

---

## Multigrid Tutorial

---

### Multigrid (MG) and Local Refinement for Elliptic Partial Differential Equations

Klaus Stüben

FhG-SCAI  
Schloss Birlinghoven  
53754 St. Augustin, Germany  
e-mail: Klaus.Stueben@scai.fraunhofer.de

---

MG\_Tutorial-1

---

## Overview

- Why multigrid?
- Basic multigrid principles
- Full multigrid (FMG)
- Nonlinear multigrid (FAS)
- Eigenproblems
- Local Refinements

MG\_Tutorial-2

# Why Multigrid?

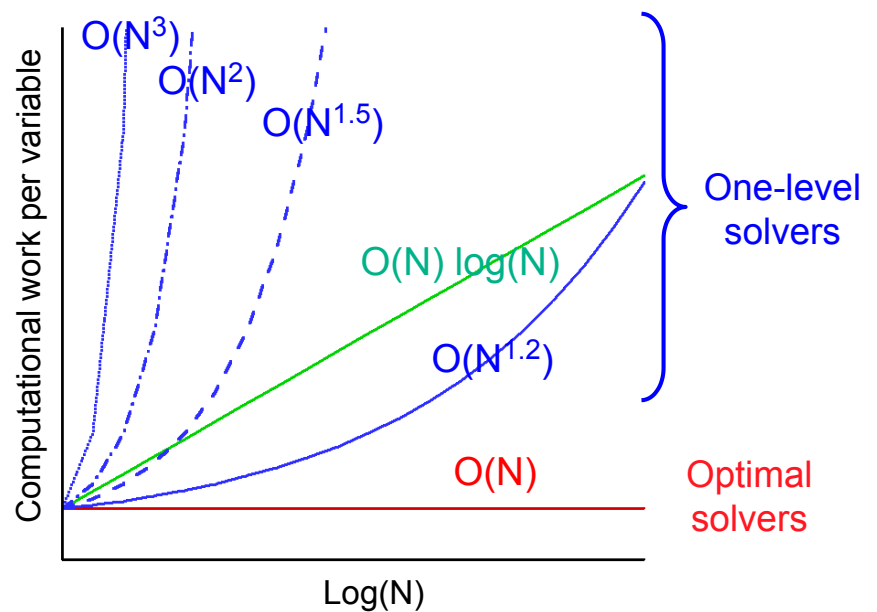
MG\_Tutorial-3

## Why Multigrid?

Large problems require  
**optimal solvers**

Optimal solvers require  
hierarchical algorithms:

- Multigrid
- Multilevel
- Multiscale

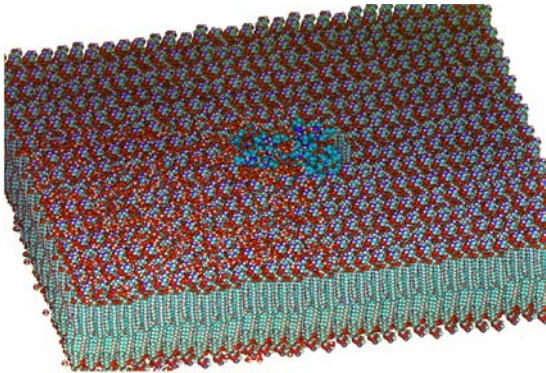


MG\_Tutorial-4



# Quantitative Example: Molecular Dynamics

Analysis of dynamical behavior of biological systems



Time integration:

$$\frac{d^2 \vec{x}_i}{dt^2} = \frac{\vec{F}_i}{q_i}$$

Computation of energy/forces:

$$\vec{F}_i = -\text{grad}_i(V)$$

Lipid-double layer membrane

Courtesy of Hoechst ZF Scientific Computing

$$E \approx V = \sum_b k_b (r_b - r_b^{eq})^2 \quad \text{bond lengths}$$

$$+ \sum_v k_v (\vartheta_v - \vartheta_v^{eq})^2 \quad \text{valence angles}$$

$$+ \sum_d k_d (1 - \cos(n_d \varphi_d - \delta_d)) \quad \text{torsion angles}$$

$$+ \sum_{i,j} \frac{q_i q_j}{4\pi\epsilon r_{i,j}} \quad \text{effective charges}$$

$$+ \sum_{i,j} \frac{A_{i,j}}{r_{i,j}^{12}} - \frac{B_{i,j}}{r_{i,j}^6} \quad \text{van der Waals interaction}$$

# Quantitative Example: Molecular Dynamics

MOLMEC: straightforward,  $O(N^2)$   
 MEGADYN: FMM approach,  $O(N)$

FMM (Fast Multipole)  
 Greengard, Rokhlin

Separate short & long range forces:

- Short-range forces are updated in each time step
- Long-range forces are treated on "coarser scales"

P	MOLMEC 7,000 atoms	MEGADYN 550,000 atoms
1	8152 sec	---
2	4481 sec	6305 sec
3	3056 sec	---
4	2427 sec	3295 sec
6	1769 sec	---
8	---	1840 sec

Estim. time for 550,000 atoms: 1.5 years!

# Basic Multigrid Principles

## Smoothing & Coarse-grid correction

MG\_Tutorial-9

### Model Problem: Gauss-Seidel Relaxation

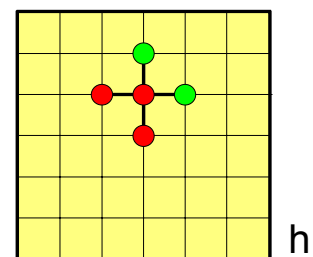
One Gauss-Seidel step:

$$u \rightarrow \bar{u}: \quad -\bar{u}_{i-1,j} - \bar{u}_{i,j-1} + 4\bar{u}_{i,j} - u_{i+1,j} - u_{i,j+1} = h^2 f_{i,j}$$

or, in terms of the error:

$$v \rightarrow \bar{v}: \quad -\bar{v}_{i-1,j} - \bar{v}_{i,j-1} + 4\bar{v}_{i,j} - v_{i+1,j} - v_{i,j+1} = 0$$

lexicographic order:



Very slow convergence:  $\rho = 1 - O(h^2)$

Asymptotic  
convergence factor

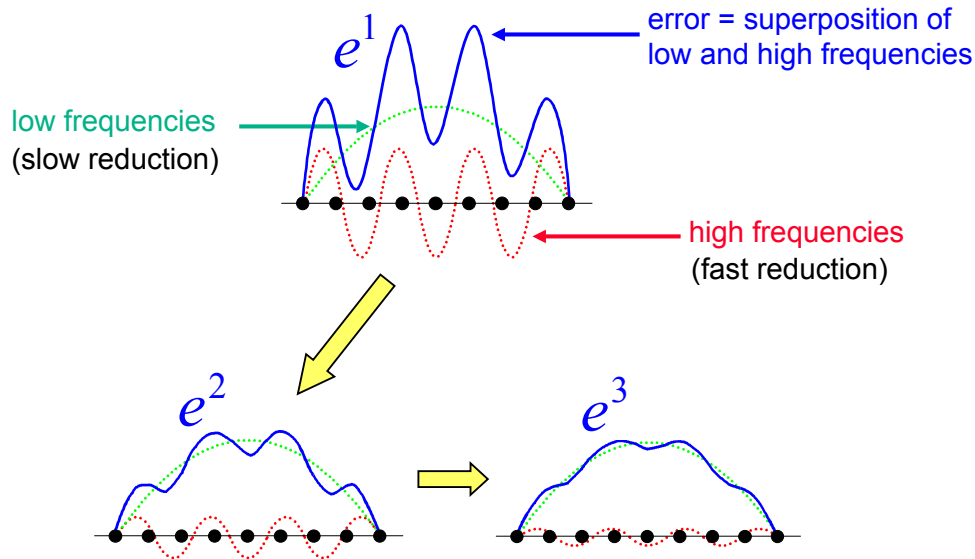
Very fast „smoothing“  
of the error:

$$\bar{v}_{ij}^h \approx \frac{1}{4} \begin{bmatrix} 1 & & \\ 1 & 0 & 1 \\ & 1 & \end{bmatrix} v_{ij}^h$$

Averaging of error

The smoother the error, the  
less efficient a further error  
reduction becomes!

