Composite Finite Elements for Jumping Coefficients

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joint work with:
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Siegburg, CdE-Seminar
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Outline

Contents

Physical problem:

- real object
- physical process

Finite Element Calculations

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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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3. Discretization (1D)

Continuous function

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Piecewise linear interpolation on a discrete grid

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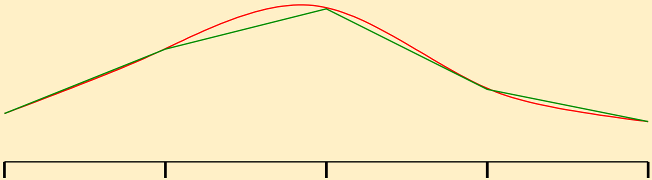
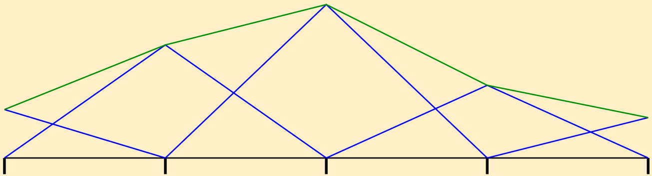
Piecewise linear interpolation on a discrete grid

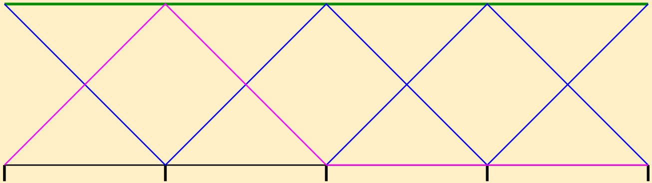


Piecewise linear interpolation on a discrete grid



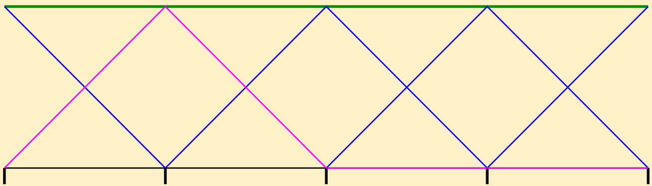
Discrete interpolation as sum of “hat” functions

3. Discretization (1D)



The basis of “hat” functions:

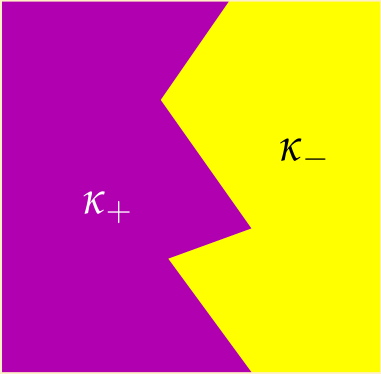
- piecewise linear
- nodal
- partition of unity



The basis of “hat” functions:

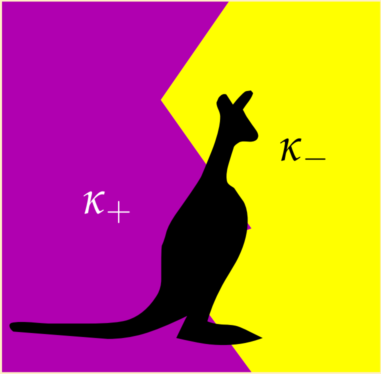
- piecewise linear
- nodal
- partition of unity
- interpolation of continuous function given by coefficient vector

Example Setting



Geometrically complicated interface between regions Ω_- and Ω_+
Material coefficient κ jumps across interface Γ.

Example Setting



Geometrically complicated interface between regions Ω_- and Ω_+
Material coefficient κ jumps across interface Γ.

Composite Finite Elements

Classical FE:

- mesh with geometric complexity
- simple basis functions.

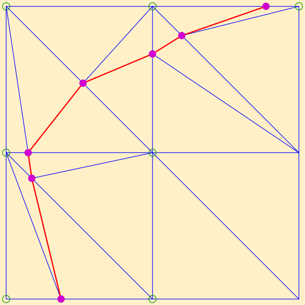
Composite FE:

- regular mesh
- complicated basis functions

Jumping Coefficients

- coefficient discontinuous across interface
- solution continuous but has kink
- want to represent kink by CFE basis functions on regular mesh

Notation



- regular cubes and triangles
- virtual nodes
- virtual triangles
- (geometrically) constraining nodes
- extrapolation

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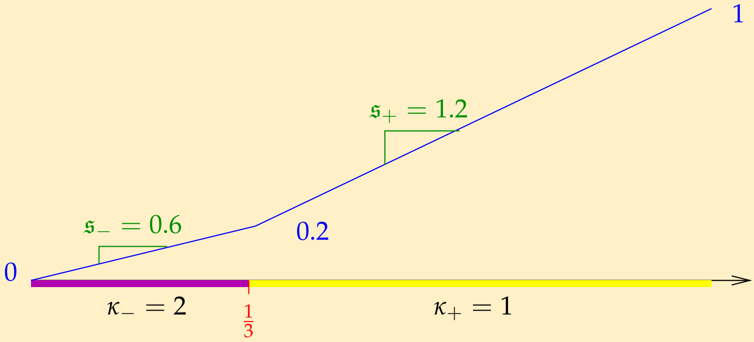
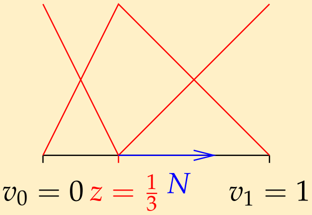
Example Setting

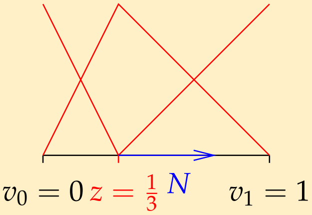


Kink ratio (“slope outside over slope inside”)

$$\kappa = \frac{\kappa_-}{\kappa_+} = \frac{\mathfrak{s}_+}{\mathfrak{s}_-} = 2 \tag{1}$$

Construction of CFE Basis Functions in 1D





Want to be able to extrapolate all functions

$$\mathcal{E} := \left\{ u : x \mapsto \begin{cases} b(x-z)+d & x \le z \\ \kappa b(x-z)+d & x > z \end{cases} : b, d \in \mathbb{R} \right\} \tag{2}$$

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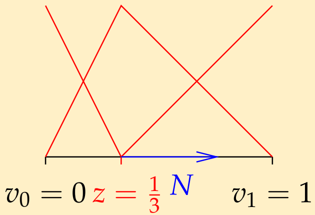

