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Multigrid Solvers for Complicated Geometries

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Bremen, 2007–11–15

Outline

Finite Element Calculations

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Physical problem:

- real object
- physical process

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FE Simulation:

1. representation of object, PDE for physical process
2. geometric discretization: mesh (grid points and connectivity)
3. basis functions for discretization of continuous quantity
4. PDE leads to system of equations
5. solve
6. interpret and visualize result

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1. Objects / Physical Processes

Representation of objects:

- CAD model
- discrete image / volume dataset (CT, MRT, . . .)
- other levelset description

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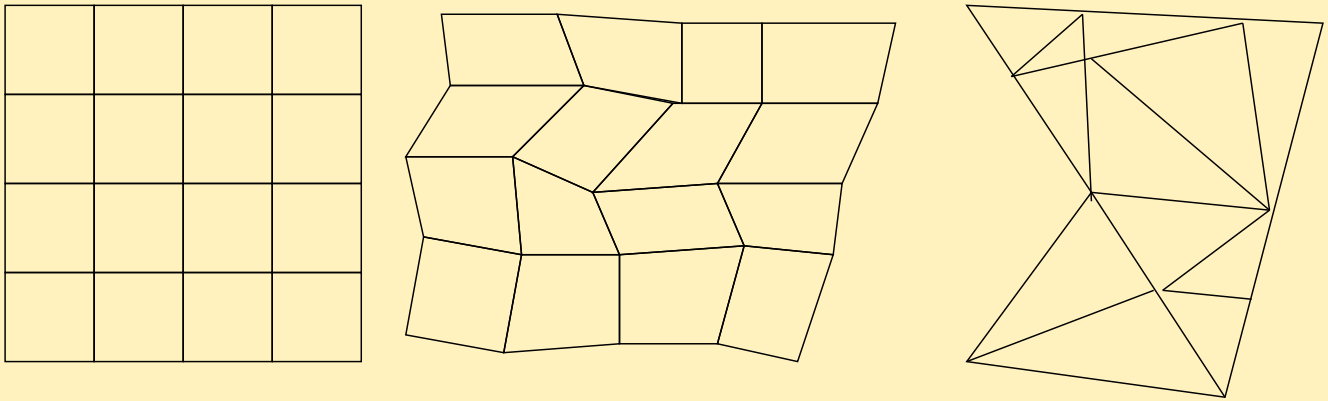
Physical process:

- process typically described by conservation principle
- can derive PDE

2. Grids



Different types of grids:

- uniform
- structured
- unstructured

3. Discretization (1D)

Continuous function

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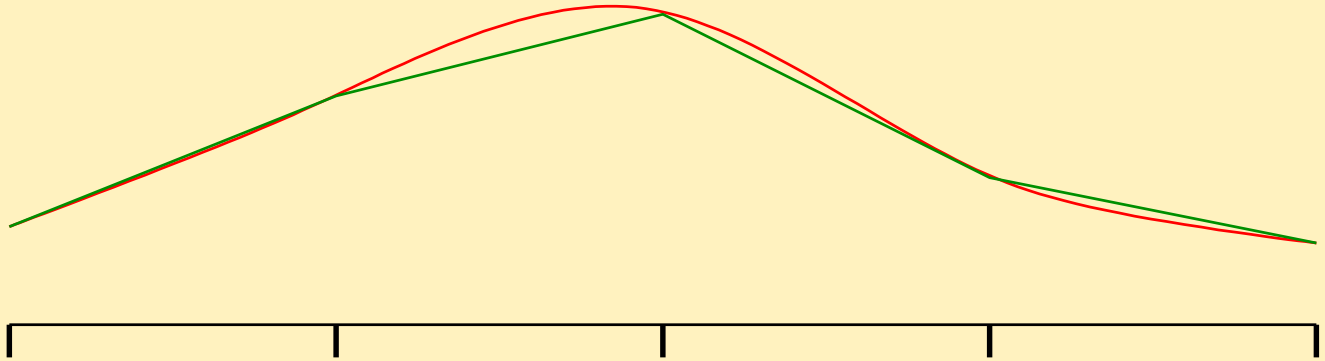

Piecewise linear interpolation on a discrete grid

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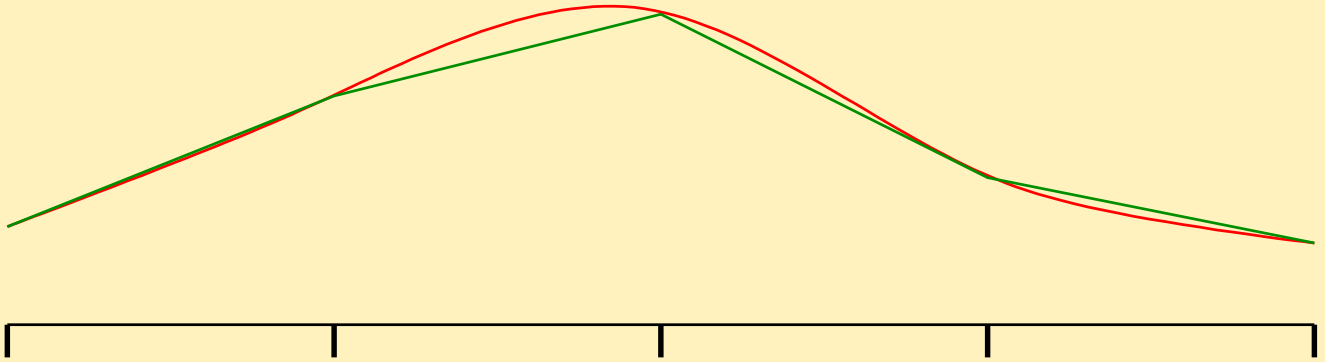

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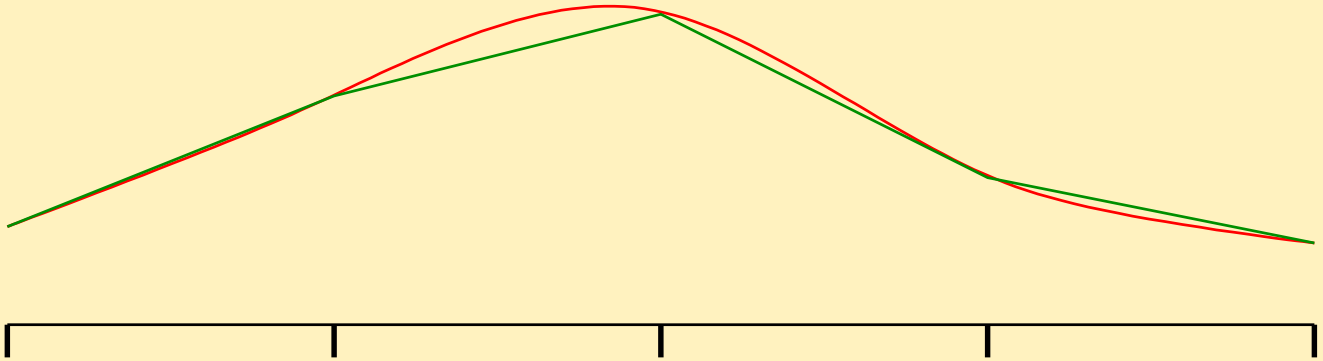

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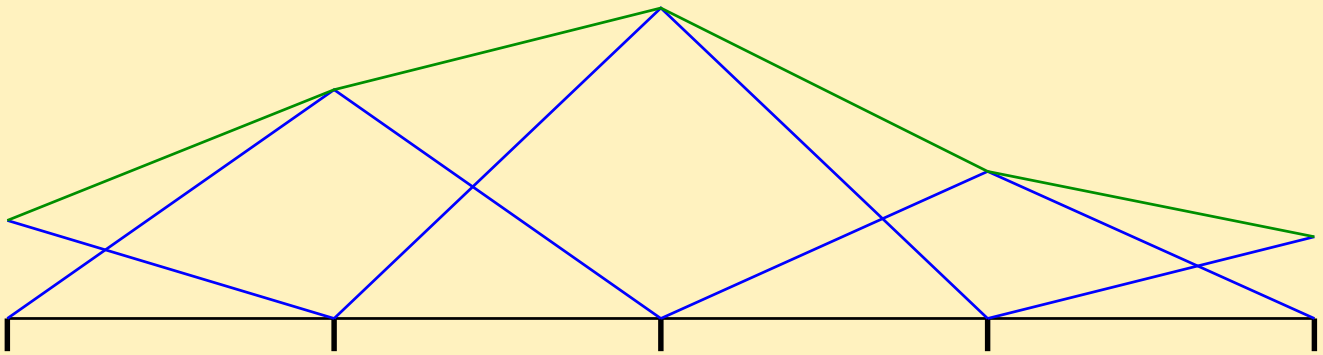
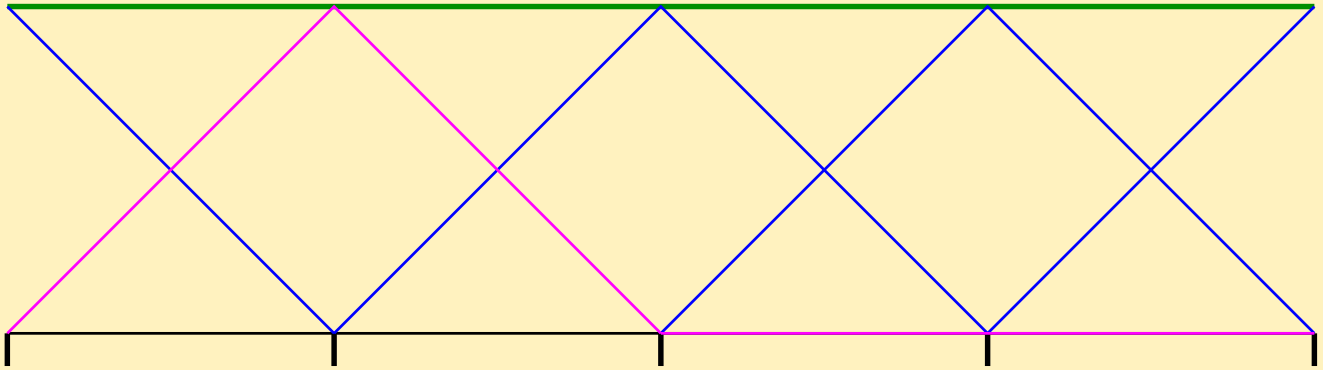


Discrete interpolation as sum of “hat” functions

3. Discretization (1D)



The basis of “hat” functions:

- piecewise linear
- nodal
- partition of unity

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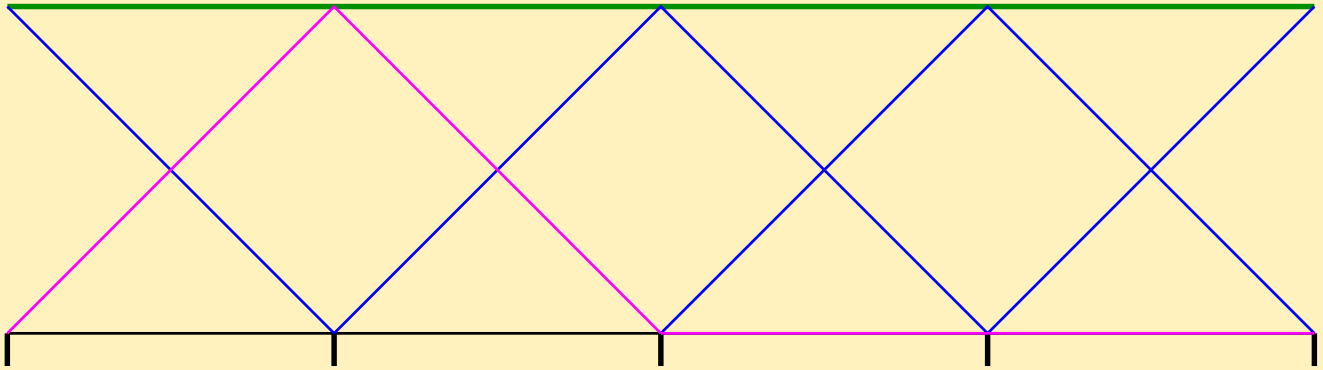
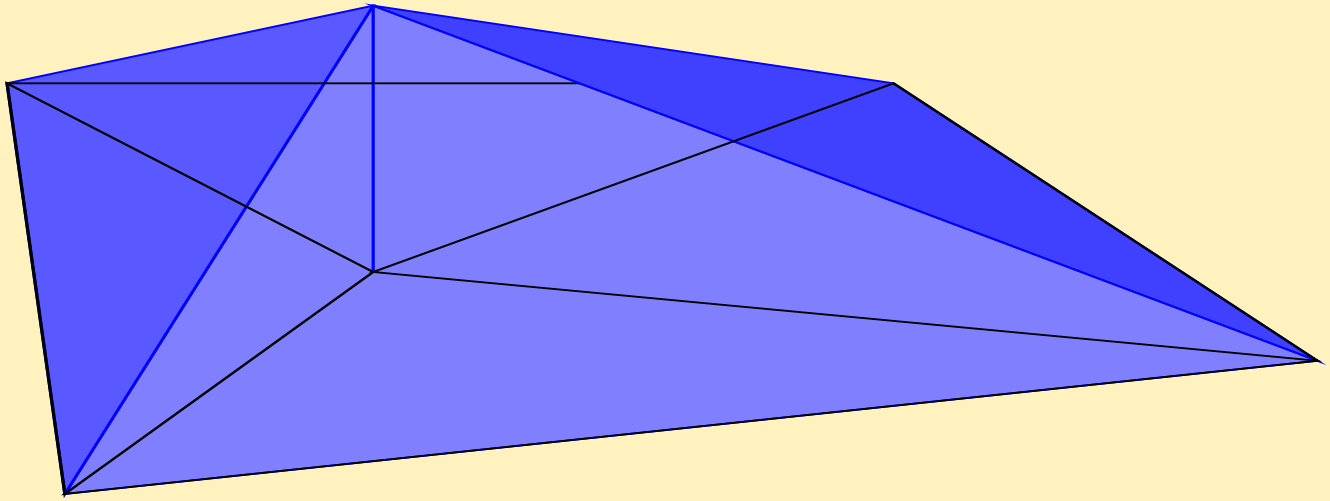


The basis of “hat” functions:

- piecewise linear
- nodal
- partition of unity
- interpolation of continuous function given by coefficient vector

3. Discretization (2D)



For triangular grids, “piecewise linear” can be generalized to 2D.

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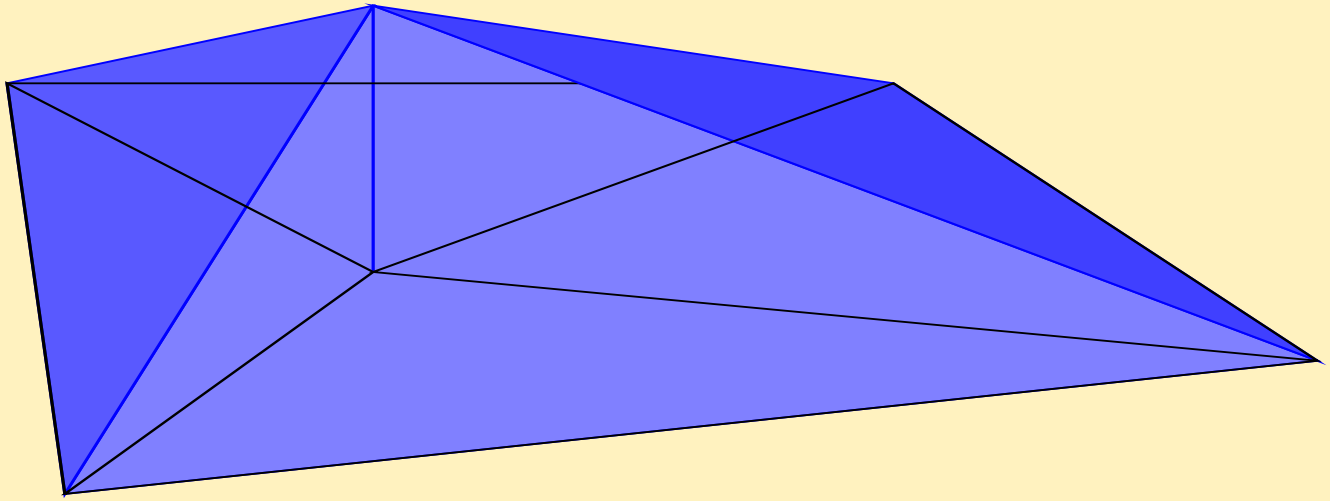

For triangular grids, “piecewise linear” can be generalized to 2D.