Relaxation methods converge slowly  
but smooth the error quickly!



MG\_Tutorial-11

## Infinite Grid Smoothing Analysis

Fourier components on infinite grid

$$e^{i\Theta x/h} \quad (|\Theta| \leq \pi) \quad \begin{cases} |\Theta| := \max(|\Theta_1|, |\Theta_2|) \\ \Theta x := \Theta_1 x_1 + \Theta_2 x_2 \end{cases}$$

Amplification factor per relaxation step

$$e^{i\Theta x/h} \longrightarrow \mu(\Theta) e^{i\Theta x/h}$$

Distinguish low & high frequencies

$$e^{i\Theta x/h} \quad \begin{cases} |\Theta| < \pi/2 & \text{low (smooth) frequencies} \\ |\Theta| \geq \pi/2 & \text{high (non-smooth) frequencies} \end{cases}$$

Smoothing factor

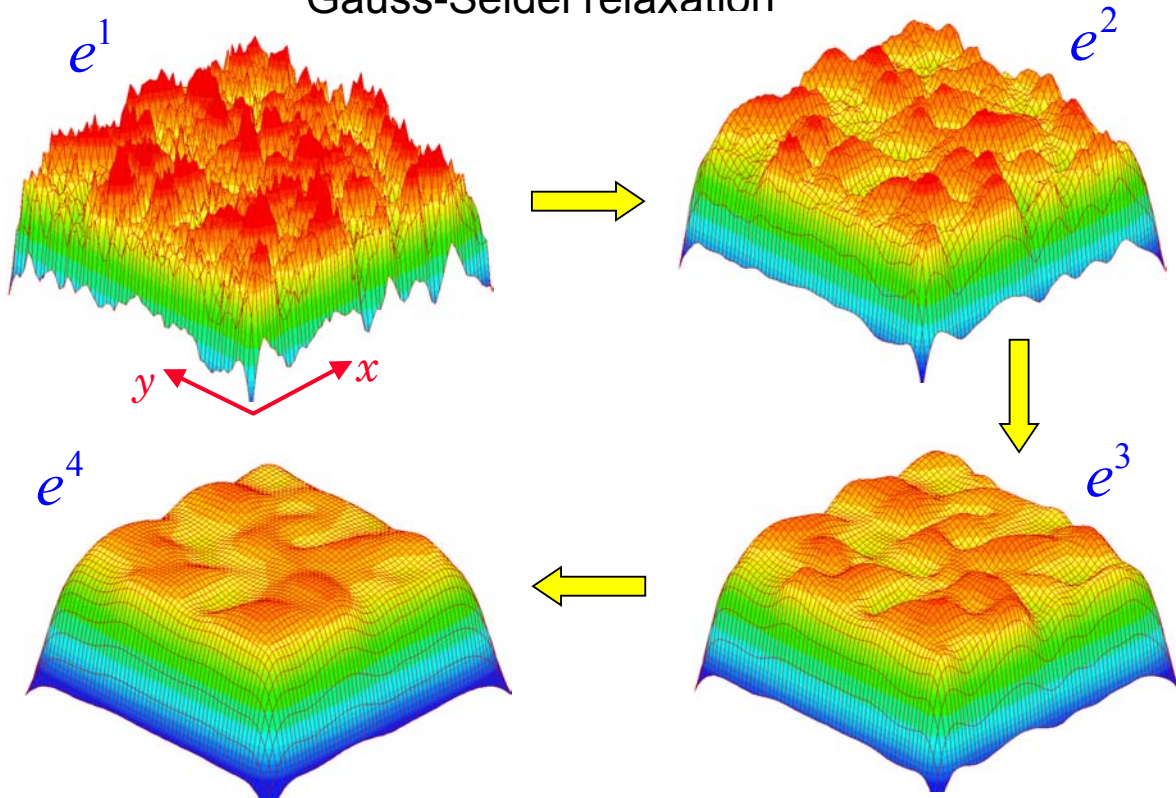
$$\mu^* = \max \{ |\mu(\Theta)| : |\Theta| \geq \pi/2 \}$$

Model problem, Gauss-Seidel

$$\mu^* = 0.5, \text{ h-independent!}$$

MG\_Tutorial-12

Smoothing by  
Gauss-Seidel relaxation



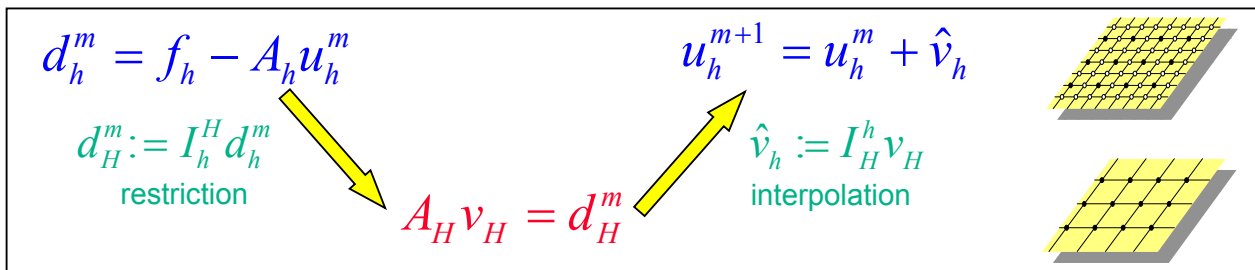
MG\_Tutorial-13

## Coarse-Grid Correction

Defect equation:

$$d_h^m = f_h - A_h u_h^m \implies A_h v_h = d_h^m \implies u_h^* = u_h^m + v_h$$

Coarse-grid correction:

