

EM Field Simulation Based on Volume Discretization: Finite Integration and Related Approaches

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ICAP 2006

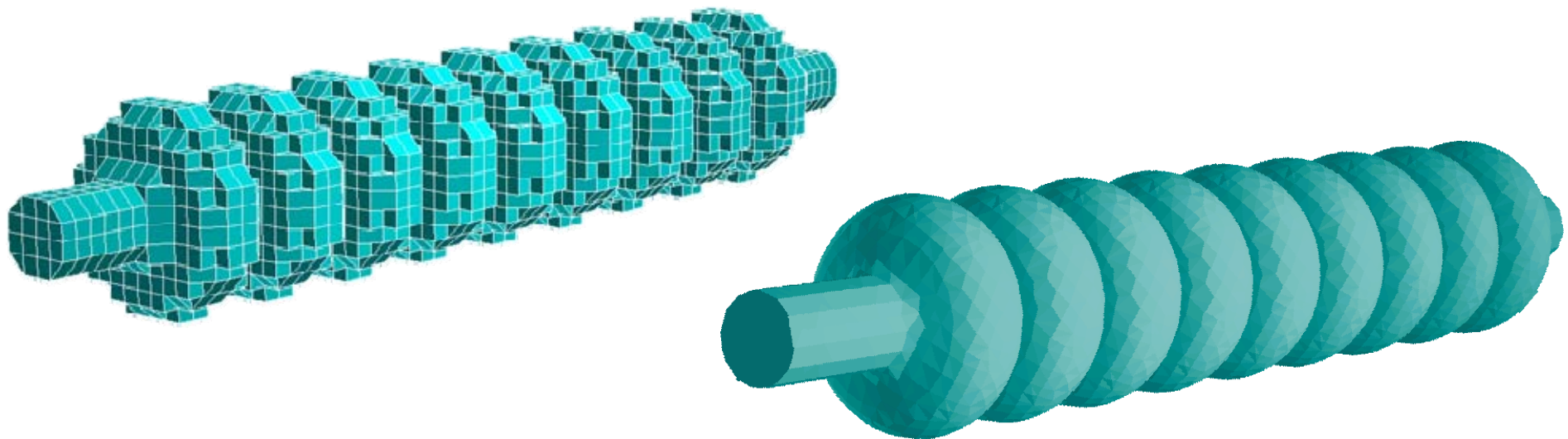


Basic Approaches of Volume-Grid Methods

- Finite Integration / Finite Differences / Finite Elements
- *Pros and Cons ...*
- *Similarities and Differences ...*

Advanced Topic

- Conformal Modeling (*with Igor Zagorodnov*)



