A fast and accurate method for grid deformation

Matthias Grajewski

Matthias.Grajewski@math.uni-dortmund.de

University of Dortmund

Overview

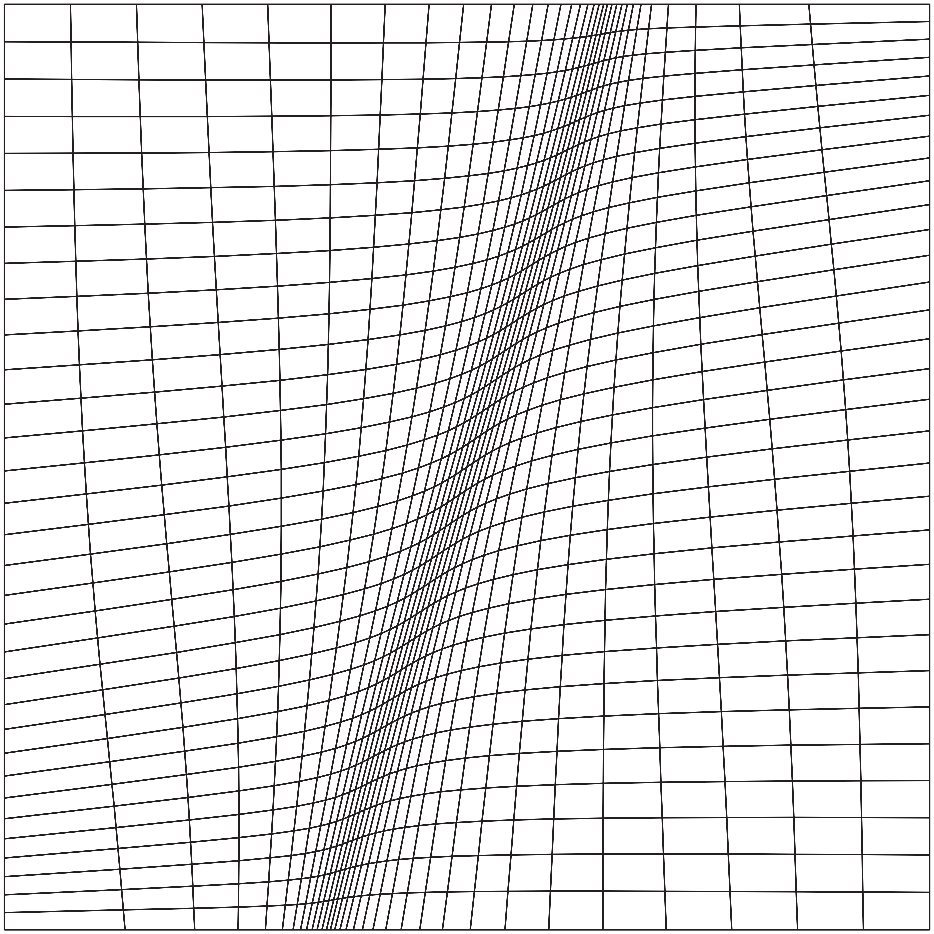
- Motivation
- Grid deformation: derivation and convergence aspects
- Multilevel deformation
- r-adaptivity

Why Grid Deformation?

main reason: building block for r-adaptivity

Why r-Adaptivity?

1. reason: flexibility



Why r-Adaptivity?

2. reason: **SPEED**

FEM example:

- tensor product mesh
- Q_1 FE, Laplace eq., equidistant grid
- for lexicographical ordering: 9 nonzero bands

Why r-Adaptivity?

2. reason: **SPEED**

FEM example:

- tensor product mesh
- Q_1 FE, Laplace eq., equidistant grid
- for lexicographical ordering: 9 nonzero bands

MV-multiplication in **FEATFLOW** (F77-code):

	N	SP-MOD	SP-STO	SBB-V
AMD Opteron 852	4.225	557	561	1805
2,6 Ghz	66.049	395	223	660
4280 MFLOP/s	1.050.625	391	75	591

from: PhD thesis Chr. Becker 2007

Why r-Adaptivity?

2. reason: **SPEED**

FEM example:

- tensor product mesh
- Q_1 FE, Laplace eq., equidistant grid
- for lexicographical ordering: 9 nonzero bands

MV-multiplication in **FEATFLOW** (F77-code):

	N	SP-MOD	SP-STO	SBB-V
AMD Opteron 852	4.225	557	561	1805
2,6 Ghz	66.049	395	223	660
4280 MFLOP/s	1.050.625	391	75	591

from: PhD thesis Chr. Becker 2007

observation: AFEM: MFlop/s-Rate $\ll$ peak performance

Why r-Adaptivity?

Reference machine: AMD Opteron 852

- peak performance: 4.3 GFlop/s
- peak memory bandwidth: 5.96 GB/s

$\Rightarrow$ peak performance, if ≈ 6 flops per memory access

Why r-Adaptivity?

Reference machine: AMD Opteron 852

- peak performance: 4.3 GFlop/s
- peak memory bandwidth: 5.96 GB/s

$\Rightarrow$ peak performance, if ≈ 6 flops per memory access

$y = Ax$, N unknowns:

	classical CSR	FEAST (bands)
flops	17 N	17 N
loads	27 N	18 N
stores	1 N	1 N

arithmetic intensity:

- CSR: $17/28 \ll 1 \Rightarrow \approx 9\%$ of peak performance
- FEAST: $17/19 \leq 1 \Rightarrow \approx 15\%$ of peak performance

Why r-Adaptivity?

Reference machine: AMD Opteron 852

- peak performance: 4.3 GFlop/s
- peak memory bandwidth: 5.96 GB/s

$\Rightarrow$ peak performance, if ≈ 6 flops per memory access

$y = Ax$, N unknowns:

	classical CSR	FEAST (bands)
flops	17 N	17 N
loads	27 N	18 N
stores	1 N	1 N

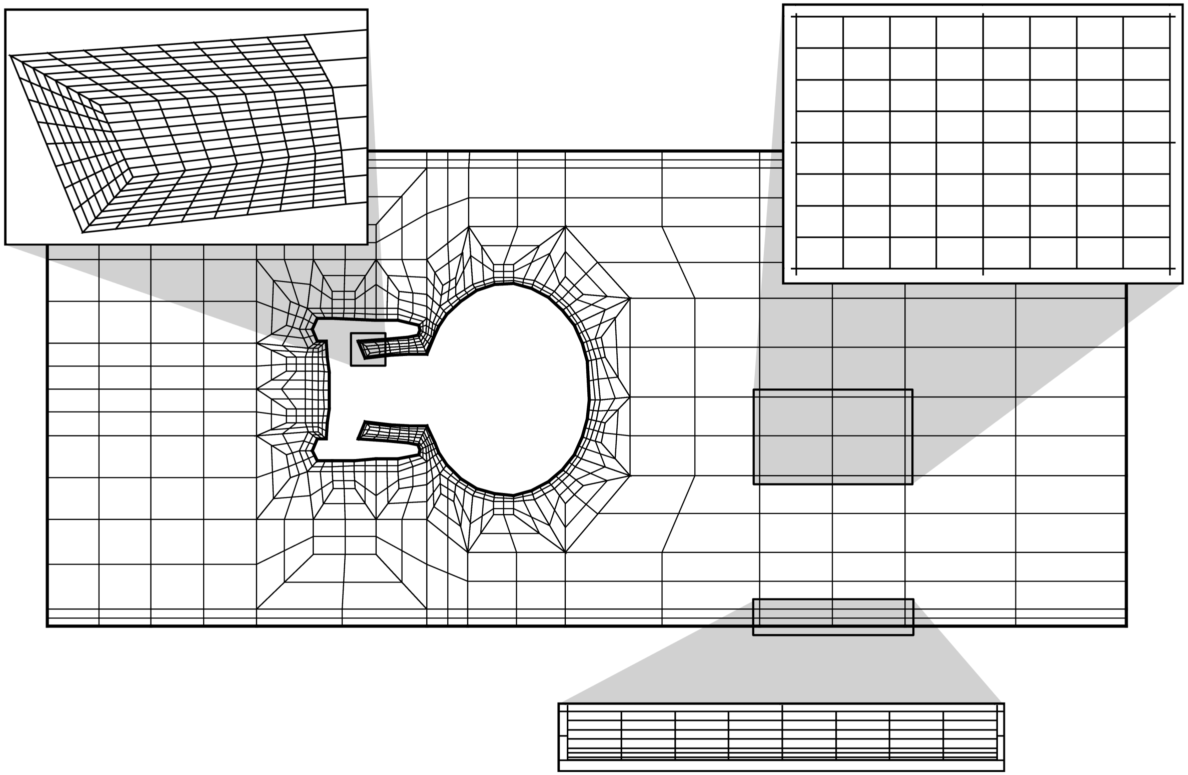
arithmetic intensity:

- CSR: $17/28 \ll 1 \Rightarrow \approx 9\%$ of peak performance
- FEAST: $17/19 \leq 1 \Rightarrow \approx 15\%$ of peak performance

Avoid unstructured meshes!

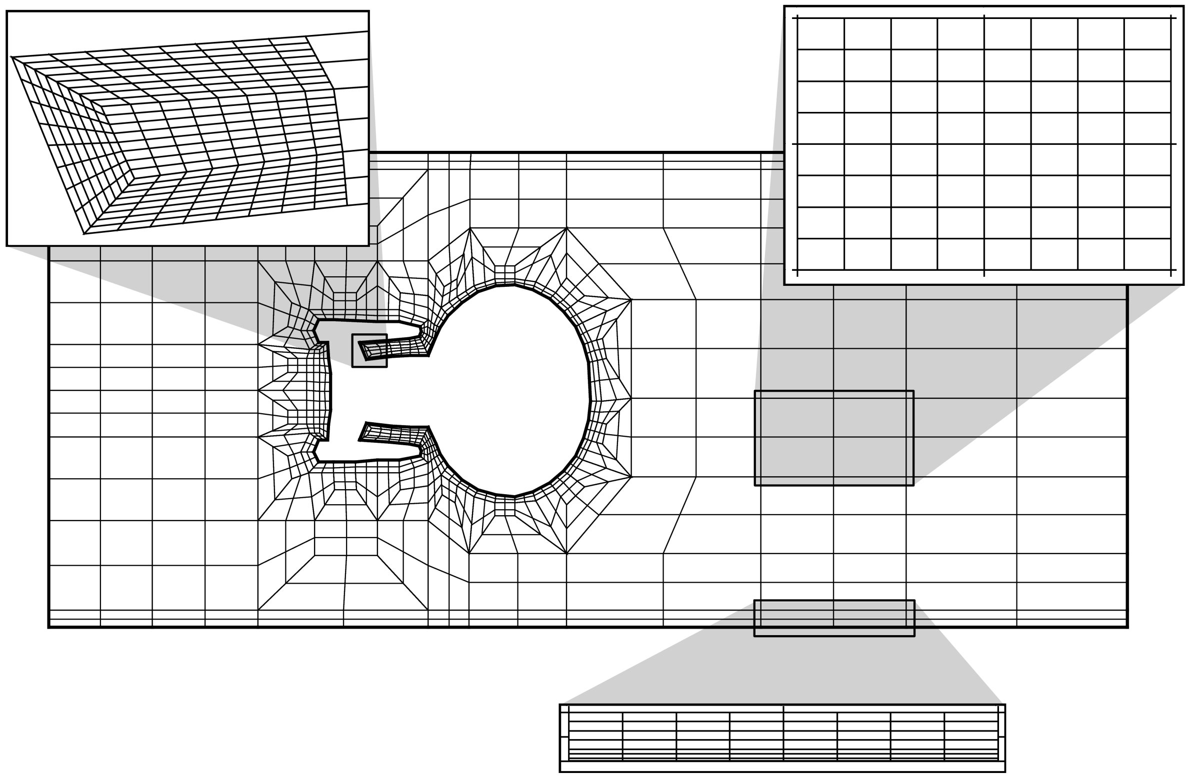
FEAST-Concept (Grid-Related Part)

global grid: “many” local generalised tensor product meshes (“macros”).



FEAST-Concept (Grid-Related Part)

global grid: "many" local generalised tensor product meshes ("macros").



r-adaptivity

Derivation

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

goal: transformation $\Phi : \Omega \to \Omega$ 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

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

Derivation

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

1×1 Gauss-formula:

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

Derivation

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

1×1 Gauss-formula:

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

If

$$g(x) = c(h)\, m(T) + \mathcal{O}(h), x \in T$$

holds, then

Derivation

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

1×1 Gauss-formula:

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

If

$$g(x) = c(h)\, m(T) + \mathcal{O}(h), x \in T$$

holds, then

$$c\, m(\Phi(T)) = f(\Phi(x_c)) + \mathcal{O}(h)$$

Grid Deformation Method

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

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

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

ENDDO

END Deformation

Theoretical Results

Theorem(Moser) Let $0 \geq k \in \mathbb{N}$, $\alpha > 0$. Let $\Omega \subset \mathbb{R}^n$ a domain with $\mathcal{C}^{3+k,\alpha}$-smooth boundary. Let $f, g \in \mathcal{C}^{k,\alpha}(\bar{\Omega})$ with $\int_\Omega f = \int_\Omega g$. Then there is a $\mathcal{C}^{k+1,\alpha}$-diffeomorphism $\Phi : \bar{\Omega} \to \mathbb{R}^n$ with

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

and

$$\Phi(x) = x \quad \forall x \in \partial\Omega.$$

Theoretical Results

Theorem(Moser) Let $0 \geq k \in \mathbb{N}$, $\alpha > 0$. Let $\Omega \subset \mathbb{R}^n$ a domain with $\mathcal{C}^{3+k,\alpha}$-smooth boundary. Let $f, g \in \mathcal{C}^{k,\alpha}(\bar{\Omega})$ with $\int_\Omega f = \int_\Omega g$. Then there is a $\mathcal{C}^{k+1,\alpha}$-diffeomorphism $\Phi : \bar{\Omega} \rightarrow \mathbb{R}^n$ with

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

and

$$\Phi(x) = x \quad \forall x \in \partial\Omega.$$

Theorem Let be Ω as above. If $\Phi : \Omega \rightarrow \Omega$ exists, it fulfills the aforementioned conditions.

