \stackrel{!}{\approx} 0 \Rightarrow$

$$Q_0 := ||q||_{L^2(\Omega)}, \quad Q_\infty := ||q||_{L^\infty(\Omega)}$$

convergence: $\Leftrightarrow$

$$Q_0 \rightarrow 0, Q_\infty \rightarrow 0 \text{ for } h \rightarrow 0$$

Let $(\mathcal{T}_i)_{i\in I}$ be edge-length regular and fulfil the similarity condition, $0 < \varepsilon < f \in \mathcal{C}^1(\bar{\Omega})$. Further, $||\nabla w - G_h w_h||_\infty = \mathcal{O}(h^{1+\delta})$, $\delta > 0$ and $||X_h - \tilde{X}|| = \mathcal{O}(h^{1+\delta})$.

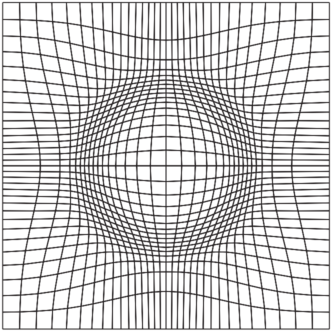
Then:

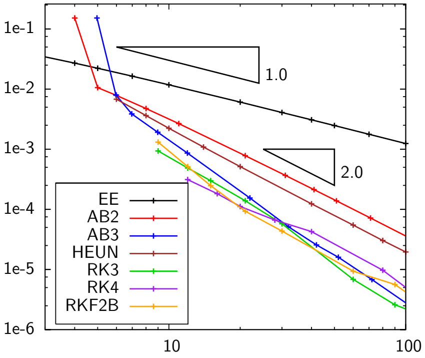
- $(\tilde{\mathcal{T}}_i)_{i\in I}$ is edge-length regular.
- $(\tilde{\mathcal{T}}_i)_{i\in I}$ is size regular.
- $\exists c > 0$:
$$Q_0 \leq ch^{\min\{1,\delta\}}, \quad Q_\infty \leq ch^{\min\{1,\delta\}}.$$

$\Omega = [0,1]^2$, tensor product mesh,

$$f(x) = \min\left\{1, \max\left\{\frac{|d - 0,25|}{0,25}, \varepsilon\right\}\right\}, \quad d := \sqrt{\left(x_1 - \tfrac{1}{2}\right)^2 + \left(x_2 - \tfrac{1}{2}\right)^2}$$

convergence of IVP solvers



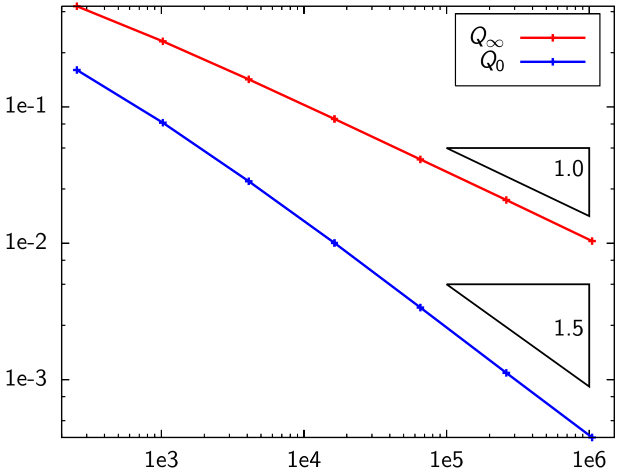


assumption:

$||\nabla w - G_h(w_h)||_\infty = \mathcal{O}(h^2) \Rightarrow \delta = 1$

$\delta = 1 \Rightarrow \Delta t = \mathcal{O}(1/\sqrt{N})$

test problem: convergence



$$Q_\infty = \mathcal{O}(h), \quad Q_0 = \mathcal{O}(h^{3/2})$$

Overview

deformation IVPs:

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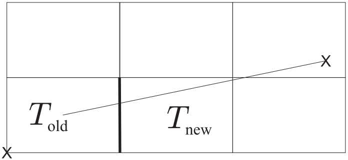
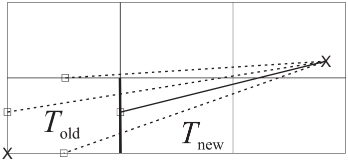
evaluation of FEM functions $\Rightarrow$ grid search



raytracing search



distance search

searching times [s]