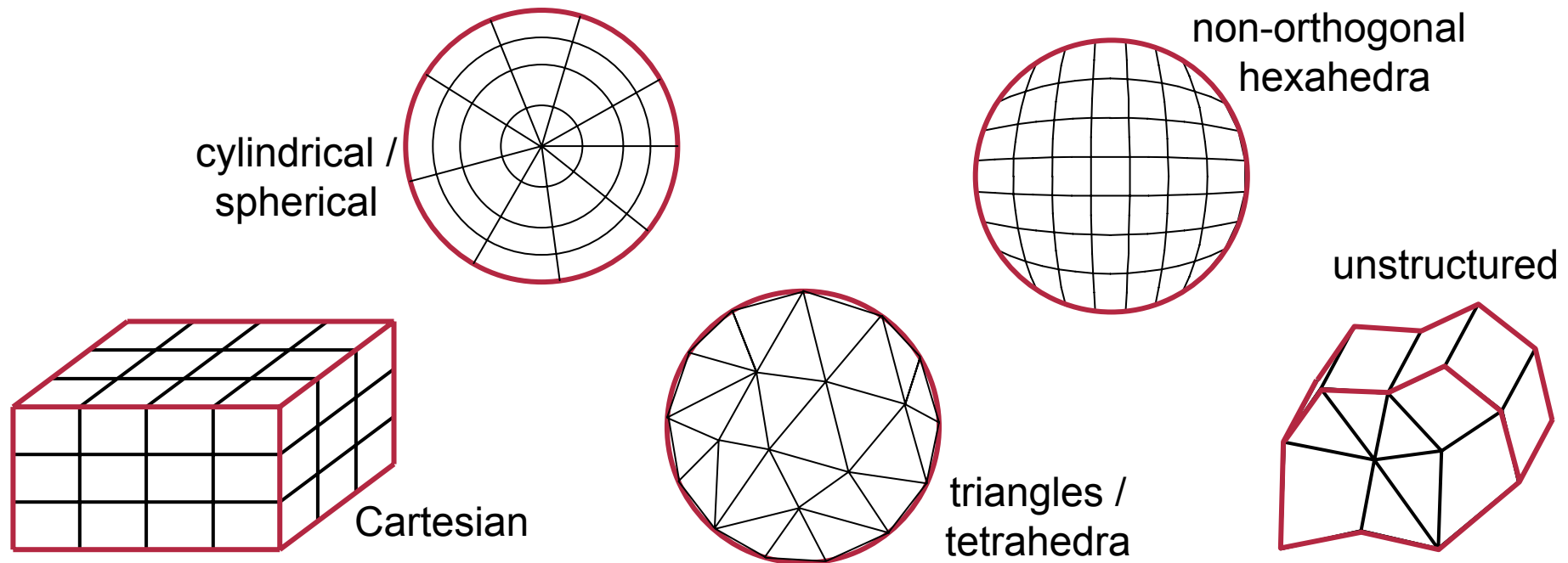


Computational Grids

Tasks of computational grids

- Allocation of state variables (DoF) of the method: potentials, field components, basis functions, ...
- Geometric Modeling (materials, boundaries)

not necessarily the same grid!





Finite Integration (FIT)

[Weiland 1977]

Idea of FIT: Geometrical Discretization

– Faraday's Law

$$\oint_{\partial A} \vec{E}(\vec{r}, t) \cdot d\vec{s} = -\frac{d}{dt} \int_A \vec{B}(\vec{r}, t) \cdot d\vec{A}$$

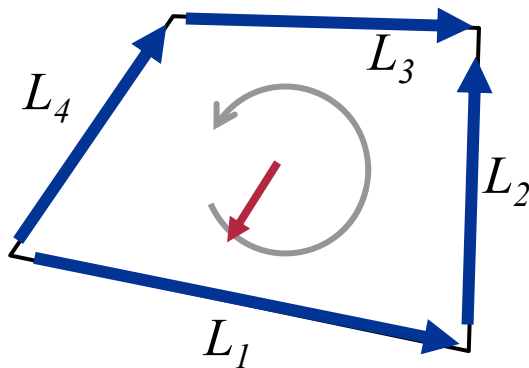
$$\forall A \subset \Omega$$

(arbitrary faces)

$$\oint_{\partial A_n} \vec{E}(\vec{r}, t) \cdot d\vec{s} = -\frac{d}{dt} \int_{A_n} \vec{B}(\vec{r}, t) \cdot d\vec{A}$$

$$\forall A_n \in G$$

(facets of the grid)



“Discretization” = reduce to a finite number of unknowns

$$\widehat{b}_n := \int \vec{B} \cdot d\vec{A} = \text{grid flux}$$

$$\widehat{e}_n := \int_{L_n} \vec{E} \cdot d\vec{s} = \text{grid voltage}$$

$$\oint_{\partial A_n} \vec{E} \cdot d\vec{s} = \oint_{L_1} + \oint_{L_2} - \oint_{L_3} - \oint_{L_4} = -\int \dot{\vec{B}} \cdot d\vec{A}$$



$$+\widehat{e}_1 + \widehat{e}_2 - \widehat{e}_3 - \widehat{e}_4 = -\frac{d}{dt} \widehat{b}_n \quad (\text{exact})$$



Finite Integration (FIT)

[Weiland 1977]

Idea of FIT: Geometrical Discretization

– Faraday's Law

$$+\hat{e}_1 + \hat{e}_2 - \hat{e}_3 - \hat{e}_4 = -\frac{d}{dt} \hat{b}_n$$

all grid facets \Rightarrow

$$\mathbf{C}\hat{\mathbf{e}} = -\frac{d}{dt} \hat{\mathbf{b}}$$

discrete Faraday's law

Building Blocks:

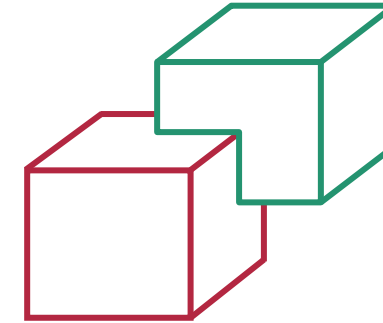
- “Curl Matrix” \mathbf{C} ($\{0, \pm 1\}$): edge orientations – role in local circulation
 - topological: describes structure of the grid (incidence matrix)
 - no metrics
 - Integral state variables
 - grid voltage, grid flux
 - not further resolved at this point
- \rightarrow generally available for arbitrary grid types



Finite Integration (FIT)

Further Steps:

- Primary and dual grid (*Cartesian or others*)
- extend set of state variables:

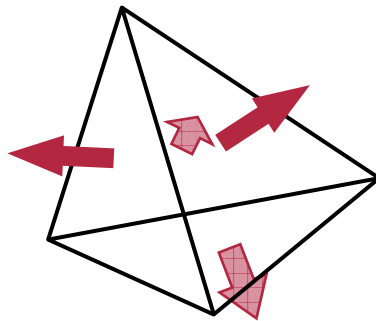


$$\widehat{d}_n := \int_{\tilde{A}_n} \vec{D} \cdot d\vec{A} \quad \widehat{j}_n := \int_{\tilde{A}_n} \vec{J} \cdot d\vec{A} \quad \widehat{h}_n := \int_{\tilde{L}_n} \vec{H} \cdot d\vec{s} \quad q_n := \int_{\tilde{V}_n} \rho \cdot dV$$

- „dual curl matrix“ $\tilde{\mathbf{C}} = \mathbf{C}^T$

$$\tilde{\mathbf{C}}\widehat{\mathbf{h}} = \frac{d}{dt}\widehat{\mathbf{d}} + \widehat{\mathbf{j}} \quad \text{discrete Ampere's law}$$

- “div”-operations: Surface integrals around cells



$$\tilde{\mathbf{S}}\widehat{\mathbf{d}} = \mathbf{q}$$

$$\mathbf{S}\widehat{\mathbf{b}} = \mathbf{0}$$

- ‘Topological’ consistency properties (for arbitrary grids):

e.g. $\mathbf{S}\mathbf{C} = \mathbf{0}$

(corresponding to $\text{div curl} \equiv 0$)

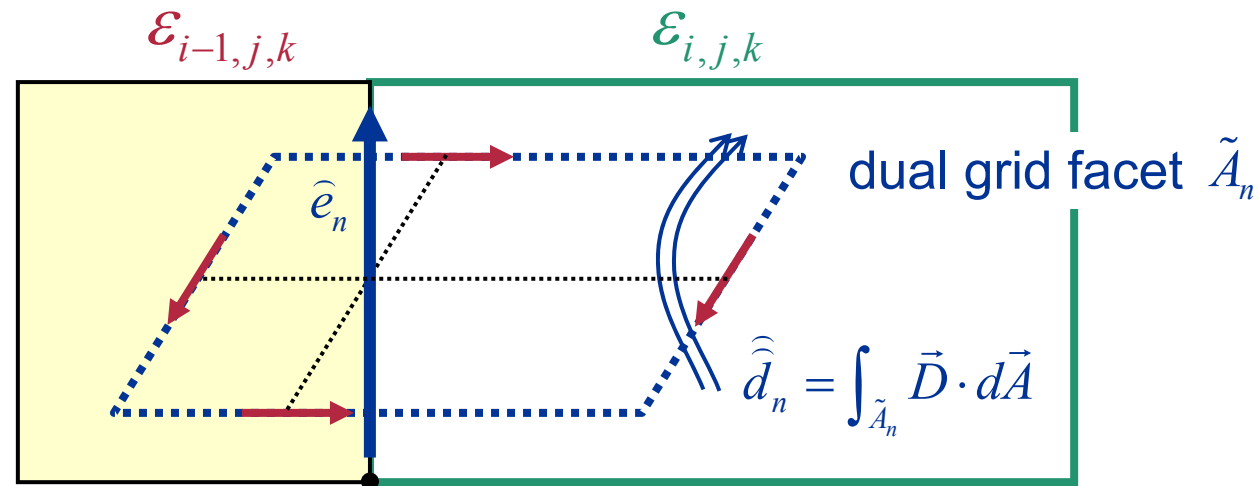


Finite Integration (FIT)