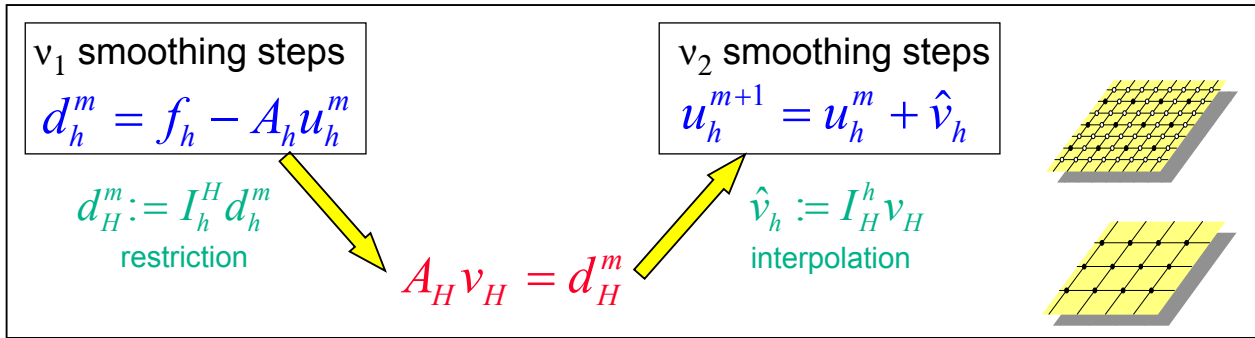


$$M_{h,H} = I_h - \underbrace{I_H^h A_H^{-1} I_h^H}_{\text{not full rank}} A_h$$

$$\rho(M_{h,H}) \geq 1 !$$



MG\_Tutorial-14



$$M_{h,H} = S_h^{v_2} (I_h - I_H^h A_H^{-1} I_h^H A_h) S_h^{v_1}$$

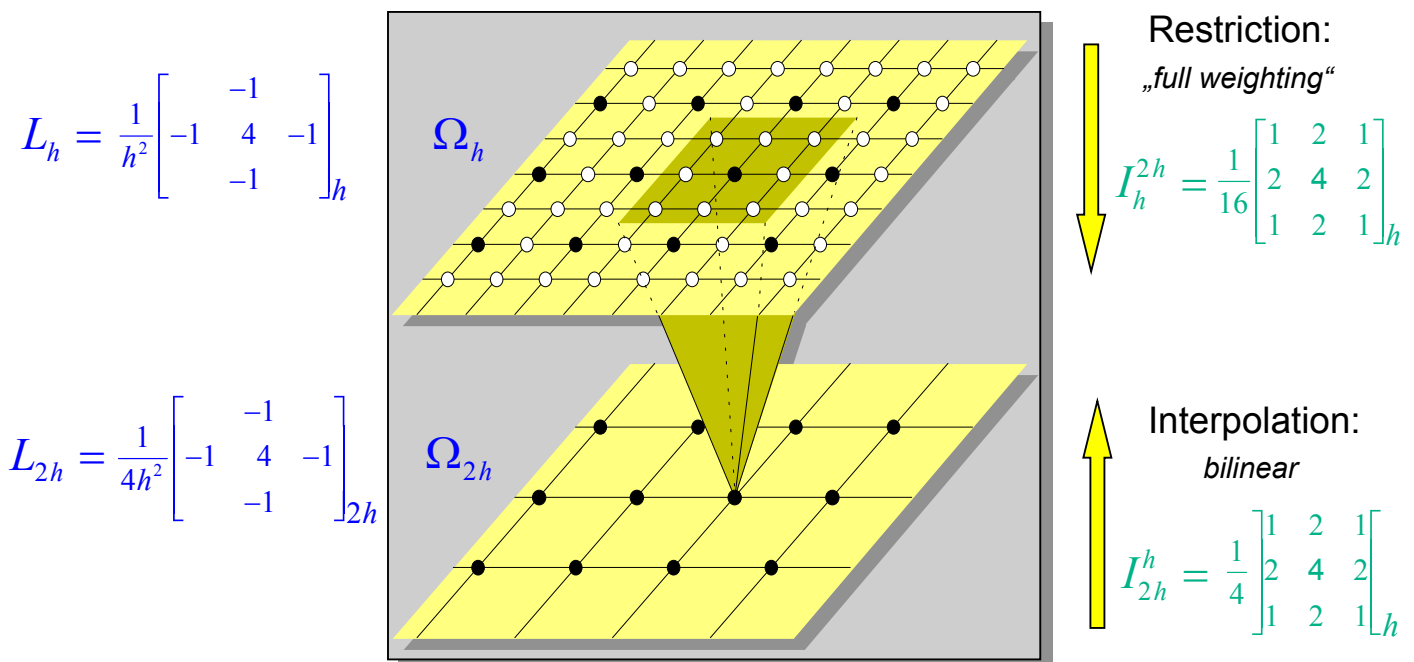
$\rho(M_{h,H}) \ll 1$

independent of h!

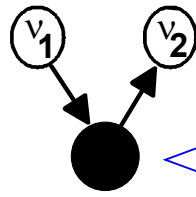
## Example: Model Problem

Standard coarsening:  $\Omega_h \rightarrow \Omega_{2h}$

Smoothing: Gauss-Seidel relaxation

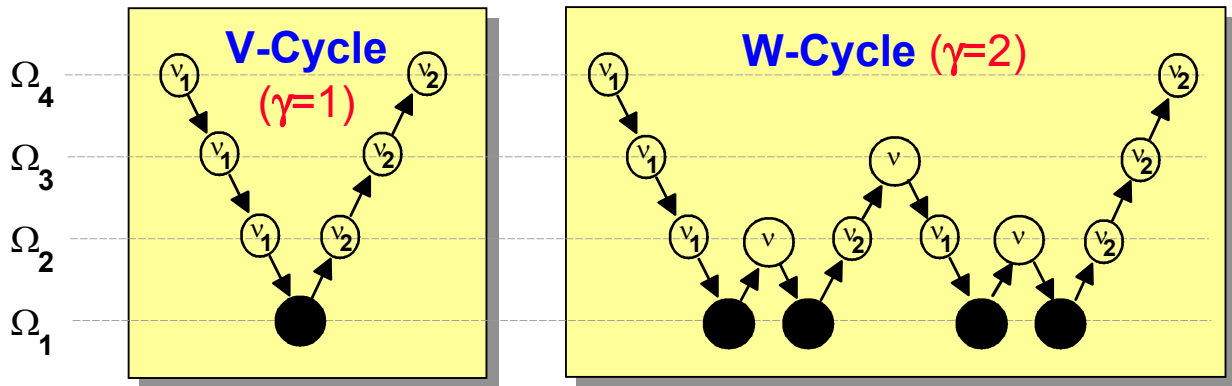






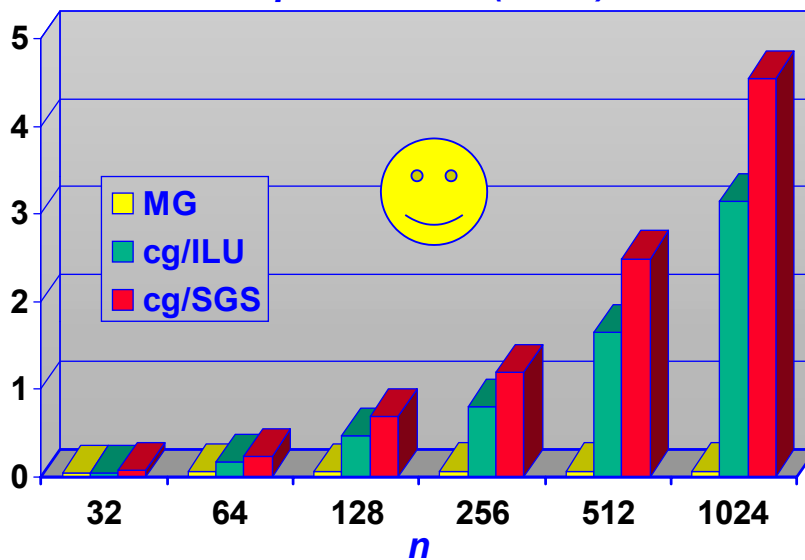
Recursive extension  
of two-grid cycle

Approximate solution by  $\gamma$  two-grid cycles using still coarser grids, .....



## MG Performance for Model Problem

Time per variable (msec)



Residual reduction:  $\epsilon = 10^{-12}$

---

# General Remarks

---

## MG Components

### What is multigrid **not**?

A particular solver

### What **is** multigrid?

A general strategy for constructing hierarchical solvers

### MG components

- Smoothing process (type, number of steps, ...)
- Coarsening process (type of hierarchy, speed of coarsening, ...)
- Intergrid transfer processes (interpolation, restriction)
- Coarser-level operators
- Coarsest-level solver
- More advanced techniques
- .....