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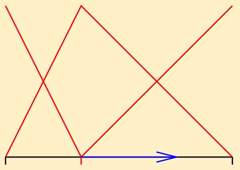
Basis of $\mathcal{E}$:

$$\eta_0(x) = 1 \tag{3}$$

$$\eta_1(x) = \begin{cases} (x-z) & x \le z \\ \kappa(x-z) & x > z \end{cases} \tag{4}$$

Construction of CFE Basis Functions in 1D



Problem: find extrapolation weights $\mathfrak{w}_z^{v_0}, \mathfrak{w}_z^{v_1}$ such that

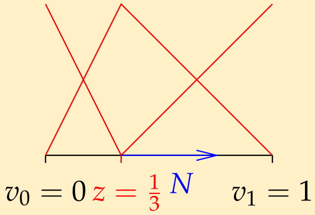
$$u(z) = \mathfrak{w}_z^{v_0} u(v_0) + \mathfrak{w}_z^{v_1} u(v_1) \qquad \forall u \in \mathcal{E} \tag{2}$$

Then let

$$\varphi_{v_0}^{\mathsf{CFE}} = 1 \cdot \varphi_{v_0}^{\mathsf{virt}} + \mathfrak{w}_z^{v_0} \cdot \varphi_z^{\mathsf{virt}} \qquad \text{and} \tag{3}$$

$$\varphi_{v_1}^{\mathsf{CFE}} = \mathfrak{w}_z^{v_1} \cdot \varphi_z^{\mathsf{virt}} + 1 \cdot \varphi_{v_0}^{\mathsf{virt}} \tag{4}$$

Construction of CFE Basis Functions in 1D



Set up system of equations (nonsymmetric):

$$\eta_0(z) = \mathfrak{w}_z^{v_0} \cdot \eta_0(v_0) + \mathfrak{w}_z^{v_1} \cdot \eta_0(v_1) \tag{2}$$

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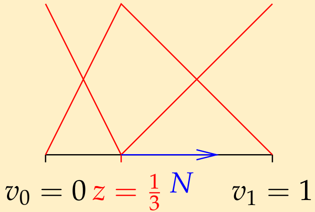

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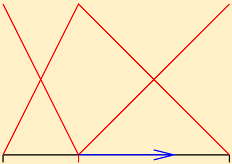
where

$$\eta_0(v_0) = 1 \qquad \eta_0(v_1) = 1 \qquad \eta_0(z) = 1 \tag{4}$$

$$\eta_1(v_0) = (x - v_0) \cdot N = -\frac{1}{3} \qquad \eta_1(v_1) = \kappa(x - v_1) \cdot N = 2 \cdot \frac{2}{3} \qquad \eta_0(z) = (z - z) \cdot N = 0 \tag{5}$$

Construction of CFE Basis Functions in 1D

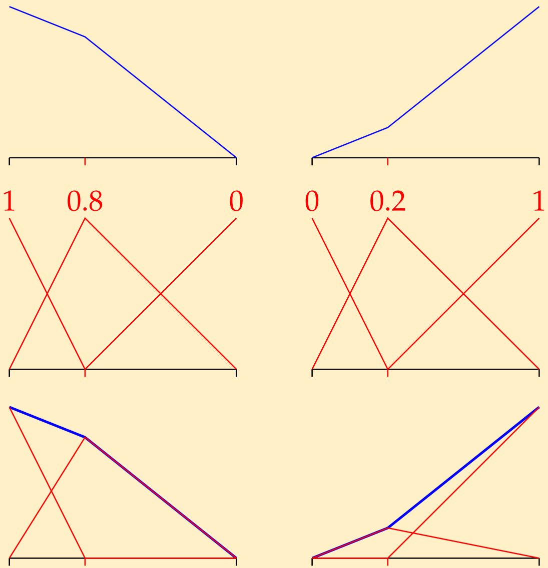


System of equations:

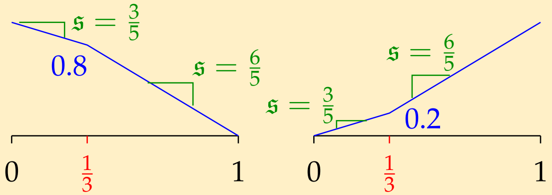
$$\begin{bmatrix} 1 & 1 \\ -\frac{1}{3} & \frac{4}{3} \end{bmatrix} \begin{bmatrix} \mathfrak{w}_z^{v_0} \\ \mathfrak{w}_z^{v_1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{2}$$

$$\Rightarrow \begin{bmatrix} \mathfrak{w}_z^{v_0} \\ \mathfrak{w}_z^{v_1} \end{bmatrix} = \begin{bmatrix} \frac{4}{5} \\ \frac{1}{5} \end{bmatrix} = \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix} \tag{3}$$

Construction of CFE Basis Functions in 1D



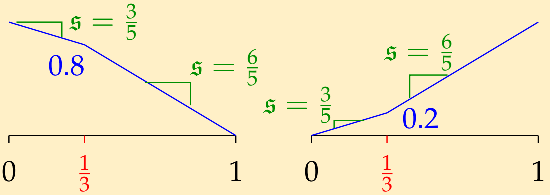
1D CFE Basis Functions on Grid Level 0



These CFE basis functions

- ✔ form partition of unity
- ✔ are nodal
- ✔ are piecewise affine

1D CFE Basis Functions on Grid Level 0



These CFE basis functions

- ✔ form partition of unity
- ✔ are nodal
- ✔ are piecewise affine
- are positive
- have the same support as standard affine basis functions
- satisfy the kink condition exactly

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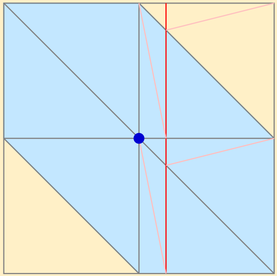
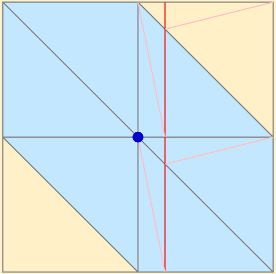
First Idea: Modified Standard Basis Functions



First (bad) idea: Keep same support as for standard affine basis functions, introduce kink along regular edges.

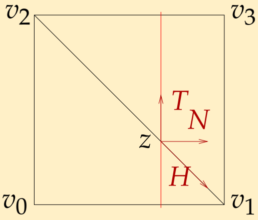
First Idea: Modified Standard Basis Functions



First (bad) idea: Keep same support as for standard affine basis functions, introduce kink along regular edges.

$\Rightarrow$ only geometrically constraining nodes constrain virtual node.