Finite Integration Technique

(still missing:)

- Material relations, e.g. $\hat{\mathbf{e}}_n \leftrightarrow \hat{\mathbf{d}}_n$



- Integral interpretation leads to canonical transformation formula
(incl. area-averaging of permittivity over dual facet)

➔ $\hat{\mathbf{d}} = \mathbf{M}_\varepsilon \hat{\mathbf{e}}$ with $\mathbf{M}_\varepsilon = \text{diag} \left(\frac{\bar{\varepsilon} \tilde{\mathbf{A}}_n}{L_n} \right)$ (here: diagonal matrix)



Finite Integration: Matrix operators

– “Topological operators”

- incidence matrices of the grids can be used as “discrete curl” and “discrete divergence”
- *discretization, no approximation* → all continuous properties still valid

Some catchwords:

- a “natural discretization” of Maxwell’s Equations
- a *general framework* for “discrete electromagnetism on a grid”

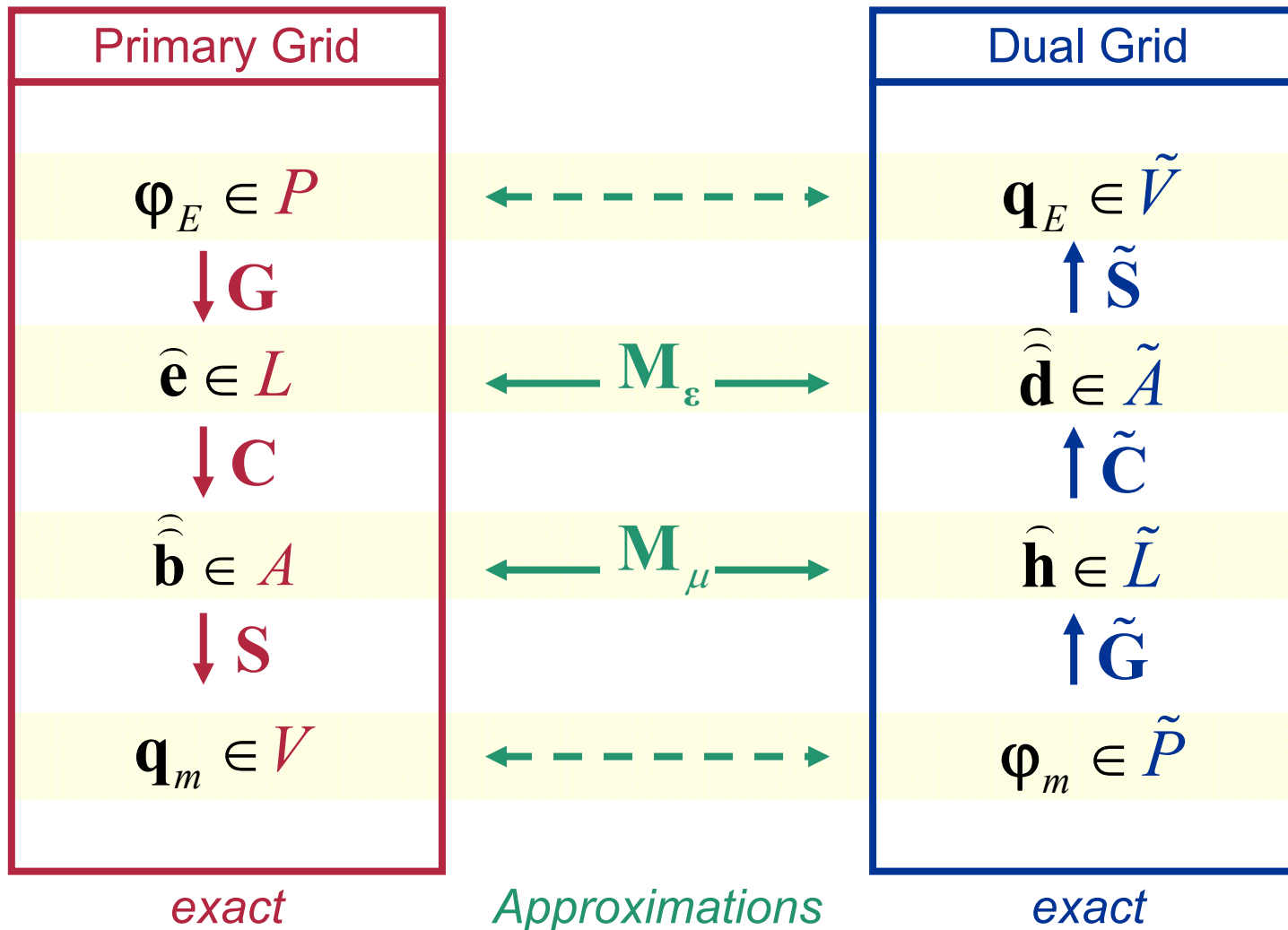
– “Material operators”