Measuring the Error and Convergence

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

$$h_i := \max_{e \in \mathcal{E}_i} |e| = \mathcal{O}(N_i^{-0.5}) \quad \forall i \in I \text{ (edge-length regularity)}$$

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

Measuring the Error and Convergence

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

$$h_i := \max_{e \in \mathcal{E}_i} |e| = \mathcal{O}(N_i^{-0.5}) \quad \forall i \in I \text{ (edge-length regularity)}$$

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

similarity condition: $\exists 0 < g_{\min} < g < g_{\max} < \infty$ with

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

Measuring the Error and Convergence

1. approach: comparison with "reference deformation":

$||\Phi_h - \Phi|| \longrightarrow 0$

Measuring the Error and Convergence

1. approach: comparison with “reference deformation”:
$||\Phi_h - \Phi|| \longrightarrow 0$

problems:

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

Measuring the Error and Convergence

1. approach: comparison with “reference deformation”:
$||\Phi_h - \Phi|| \to 0$

problems:

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

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

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

Measuring the Error and Convergence

1. approach: comparison with “reference deformation”:
$||\Phi_h - \Phi|| \longrightarrow 0$

problems:

- Φ unique only by $\mathrm{curl} v \stackrel{!}{=} 0$
- $||\Phi_h - \Phi||$ difficult 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 $:\Leftrightarrow Q_0 \rightarrow 0, Q_\infty \rightarrow 0, h \rightarrow 0$

Convergence Theorem

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

Then:

a) $(\tilde{\mathcal{T}}_i)_{i\in I}$ is edge-length regular.

b) $(\tilde{\mathcal{T}}_i)_{i\in I}$ is size regular.

c) $\exists c > 0$:

$$Q_0 \leq c h^{\min\{1,\delta\}}, \quad Q_\infty \leq c h^{\min\{1,\delta\}}.$$

Test Problem

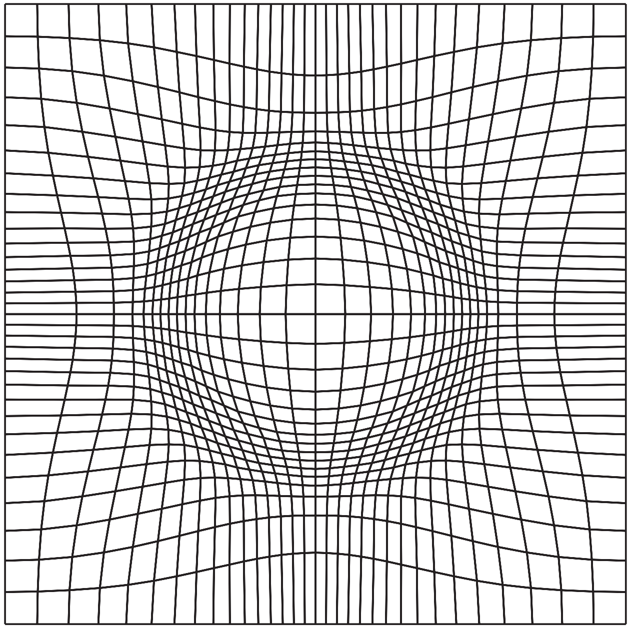
$\Omega = [0,1]^2$, tensor product mesh

$$f(x) = \min\left\{1, \max\left\{\frac{|d-0.25|}{0.25}, \varepsilon\right\}\right\}, \quad d := \sqrt{\left(x_1 - \tfrac{1}{2}\right)^2 + \left(x_2 - \tfrac{1}{2}\right)^2}$$

Test Problem

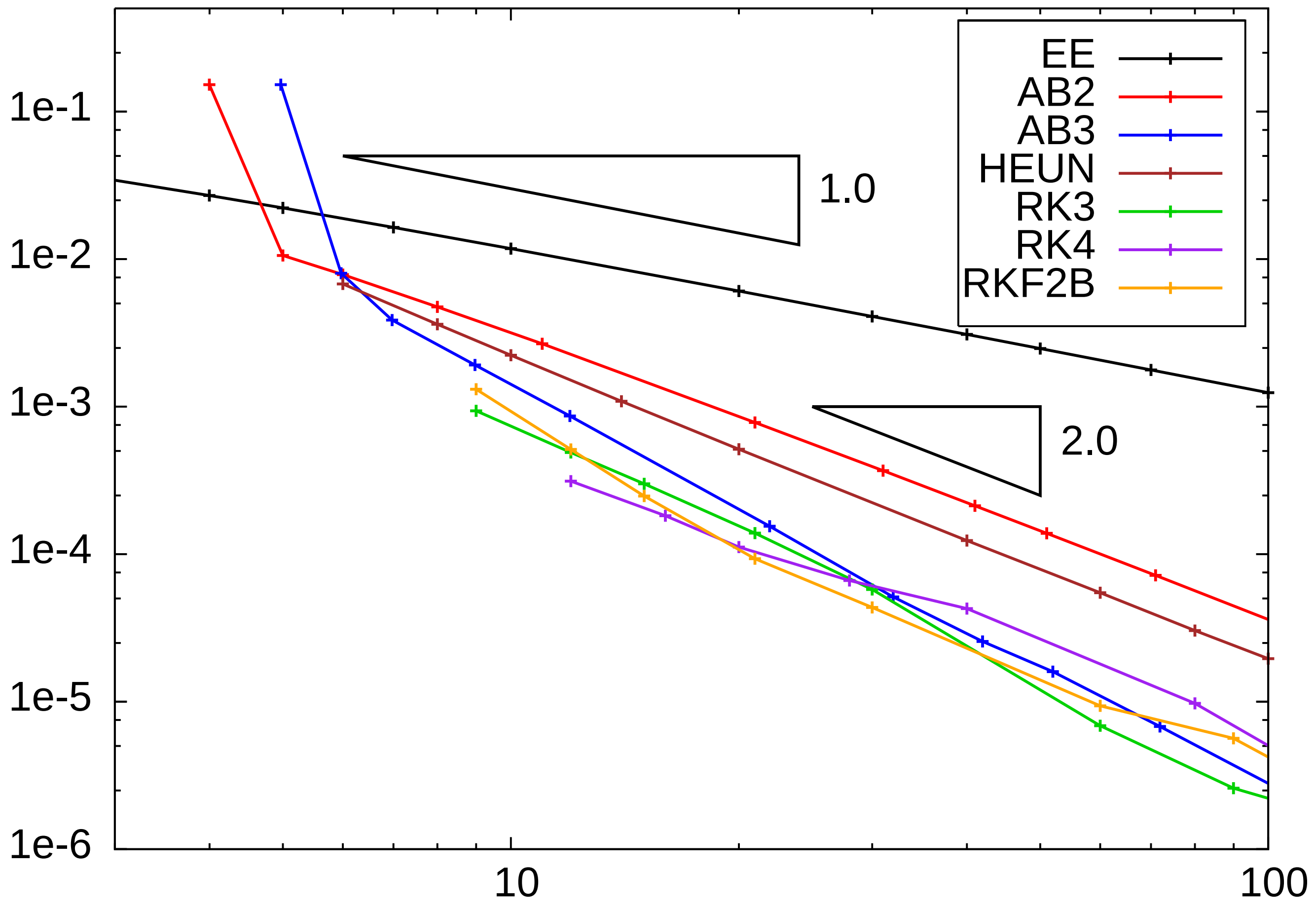
$\Omega = [0,1]^2$, tensor product mesh

$$f(x) = \min\left\{1, \max\left\{\frac{|d-0.25|}{0.25}, \varepsilon\right\}\right\}, \quad d := \sqrt{\left(x_1 - \tfrac{1}{2}\right)^2 + \left(x_2 - \tfrac{1}{2}\right)^2}$$