For quadrilateral grids, it becomes “piecewise multilinear”.

4. From PDE to Linear Equations

- weak / variational form of PDE problem
- “combination” of discrete basis functions
- integrals of (derivatives of) pairs of basis functions

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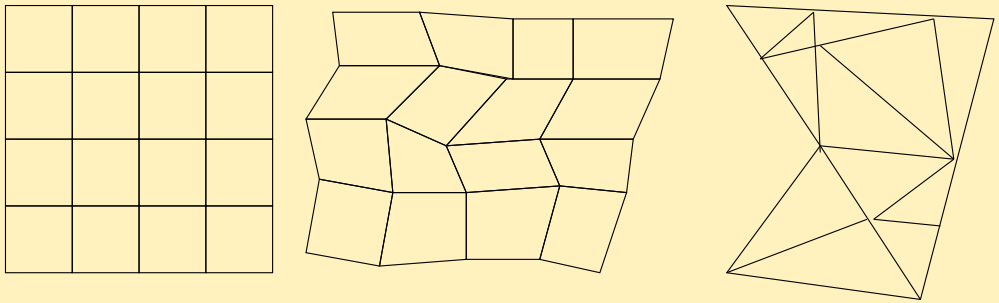
Consequences:

- matrix entry nonzero if supports overlap
- matrix is sparse
- sparsity structure reflects connectivity of the grid



Solving a system of equations

$$Ax = b$$

for $A \in \mathbb{R}^{n \times n}$

$$\begin{bmatrix} * & * & \dots & * \\ * & * & & * \\ \vdots & & \ddots & \\ * & * & & * \end{bmatrix} \begin{bmatrix} ? \\ ? \\ \vdots \\ ? \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \vdots \\ \star \end{bmatrix}$$

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Different methods:

- direct
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Different methods:

- direct
- iterative
- conjugate gradient
- multigrid

Gaußian Elimination

Simple direct method to compute the solution.

$$\begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \end{bmatrix} \begin{bmatrix} ? \\ ? \\ ? \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix} \rightarrow \begin{bmatrix} 1 & * & * \\ & * & * \\ & * & * \end{bmatrix} \begin{bmatrix} ? \\ ? \\ ? \end{bmatrix} = \begin{bmatrix} \star \\ \star \\ \star \end{bmatrix}$$

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- full matrix storage required, even for sparse matrices: $O(n^2)$ memory
- $O(n^3)$ algorithmic complexity
- propagation of numerical errors

Iterative Methods

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Properties:

- typically no storage of matrix necessary
- can stop if $\|Ax^n - b\|$ "sufficiently small"

Iterative Method: Jacobi

[Jacobi 1844]
Let $D = \text{diag}(A)$ have nonzero entries.

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Jacobi iteration:

$$x^{n+1} = D^{-1}\left(D - A\right)x^{n} + D^{-1}b$$

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Properties:

- no need to store $A, D, D - A$
- convergence is slow

Iterative Method: Gauß-Seidel

Let

- D be the diagonal part of A with nonzero entries
- L be the strictly lower trianuglar part

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Properties:

- Jacobi iteration using same memory for x^n and x^{n+1}
- no need to store $A, L, D + L - A$
- convergence is better than for Jacobi, but still slow

Solving as an Optimization Problem

Let A be symmetric and positive definite (SPD), then

$$Ax = b \Leftrightarrow Ax - b = 0 \Leftrightarrow x \text{ minimizes } \frac{1}{2}Ay \cdot y - b \cdot y$$

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solving the system is equivalent to a convex minimization problem.

Conjugate Gradient Method

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[Hestenes, Stiefel 1952]
In each step, find optimal descent direction based on old directions.

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Properties:

- direct method (n iterations)
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- convergence depends on condition number $\kappa(A)$

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[Hestenes, Stiefel 1952]
In each step, find optimal descent direction based on old directions.

Properties:

- direct method (n iterations)
- typically used as iterative method
- convergence depends on condition number $\kappa(A)$ and on full spectrum

Condition Number

$$\kappa := \frac{|\text{largest eigenvalue of } A|}{|\text{smallest eigenvalue of } A|}$$

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Example:

$$\begin{bmatrix} 1 & \\ & 1000 \end{bmatrix} \begin{bmatrix} ? \\ ? \end{bmatrix} = \begin{bmatrix} \star \\ \star \end{bmatrix} \qquad \kappa = 1000$$

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$$\left\| \begin{bmatrix} 1 & \\ & 1000 \end{bmatrix} \begin{bmatrix} ? \\ ? \end{bmatrix} - \begin{bmatrix} \star \\ \star \end{bmatrix} \right\|$$

Preconditioning

For nonsingular P,

$$Ax = b \Leftrightarrow (P^{-1}A)x = P^{-1}b$$

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Need

- P “easy to invert”
- $P^{-1}A$ has “small condition number” (for fast CG convergence)

Preconditioning

For nonsingular P,

$$Ax = b \Leftrightarrow (P^{-1}A)x = P^{-1}b$$

Need

- P "easy to invert" $P = \mathbb{1}$
- $P^{-1}A$ has "small condition number" (for fast CG convergence) $P = A^{-1}$

Preconditioning

For nonsingular P,

$$Ax = b \Leftrightarrow (P^{-1}A)x = P^{-1}b$$

Need

- P "easy to invert"
- $P^{-1}A$ has "small condition number" (for fast CG convergence)

Simplest choice: $P = \text{Diag}(A)$, other methods (SSOR, ILU0, ...)

Smoothing by Gauß-Seidel

Consider the Poisson problem (steady state of heat conduction)

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega \\ u &= 0 && \text{on } \partial\Omega \end{aligned}$$

for given source term f.
Again leading to system

$$Ax = b$$

Smoothing by Gauß-Seidel

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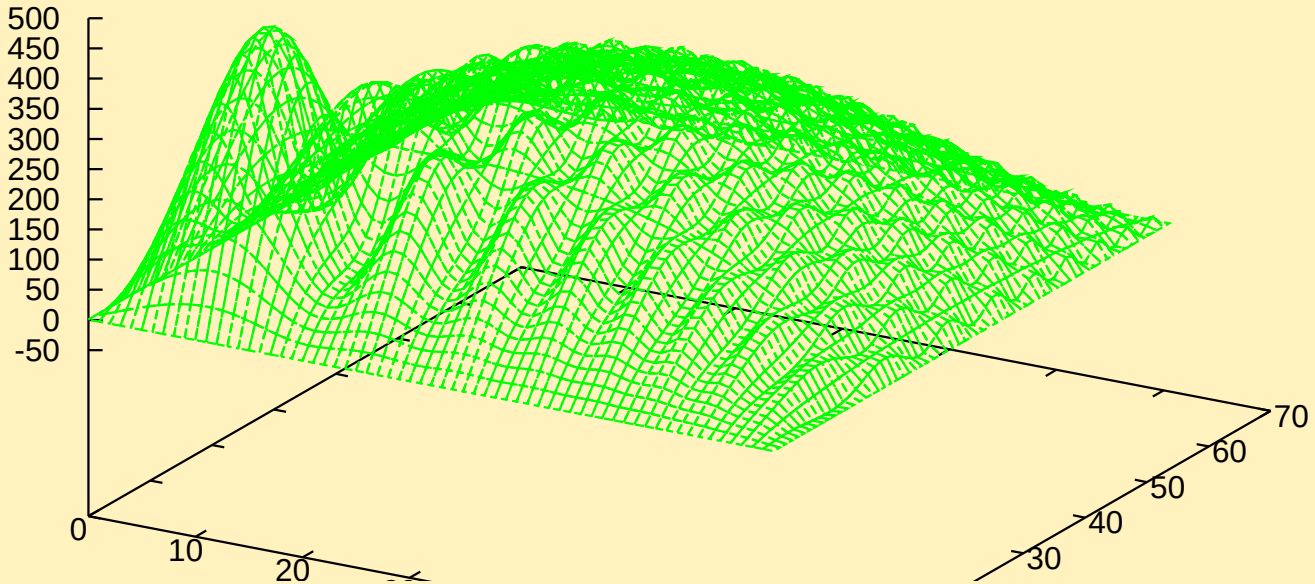
Known solution:



Smoothing by Gauß-Seidel

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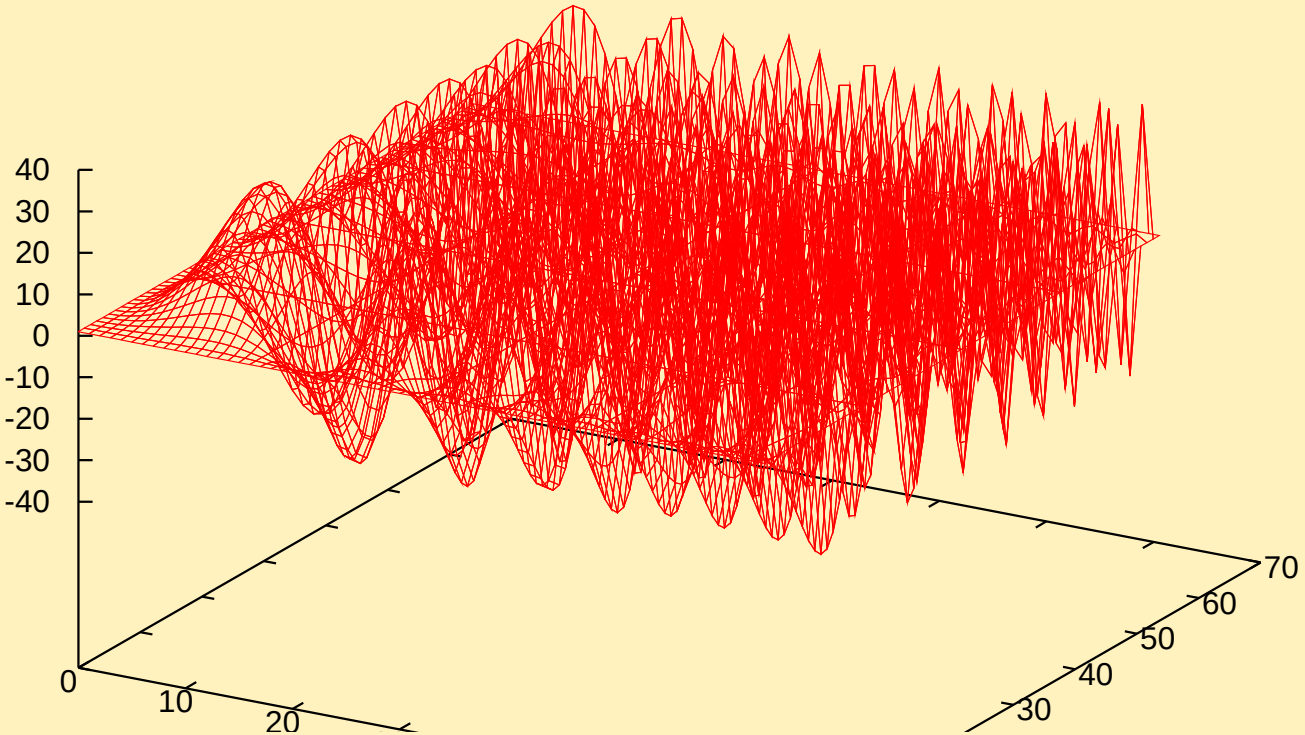
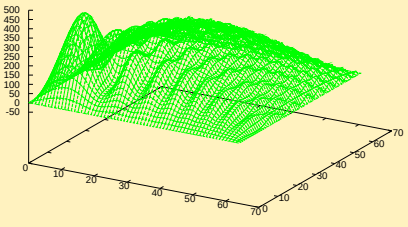
Right hand side:





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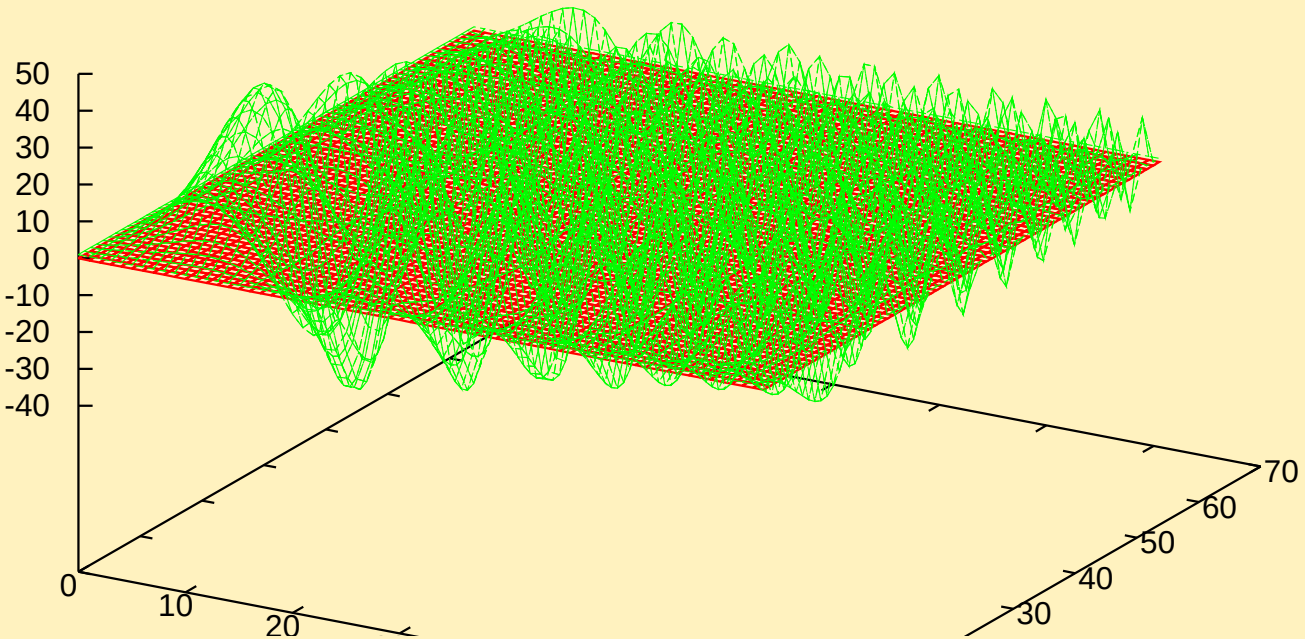
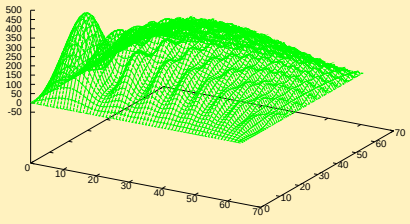
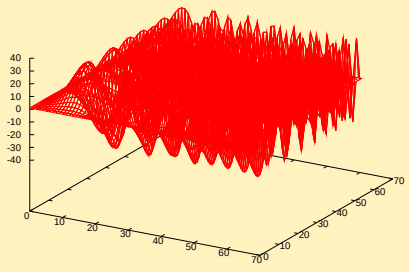
Initial guess (red) and “solution” after two Gauß-Seidel iterations:







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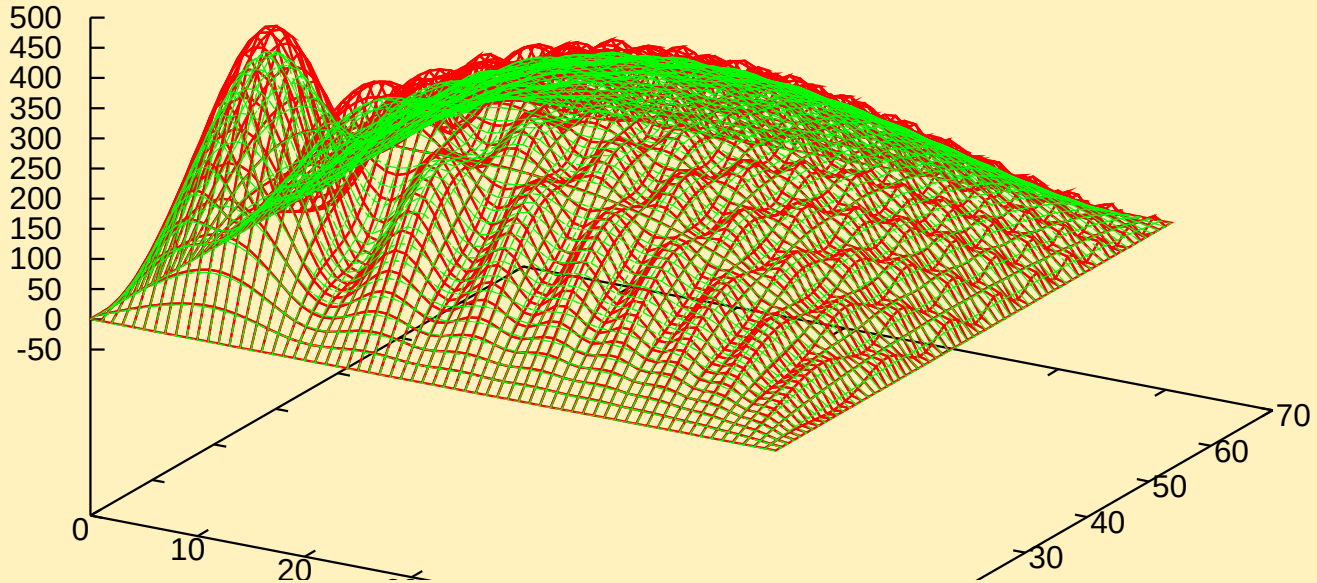
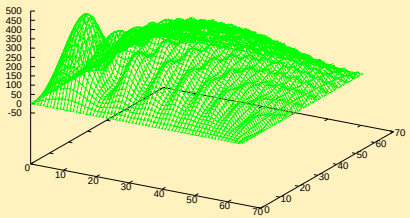
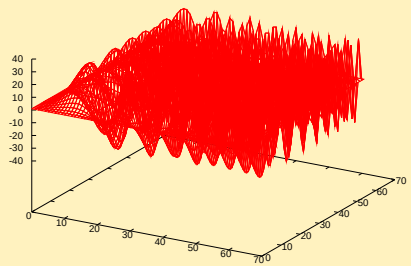
Initial error (red) and error after two Gauß-Seidel iterations:







Smoothing by Gauß-Seidel

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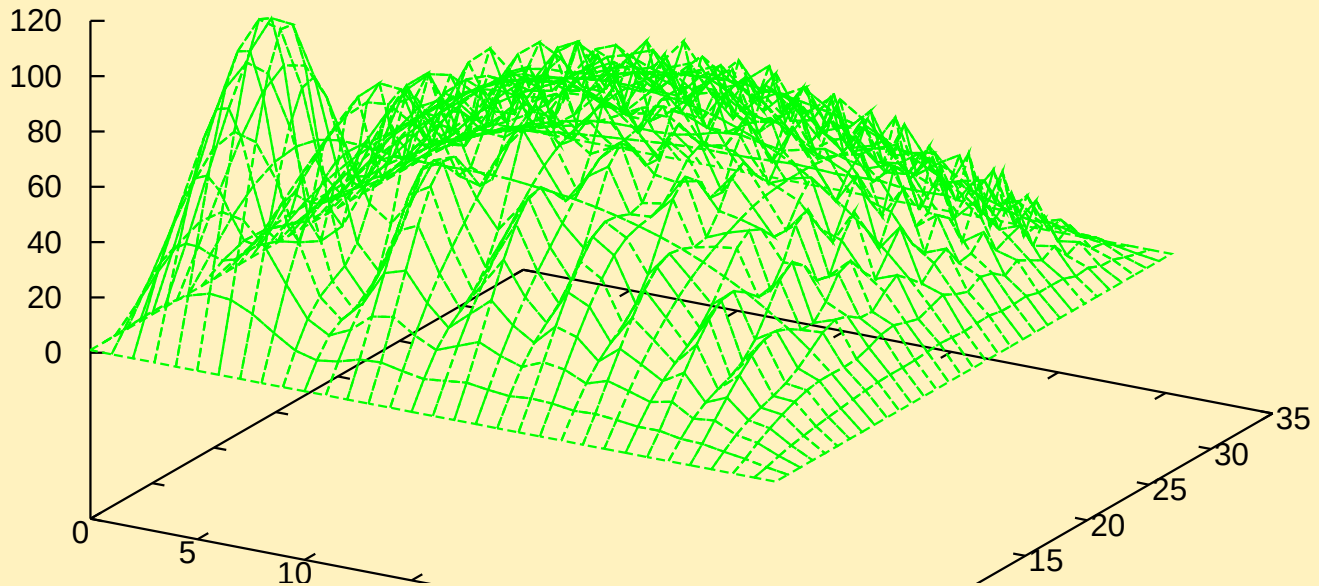
Known solution on coarser grid:



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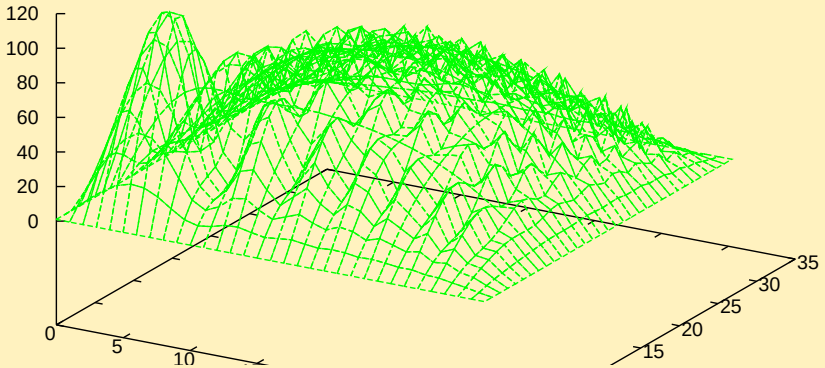
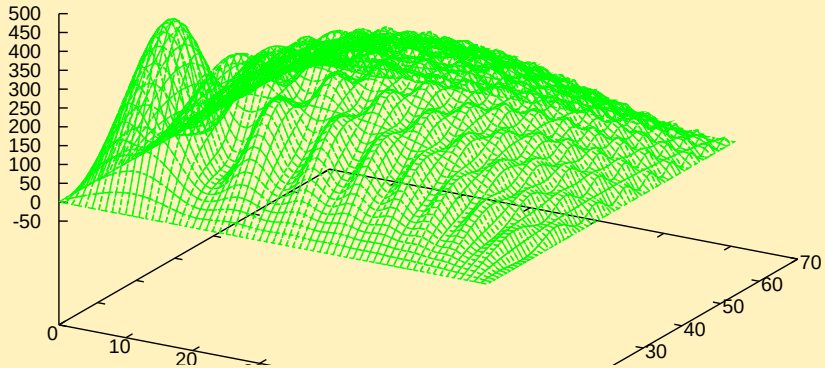
Compare coarse and fine grid:





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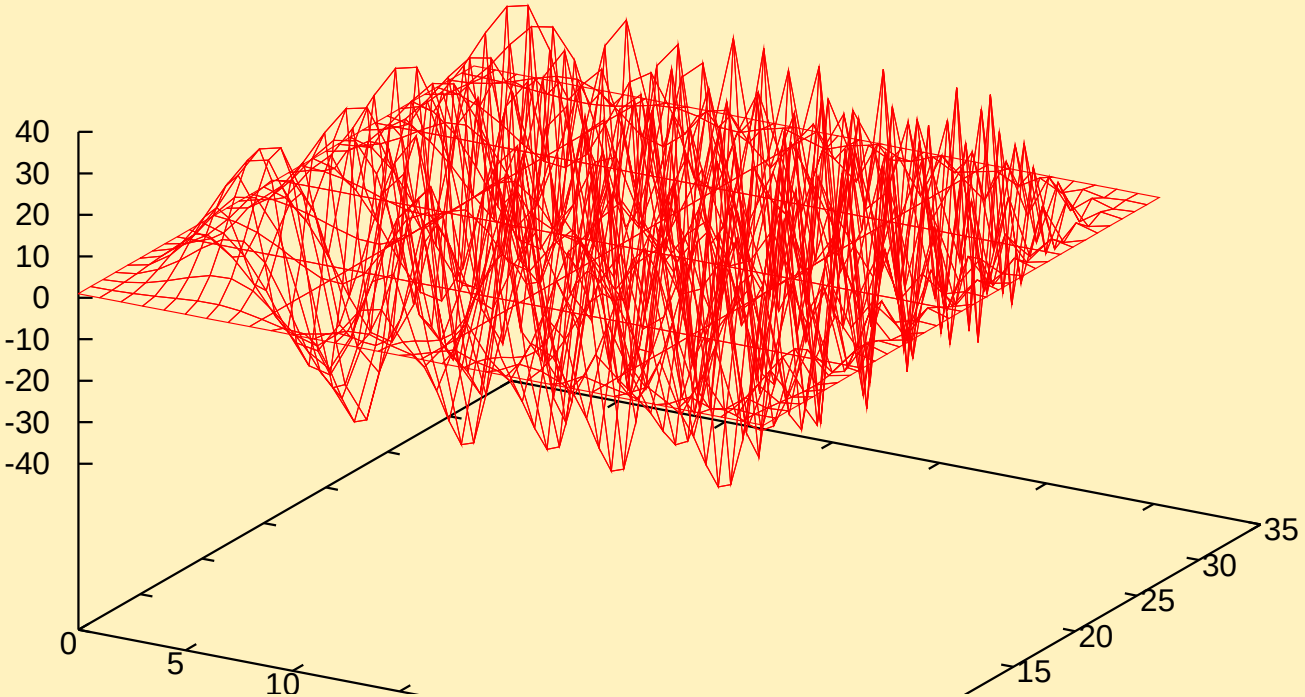

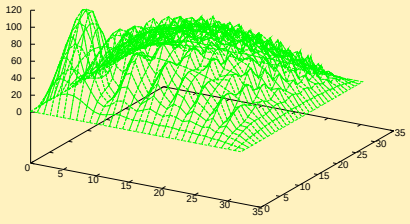

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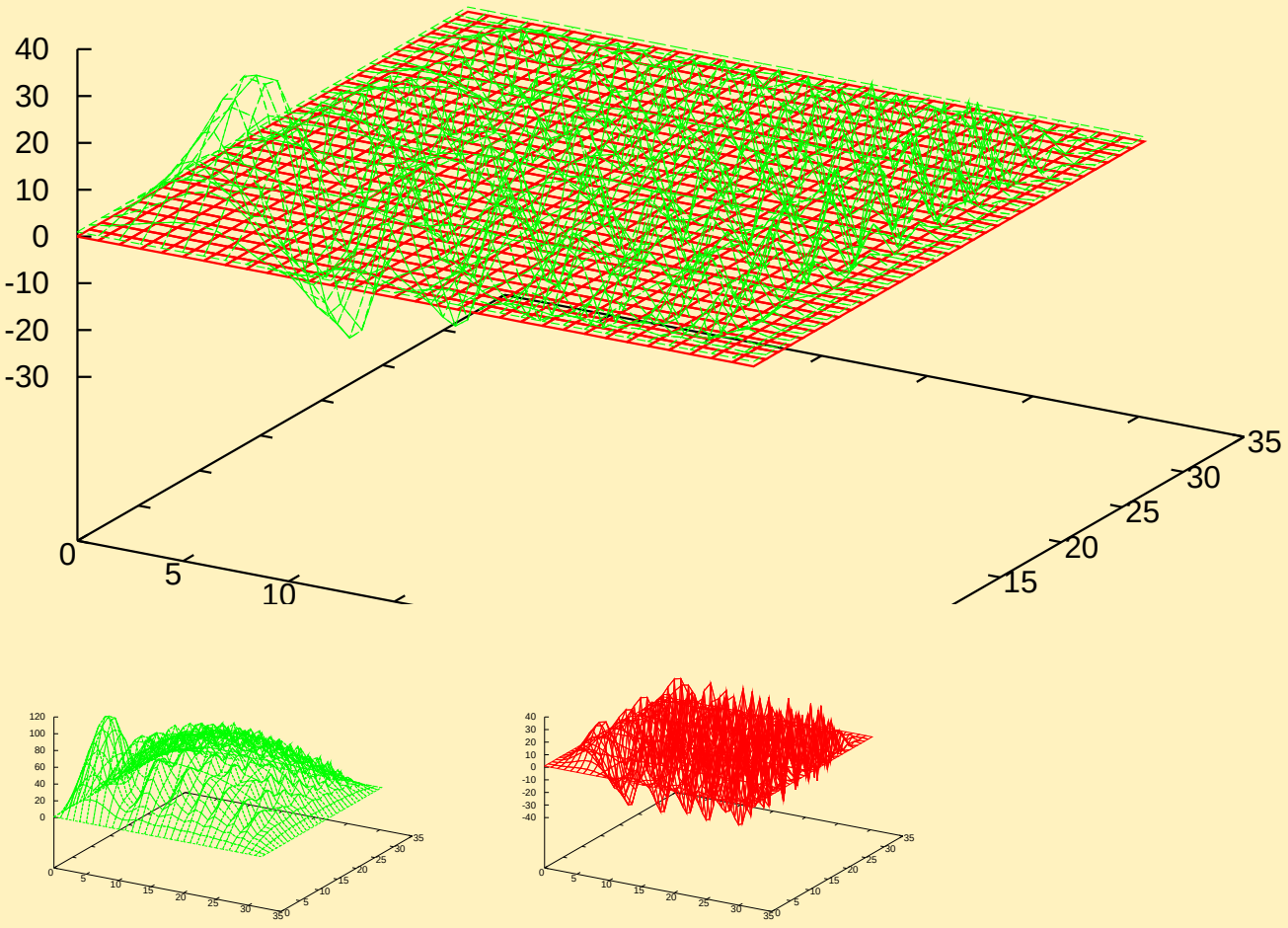

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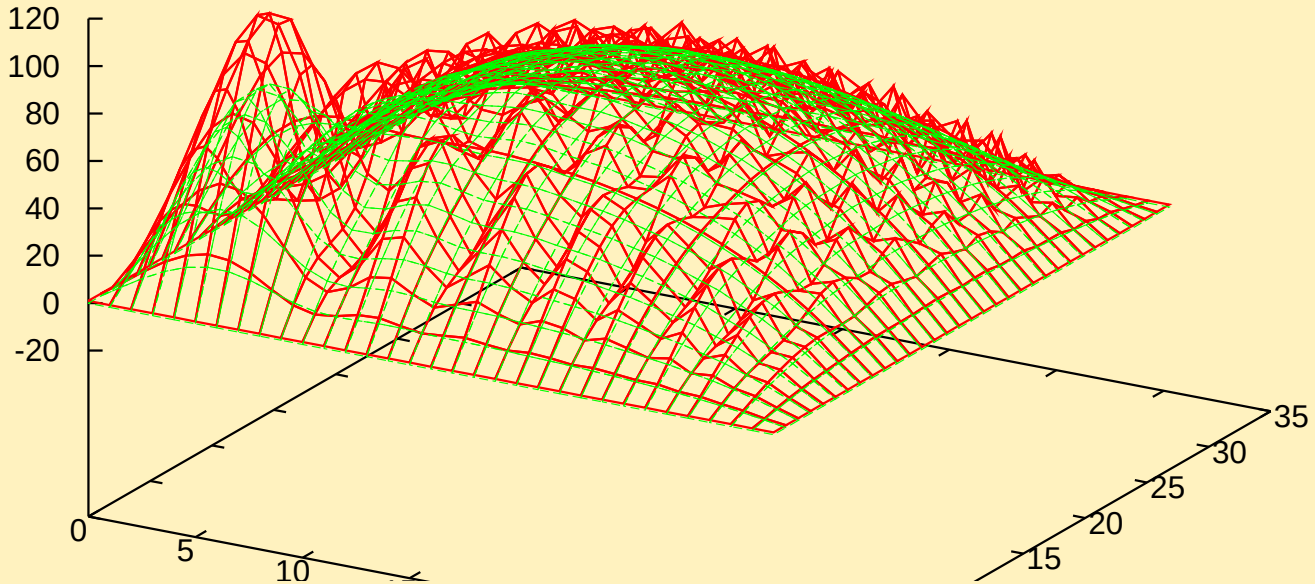

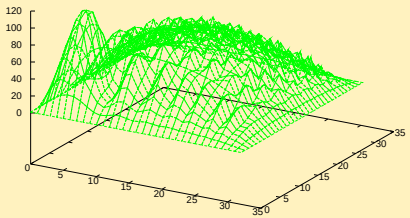

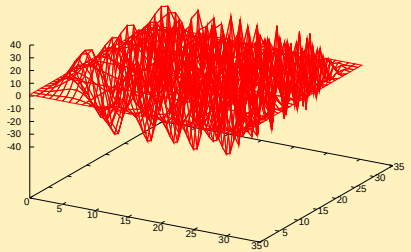

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Observations:

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Conclusion:

- Treat different frequencies at different resolutions!