- the approximations of the method
- many ways to derive them
- must fulfill key properties: *consistent, symmetric positive definite*



Finite Integration (FIT)

Finite Integration: Matrix operators

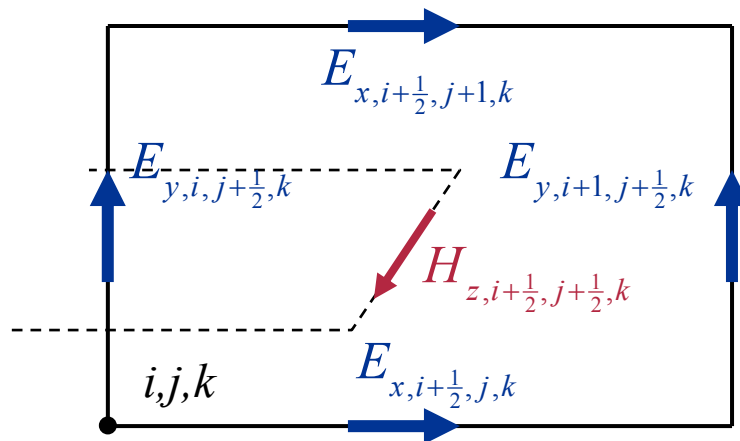




Finite Differences

for RF-fields: **Finite Difference Time Domain (FDTD)**

- start with Maxwell's equations **in their differential form**: curl, $\partial/\partial t$ - operators
- 'Staggered grids' in time and space (Cartesian) [Yee 1966]



$$-\frac{\partial}{\partial t}(\mu H_z) = \text{curl } \vec{E} \Big|_z = -\frac{\partial E_x}{\partial y} + \frac{\partial E_y}{\partial x}$$

↓
staggered
time
grid

↓
staggered spatial
grid ('dual grid')

$$\frac{\partial}{\partial t} H_z \Big|_{n+\frac{1}{2}} \approx \frac{H_z^{n+1} - H_z^n}{\Delta t}$$

$$\frac{\partial E_x}{\partial y} \Big|_{j+\frac{1}{2}} \approx \frac{E_{x,i+\frac{1}{2},j+1,k} - E_{x,i+\frac{1}{2},j,k}}{\Delta y}$$

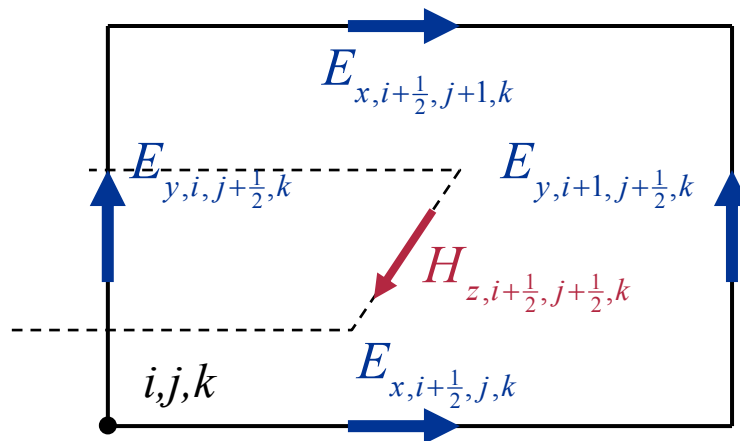
Discretization + Approximation in 1 step