## Advanced techniques

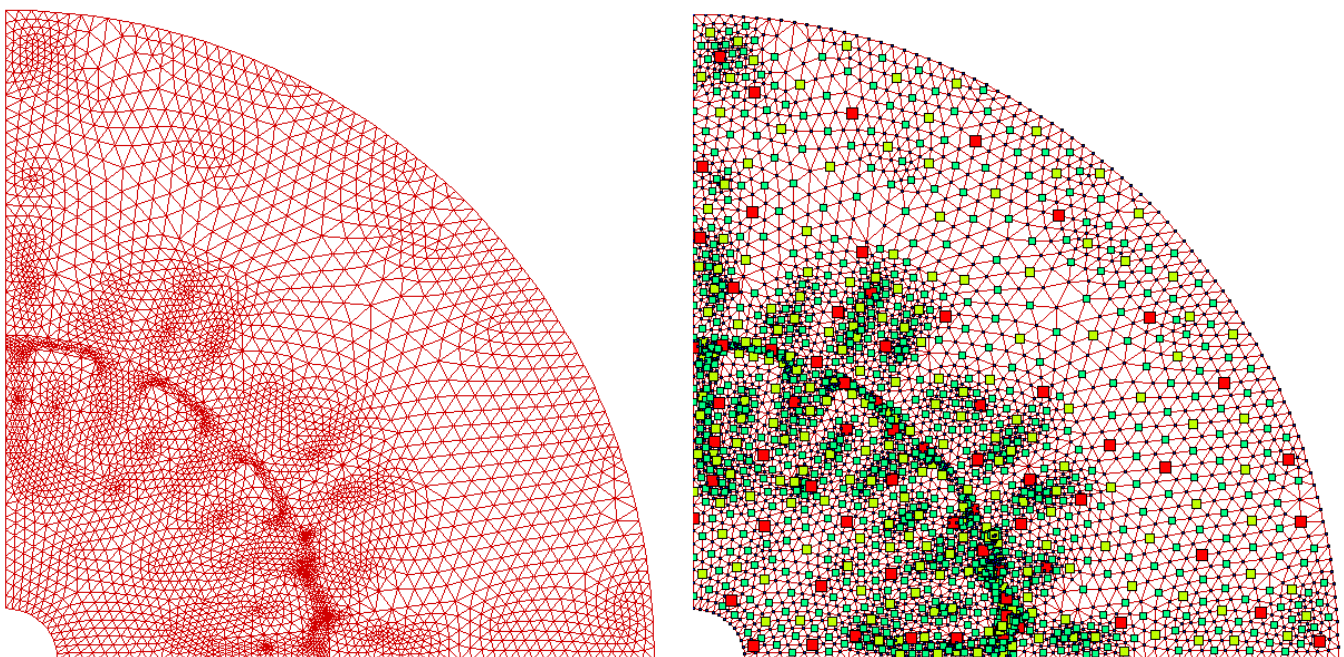
- Full multigrid (FMG)
- Nonlinear multigrid (FAS)
- Local refinements
- Multigrid for eigenproblems
- Parallel multigrid
- Algebraic multigrid (AMG)

## Applications

- General domains and BCs
- Variable coefficients
- Singular perturbed problems
- Discontinuous coefficients
- Systems of PDEs
- Non-elliptic PDEs
- Algebraic problems
- .....

MG\_Tutorial-21

# Unstructured Grids

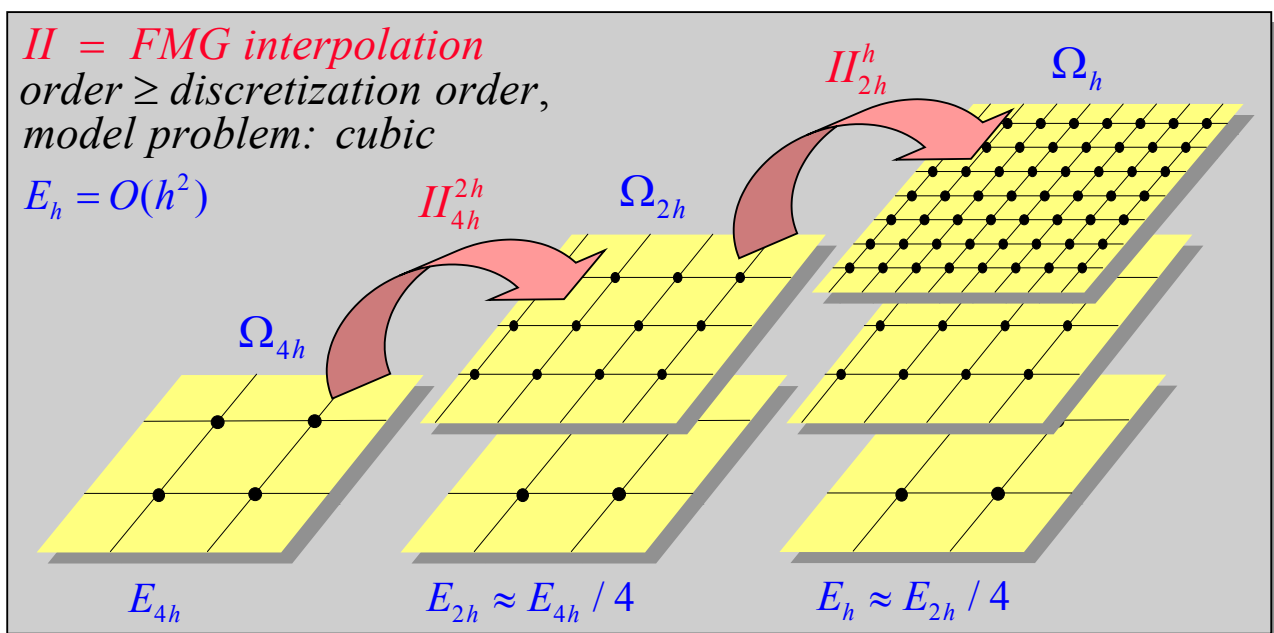


MG\_Tutorial-22

# Full Multigrid (FMG)

MG\_Tutorial-23

## Nested Iteration + MG = Full Multigrid (FMG)



On each level, a fixed number of cycles,  $\kappa$ , is sufficient  
(typically,  $\kappa = 1$  or  $\kappa = 2$ )  $\rightarrow$   **$O(N)$  complexity!**

MG\_Tutorial-24

# Nonlinear Multigrid (FAS)

$$L[u](\vec{x}) = f(\vec{x})$$

$$\text{discrete: } \begin{cases} L_h[u_h](\vec{x}) = f_h(\vec{x}) \\ A_h[u_h] = f_h \end{cases}$$

MG\_Tutorial-25

## Nonlinear Problems: Two Approaches

### Straightforward approach

1. Global linearization (outer iteration)
2. Linear multigrid (inner iteration)



- Global Jacobian needs to be computed (and stored!)
- Inner and outer iterations have to be matched

### Full approximation scheme (FAS)

1. Nonlinear relaxation (local linearization)
2. Nonlinear defect equation



- No global linearization (except for coarsest level?)
  - Same cycle structure as in the linear case
  - No matching of different iterations required
  - Advantages also for linear problems

MG\_Tutorial-26

$$i = 1, \dots, N: \begin{cases} a_i[u_1, \dots, u_{i-1}, \bar{u}_i, u_{i+1}, \dots, u_N] = f_i & \text{Jacobi} \\ u_i \rightarrow \bar{u}_i & \\ a_i[\bar{u}_1, \dots, \bar{u}_{i-1}, \bar{u}_i, u_{i+1}, \dots, u_N] = f_i & \text{Gauss-Seidel (GS)} \end{cases}$$

## Example for nonlinear GS

$$L[u] = -\Delta u + g(x, y, u) = f \quad (g_u(x, y, u) \geq 0)$$

$$-\bar{u}_{i-1,j} - \bar{u}_{i,j-1} + 4\bar{u}_{i,j} - u_{i+1,j} - u_{i,j+1} + h^2 g(x_i, y_j, \bar{u}_{i,j}) = h^2 f_{i,j}$$

GS-Picard:  $\rightarrow g(x_i, y_j, u_{i,j})$  (reasonable if  $h^2 g_u < 1$ )

GS-Newton:  $\rightarrow g(x_i, y_j, u_{i,j}) + g_u(x_i, y_j, u_{i,j})(\bar{u}_{i,j} - u_{i,j})$