NEL	distance	β	raytracing	β	brute force	β
256	$5.15 \cdot 10^{-3}$	-	$5.40 \cdot 10^{-3}$	-	$1.34 \cdot 10^{-1}$	-
1,024	$2.27 \cdot 10^{-2}$	4.41	$2.20 \cdot 10^{-2}$	4.07	$2.13 \cdot 10^{0}$	15.9
4,096	$9.48 \cdot 10^{-2}$	4.17	$9.52 \cdot 10^{-2}$	4.32	$3.53 \cdot 10^{1}$	16.6
16,384	$4.27 \cdot 10^{-1}$	4.50	$4.55 \cdot 10^{-1}$	4.78	$5.59 \cdot 10^{2}$	15.8
65,536	$2.05 \cdot 10^{0}$	4.80	$2.38 \cdot 10^{0}$	5.23	$9.79 \cdot 10^{3}$	17.5
262,144	$1.12 \cdot 10^{1}$	5.46	$1.41 \cdot 10^{1}$	5.92	-	-
1,048,576	$6.77 \cdot 10^{1}$	6.05	$9.33 \cdot 10^{1}$	6.61	-	-

Overview

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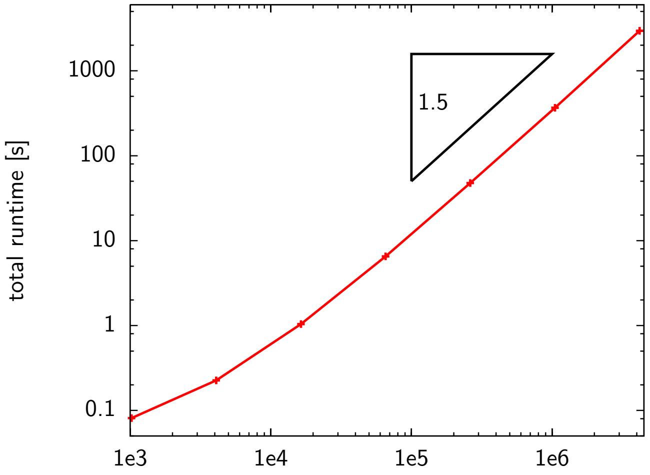

complexity: $\mathcal{O}(N^{3/2})$

- deformation on coarse grid
- regular refinement
- deformation on fine grid (correction step)

assumption 1:

$$d_k := \max_{x \in \mathcal{X}_k} ||x - \Phi(x)|| \stackrel{?!}{=} \mathcal{O}(h^2)$$

assumption 2:

$$\frac{||X_h - \tilde{X}||}{||x - \Phi(x)||} \leq c$$

$$\Rightarrow ||X_h - \tilde{X}|| = \mathcal{O}(h^2)$$

under these assumptions:

convergence + complexity $\mathcal{O}(N)$

multilevel def: basic idea

- deformation on coarse grid
- regular refinement
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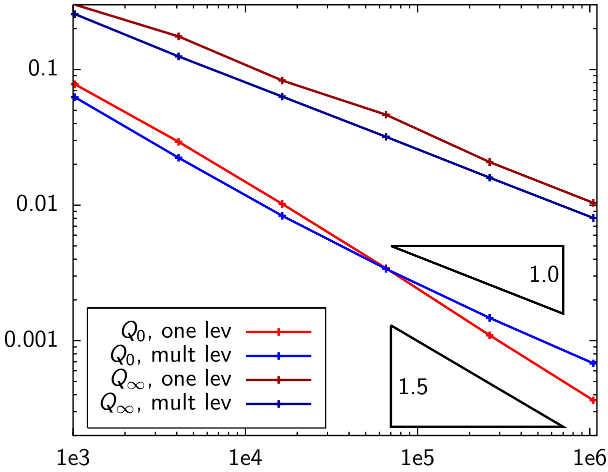
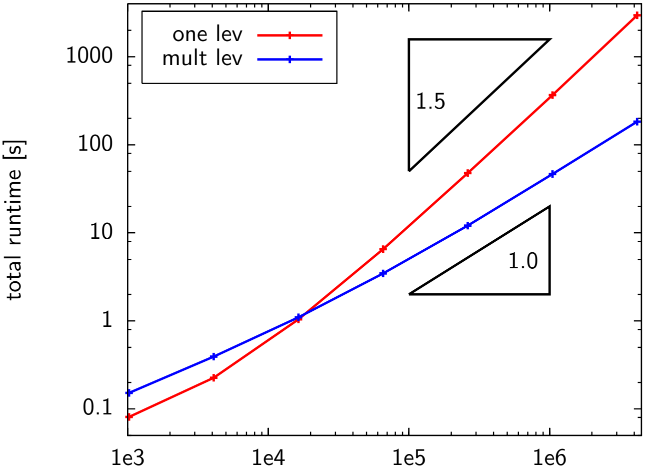


convergence despite of fixed time step size

multilevel deformation: complexity



optimal complexity

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r-AFEM

$GRID_1 := GRID$

DO $i = 1,\ i_{\max}$

$u_i :=$ **SOLVE**$(f, g, GRID_i)$

$\eta_i :=$**ESTIMATE**(u_i, J)