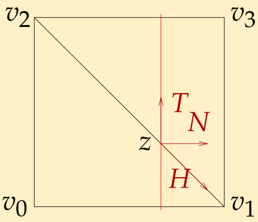
What to do Better



We require our scheme to correctly extrapolate any piecewise affine function with appropriate kink: (Taylor expansion at z)

$$\mathcal{E} = \left\{ u : x \mapsto \begin{cases} b(x-z) \cdot N + c(x-z) \cdot T + d & x \in \Omega_- \\ \kappa b(x-z) \cdot N + c(x-z) \cdot T + d & x \in \Omega_+ \end{cases} \right\} \tag{4}$$

with $b, c, d \in \mathbb{R}$.



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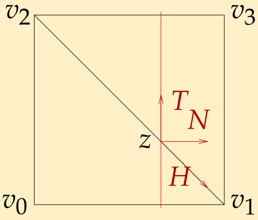
with $b, c, d \in \mathbb{R}$.

$\Rightarrow \dim \mathcal{E} = 3 \Rightarrow$ two constraining nodes are insufficient!

What to do Better



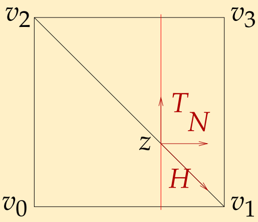
Basis of $\mathcal{E}$:

$$\eta_0(x) = 1 \tag{4}$$

$$\eta_1(x) = (x - z) \cdot T \tag{5}$$

$$\eta_2(x) = \begin{cases} (x - z) \cdot N & x \in \Omega_- \\ \kappa(x - z) \cdot N & x \in \Omega_+ \end{cases} \tag{6}$$

What to do Better



Consider the triangle $\Delta(v_0, v_1, v_2)$:

$$\begin{bmatrix} \eta_0(v_0) & \eta_0(v_1) & \eta_0(v_2) \\ \eta_1(v_0) & \eta_1(v_1) & \eta_1(v_2) \\ \eta_2(v_0) & \eta_2(v_1) & \eta_2(v_2) \end{bmatrix} \begin{bmatrix} \mathfrak{w}_z^{v_0} \\ \mathfrak{w}_z^{v_1} \\ \mathfrak{w}_z^{v_2} \end{bmatrix} = \begin{bmatrix} \eta_0(z) \\ \eta_1(z) \\ \eta_2(z) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

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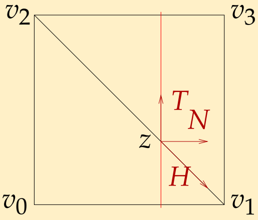

Consider the triangle $\Delta(v_1, v_2, v_3)$:

$$\begin{bmatrix} \eta_0(v_1) & \eta_0(v_2) & \eta_0(v_3) \\ \eta_1(v_1) & \eta_1(v_2) & \eta_1(v_3) \\ \eta_2(v_1) & \eta_2(v_2) & \eta_2(v_3) \end{bmatrix} \begin{bmatrix} \mathfrak{w}_z^{v_1} \\ \mathfrak{w}_z^{v_2} \\ \mathfrak{w}_z^{v_3} \end{bmatrix} = \begin{bmatrix} \eta_0(z) \\ \eta_1(z) \\ \eta_2(z) \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Modified-Support Basis Functions

Evaluate basis function η_i at nodes v_j, z:

$$
\begin{array}{lllll}
\eta_0(v_0) = 1 & \eta_0(v_1) = 1 & \eta_0(v_2) = 1 & \eta_0(v_3) = 1 & \eta_0(z) = 1 \\
\eta_1(v_0) = \frac{-1}{3} & \eta_1(v_1) = \frac{-1}{3} & \eta_1(v_2) = \frac{2}{3} & \eta_1(v_3) = \frac{2}{3} & \eta_1(z) = 0 \\
\eta_2(v_0) = \frac{-2}{3} & \eta_2(v_1) = \frac{2}{3} & \eta_2(v_2) = \frac{-2}{3} & \eta_2(v_3) = \frac{2}{3} & \eta_2(z) = 0
\end{array}
$$

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\end{array}$$

So our two systems of equations are:

$$\begin{bmatrix} 1 & 1 & 1 \\ \frac{-1}{3} & \frac{-1}{3} & \frac{2}{3} \\ \frac{-2}{3} & \frac{2}{3} & \frac{-2}{3} \end{bmatrix} \begin{bmatrix} \mathfrak{w}_z^{v_0} \\ \mathfrak{w}_z^{v_1} \\ \mathfrak{w}_z^{v_2} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \Rightarrow \begin{bmatrix} \mathfrak{w}_z^{v_0} \\ \mathfrak{w}_z^{v_1} \\ \mathfrak{w}_z^{v_2} \end{bmatrix} = \begin{bmatrix} \frac{1}{6} \\ \frac{1}{2} \\ \frac{1}{3} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 1 \\ \frac{-1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{-2}{3} & \frac{2}{3} \end{bmatrix} \begin{bmatrix} \mathfrak{w}_z^{v_1} \\ \mathfrak{w}_z^{v_2} \\ \mathfrak{w}_z^{v_3} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad \Rightarrow \begin{bmatrix} \mathfrak{w}_z^{v_1} \\ \mathfrak{w}_z^{v_2} \\ \mathfrak{w}_z^{v_3} \end{bmatrix} = \begin{bmatrix} \frac{2}{3} \\ \frac{1}{2} \\ \frac{-1}{6} \end{bmatrix}$$

Modified-Support Basis Functions

On the triangles $\Delta(v_0, v_1, v_2)$ and $\Delta(v_1, v_2, v_3)$, we have

$$\mathfrak{w}_z^{v_0} = \frac{1}{6} \qquad \mathfrak{w}_z^{v_1} = \frac{1}{2} \qquad \mathfrak{w}_z^{v_2} = \frac{1}{3} \qquad \mathfrak{w}_z^{v_3} = \text{n/a},$$

$$\mathfrak{w}_z^{v_0} = \text{n/a} \qquad \mathfrak{w}_z^{v_1} = \frac{2}{3} \qquad \mathfrak{w}_z^{v_2} = \frac{1}{2} \qquad \mathfrak{w}_z^{v_3} = \frac{-1}{6}$$

- each scheme by itself allows correct extrapolation
- any convex combination allows correct extrapolation
- easiest convex combination is arithmetic mean:

$$\mathfrak{w}_z^{v_0} = \frac{1}{12} \qquad \mathfrak{w}_z^{v_1} = \frac{7}{12} \qquad \mathfrak{w}_z^{v_2} = \frac{5}{12} \qquad \mathfrak{w}_z^{v_3} = \frac{-1}{12}$$

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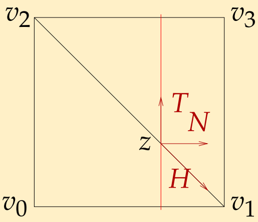
- any convex combination generally better??