Finite Differences

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↓
staggered
time
grid

↓
staggered spatial
grid ('dual grid')

$$H_{z,i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = H_{z,i+\frac{1}{2},j+\frac{1}{2},k}^n - \frac{\Delta t}{\mu} \left(-\frac{E_{x,i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - E_{x,i+\frac{1}{2},j,k}^{n+\frac{1}{2}}}{\Delta y} + \frac{E_{y,i+1,j+\frac{1}{2},k}^{n+\frac{1}{2}} - E_{y,i,j+\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta x} \right)$$

„Update Equations“



Finite Integration (FIT) and Finite Differences (FDTD)

- FIT on Cartesian grids + leapfrog time discretization:

$$\hat{\mathbf{h}}^{n+1} = \hat{\mathbf{h}}^n - \Delta t \mathbf{M}_\mu^{-1} \mathbf{C} \hat{\mathbf{e}}^{n+\frac{1}{2}}$$

– update



conceptually different, but
„*computationally equivalent*“



$$\hat{h}_z \approx H_z \cdot \Delta \tilde{z}$$

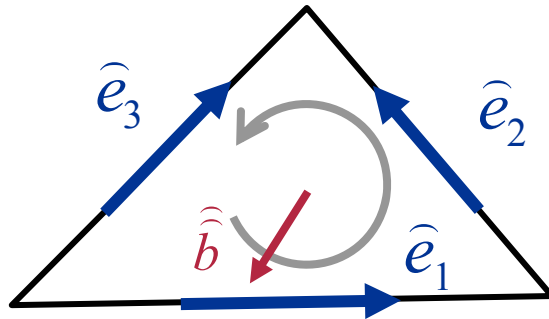
$$\underbrace{\mu \Delta x \Delta y}_{\mathbf{M}_\mu^{-1}} \underbrace{\mathbf{C} \hat{\mathbf{e}}^{n+\frac{1}{2}}}$$

$$H_{z,i+\frac{1}{2},j+\frac{1}{2},k}^{n+1} = H_{z,i+\frac{1}{2},j+\frac{1}{2},k}^n - \frac{\Delta t}{\mu} \left(-\frac{E_{x,i+\frac{1}{2},j+1,k}^{n+\frac{1}{2}} - E_{x,i+\frac{1}{2},j,k}^{n+\frac{1}{2}}}{\Delta y} + \frac{E_{y,i+1,j+\frac{1}{2},k}^{n+\frac{1}{2}} - E_{y,i,j+\frac{1}{2},k}^{n+\frac{1}{2}}}{\Delta x} \right)$$



Triangular (tetrahedral) grids:

(FDTD ??)



$$\oint_{\partial A} \vec{E} \cdot d\vec{s} = -j\omega \int_A \vec{B} \cdot d\vec{A}$$