Basic Two-Grid Scheme

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[Bakhalov; Fedorenko; Brandt 1977]

1. **Presmooth**: Perform ν_1 Gauß-Seidel iterations: $x^{(1)}$

Basic Two-Grid Scheme

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4. **Solve** $\tilde{A}\tilde{e} = \tilde{r}$ 
5. **Prolongate** the result: compute fine e
6. Add the coarse grid correction: $x^{(2)} = x^{(1)} + e$

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[Bakhalov; Fedorenko; Brandt 1977]

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System Coarsening $\tilde{A} = \mathcal{R}A\mathcal{P}$

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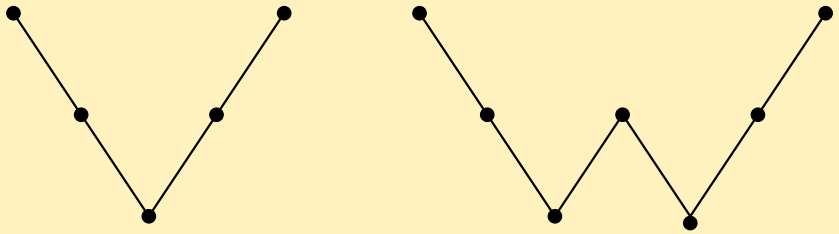
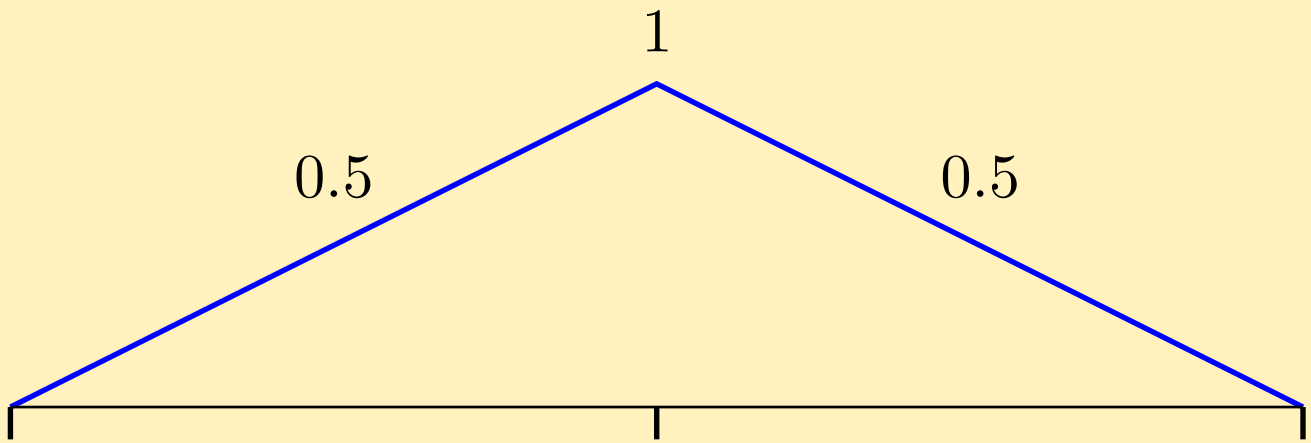
Solve can recursively call this procecdure: Multigrid.
V-cycle vs. W-cycle:



Prolongation

Evaluate coarse grid basis functions at fine grid points.



Can be interpreted as interpolation based on basis functions.

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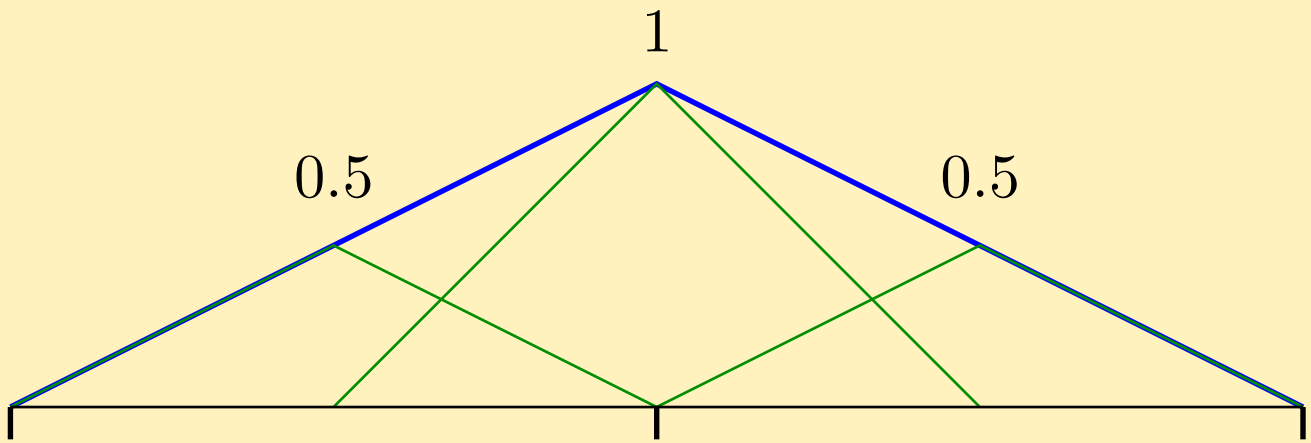

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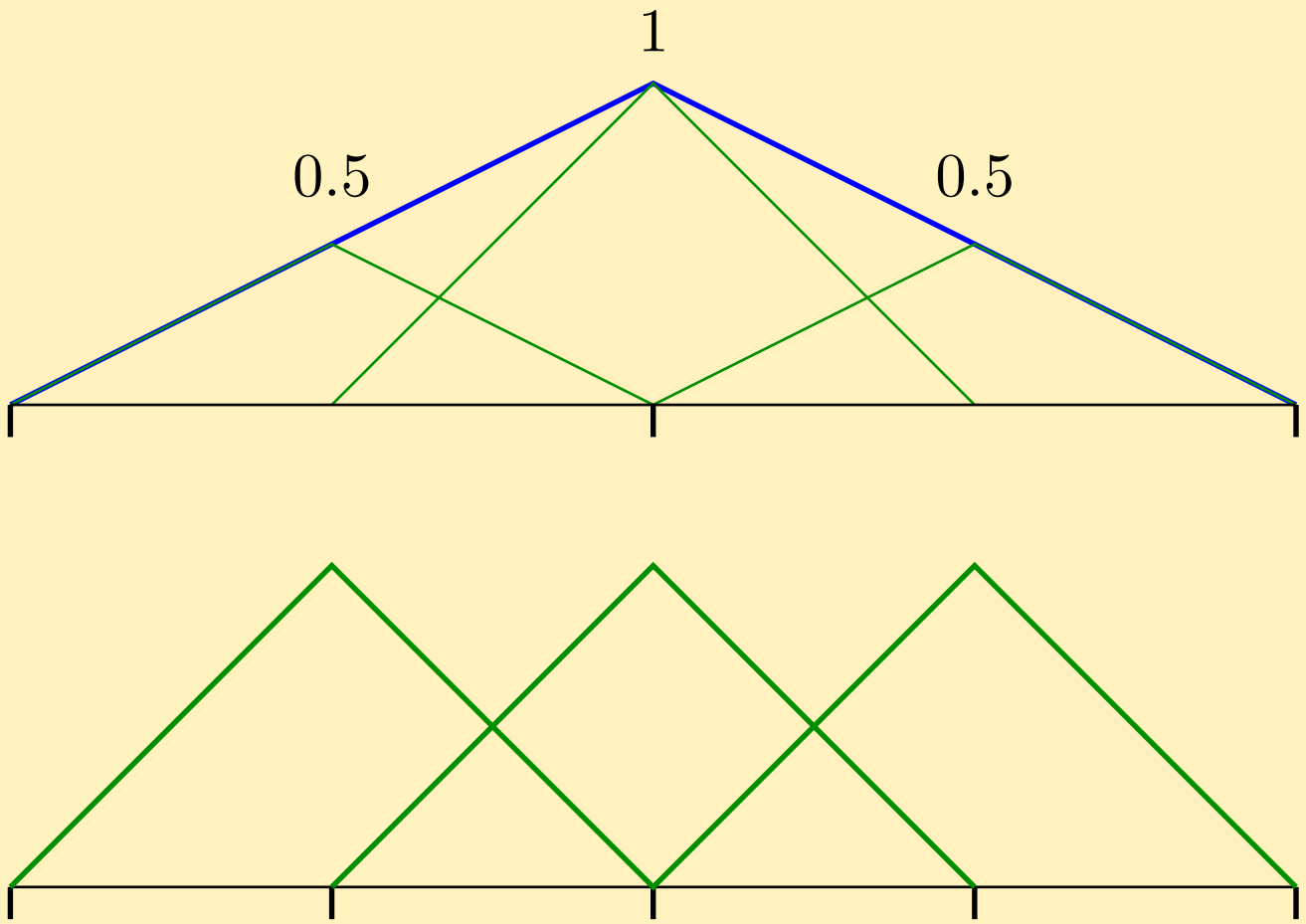

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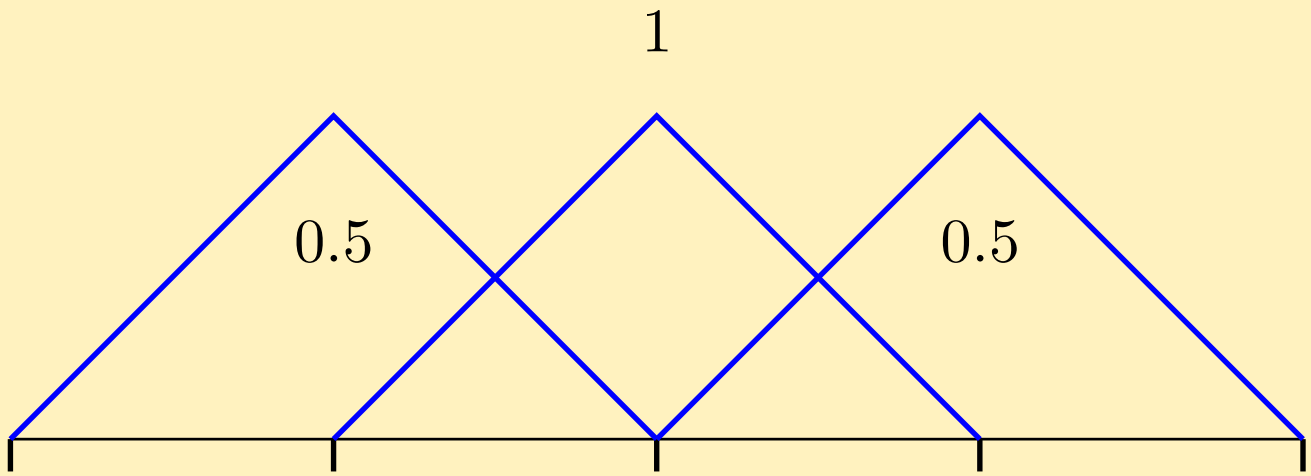
Restriction

Transpose of prolongation.



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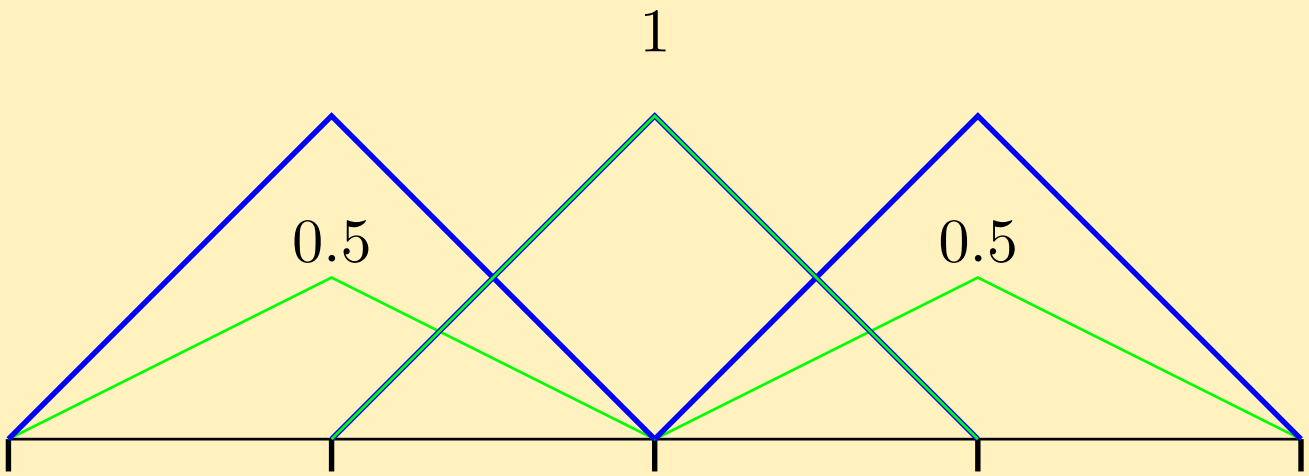