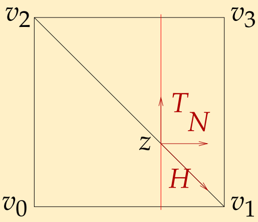
Modified-Support Basis Functions



Again construct CFE basis functions as weighted sum of virtual basis functions.

- $v_{0,1,2,3}$ constrain z, thus support of v_0 and v_3 is now bigger

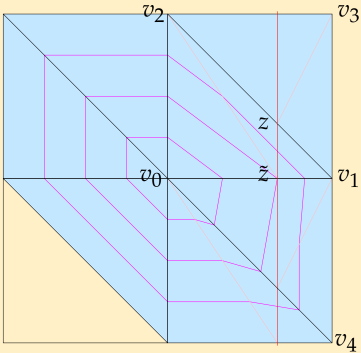
Modified-Support Basis Functions



Again construct CFE basis functions as weighted sum of virtual basis functions.

- $v_{0,1,2,3}$ constrain z, thus support of v_0 and v_3 is now bigger
- kink ratio is not satisfied along edge H for the basis functions

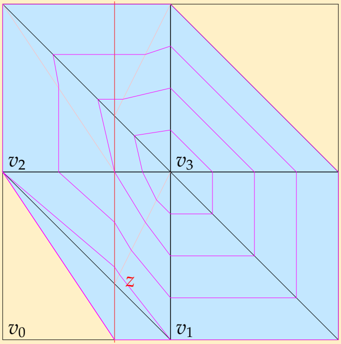
Modified-Support Basis Functions



For $\tilde{z}$ = virtual node on edge $[v_0, v_1]$, $\mathfrak{w}_{\tilde{z}}^{v_2}$ turns out to be zero (support does not grow downwards).

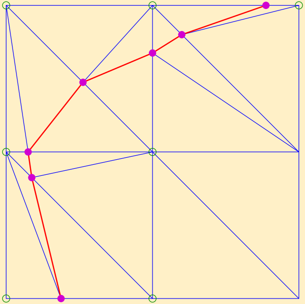
Magenta lines are $\frac{3}{4}, \frac{1}{2}, \frac{1}{4}$ isolines of CFE basis function.

Modified-Support Basis Functions



Magenta lines are $\frac{3}{4}, \frac{1}{2}, \frac{1}{4}, 0$ isolines of CFE basis function.

Normals for Non-Planar Interfaces



In case of non-planar interface, use per-triangle normal.

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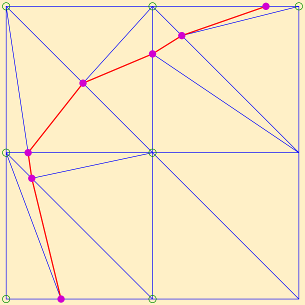


In case of non-planar interface, use per-triangle normal.
May encounter numerical problems in solution of 4×4 systems in 3D: omit unreliable tetrahedra.

Properties of CFE Basis Functions

universitätbonn

- ✔ nodality
- ✔ partition of unity
- ✔ piecewise affine
- ✘ may have negative values
- ✘ may have bigger support standard affine basis functions
- ✘ basis functions do not satisfy kink condition

Contents

Approximation Tests

Compute L^∞, L^2, H^1 differences between analytically given function and CFE interpolation

$$\|e\|_{L^\infty} = \text{“}\max_\Omega\text{''} |e|$$

$$\|e\|_{L^2} = \sqrt{\int_\Omega e^2 \,\mathrm{d}x}$$

$$\|e\|_{H^1} = \sqrt{\int_\Omega e^2 \,\mathrm{d}x + \sum_i \int_\Omega (\partial_i e)^2 \,\mathrm{d}x}$$

for decreasing grid spacing h.

Approximation Tests: Expected Results

Expected orders of convergence:

- L^∞: 2
- L^2: 2

in contrast to standard Affine and Multilinear Finite Elements (ignoring kink):

- L^∞: 1
- L^2: 1.5

Contents

Planar Interface and Test Functions

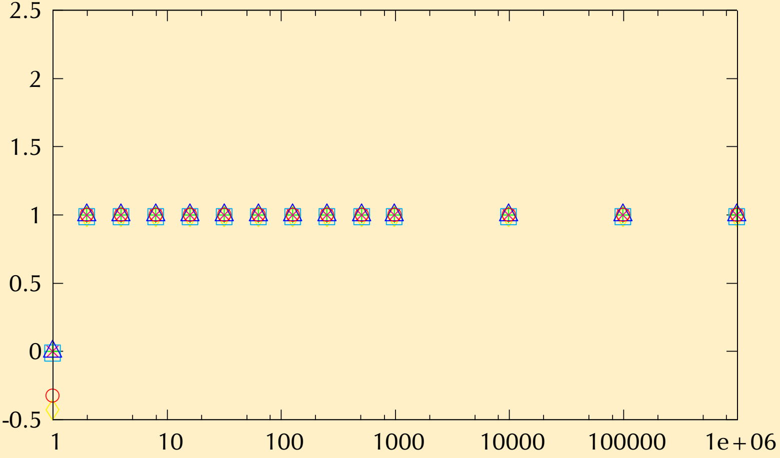
Consider a planar interface (not aligned with coordinate axes) and an affine function with kink across the interface.

Planar Interface and Test Functions

Consider a planar interface (not aligned with coordinate axes) and an affine function with kink across the interface.

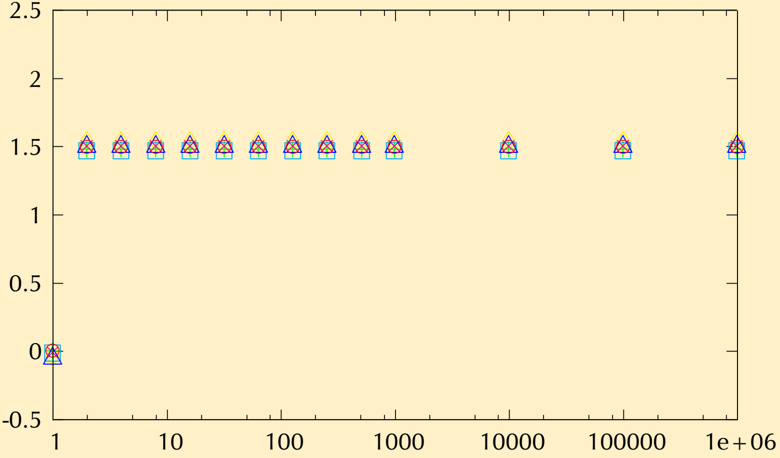
In this case, CFE approximation should be exact.