↓

$$\hat{e}_1 + \hat{e}_2 - \hat{e}_3 = -j\omega \hat{b}$$

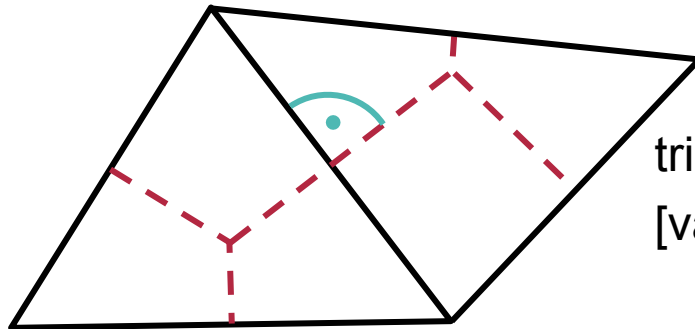
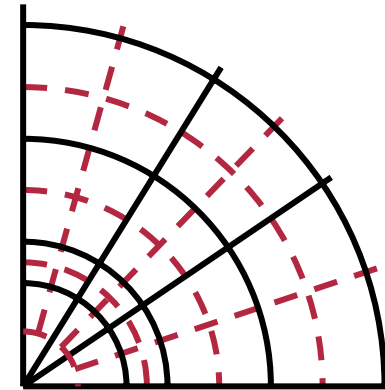
- Operators S,C canonical ➡ all topological properties fulfilled
 - “Only” needed: new material matrices
-
- Orthogonality of primary and dual grid: Standard-approach (→ diagonal matrix)
 - Loss of this orthogonality: special solution needed
 - Necessary for stability: symmetric positive definite



Extension to other grids

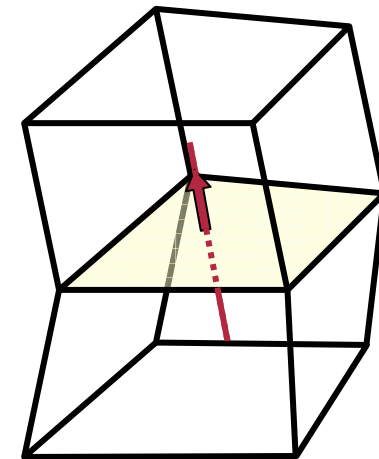
☞ So far implemented:

Cartesian, cylindrical (2D/3D)
[1983]



triangular (with orth. dual grid)
[van Rienen 1985]

non-orthogonal hexahedral
[1998]





FIT: History of Notations

1966 Yee's Method (FDTD)

1975 E. Tonti: "On the Formal Structure of Physical Theories"

$$\begin{aligned} j\omega D_{\tilde{G}} D_{\epsilon} \underline{e} - R_{\tilde{G}} D_{\mu}^{-1} \underline{b} &= \underline{c}, \\ j\omega D_G \underline{b} + R_G \underline{e} &= \underline{0}. \end{aligned}$$

$$D_h (-\mu_0 \dot{\underline{h}}) = R_e \underline{e}$$

$$D_e (\epsilon_0 \dot{\underline{e}} + \underline{j}) = R_h \underline{h}$$

30 years of FIT
in 2007!

1977 (1st paper)
AEÜ 31

1980, „Finite Integration“
Proc. XI Conf. High Energy Acc, Geneva.



FIT: History of Notations

1980 Taflove: Yee's Method named "FDTD" IEEE T-EMC 22

1980/1986 Nedelec: Edge elements in FE Num.Math. 35/50

$$\mathbf{C} \mathbf{D}_s \mathbf{e} = -\mathbf{D}_A \mathbf{b}$$

1986: Curl matrix notated "C"

URSI EMTS Budapest

$e_i = \int_{L_i} \vec{E} \cdot d\vec{s}$	$-\dot{\mathbf{b}} = \mathbf{C} \mathbf{e}$
$b_i = \int_{A_i} \vec{B} \cdot d\vec{A}$	$\mathbf{S} \mathbf{b} = 0$
	$\mathbf{i} + \dot{\mathbf{d}} = \tilde{\mathbf{C}} \mathbf{h}$
	$\tilde{\mathbf{S}} \mathbf{d} = \mathbf{q}$

1996: Grid voltages and fluxes

Int. J. Num Mod. 9

(in PhD-Theses since 1992)

but still the same basic formulas and discretization approach as in 1977 !



Back to time domain:

$\widehat{\mathbf{h}}^{n+1} = \widehat{\mathbf{h}}^n - \Delta t$	\mathbf{M}_{μ}^{-1}	$\mathbf{C}\widehat{\mathbf{e}}^{n+\frac{1}{2}}$
$\widehat{\mathbf{e}}^{n+\frac{3}{2}} = \widehat{\mathbf{e}}^{n+\frac{1}{2}} + \Delta t$	$\mathbf{M}_{\varepsilon}^{-1}$	$\tilde{\mathbf{C}}\widehat{\mathbf{h}}^{n+1}$

Update-Equations of explicit scheme

Inverse material operators needed !