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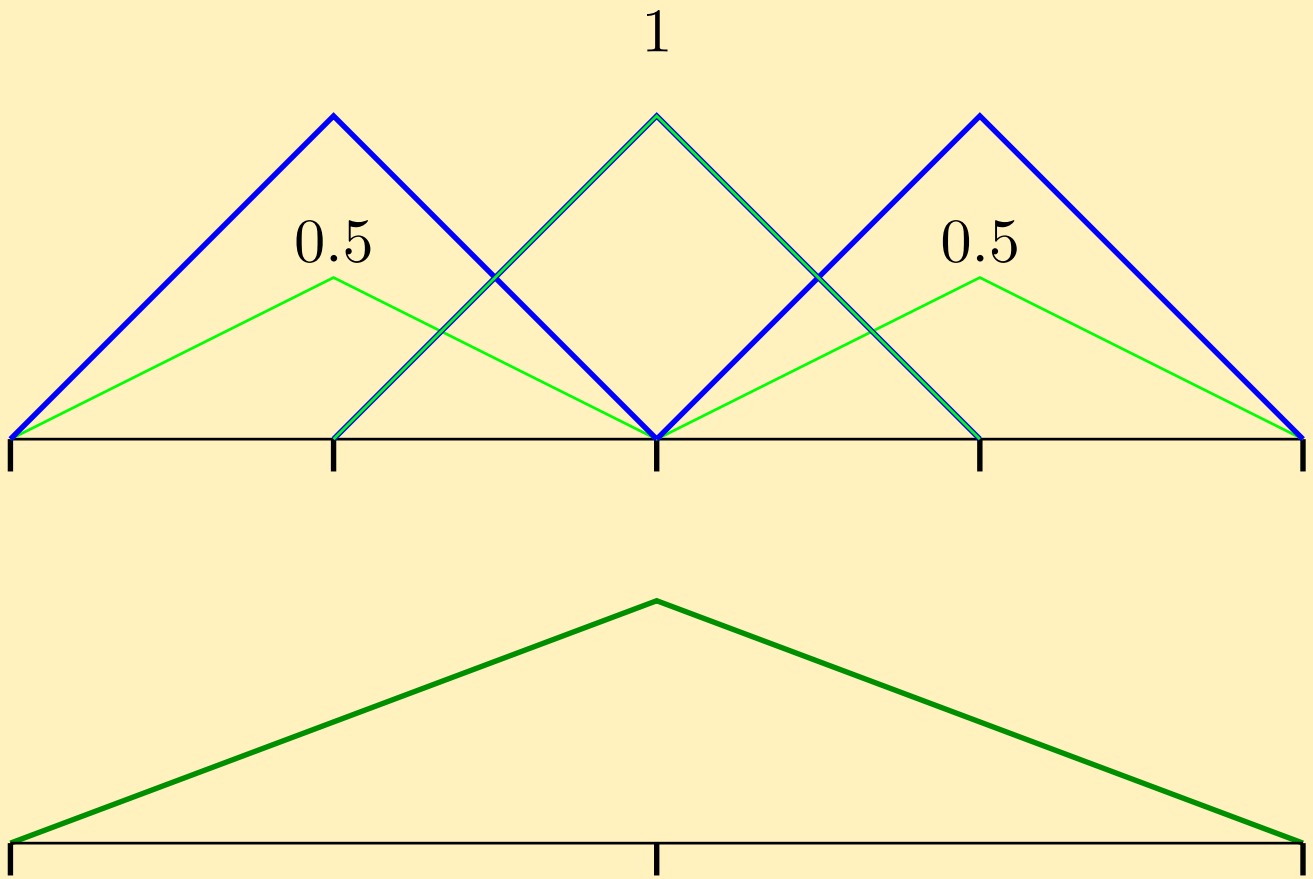

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Algorithmic Complexity

For $A \in \mathbb{R}^{n \times n}$ with β nonzero bands, solve

$$Ax = b$$

to accuracy ϵ, e. g.

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method	**complexity**	**convergence rate**
Gaußian elimination	$O(n^3)$	—
Jacobi, Gauß-Seidel	$O(\beta n \lvert \log \epsilon \rvert)$	$O\left(\frac{\kappa-1}{\kappa+1}\right)$
conjugate gradient	$O(\beta n \lvert \log \epsilon \rvert)$	$O\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)$
multigrid	$O(\beta n \lvert \log \epsilon \rvert)$	not destroyed by large κ

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Algebraic Multigrid Methods

If no geometric coarse scales available, purely algebraic coarsening can be used:

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If no geometric coarse scales available, purely algebraic coarsening can be used:

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- can define coarsening only based on this information

Composite FE for Complicated Geometries

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Finite Elements:

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- structured cubic grids:
  - efficient
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Composite Finite Elements:

- combine advantages of both
- use simple grid with complicated basis functions

Composite FE in 1D

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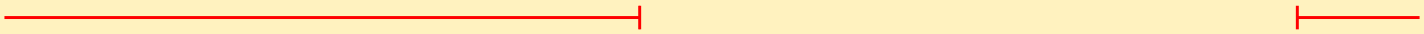
[Hackbusch, Sauter 1997]



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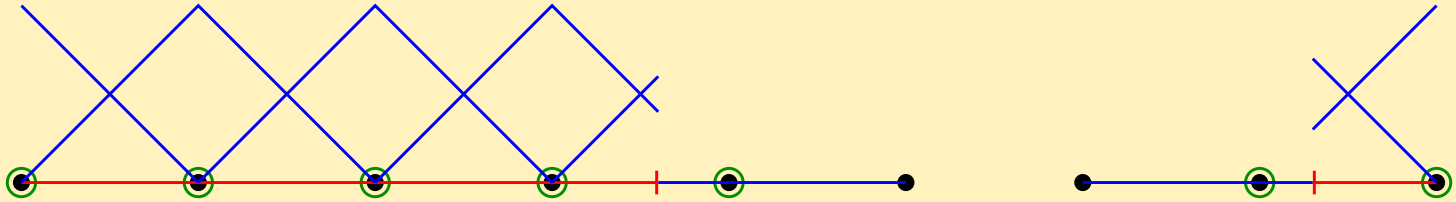

- equidistant grid for complicated geometry, based on image data
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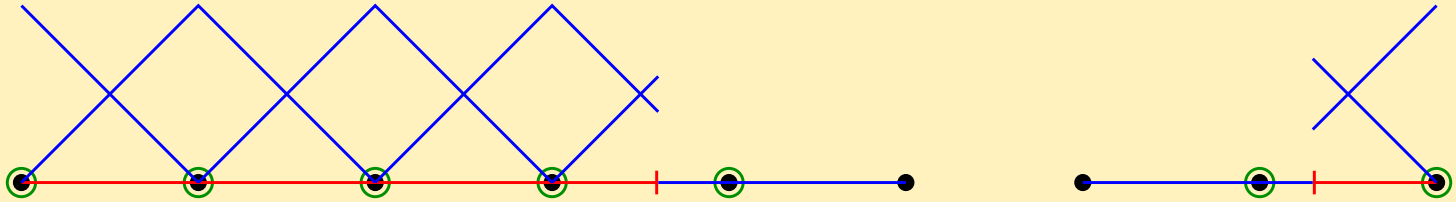

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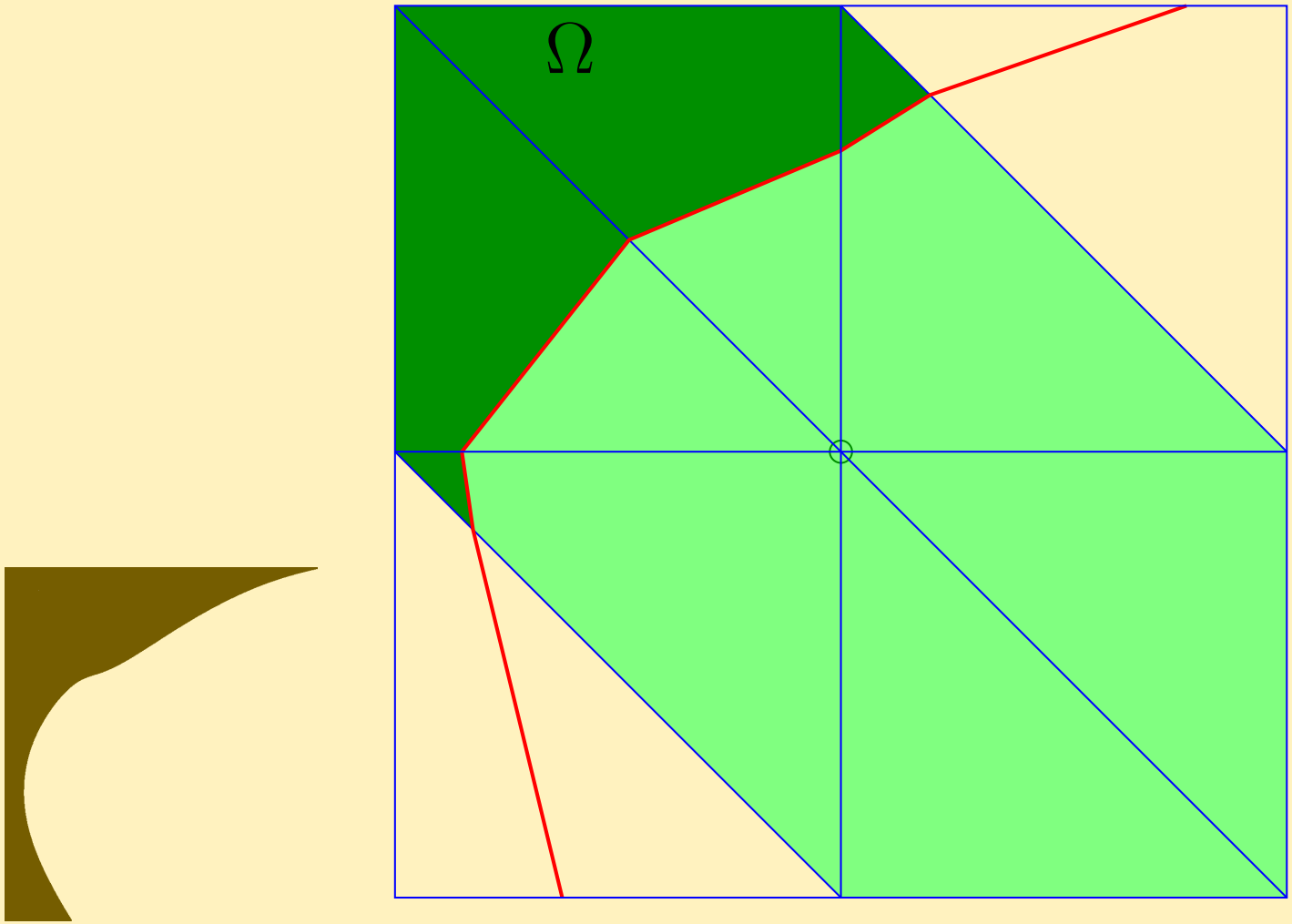
CFE basis functions are

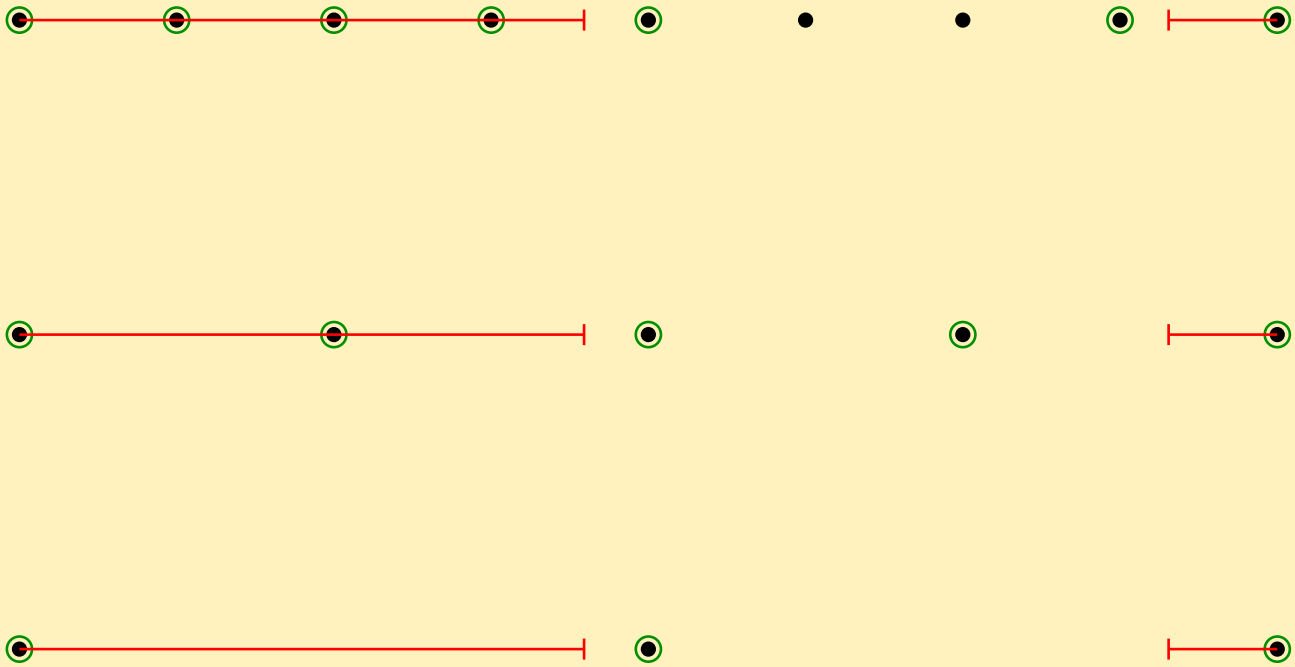
- piecewise linear
- nodal
- partition of unity

Composite FE in 2D



Basis function supported in dark green region and set to zero in light green region

Multigrid: Coarsening in 1D



- natural grid hierarchy

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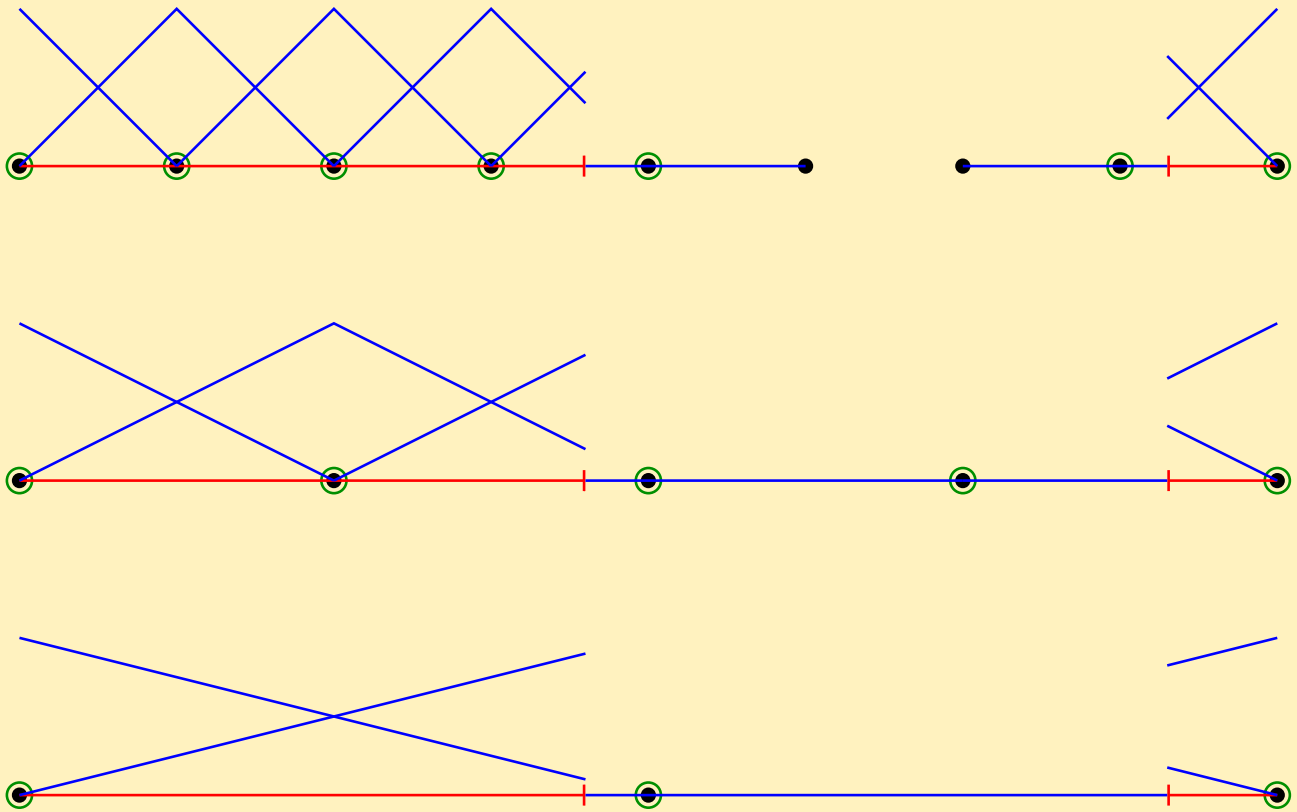