L^∞ error for Multilinear FE



convergence rate ($2-3, \ldots,$ △$6-7$, ◯$7-8$) vs. kink ratio

L^2 error for Multilinear FE



convergence rate $(2-3, \ldots, \triangle 6-7, \bigcirc 7-8)$ vs. kink ratio

L^∞ error for CFE

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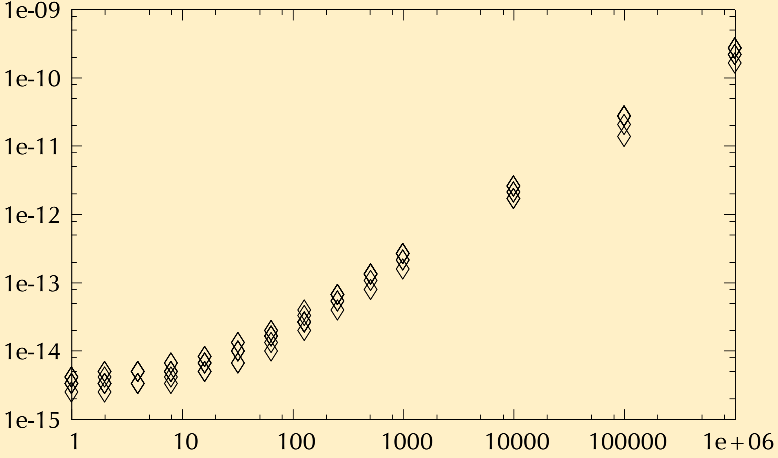
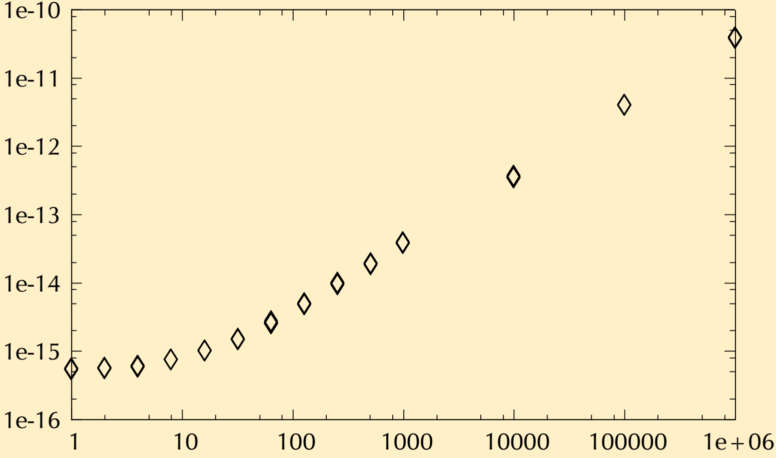


(L^∞ norm of error relative to L^2 norm of function) vs. kink ratio

L^2 error for CFE



(L^2 norm of error relative to L^2 norm of function) vs. kink ratio

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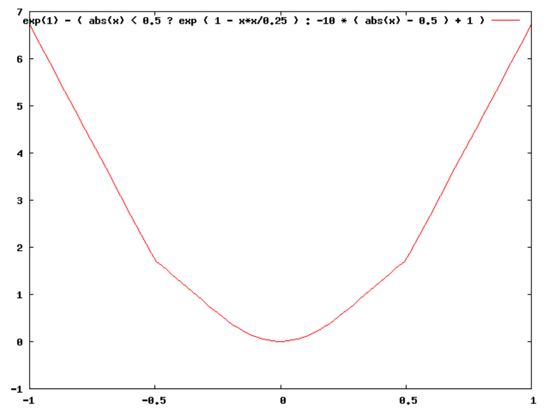
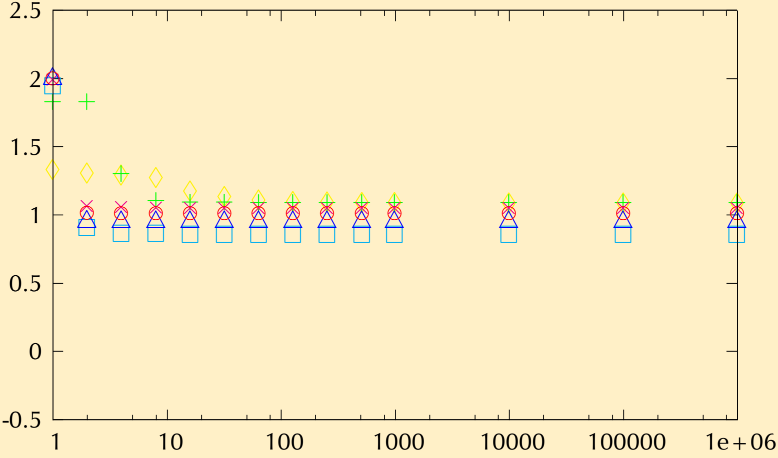
Cylindrical Test Function

Consider



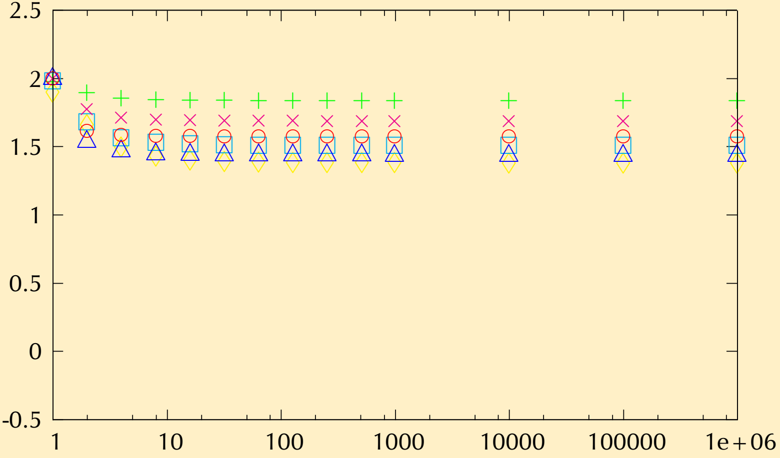
made "cylindrically symmetric".