$\varepsilon = 0.1$

Convergence of ODE-Solvers



$NEL = 65536$

ODE-error: $\mathcal{O}(\Delta t^2)$

convergence for the Test Problem

Corollary Let us assume that

$$||\nabla w - G_h w_h||_{L^\infty} = \mathcal{O}(h^2), \quad \Delta t = \mathcal{O}(h).$$

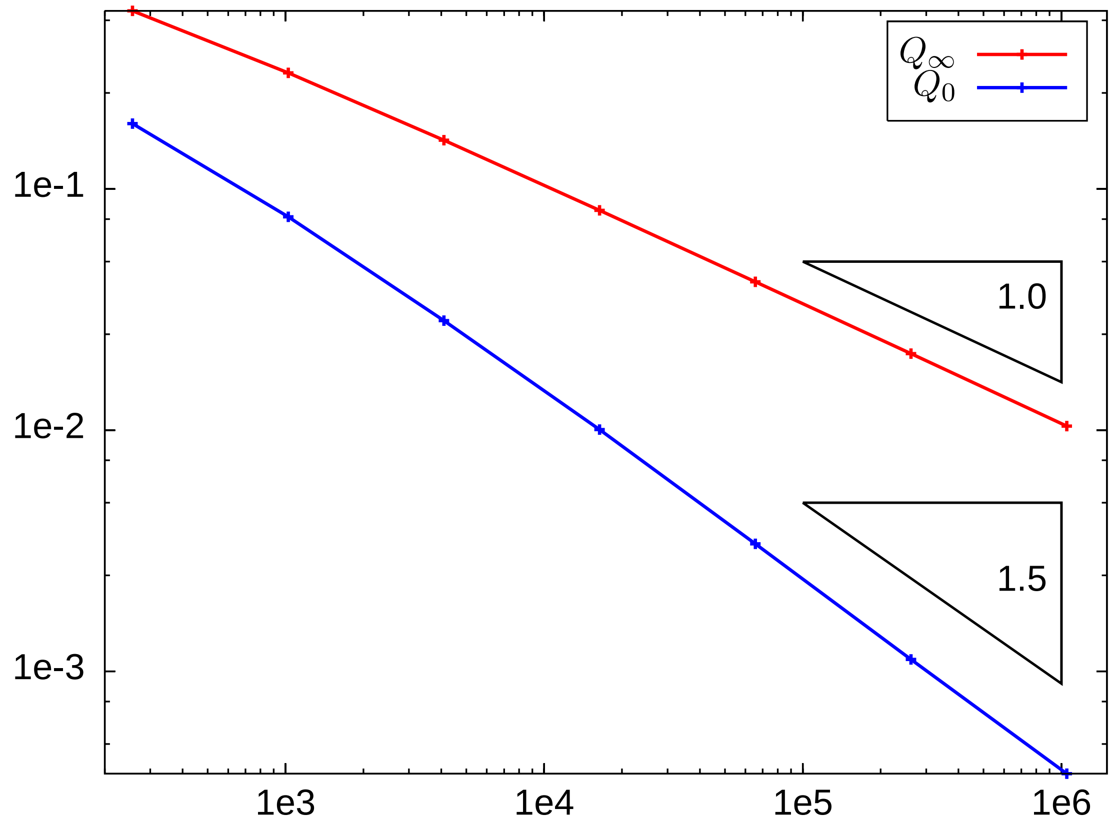
$$\Rightarrow \quad Q_0 = \mathcal{O}(h), \quad Q_\infty = \mathcal{O}(h)$$

convergence for the Test Problem

Corollary Let us assume that

$$||\nabla w - G_h w_h||_{L^\infty} = \mathcal{O}(h^2), \quad \Delta t = \mathcal{O}(h).$$

$$\Rightarrow \quad Q_0 = \mathcal{O}(h), \quad Q_\infty = \mathcal{O}(h)$$

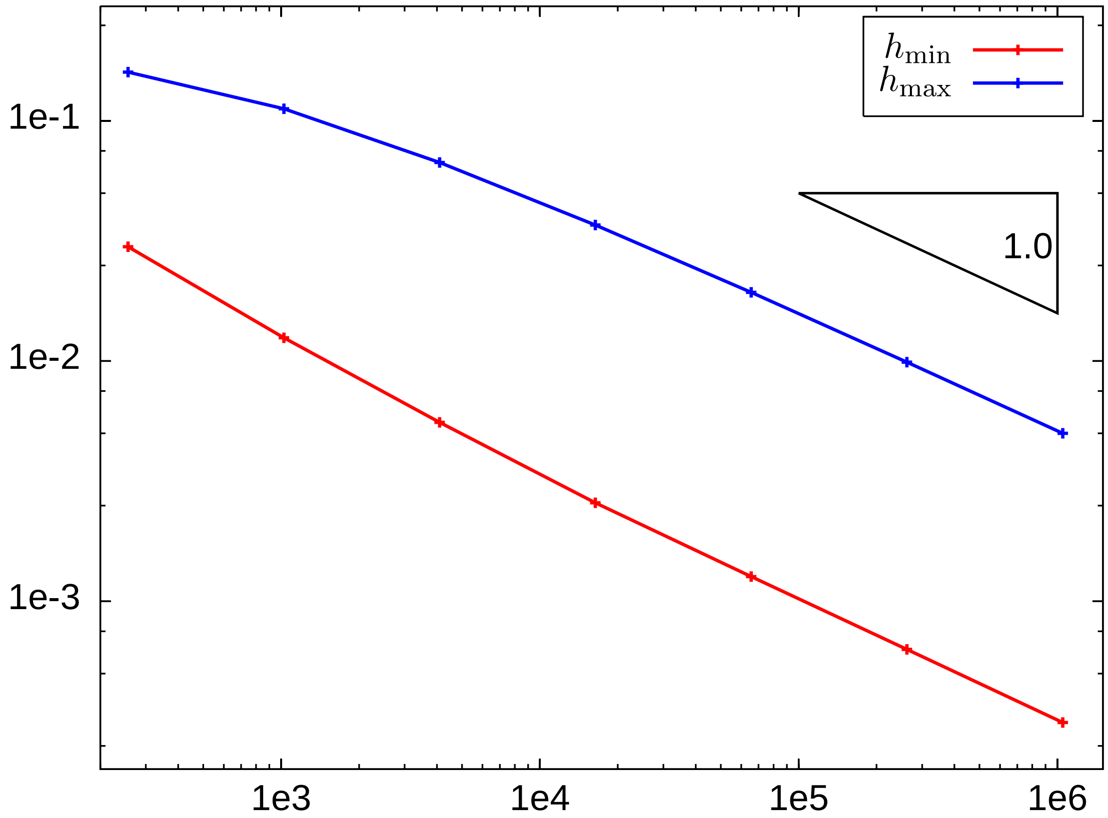


convergence for the Test Problem

Corollary Let us assume that

$$||\nabla w - G_h w_h||_{L^\infty} = \mathcal{O}(h^2), \quad \Delta t = \mathcal{O}(h).$$