IF $(\eta_i < TOL)$ EXIT LOOP

$f_{mon,i} :=$**MON**(η_i)

$GRID_{i+1} :=$ **DEFORM**$(f_{mon,i},\ GRID_i)$
IF ($\exists$ non-convex elements) RETURN

END DO

$J(u_h) := J(u_i);\ \eta := \eta_i$

RETURN $J(u_h), \eta$

END r-AFEM

$$Mon(v)(x) := [-c_1 \ln(\mathbf{Smooth}_i(v(x))) + c_2] \cdot \mathrm{area}(x)$$

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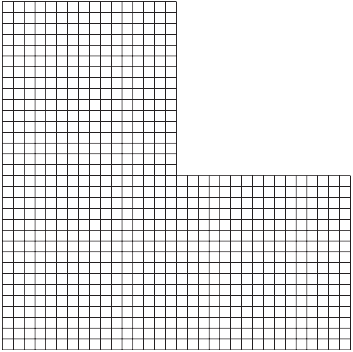


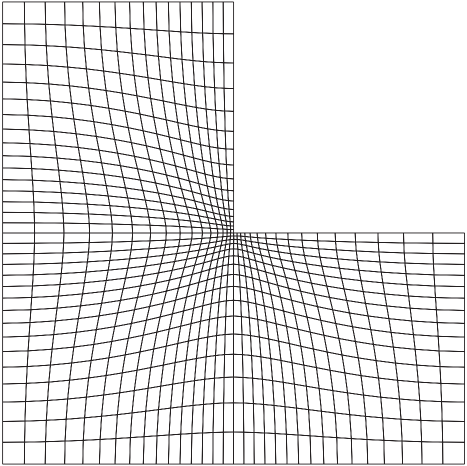
Poisson equation

$\Omega = [-0.5, 0.5]^2 / [0, 0.5]^2$

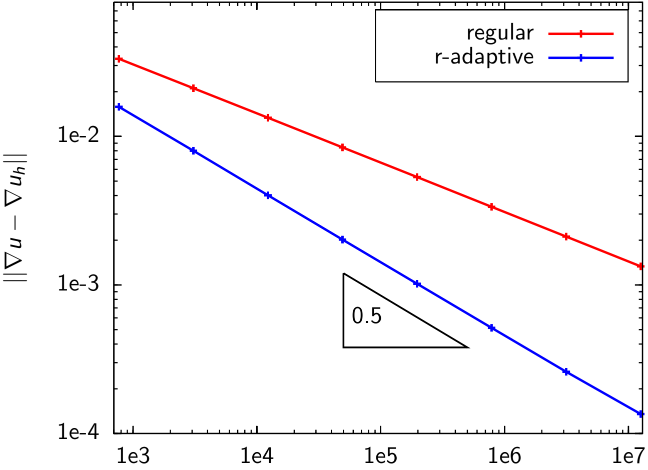
$u(r, \varphi) = r^{2/3} \sin(2/3\varphi)$