L^∞ error for Multilinear FE



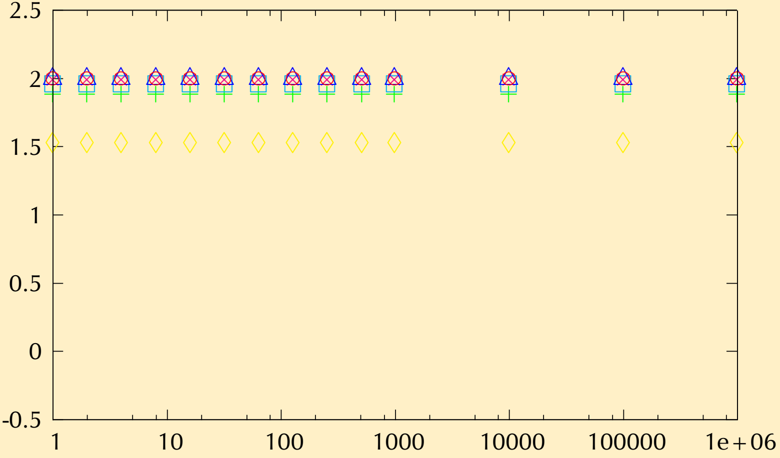
convergence rate (2 − 3, . . . , △6 − 7, ◯7 − 8) vs. kink ratio

L^2 error for Multilinear FE



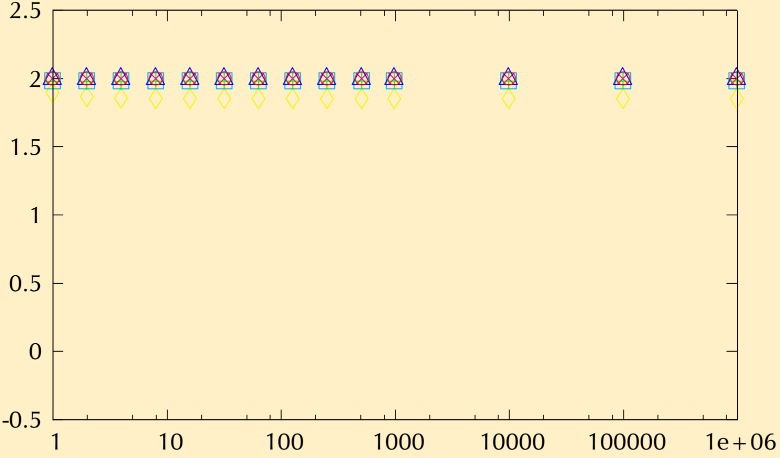
convergence rate $(2-3, \ldots, \triangle 6-7, \bigcirc 7-8)$ vs. kink ratio

L^{∞} error for CFE



convergence rate $(2-3, \ldots, \triangle 6-7, \bigcirc 7-8)$ vs. kink ratio

L^2 error for CFE



convergence rate (2 − 3, . . . , △6 − 7, ◯7 − 8) vs. kink ratio

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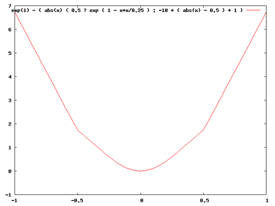
Spherical Test Function

Consider again



made spherically symmetric, modulated by

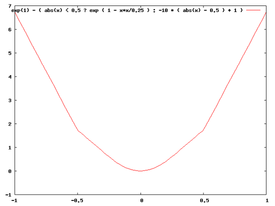
$$\gamma(x,y) = \frac{y}{\sqrt{(x-c)^2 + (y-c)^2}}$$

$$m(x,y,z) = 1 - t \cdot \gamma(x,y) \cdot \gamma(y,z) \cdot \gamma(z,x)$$

for nontrivial tangential derivatives at interface.

Spherical Test Function

Consider again



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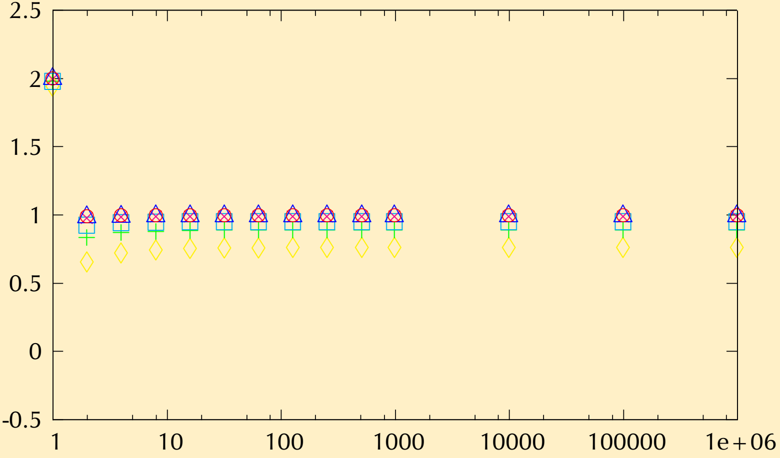
for nontrivial tangential derivatives at interface.

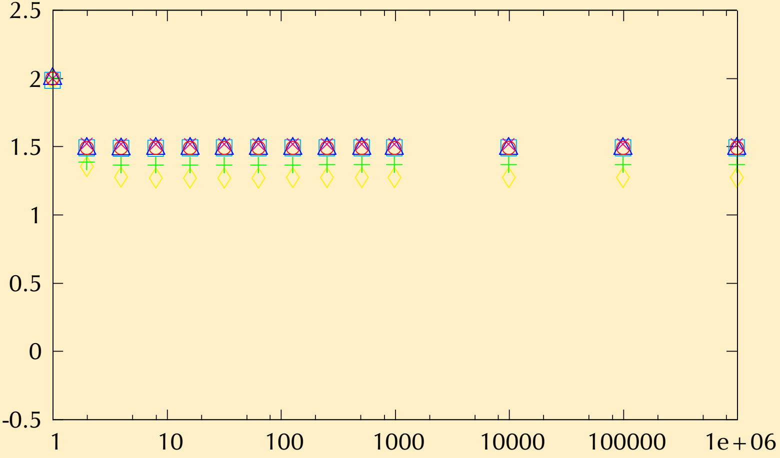
We now consider the case c being outside of the computational domain Ω and R such that the interface is inside Ω.