$$\Rightarrow \quad Q_0 = \mathcal{O}(h), \quad Q_\infty = \mathcal{O}(h)$$



Runtime

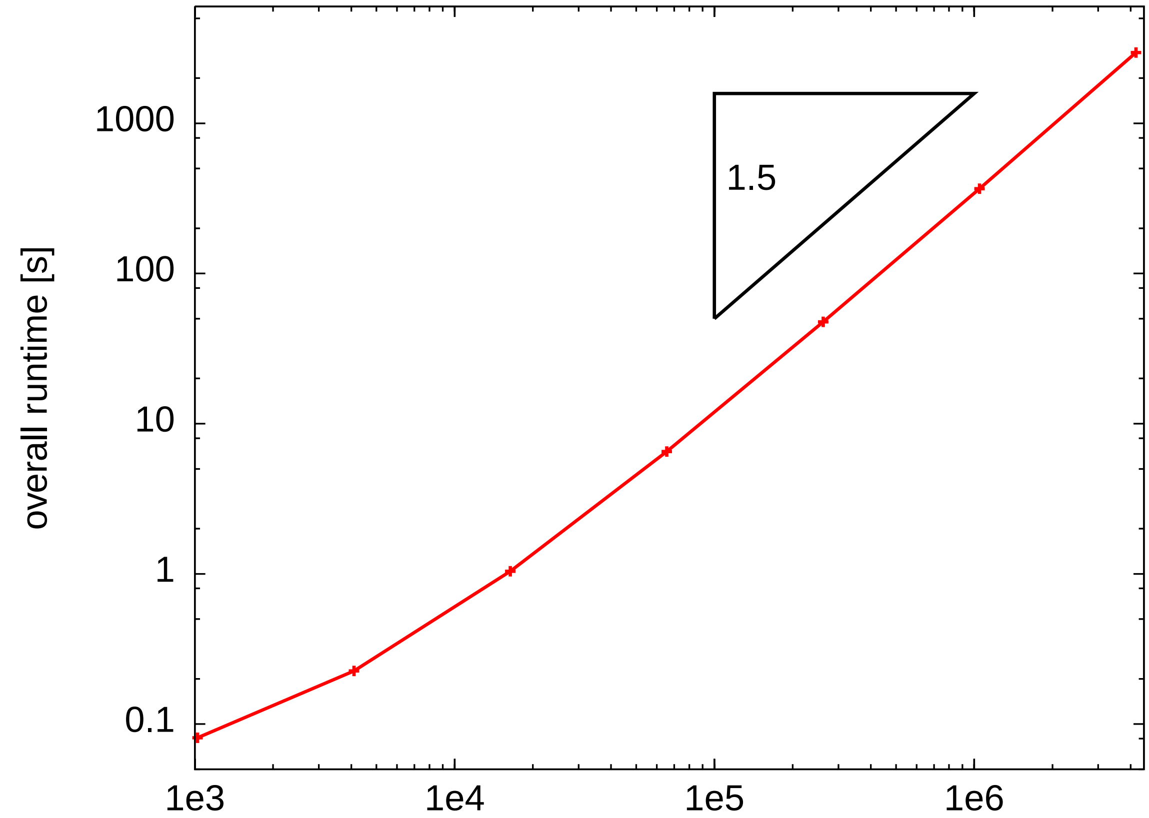
convergence: time step size $\Delta t = \mathcal{O}(h) = \mathcal{O}(N^{-1/2})$

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

Runtime

convergence: time step size $\Delta t = \mathcal{O}(h) = \mathcal{O}(N^{-1/2})$

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



Multilevel Deformation

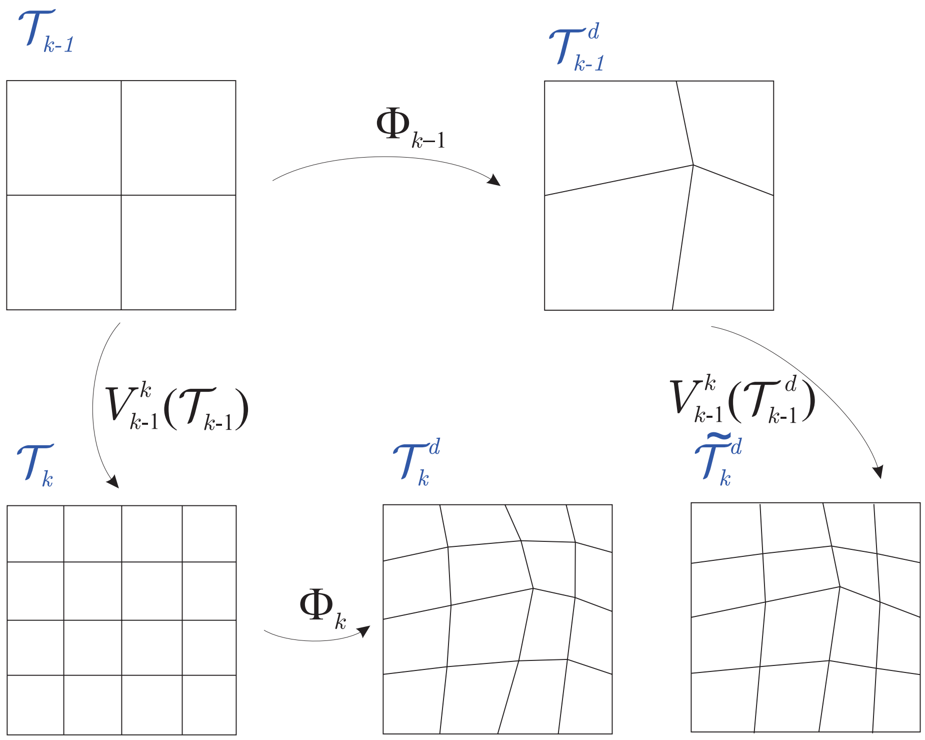
goal: fixed time step size + convergence