# Nonlinear Defect Equation

Linear defect equation:  $A_h v_h = d_h^m \quad (= f_h - A_h u_h^m)$

Nonlinear analog:  $A_h[v_h + u_h^m] - A_h[u_h^m] = d_h^m$



## Coarse-grid approximation

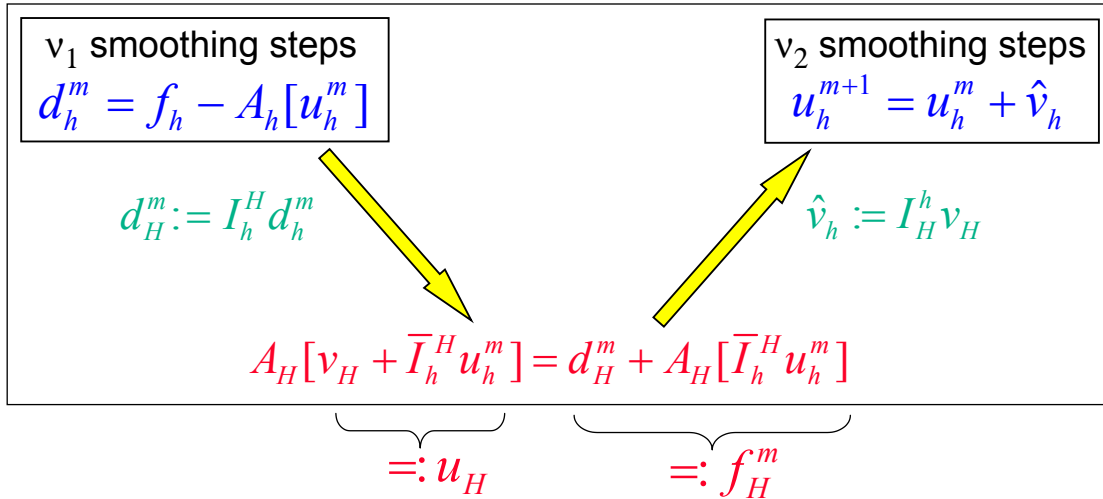
$$A_H[v_H + \bar{I}_h^H u_h^m] - A_H[\bar{I}_h^H u_h^m] = I_h^H d_h^m$$

$\bar{I}_h^H$  and  $I_h^H$  not necessarily the same!

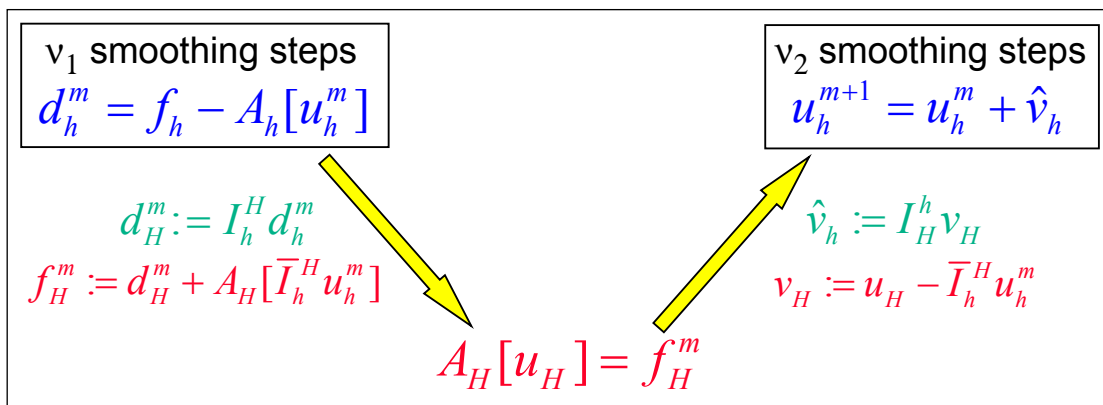
## Standard coarsening

Typical choice:  $\bar{I}_h^{2h} = \text{straight injection}$

# Full Approximation Scheme (FAS)



# Full Approximation Scheme (FAS)



$$u_h^m \rightarrow u_h^* \longrightarrow u_H \rightarrow \bar{I}_h^H u_h^*$$

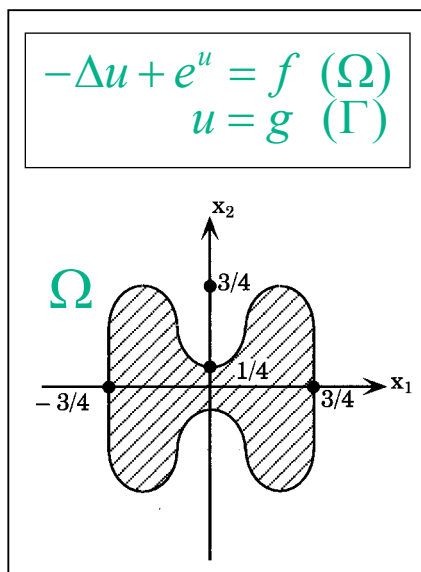
$$\left. \begin{array}{l} \text{Standard coarsening} \\ \bar{I}_h^{2h} = \text{straight injection} \end{array} \right\} \longrightarrow u_{2h} \rightarrow u_h^*$$

## Remarks

- If  $A$  linear:
  - FAS identical to linear cycle („correction scheme“)
  - however: different point of view
- Recursive extension to multigrid as in the linear case
- In general, continuation required
  - approach the range of attraction
  - most natural: combination with FMG
- Natural for solving eigenvalue problems

MG\_Tutorial-31

## Example



$m$	<i>Method I</i>	<i>Method II</i>	<i>FAS</i>
1	.18(+2)	.18(+2)	.14(+2)
2	.29	.20	.20
3	.86(-2)	.55(-2)	.54(-2)
4	.14(-3)	.14(-3)	.14(-3)
5	.43(-5)	.42(-5)	.42(-5)
6	.13(-6)	.13(-6)	.13(-6)
7	.47(-8)	.39(-8)	.38(-8)
8	.13(-9)	.12(-9)	.12(-9)
9	.42(-11)	.40(-11)	.39(-11)

$\|u_h^* - u_h^m\|_2$  as a function of  $m$

Method I: Global Newton linearization, number of MG cycles doubled

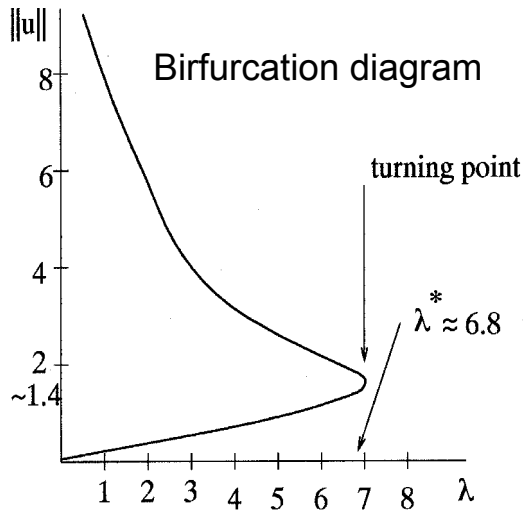
Method II: Global Newton linearization, one MG cycle per Newton step

MG\_Tutorial-32



## Bratu's problem (bifurcation)

$$\begin{aligned} -\Delta u - \lambda e^u &= 0 \quad (\Omega = (0,1)^2) \\ u &= 0 \quad (\Gamma) \end{aligned}$$



Continuation via  $\lambda$  :  
gives only lower branch  
solutions (up to  $\lambda \sim 6.5$ )

Other solutions require  
more sophisticated  
continuation techniques!