desired: gradient error

r-adapted mesh



gradient error

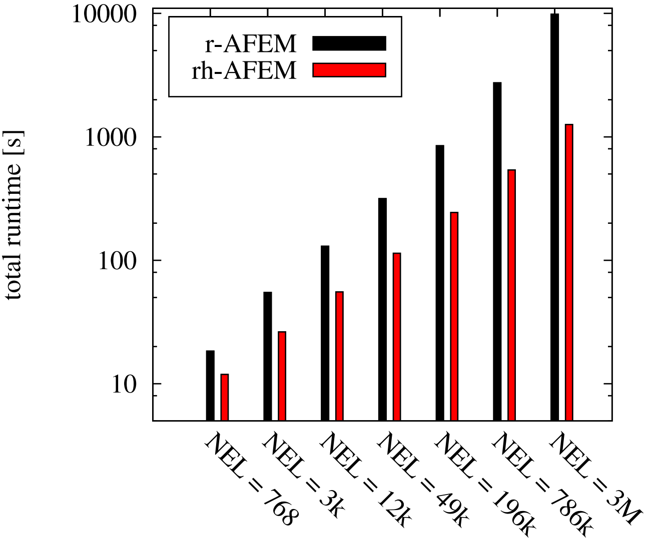


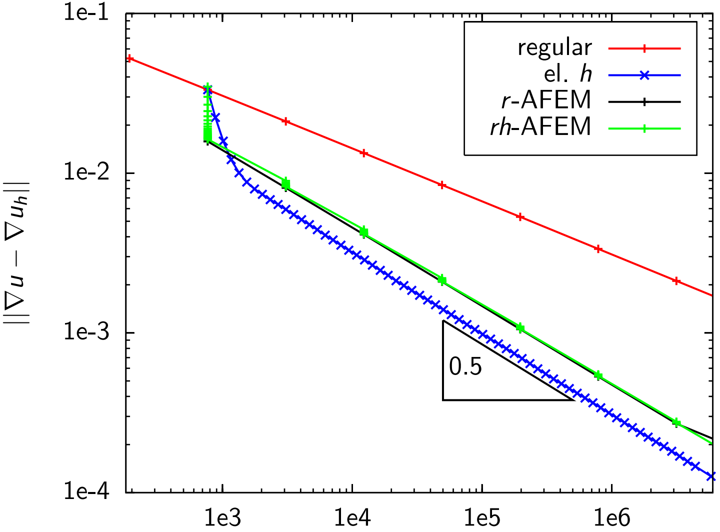
optimal rate of convergence by r-adaptivity

rh-**AFEM**

```
η_0 := ∞
GRID_1 := GRID
DO i = i_{lev,min}, i_{lev,max}
    DO j = 1, i_{max,r}
        u_j := SOLVE(f, g, GRID_j)
        η_j := ESTIMATE(u_j, J)
        IF (η_j < TOL) THEN
           J(u_h) := J(u_j); η := η_j
           RETURN J(u_h), η
        END IF
        IF (η_j > c_r η_{j-1}) EXIT LOOP
        f_{mon,j} := MON(η_j)
        GRID_{j+1} := DEFORM(f_{mon,j}, GRID_j)
        IF (∃ non-convex elements) RETURN
    END DO
    GRID_1 := PROLONGATE(GRID_j)
END DO
J(u_h) := J(u_j); η := η_j
END rh-AFEM
```

comparison of runtime




1e-1
1e-2
1e-3
1e-4
1e3
1e4
1e5
1e6
$||\nabla u - \nabla u_h||$
regular
el. h
r-AFEM
rh-AFEM
0.5

Overview

problem setting and example

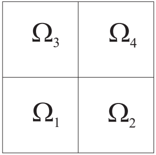
generalised Poisson equation:

$$-\mathrm{div}(D\cdot\nabla u) = f, \quad D = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

weak formulation:

$$(D \cdot \nabla u, \nabla\varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1.$$

test example: $\Omega = [0,1]^2, k_1 = 1000, k_2 = 1$



$$\theta = \begin{cases} -\pi/6 & , \quad x \in \Omega_1 \cup \Omega_4 \\ \pi/6 & , \quad x \in \Omega_2 \cup \Omega_3 \end{cases}.$$

$$f(x) = \begin{cases} \frac{1}{|\omega|} & , \quad x \in \omega \\ 0 & , \quad x \notin \omega \end{cases}, \quad \omega = [7/18, 11/18]^2.$$

desired: point error in $(1/4, 1/4)$

$$(\nabla u, \nabla \varphi) = (f, \varphi) \quad \forall \varphi \in H_0^1, u|_{\partial\Omega} = 0$$

desired: evaluation of derived quantities

- $J_{x_0}(\varphi) := \varphi(x_0)$ (point evaluation),
- $J_\Gamma(\varphi) := \int_\Gamma \partial_\mathfrak{n} \varphi ds$ (evaluation along a line),
- $J_{D/L}(\varphi, \chi) := \int_\Gamma \mathfrak{n} \cdot \sigma(\varphi, \chi) \cdot \mathfrak{e}_{x/y}\, ds$ (lift /drag computation).

dual problem:

$$(\nabla z, \nabla \varphi) = J(\varphi) \quad \forall \varphi \in H_0^1$$

$$\begin{aligned}
|J(u-u_h)| &= |(\nabla u, \nabla z) - (\nabla u_h, \nabla z)| \\
&= |(f, z-\varphi_h) - (\nabla u_h, \nabla(z-\varphi_h))| \quad \forall \varphi_h \in V_h \\
&= \left| \sum_{T\in\mathbb{T}} (f, z-\varphi_h)_T - (\nabla u_h, \nabla(z-\varphi_h))_T \right| \forall \varphi_h \in V_h \\
&\approx \left| \sum_{T\in\mathbb{T}} (f, \tilde{z}-z_h)_T - (\nabla u_h, \nabla(\tilde{z}-z_h))_T \right|
\end{aligned}$$