in practical computations: sequence of grids by successive regular refinement

Multilevel Deformation

goal: fixed time step size + convergence

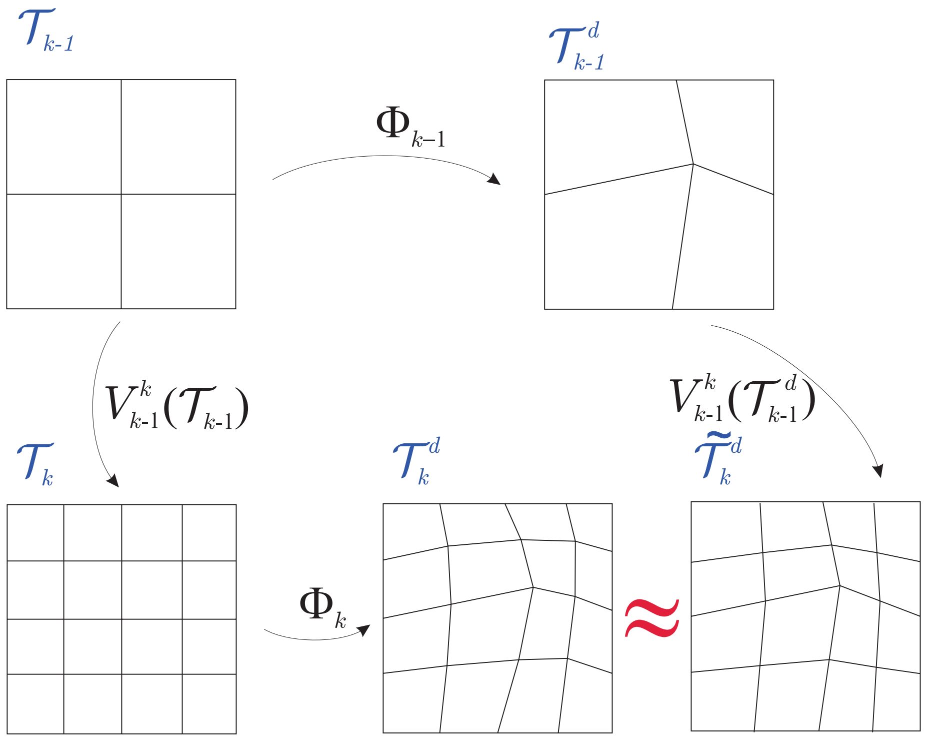
in practical computations: sequence of grids by successive regular refinement



Multilevel Deformation

goal: fixed time step size + convergence

in practical computations: sequence of grids by successive regular refinement



Multilevel Deformation

idea:

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

Multilevel Deformation

idea:

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

assumption 1:

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

assumption 2:

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

Multilevel Deformation

idea:

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

assumption 1:

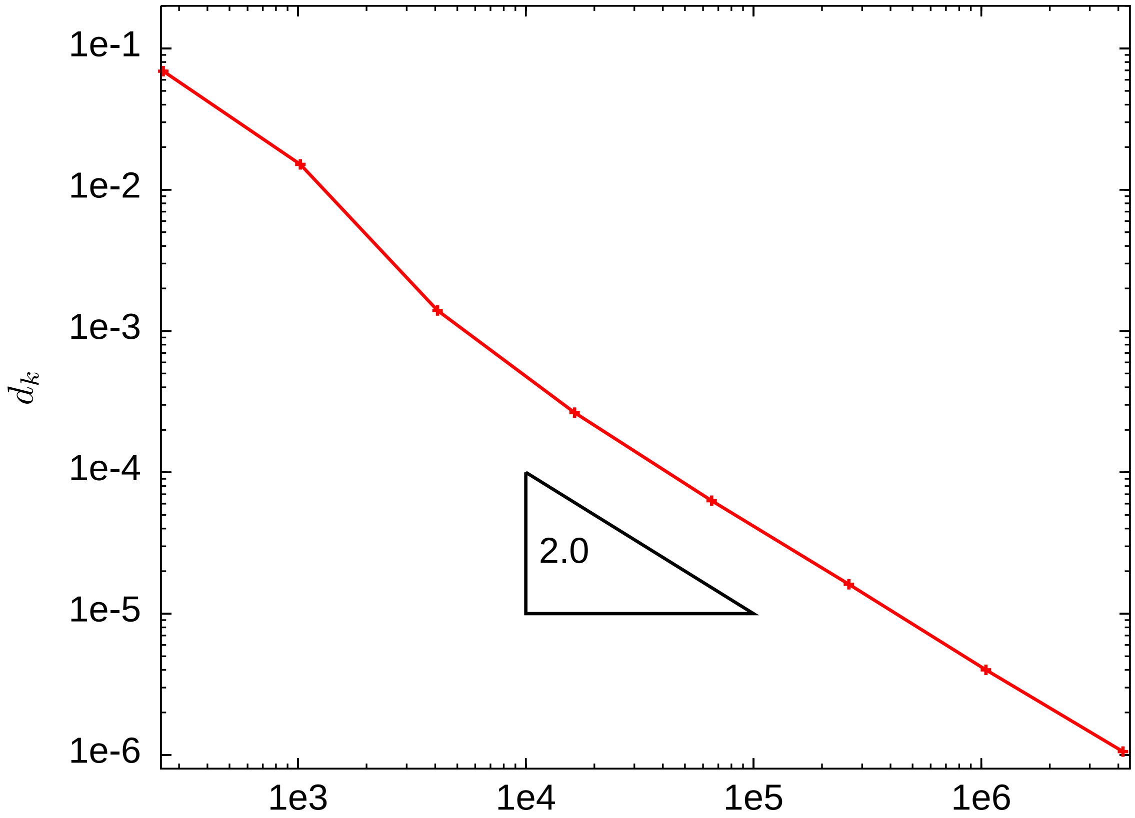
$$d_k := \max_{x \in \mathcal{X}_k} ||x - \Phi(x)|| \overset{?!}{=} \mathcal{O}(h^2)$$

assumption 2:

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

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

Multilevel Deformation



Multilevel Deformation (Algorithm)

MultilevelDef(f, $\mathcal{T}$, N_{pre}) : $\mathcal{T}$

$\mathcal{T}_{i_{\min}}$:= R ($\mathcal{T}, i_{\min}$)

DO i = $i_{\min}, i_{\max}, i_{\text{incr}}$

$\mathcal{T}_i$:= PreSmooth($\mathcal{T}_i$, $N_{\text{pre}}(i)$)

$\mathcal{T}_i$:= Deformation(f, $\mathcal{T}_i$)

IF ($i < i_{\max}$) $\mathcal{T}_{i+1}$:= V($\mathcal{T}_i$)