MG\_Tutorial-33

# Continuation Methods

## Augmented system: continuation parameter „s“

$$\left. \begin{aligned} L[u, \lambda] &= 0 \quad (\Omega) \\ u &= 0 \quad (\Gamma) \end{aligned} \right\} \longrightarrow \left\{ \begin{aligned} L[u(s), \lambda(s)] &= 0 \quad (\Omega) \\ u(s) &= 0 \quad (\Gamma) \\ C[u(s), \lambda(s), s] &= 0 \quad (\text{constraint}) \end{aligned} \right.$$

The constraint has also to be transferred  
to coarser grids in the sense of FAS



## For example: „arclength continuation“

$$C[u, \lambda, s] = \| du / ds \|_2^2 + |d\lambda / ds|^2 - 1 = 0$$

Simpler choices for Bratu:

$$\begin{aligned} C[u, \lambda, s] &= \|u\| - s \\ C[u, \lambda, s] &= u(0.5, 0.5) - s \end{aligned}$$

MG\_Tutorial-34

# Eigenproblems

Here: computation of *smallest*  
EV/EF for elliptic s.p.d. problems

MG\_Tutorial-35

## Eigenproblems + FAS

Problem: Find *smallest* EV/EF of

$$\begin{array}{l} L_h u_h - \lambda_h u_h = 0 \quad (=: f_h) \\ \eta_h(u_h) = \sigma_h \end{array} \quad \leftarrow \begin{cases} \text{normalization,} \\ \text{e.g. } \|u_h\| = 1 \end{cases}$$

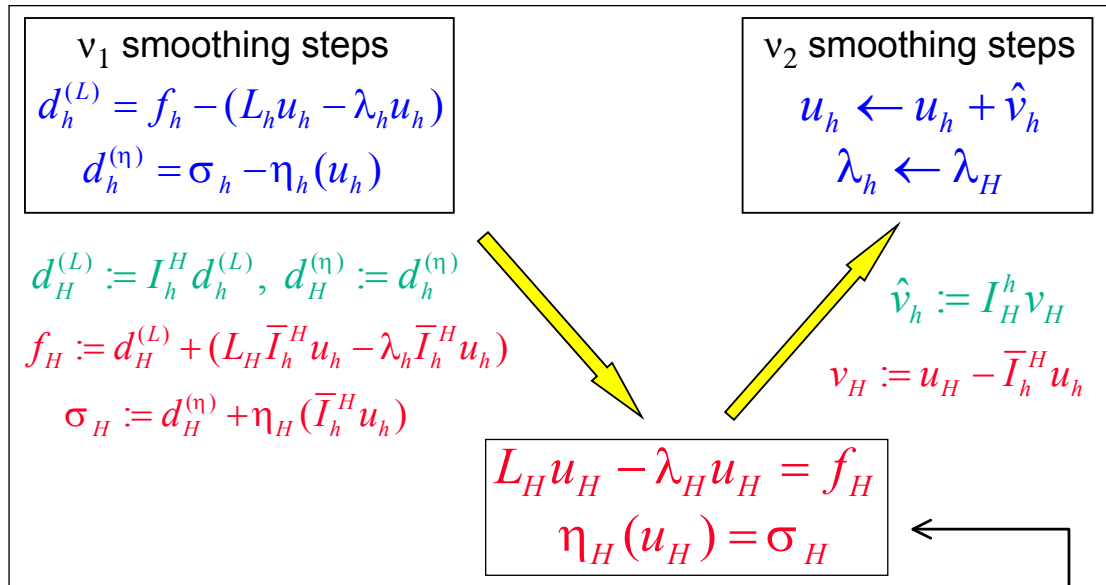
One step of a relaxation method (inefficient as solver!):

- |   |  |
|---|--|
| (1) GS relaxation step w.r.t. $u_h$ ( $\lambda_h$ fixed): | $L_h u_h - \lambda_h u_h = f_h$                      |
| (2) Scale $u_h$ :   | $\eta_h(u_h) = \sigma_h$                             |
| (3) Update of $\lambda_h$ ( $u_h$ fixed):                 | $(L_h u_h, u_h) - \lambda_h (u_h, u_h) = (f_h, u_h)$ |

### Two multigrid approaches

- (a) Replace (1) by *linear* MG cycle  $\longrightarrow$  **inefficient**
- (b) Use (1-3) as smoother in (non-linear) FAS process  
(can be simplified, see later)

MG\_Tutorial-36



At convergence:

$$u_H = \bar{I}_h^H u_h, \lambda_H = \lambda_h$$

If coarse enough, e.g.,  
solution by relaxation (1-3)

## Remarks

- Straightforward: recursive extension to more levels
- Solution on coarsest level: e.g. by relaxation (1-3)
- Generally sufficient:
  - $\lambda$ -update only on coarsest level
  - normalization only on coarsest level
- Natural combination with FMG
- No more expensive than MG for regular problems
- Generalization to several (many) eigenvalues

---

# Local Refinement (MLAT)

MG\_Tutorial-39

---

## Adaptivity

### Adaptivity

grid resolution,  
order of discretization,  
type of discretization.

### Adaptive grids

pre-defined (static),  
self-adapting (dynamic).

### Applications

locally non-smooth solutions  
(boundary or interior layers, shocks, turbulence, ....),  
non-smooth domains,  
singularities / discontinuities in the differential problem.

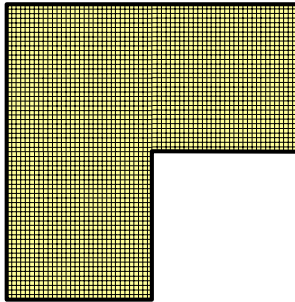
MG\_Tutorial-40

$$\begin{aligned} -\Delta u &= f & (\Omega) \\ u &= 0 & (\Gamma) \end{aligned}$$

Singular behavior near  $\mathbf{P}$ :

$$u_s(r, \phi) = r^{2/3} \sin(\frac{2}{3}\phi)$$

$(r, \phi) =$   
polar coordinates



Discretization error:

$$O(h^{4/3}) \text{ at fixed distance from } \mathbf{P}$$

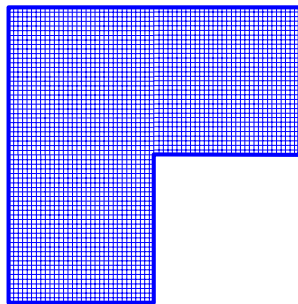
$$O(h^{2/3}) \text{ at distance } O(h) \text{ from } \mathbf{P}$$

Remedies:

- (1)  $u^* = \tilde{u} + u_s$ ,  $\tilde{u}$  smooth
- (2) local refinements

## Global grid vs. adaptive grid

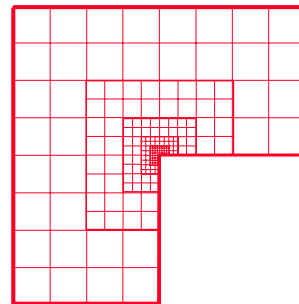
Global fine grid



49 665 points

$$\|u^* - u_h\|_\infty = 3.3(-3)$$

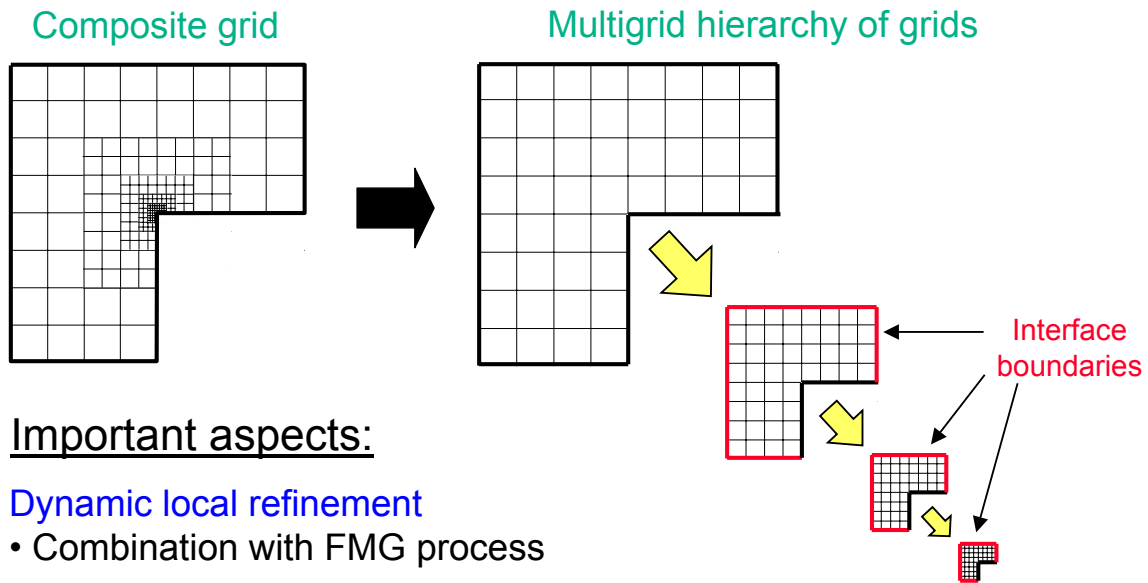
Adaptive grid



657 points

$$\|u^* - u_h\|_\infty = 3.8(-3)$$

## Natural integration into the MG approach



### Important aspects:

#### Dynamic local refinement

- Combination with FMG process

#### New aspects in MG cycling

- Treatment of interface boundaries
- Grids covering only subdomains ➔ FAS, even for linear problems!