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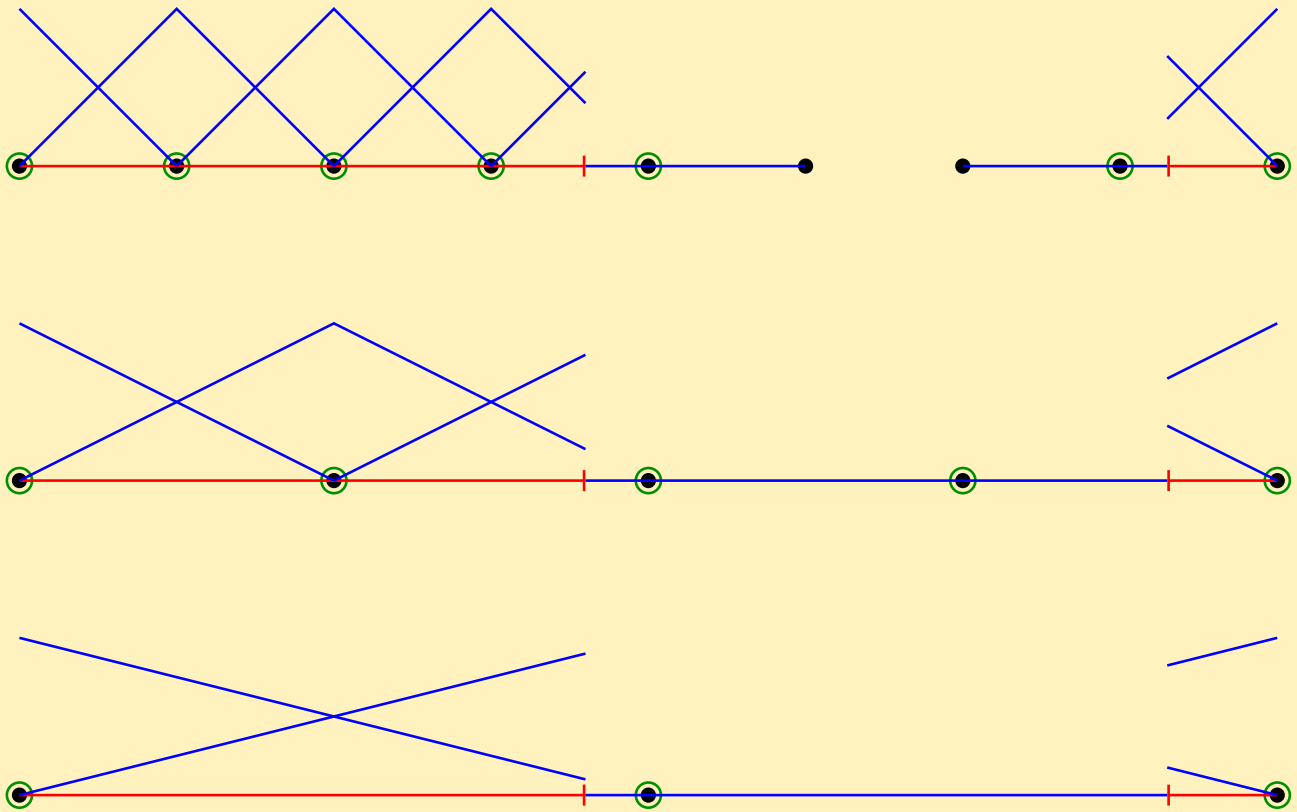

- natural grid hierarchy
- last step questionable: same DOF for separate parts

Multigrid: Artificial Coupling

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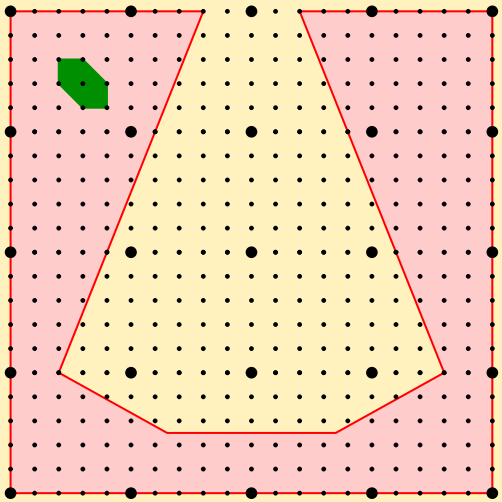
"Horseshoe" geometry



On fine scale: no problem.

Multigrid: Artificial Coupling

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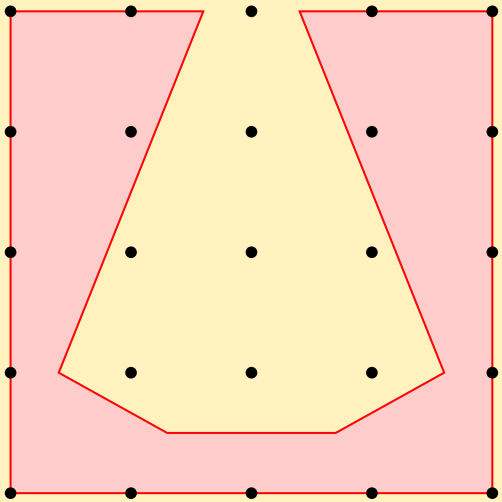

On coarse scale

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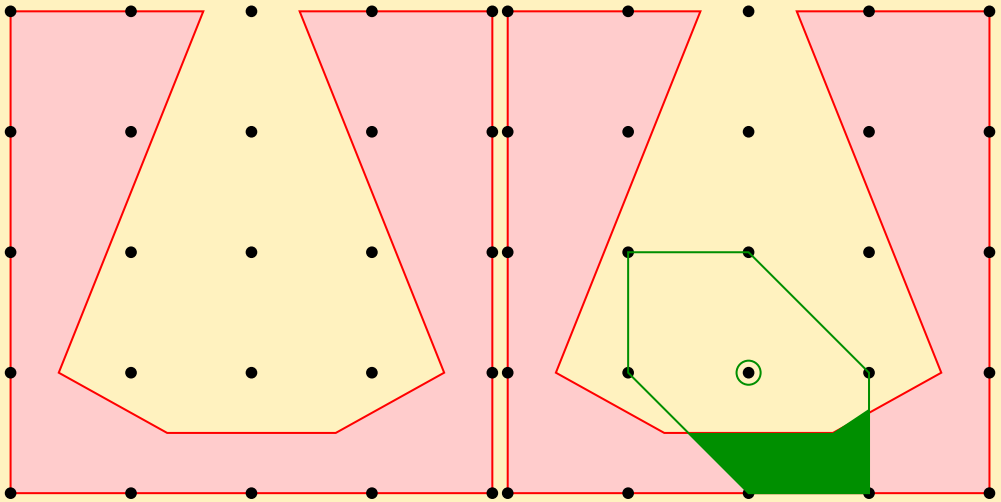

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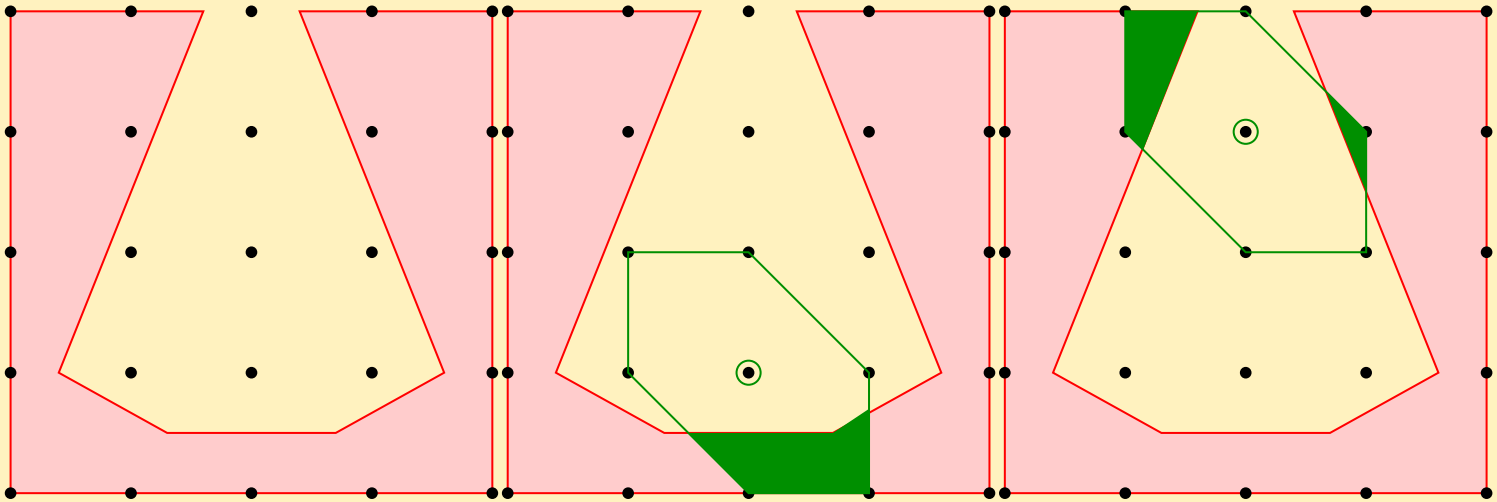
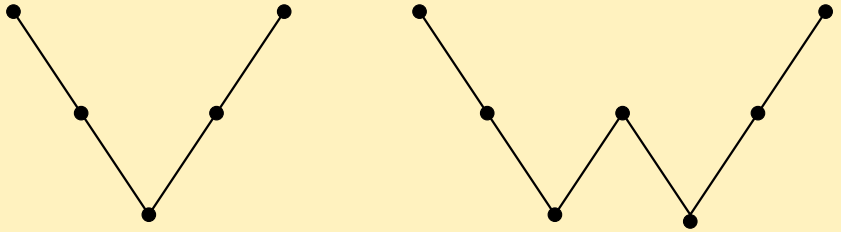


On coarse scale: FE coupling in simulations does not reflect physical coupling.

Truncated Multigrid



Globally stop coarsening process as soon as “horseshoe effect” occurs.

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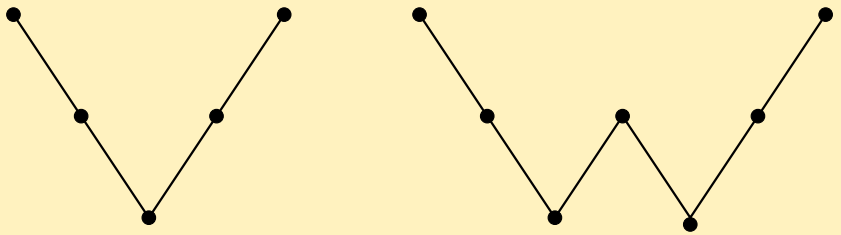

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- ✔ simple modification
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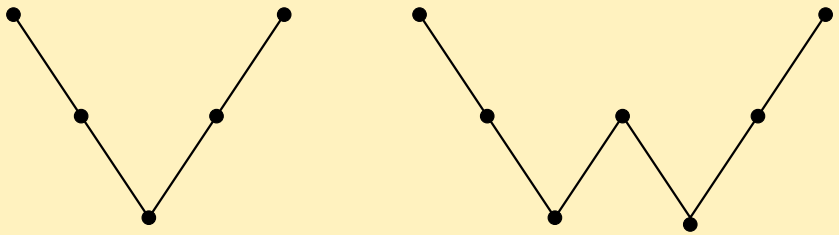
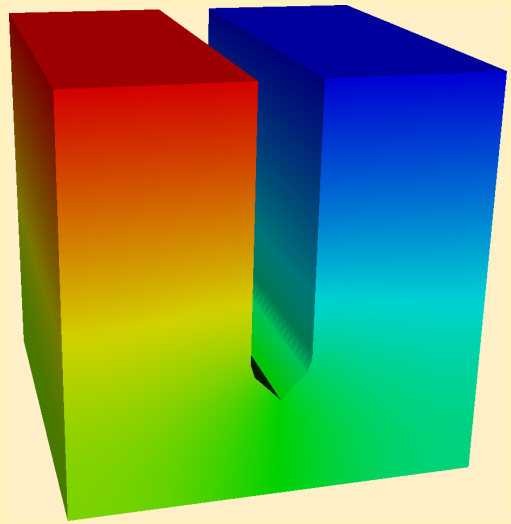


Globally stop coarsening process as soon as “horseshoe effect” occurs.

- ✔ simple modification
- ✔ good convergence rates
- ✘ slow, because large problems need to be solved directly

Truncated Multigrid, Example



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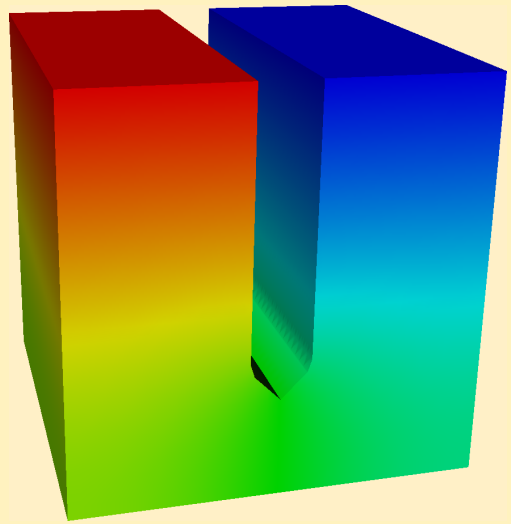

slot width	coarsest grid	convergence rate
1/7	1/16	0.117
1/7	1/8	0.451
1/14	1/64	0.107
1/14	1/32	0.171
1/14	1/16	0.650

Adaptively Stopped Coarsening

Recall basic multigrid cycle:

1. **Presmooth**: Perform ν_1 Gauß-Seidel iterations: $x^{(1)}$ 
2.
3. Compute Residual: $r = b - Ax^{(1)}$.
4. **Restrict** the residual: compute coarse version $\tilde{r}$
5. **Solve** $\tilde{A}\tilde{e} = \tilde{r}$ 
6. **Prolongate** the result: compute fine e
7. Add the coarse grid correction: $x^{(2)} = x^{(1)} + e$
8.
9. **Postsmooth**: Perform ν_2 Gauß-Seidel iterations 

Adaptively Stopped Coarsening

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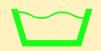
Distinguish between "standard" nodes and "horseshoe" nodes:

1. **Presmooth**: Perform ν_1 Gauß-Seidel iterations: $x^{(1)}$ 
2. Perform α_1 additional Gauß-Seidel iterations for "horseshoe" nodes only 
3. Compute Residual: $r = b - Ax^{(1)}$.
4. **Restrict** the residual: compute coarse version $\tilde{r}$ ignoring "horseshoe" nodes
5. **Solve** $\tilde{A}\tilde{e} = \tilde{r}$ 
6. **Prolongate** the result: compute fine e ignoring "horseshoe" nodes
7. Add the coarse grid correction: $x^{(2)} = x^{(1)} + e$
8. Perform α_2 additional Gauß-Seidel iterations for "horseshoe" nodes only 
9. **Postsmooth**: Perform ν_2 Gauß-Seidel iterations 

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- ✔ easy to implement
- ✘ minor or no improvement of convergence
- theoretical implications for convergence?