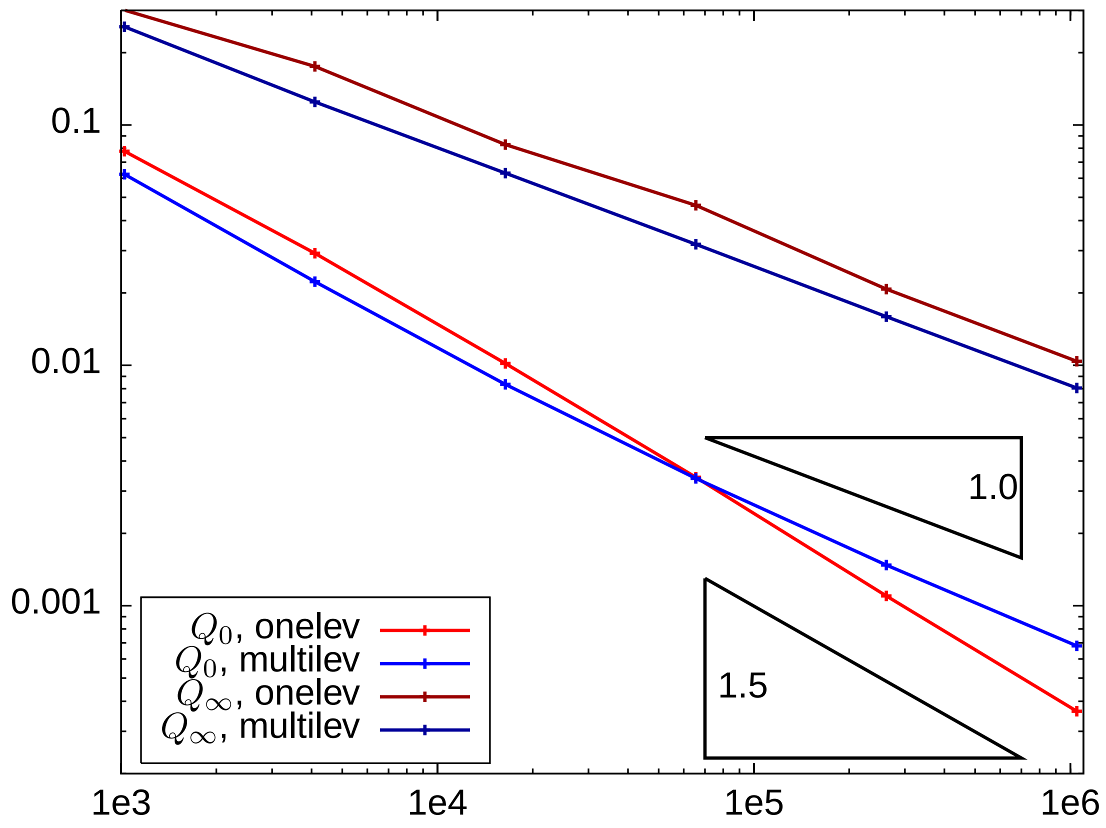
ENDDO

$\mathcal{T}$:= $\mathcal{T}_{i_{\max}}$

RETURN $\mathcal{T}$

END MultilevelDef

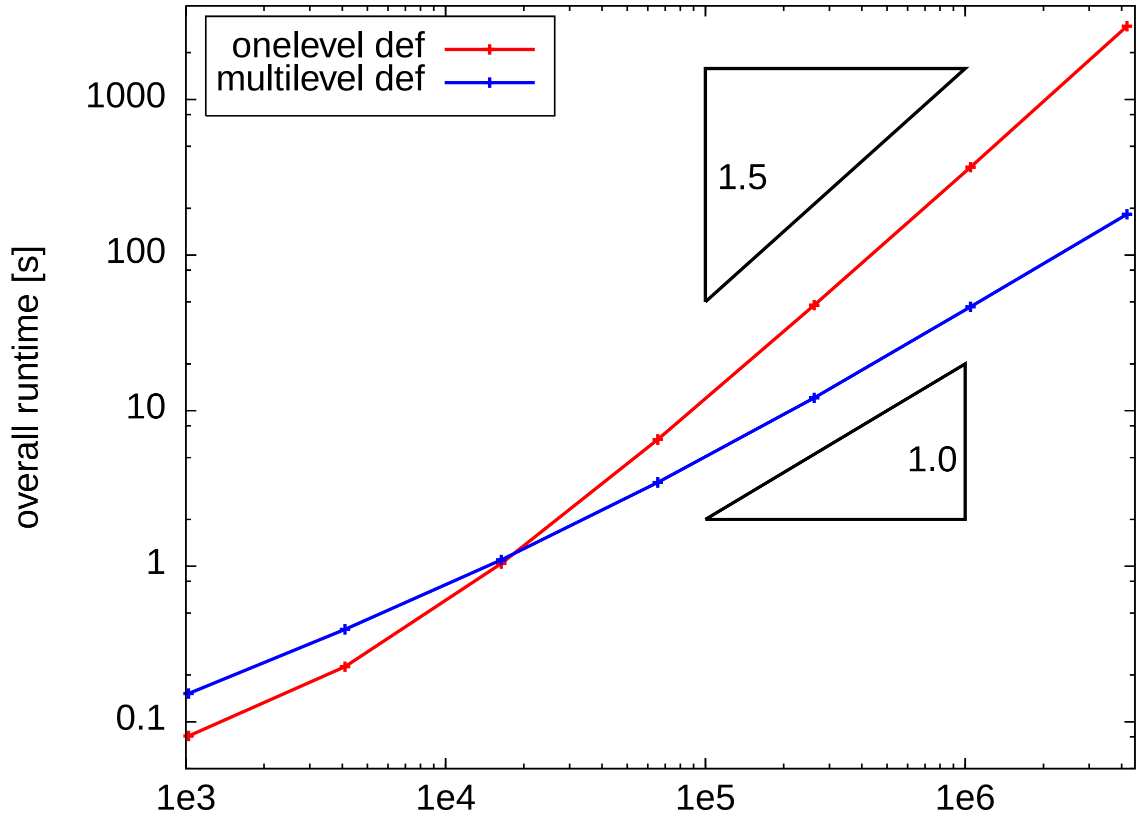
Multilevel Deformation



convergence despite of fixed time step size

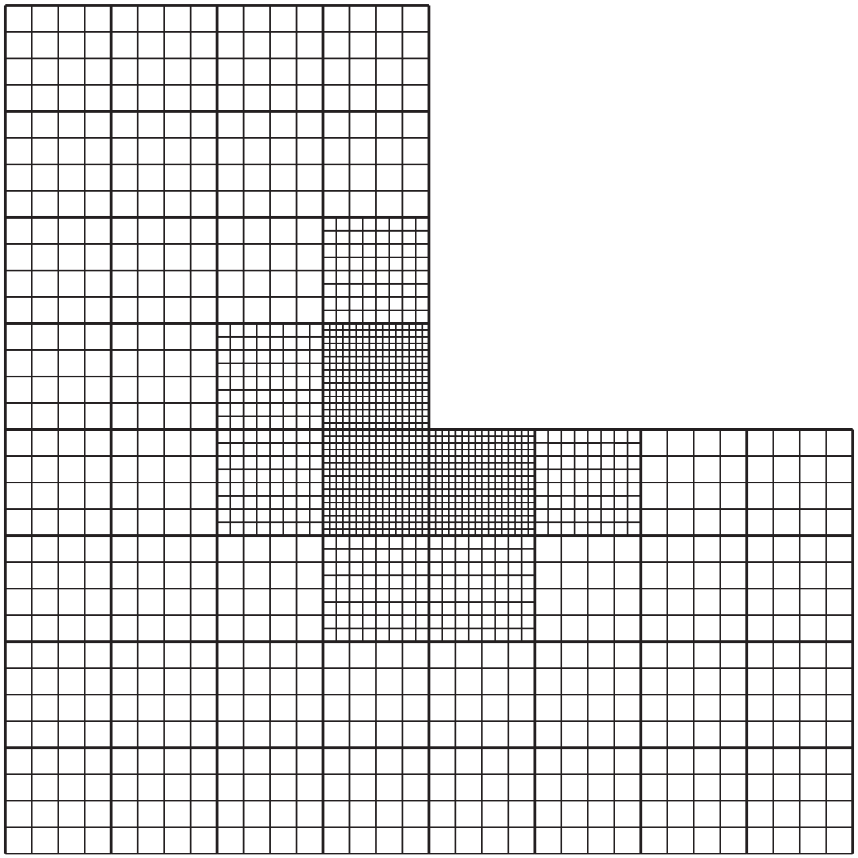
$$i_{\min} = 3,\ i_{\text{incr}} = 1,\ N_{\text{Pre}} = 2$$