MG\_Tutorial-43

# Local Refinement + FAS

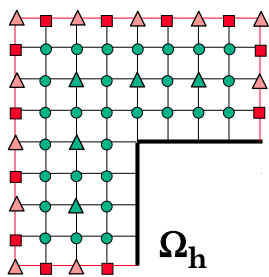
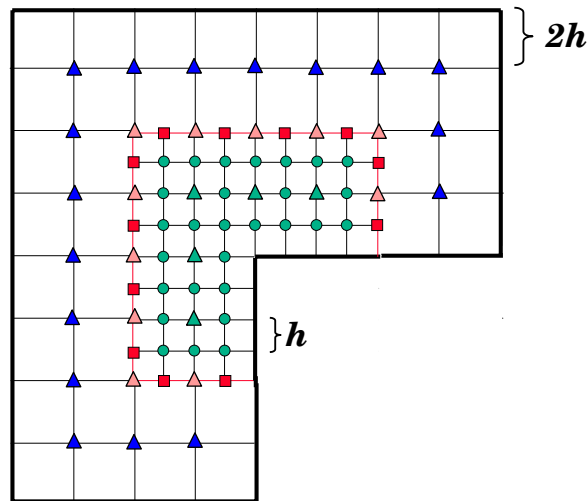
## Recall: FAS correction equation

$$\begin{aligned}
 L_{2h}[u_{2h}] &= I_h^{2h} d_h^m + L_{2h}[\bar{I}_h^{2h} u_h^m] \\
 &= I_h^{2h} f_h + L_{2h}[\bar{I}_h^{2h} u_h^m] - I_h^{2h} L_h[u_h^m] \\
 &= I_h^{2h} f_h + \tau_h^{2h} \quad (h, 2h)\text{-relative truncation error}
 \end{aligned}$$

$\bar{I}_h^{2h}$  = straight injection:

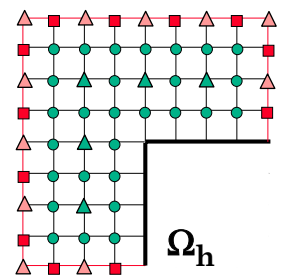
$$u_h^m \rightarrow u_h^* \quad \rightarrow \quad u_{2h} \rightarrow \bar{I}_h^{2h} u_h^* = u_h^*$$

MG\_Tutorial-44



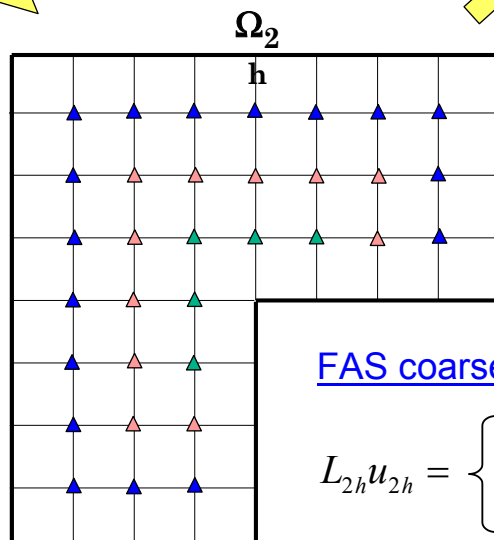
### Smoothing:

Relaxation on grid  $\Omega_h$ : ● ▲  
 Interface variables are treated as Dirichlet points: ▲ ■



### FAS correction:

At all points: ● ▲ ▲ ■



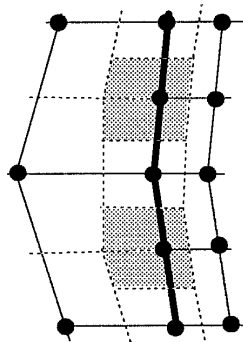
### FAS coarse-grid equations:

$$L_{2h}u_{2h} = \begin{cases} I_h^{2h} f_h + \tau_h^{2h} & \text{▲} \\ f_h & \text{▲ ▲} \end{cases}$$

## Modifications

- conservative interpolation
- conservative discretization along interface

## Modified interface treatment



Conservative FV discretization  
along interface

Smoothing by relaxation now  
includes interface variables

MG\_Tutorial-47

# Local Refinement

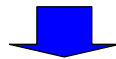
## Requirements on automatic refinement criteria

- Reliably detect local low accuracy
- Terminate automatically (!)

## A simple grid refinement criterion

$$L_{2h}u_{2h} = \begin{cases} I_h^{2h} f_h + \tau_h^{2h} \\ f_h \end{cases}$$

$\tau_h^{2h}$ : measures to which extent the fine grid solution  
is different from the coarse grid one.



refine where  $h^d \tau_h^{2h} \geq \varepsilon$  ( $d = \text{dimension}$ )

MG\_Tutorial-48



# Example: Euler Equations

## Euler Equations

$$\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = 0$$

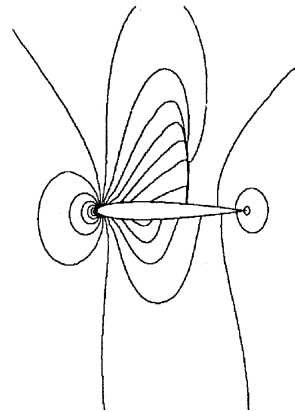
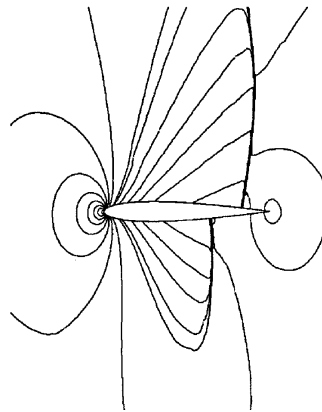
$$f = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E + p)u \end{bmatrix} \quad \text{and} \quad g = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (E + p)v \end{bmatrix}$$

$$p = (\gamma - 1) \left( E - \frac{1}{2} \rho (u^2 + v^2) \right)$$

$$M_\infty = 0.85, \alpha = 1.0^\circ$$

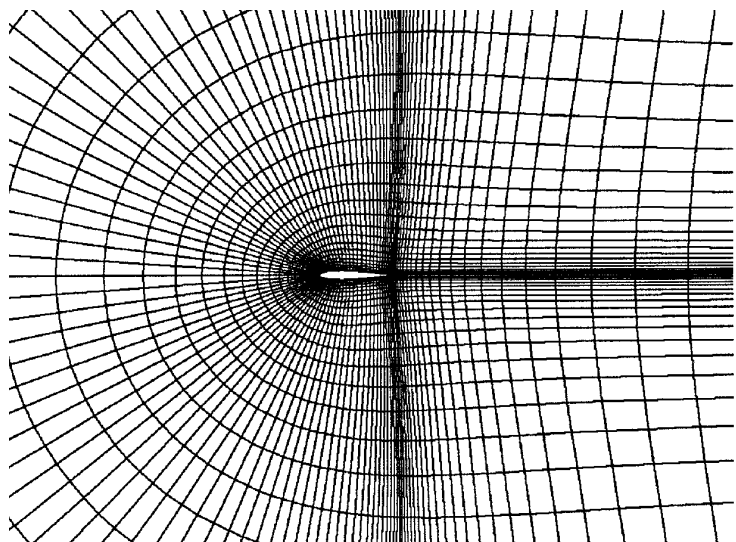
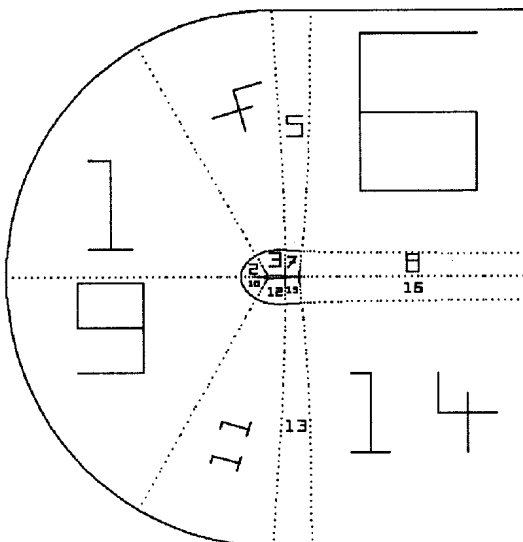
$$M_\infty = 0.80, \alpha = 1.25^\circ$$