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slot width	coarsest grid	conv. rate std MG	adapted MG
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Review: Standard Grid Coarsening (2D)

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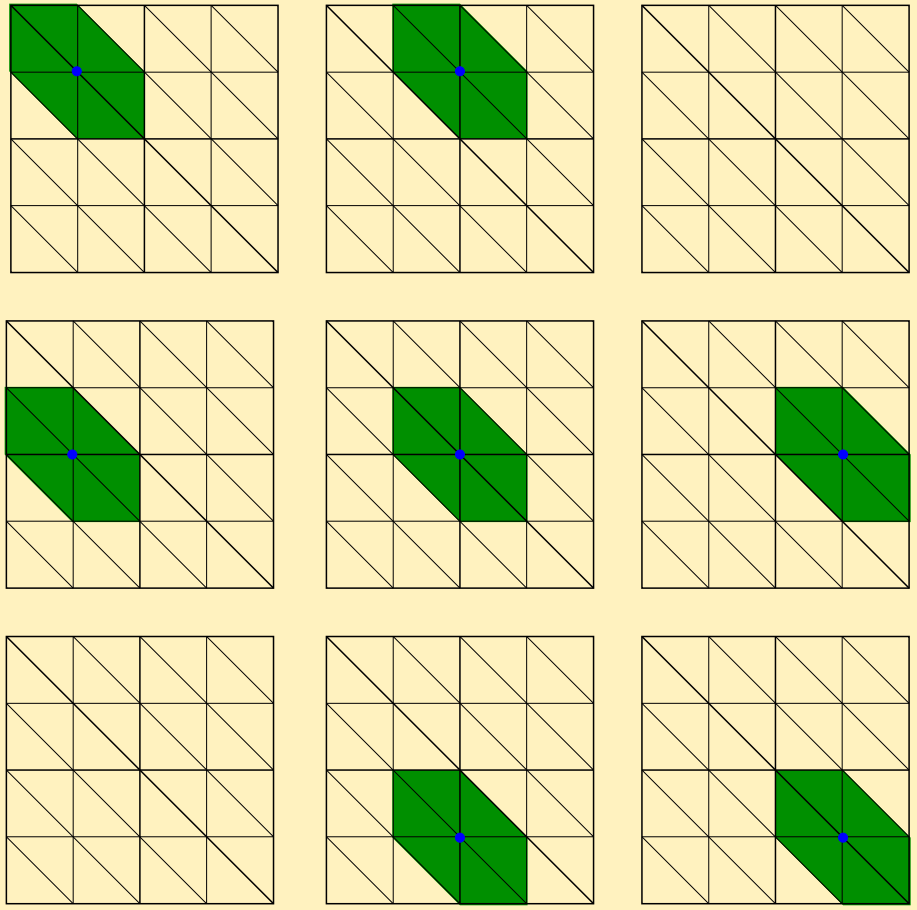

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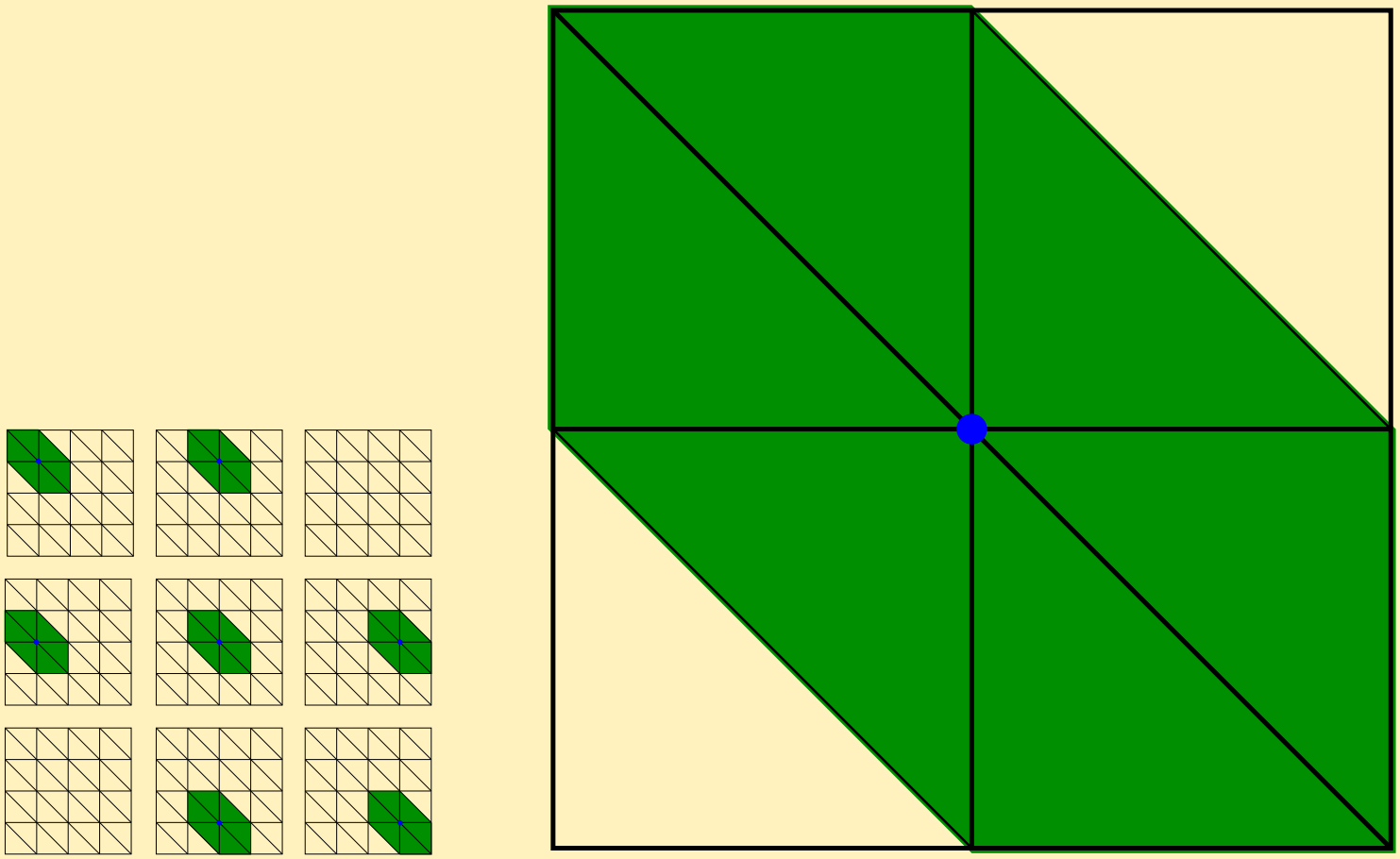
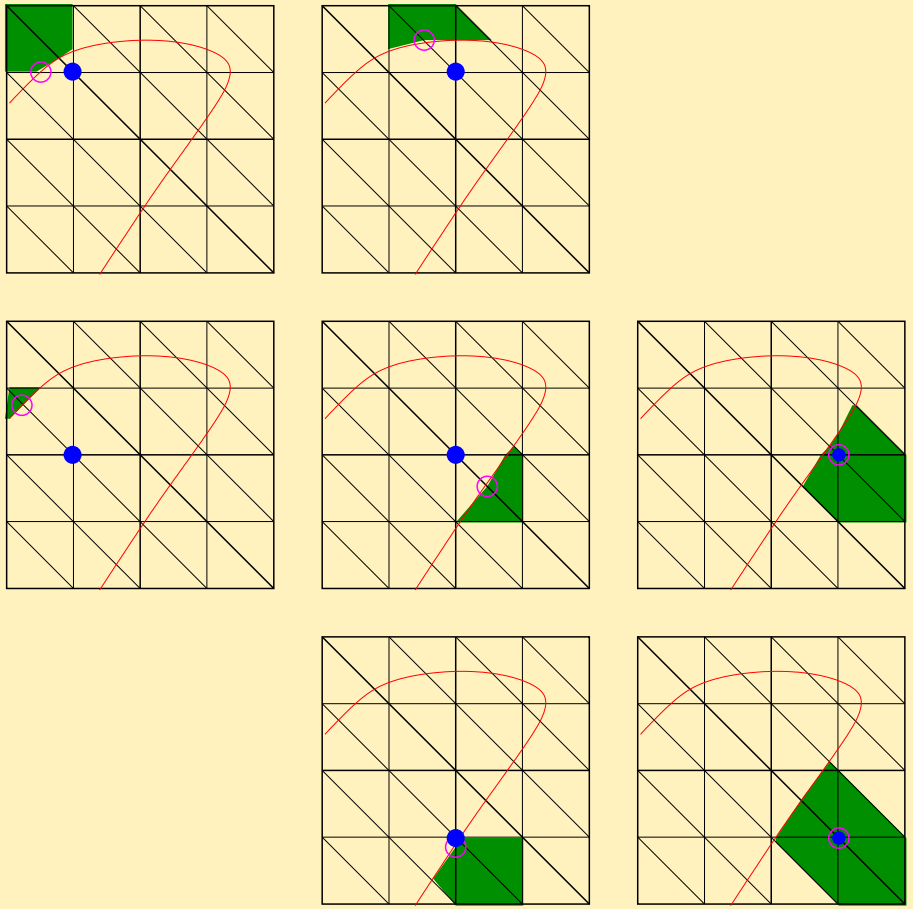


One fine basis function and its neighbors are combined to a coarse basis function.

Coarsening by Hierarchical Partitioning (2D)



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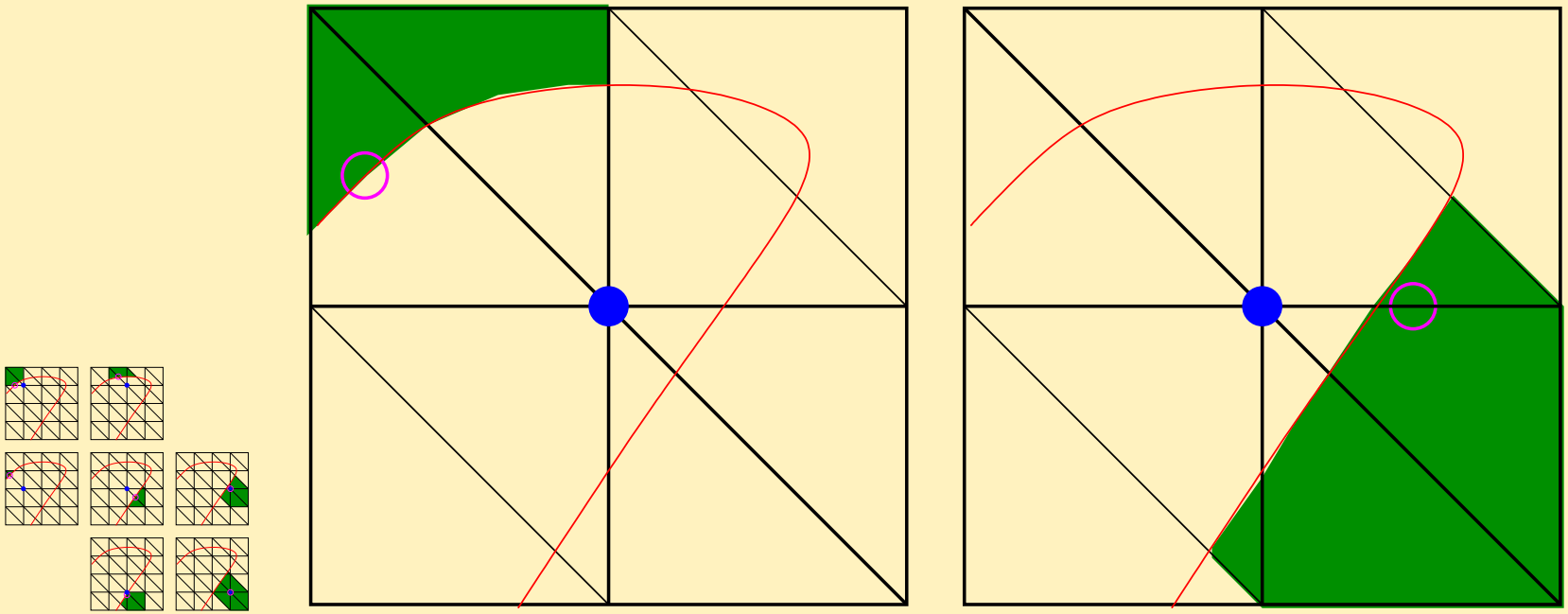
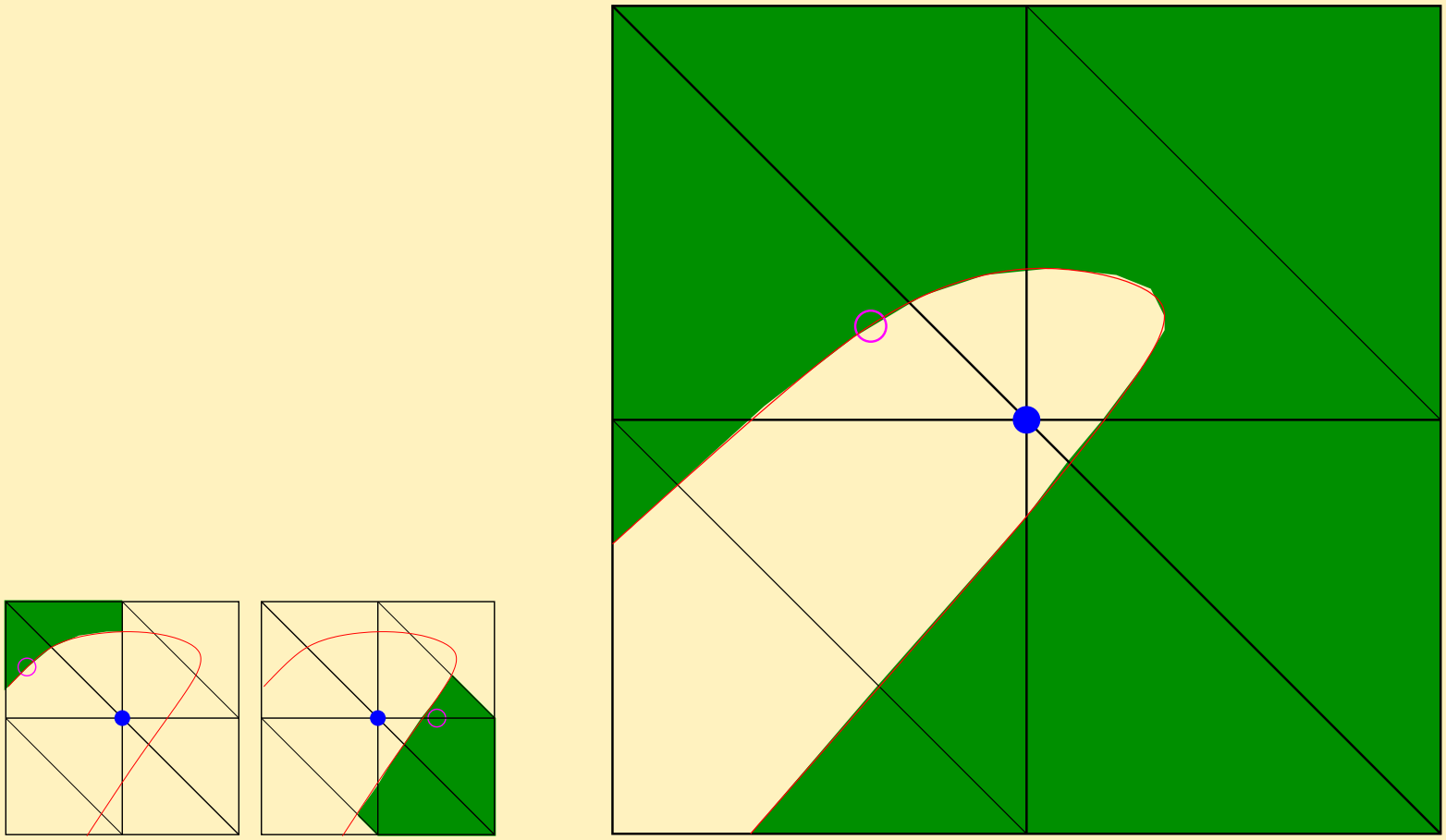