Runtime Comparison



almost optimal complexity

Test Problem: L-domain



Poisson equation

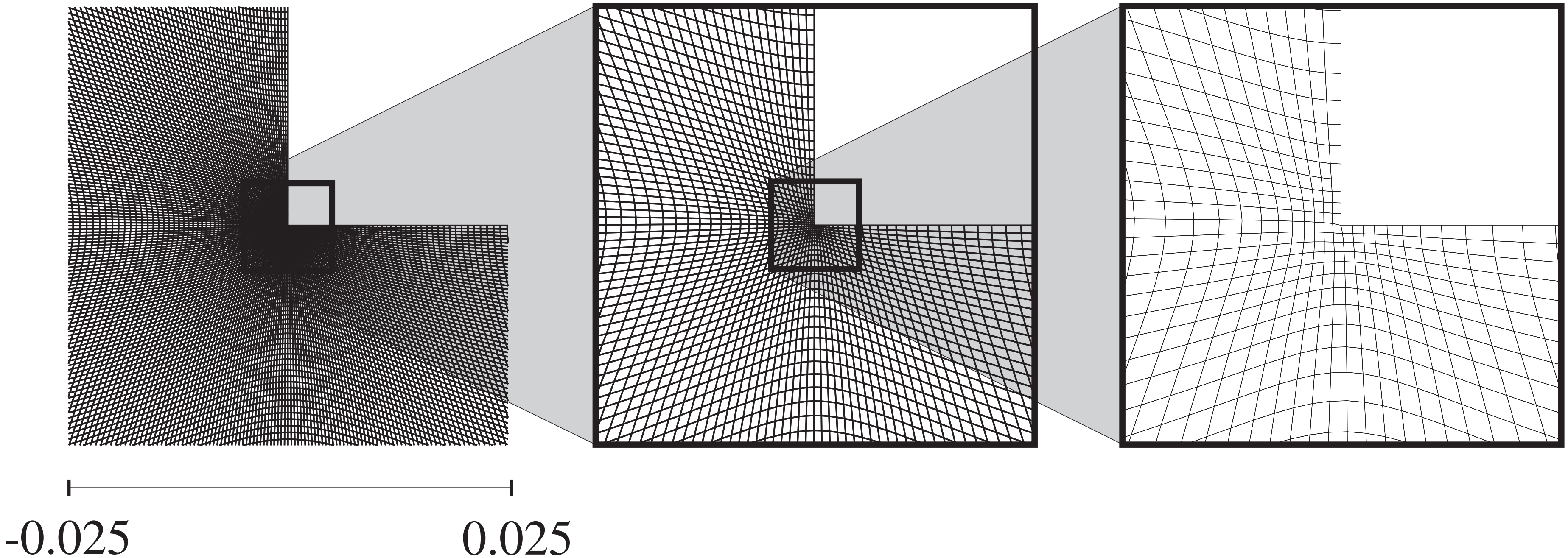
$$\Omega = [-0.5, 0.5]^2 / [0, 0.5]^2$$

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

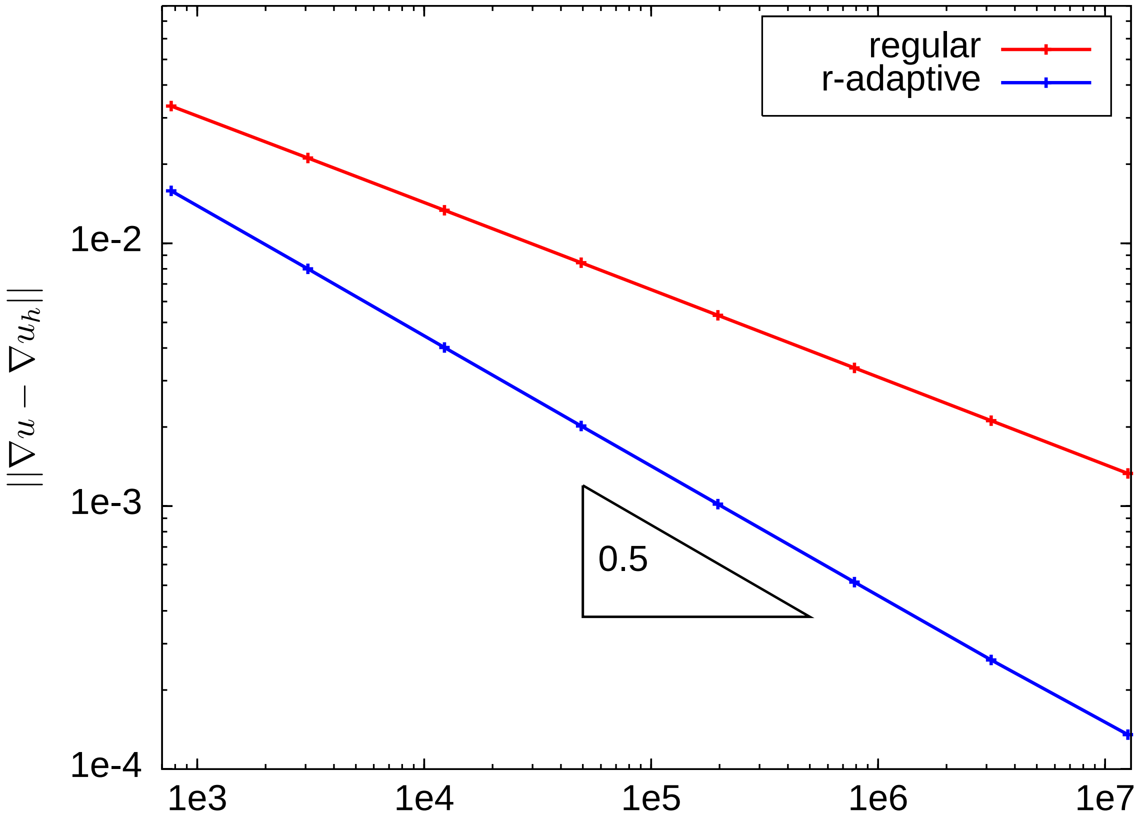
$$f(r) = \min\left\{1, \max\{c_0 h, \sqrt{2}|r|\}\right\}$$

desired: gradient error

Grid at Reentrant Corner



Discretisation Error



optimal convergence rate by deformed grids

Conclusion

- HPC: locally structured mesh
- Deformation method: derivation and convergence aspects
- Multilevel deformation
- L-domain: r-adaptivity

Thank you for your attention!