NACA0012  
airfoil:

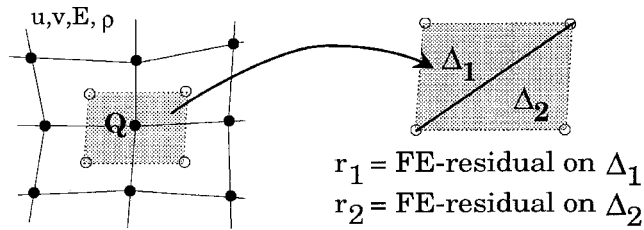


# Example: Euler Equations

Global block-structured grid  
(subdivided for parallel processing)



## Refinement criterion (FE)



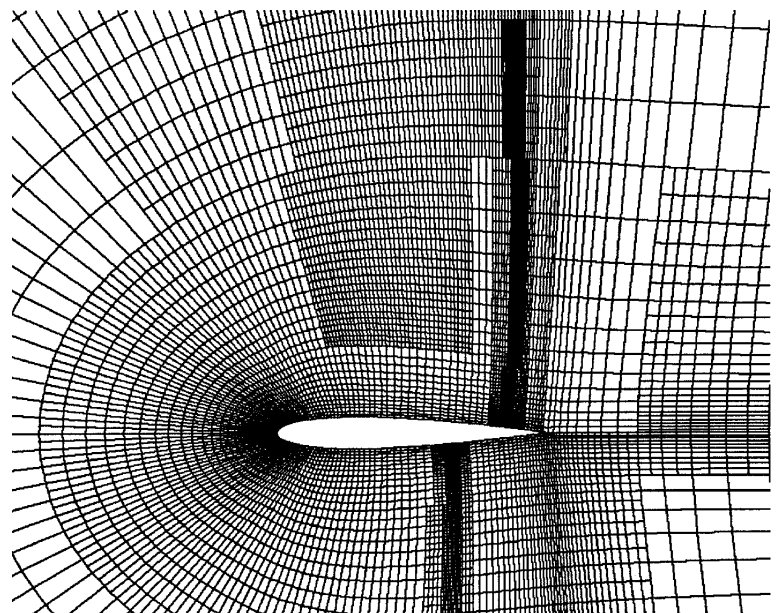
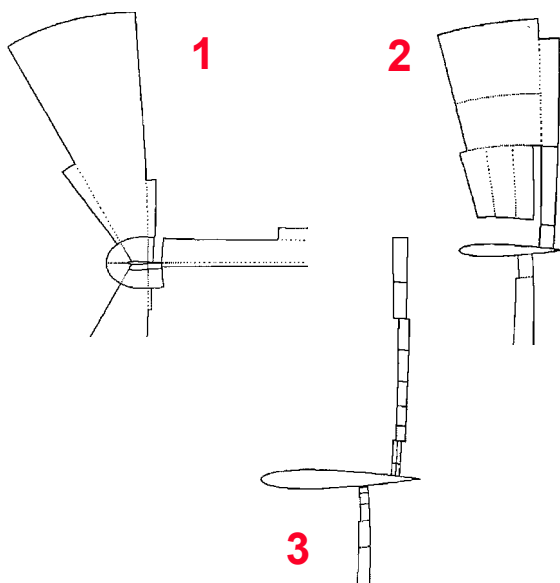
assuming *linear* shape functions

$$r^h(Q) = \sum_{i=1}^2 \sum_{j=1}^4 \int_{\Delta_i} |r_{ij}| dx$$

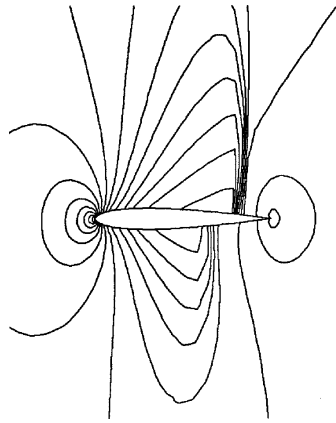
refine near  $Q$  if  $r^h(Q) \geq \varepsilon$

## Refinement areas

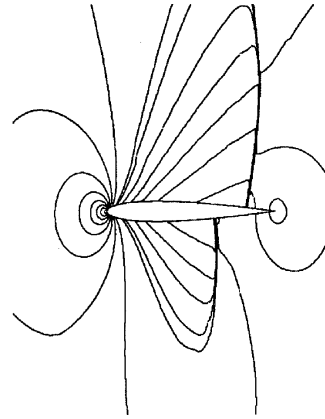
## Resulting refined grid (near the profile)



Without refinement



With refinement



	<i>Global fine grid</i>	<i>Adaptive grid</i>	<i>Factor</i>
<b># points</b>	<b>197 632</b>	<b>13 866</b>	<b>14</b>
<b>Time</b>	<b>6 115 sec</b>	<b>590 sec</b>	<b>10</b>

Comparison: global grid vs. adaptive grid  
(obtained in parallel on 16 processors)

MG\_Tutorial-53

## Literature

- **Discovery of multigrid (theoretical)**
  - **Fedorenko, R.P.:** *The speed of convergence of an iterative method*, USSR Comput. Math. and Math. Phys. 4,3 (1964).
  - **Bakhvalov, N.S.:** *On the convergence of a relaxation method with natural constraints on the elliptic operator*, USSR Comput. Math. and Math. Phys. 6,5 (1966).
- **Beginning of multigrid**
  - **Brandt, A.:** *Multi-level adaptive technique (MLAT) for fast numerical solution to boundary value problems*, Lecture Notes in Physics 18, Springer 1973.
  - **Brandt, A.:** *Multi-level adaptive solutions to boundary value problems*, Math. Comp. 31 (1977).
- **Re-discovery of multigrid**
  - **Hackbusch, W.:** *On the multigrid method applied to difference equations*, Computing 20 (1978).

## Text Books

- **Classical**
  - **Stüben, K.; Trottenberg, U.:** *Multigrid methods: Fundamental algorithms, model problem analysis and applications*, Lecture Notes in Mathematics 960, Springer (1982).
  - **Brandt, A.:** *Multigrid techniques: 1984 Guide with applications to fluid dynamics*, GMD-Studie No. 85 (1984).
- **Theory**
  - **Hackbusch, W.:** *Multigrid methods and applications*, Springer Series in Comp. Math. 4, Springer (1985).
  - **McCormick, S. (ed.):** *Multigrid methods*, Frontiers in Applied Mathematics, Vol. 5, SIAM, Philadelphia (1987).
- **Tutorial-level**
  - **Briggs, W.:** *A multigrid tutorial*, SIAM, Philadelphia (1987). New edition: 2001.
- **Engineers**
  - **Wesseling, P.:** *An introduction to multigrid methods*, Pure and Applied Mathematics Series, John Wiley and Sons (1992).
- **Engineers and Practitioners**
  - **Trottenberg, U.; Oosterlee, C.W.; Schüller, A.:** *Multigrid*, Academic Press, 2001 (with appendices by **Brandt, A., Oswald, P.** and **Stüben, K.**)