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\end{aligned}$$

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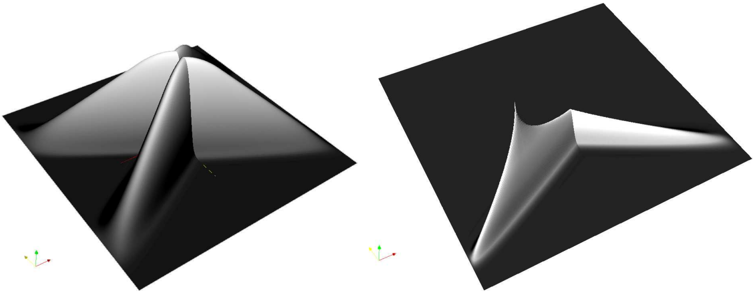
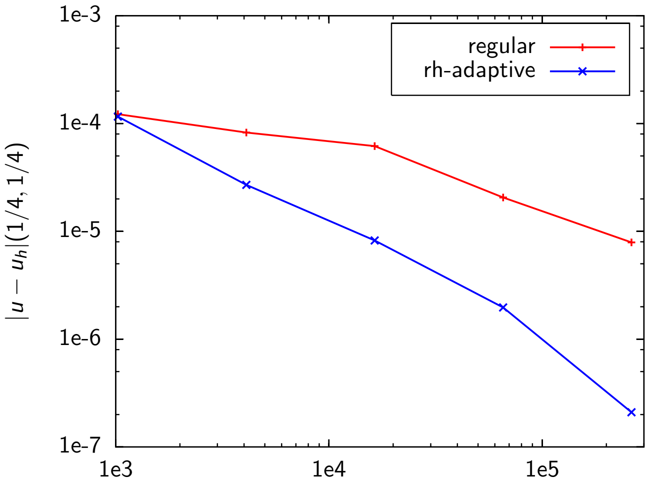
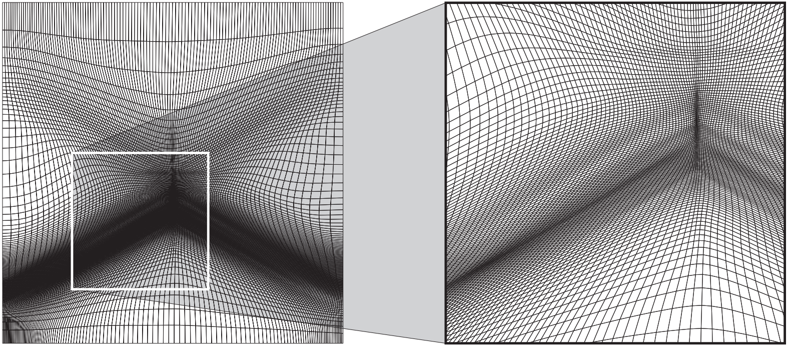
\end{aligned}$$

primal and dual solution

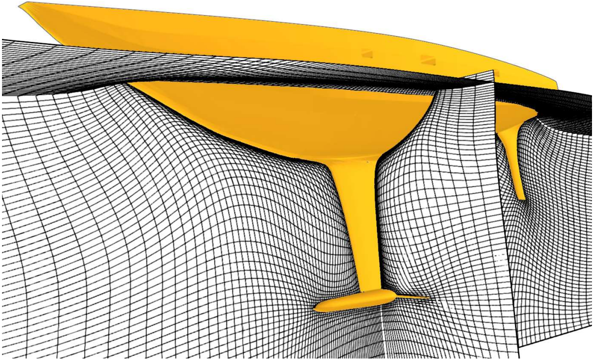



1e-3
1e-4
1e-5
1e-6
1e-7
1e3
1e4
1e5
$|u - u_h|(1/4, 1/4)$
regular
rh-adaptive

r-adapted grid



advanced application: CFD



- incompressible Navier-Stokes equation (3D)
- based upon FeatFlow
- fictitious boundary technique

[picture: Matthias Miemczyk]

the (current) core FEAST-team:

- Christian Becker (ScaRC, software design)
- Sven Buijssen (CFD, kernel development)
- Dominik Göddeke (GPU integration)
- Matthias Grajewski (error control & adaptivity, kernel development)
- Stefan Turek (founder, sponsor, SBBLAS)
- Hilmar Wobker (CSM, kernel development)

Summary

- Finite Element code
- local band matrices
- generalised DD/MG approach (ScaRC)
- GPU integration
- MFLOP/s preserving adaptivity
- grid deformation
- multilevel deformation
- *r*- and *rh*-adaptivity
- anisotropic diffusion
- www.feast.tu-dortmund.de

Thank you for your attention!