L^∞ error for Multilinear FE

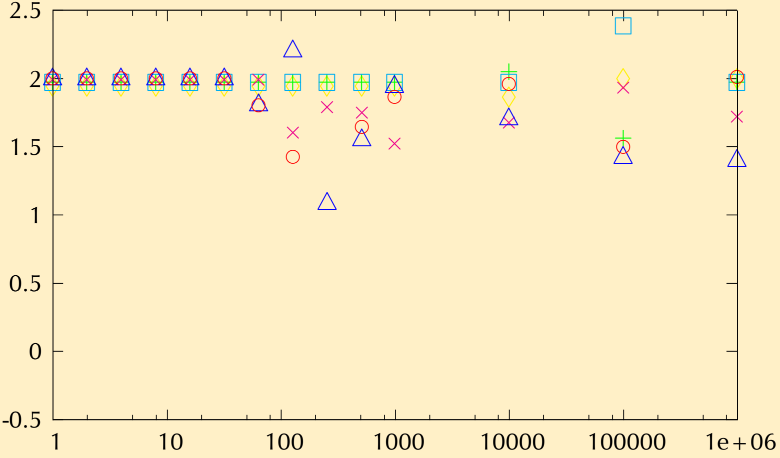


convergence rate (2 − 3, . . . , △6 − 7, ◯7 − 8) vs. kink ratio

L^2 error for Multilinear FE

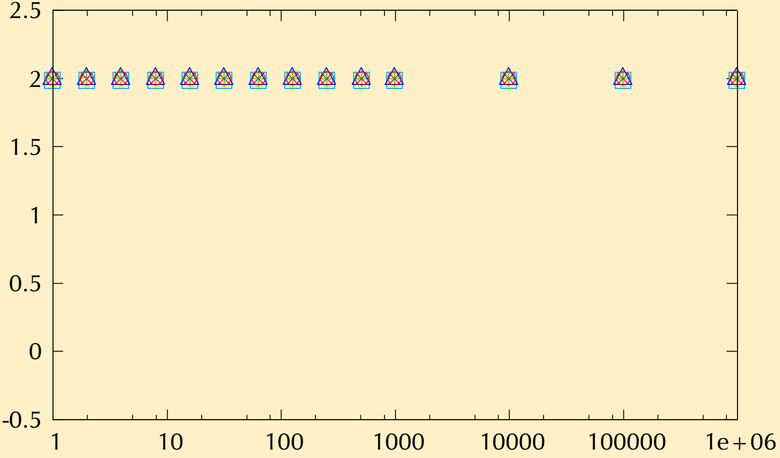


convergence rate (2 − 3, . . . , △6 − 7, ◯7 − 8) vs. kink ratio



convergence rate $(2-3, \ldots, \triangle 6-7, \bigcirc 7-8)$ vs. kink ratio

L^2 error for CFE



convergence rate ($2-3, \ldots,$ △$6-7$, ◯$7-8$) vs. kink ratio

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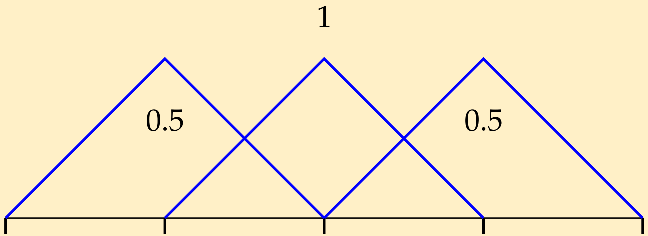
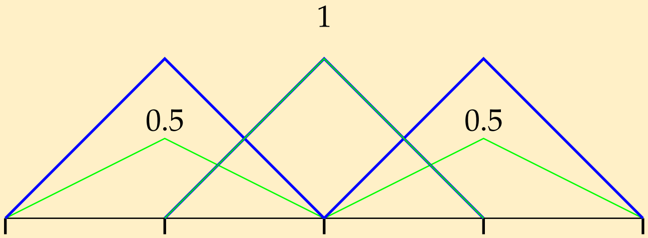
Multigrid Solvers

- key factor in cpu time: solution of systems of equations
- multigrid solvers are fast such techniques
- iterative scheme with coarse grid corrections
- requires coarsening

Standard Coarsening



Standard Coarsening



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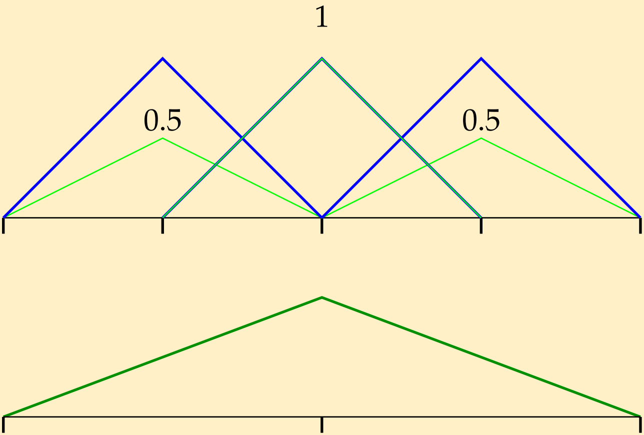

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Multigrid coarsening

Problem: Determine coarsening weights to write coarsened basis functions as linear combination of fine basis functions:

$$\varphi_{c_0}^{\mathrm{CFE,coarse}} = \sum_f \mathfrak{w}_f^{c_0} \varphi_f^{\mathrm{CFE,fine}} \tag{4}$$

Coarsened basis functions should be as similar as possible to those obtained by construction on the coarse grid.

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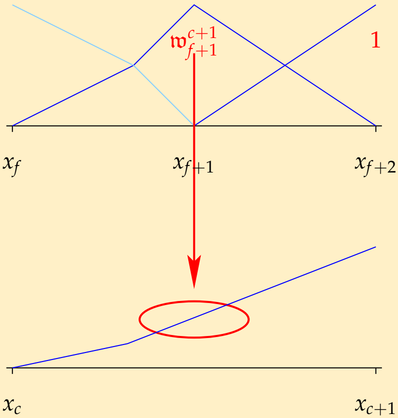
Coarsened basis functions should be as similar as possible to those obtained by construction on the coarse grid.

Necessary condition for coarsened basis functions forming partition of unity:

$$\sum_c \mathfrak{w}_{f_0}^c = 1 \tag{5}$$

The NAK Condition

Coarsening should not introduce additional kinks
(**N**o **A**dditional **K**ink condition):



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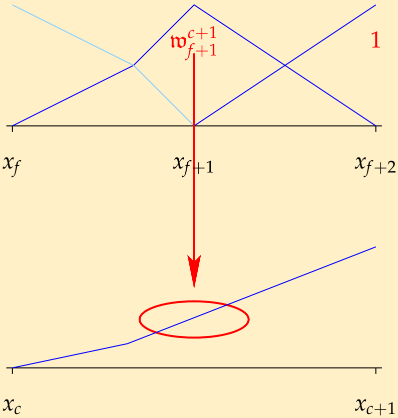
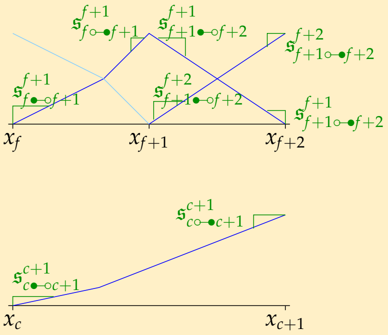


$\Rightarrow$ need to balance all “relevant” slopes at x_{f+1}.