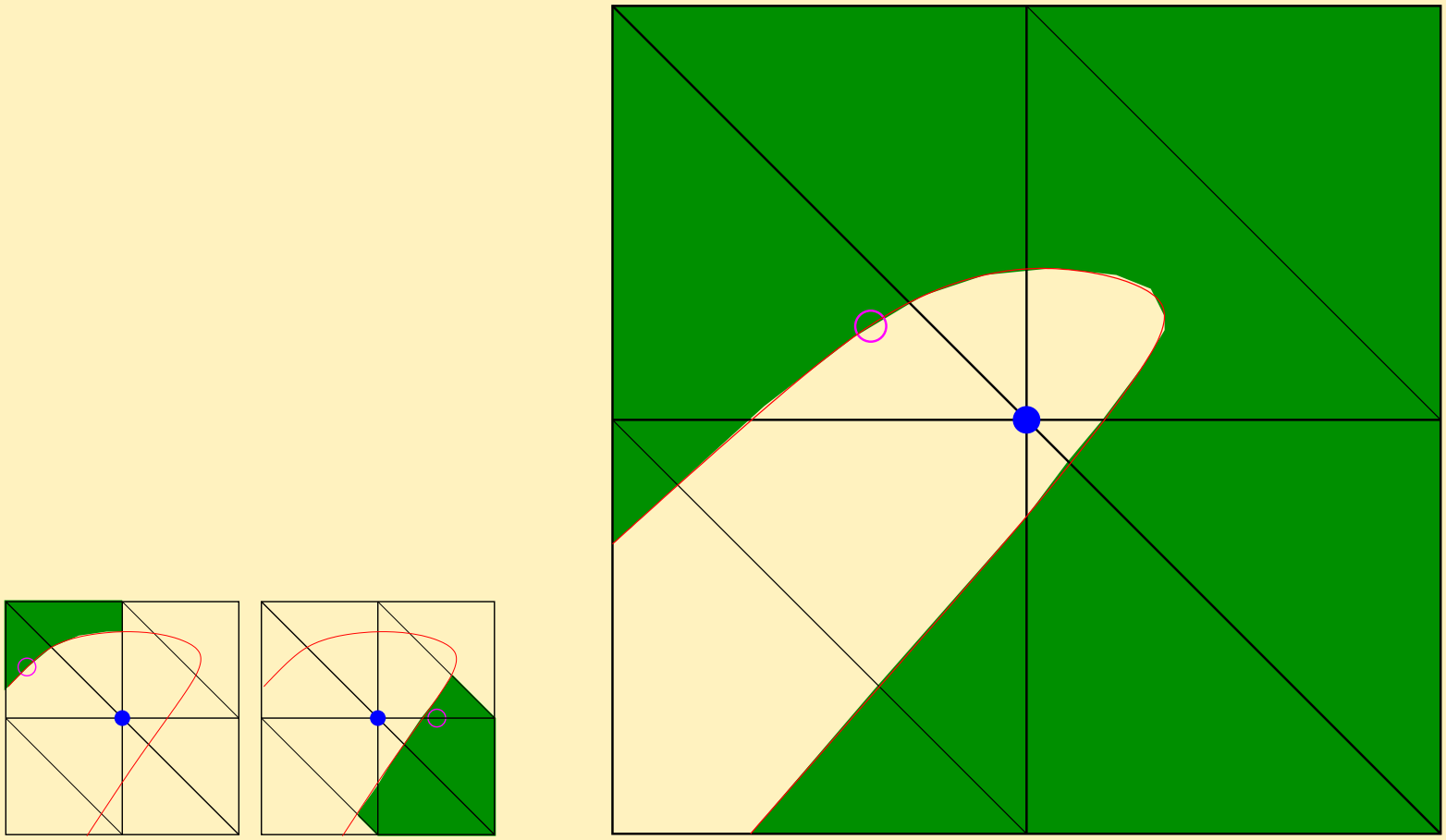
Fine DOFs and basis functions combined to *two* intermediate ones.

Coarsening by Hierarchical Partitioning (2D)



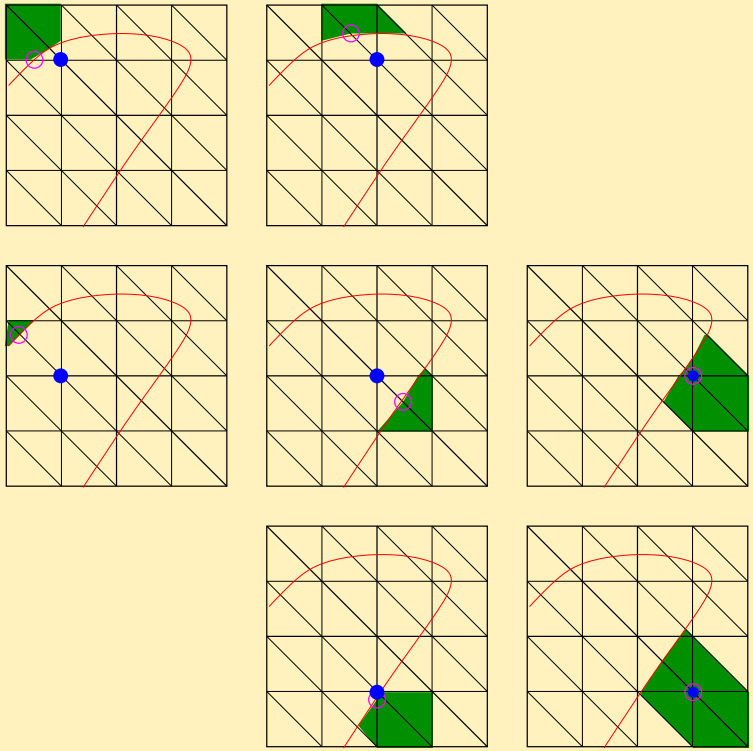
Intermediate DOFs and basis functions recombined to *same* coarse ones.

Coarsening by Hierarchical Partitioning (2D)



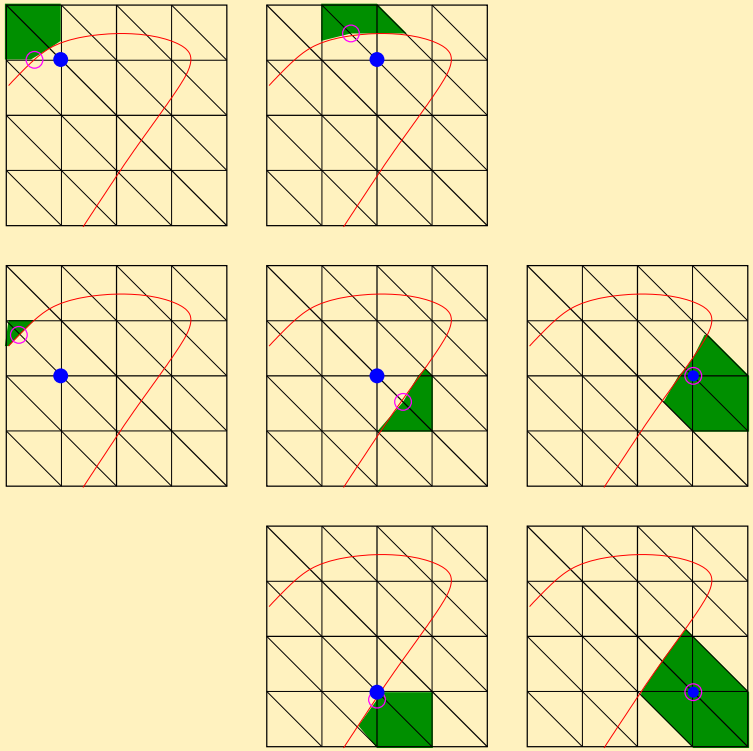
Partitioning must not be more expensive than $O(n)$ (at least not much more . . .)

Hierarchical Partitioning



- assign “seed” to each DOF

Hierarchical Partitioning



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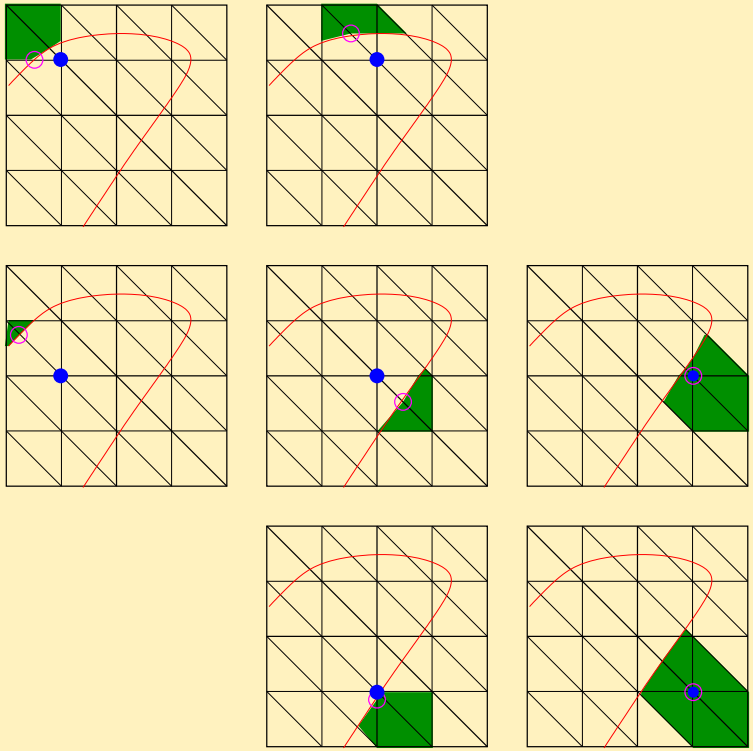
- compute geodesic distances in “neighborhoods” of seeds

Hierarchical Partitioning



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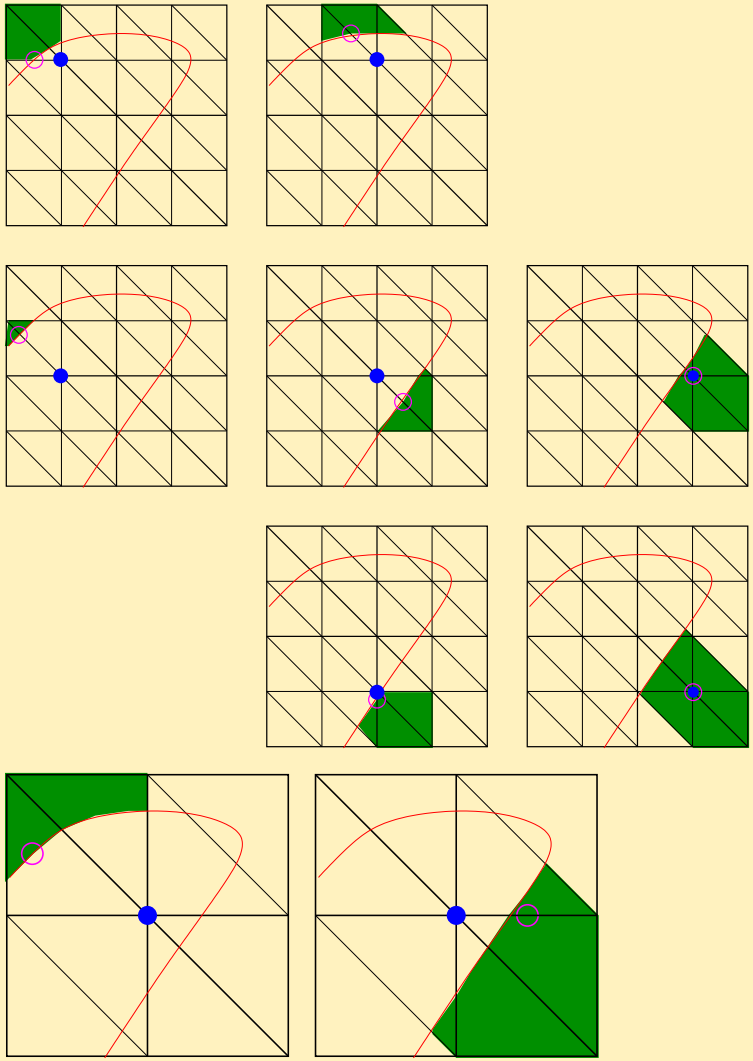

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- grid level
- DOF
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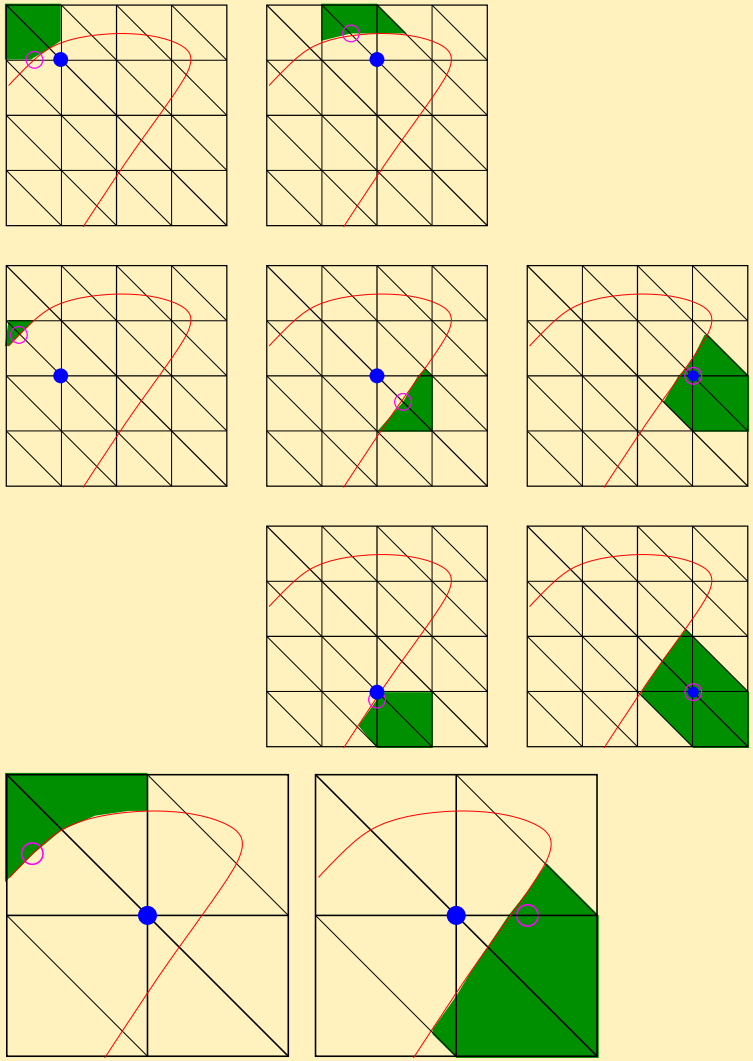

- assign “seed” to each DOF
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Component given by

- grid level
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Now grow those neighborhoods with distance information and continue . . .

Back to Multigrid

Goal: Use this hierarchy to define $\mathcal{R}$estriction and $\mathcal{P}$rolongation.

Back to Multigrid

Goal: Use this hierarchy to define $\mathcal{R}$estriction and $\mathcal{P}$rolongation.

Issues:

- (cache-) efficient algorithmical treatment of “cloned” DOFs
- keep track of different components on different levels
- overall efficiency?

Summary

1. FE Simulations and Systems of Equations
2. Solvers for Systems of Equations
   - Direct and Iterative Methods
   - Conjugate Gradient Solvers
3. Multigrid Methods
   - Smoothing Properties of Iterative Solvers
   - Multigrid for Uniform Grids
   - Algebraic Multigrid Methods
4. Multigrid Methods for Complicated Geometries
   - Composite Finite Elements
   - Multigrid for CFE
   - Improvement of the Multigrid Method
   - Hierarchical Partitioning

References

- F. Liehr, T. Preusser, M. Rumpf, S. Sauter and O. Schwen: *Composite Finite Elements for 3D Image Based Computing*, submitted to Computing and Visualization in Science, 2007
- T. Preusser, M. Rumpf and O. Schwen: *Finite Element Simulation of Bone Microstructures*, Proceedings of the 14th Finite Element Workshop, Ulm 2007

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