Slope Coarsening

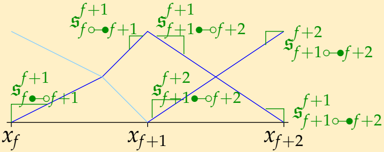


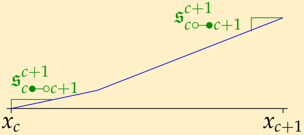
Coarsening weights (such that left slope = right slope)

$$\mathfrak{w}_{c+1}^{f+1} \cdot \mathfrak{s}_{f\circ\!-\!\bullet f+1}^{f+1} = 1 \cdot \mathfrak{s}_{f+1\bullet\!-\!\circ f+2}^{f+2} + \mathfrak{w}_{c+1}^{f+1} \cdot \mathfrak{s}_{f+1\bullet\!-\!\circ f+2}^{f+1}$$

$$\Rightarrow \mathfrak{w}_{c+1}^{f+1} = \frac{\mathfrak{s}_{f+1\bullet\!-\!\circ f+2}^{f+2}}{\mathfrak{s}_{f\circ\!-\!\bullet f+1}^{f+1} - \mathfrak{s}_{f+1\bullet\!-\!\circ f+2}^{f+1}}$$

Slope Coarsening





Coarsened slopes (in units of grid spacing)

$$\mathfrak{s}^{c+1}_{c\bullet\!-\!\circ c+1} = 2\left[\mathfrak{w}^{c+1}_{f+1}\cdot \mathfrak{s}^{f+1}_{f\bullet\!-\!\circ f+1}\right]$$

$$\mathfrak{s}^{c+1}_{c\circ\!-\!\bullet c+1} = 2\left[1\cdot \mathfrak{s}^{f+2}_{f+1\circ\!-\!\bullet f+2} + \mathfrak{w}^{f+1}_{c+1}\cdot \mathfrak{s}^{f+1}_{f+1\circ\!-\!\bullet f+2}\right]$$

Slope Coarsening

- NAK condition gives one equation per coarsening weight

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Slope Coarsening

- NAK condition gives one equation per coarsening weight
- on coarse grid, only slopes at end points of intervals are relevant
- slopes measured in units of grid spacing on different grids (standard slopes are always ± 1)
- linear construction preserves kink representability

Properties of CFE Basis Functions and Coarsening

- ✔ nodality
- ✔ partition of unity
- ✔ piecewise affine

Properties of CFE Basis Functions and Coarsening

- ✔ nodality
- ✔ partition of unity
- ✔ piecewise affine

… and properties that are no longer satisfied in 2D/3D:

- ✘ positivity
- ✘ same support as standard affine basis functions
- ✘ same neighbors in the sense of "overlapping support of basis functions", thus same sparsity structure of matrices
- ✘ exact representation of kink in basis functions
- ✘ only standard neighbors can jointly constrain virtual node
- ✘ coarsened and coarse basis functions coincide for "simple" interfaces

Contents

Multigrid Coarsening

Again want coarsened basis functions to be as similar as possible to those obtained on the fine grid.

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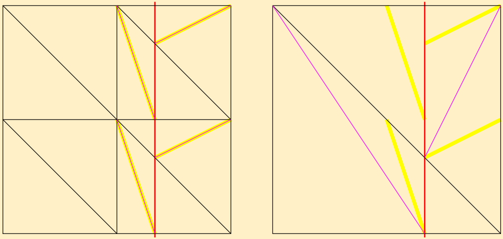

Problem:

- basis functions have kinks across virtual edges
- virtual edges not present on coarse grid
- even for simple interfaces, coarsened $\neq$ coarse basis functions

Multigrid Coarsening

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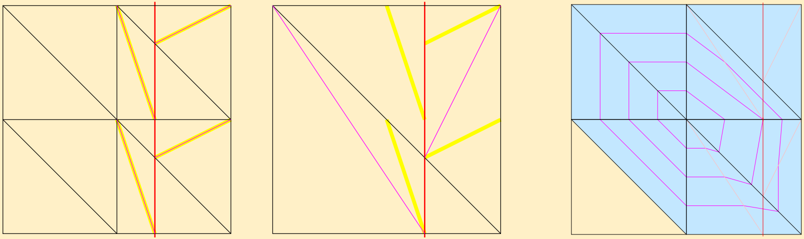
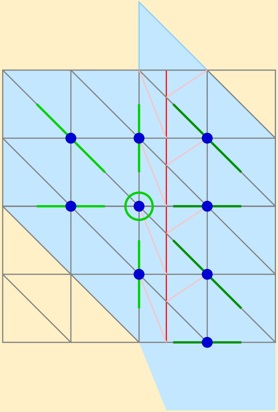


Problem:

- basis functions have kinks across virtual edges
- virtual edges not present on coarse grid
- even for simple interfaces, coarsened $\neq$ coarse basis functions
- different neighborhoods $\Rightarrow$ need other coarsening scheme

Relevant Edges for Coarsening



- relevant edges
- standard and JCV neighbors (jointly constraining virtual node)

needed for coarsening

Example System for Determining Coarsening Weights

$$
\begin{bmatrix}
2 & & & & & & & \\
-2 & * & & & & & & \\
 & \star & * & & \star & & & \\
 & & & 2 & & & & \\
 & & \star & & * & & \star & \\
 & & & & & -2 & \star & \\
 & & & & \star & & * & \star \\
 & & & & & & \star & *
\end{bmatrix}
\begin{bmatrix}
\tilde{\tilde{\mathfrak{w}}}_4^0 \\
\tilde{\tilde{\mathfrak{w}}}_4^1 \\
\tilde{\tilde{\mathfrak{w}}}_4^2 \\
\tilde{\tilde{\mathfrak{w}}}_4^3 \\
\tilde{\tilde{\mathfrak{w}}}_4^4 \\
\tilde{\tilde{\mathfrak{w}}}_4^5 \\
\tilde{\tilde{\mathfrak{w}}}_4^6 \\
\tilde{\tilde{\mathfrak{w}}}_4^7 \\
\tilde{\tilde{\mathfrak{w}}}_4^8 \\
\tilde{\tilde{\mathfrak{w}}}_4^9
\end{bmatrix}
=
\begin{bmatrix}
-1 \\ +1 \\ 0 \\ -1 \\ 1 \\ -1 \\ 1 \\ 0
\end{bmatrix}
$$

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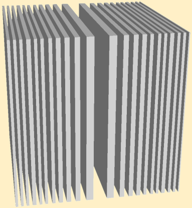
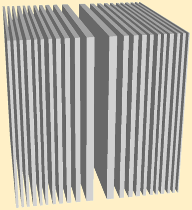


$\kappa = 5$, Ω_- shown as solid.

Example Problem: One time step ($\tau = h$) of heat diffusion, starting with noise.

$v(3, 3)$ cycle on grid level 6, coarsening up to grid level 1, reduction of squared residuum by 10^{-24}.



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Standard Coarsening 20 multigrid cycles, final convergence 0.379

NAK coarsening 16 multigrid cycles, final convergence 0.279

References

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