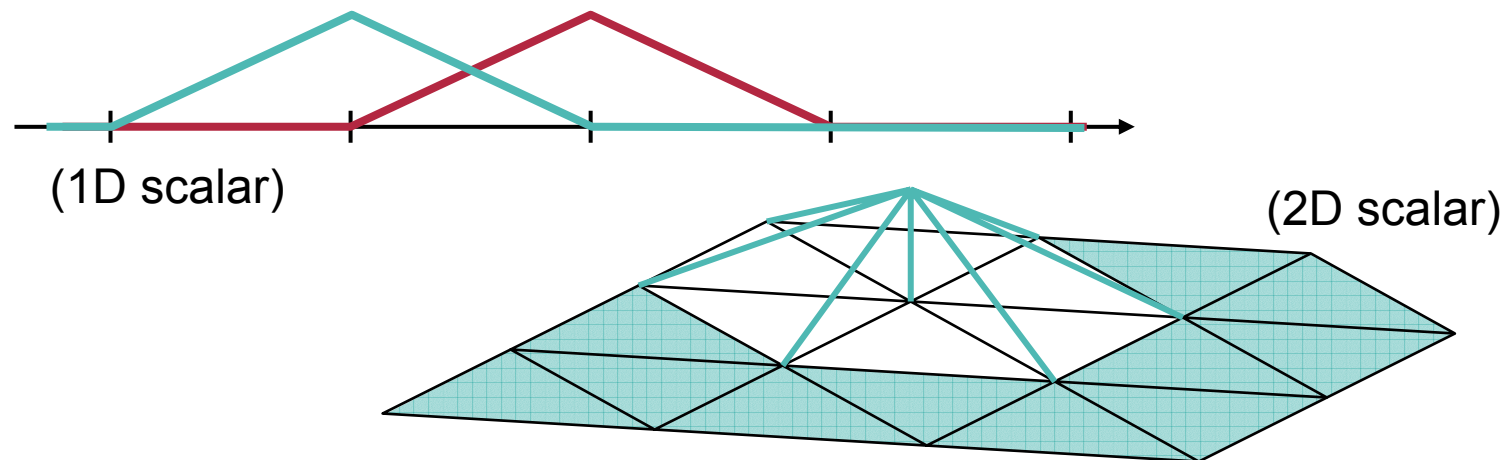
- ok for diagonal matrices, but this needs dual-orthogonal meshes

→ A motivation for research in this field:
to find an explicit time-domain scheme for general tet-grids



Finite Elements:

- represent solution by basis functions with „compact support“
- low requirements on (type of) computational grid



- low polynomial order (linear, quadratic, ...) → rate of convergence



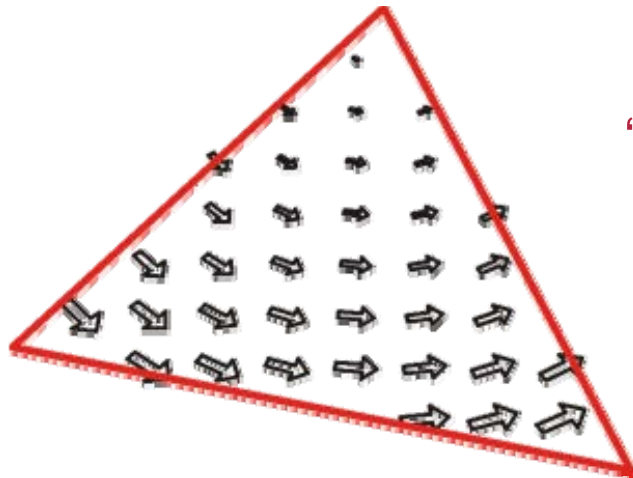
„discretization of (solution) space“

(vs. discretization of operators in FD, FIT)



Edge Elements (Whitney forms)

- A set of functions for vector-valued problems on simplicial meshes [Whitney 1957, Nédélec 1980]
- tangential continuity



“edge functions”: $\int_{L_i} \vec{w}_j \cdot d\vec{s} = \delta_{ij}$

FE FIT

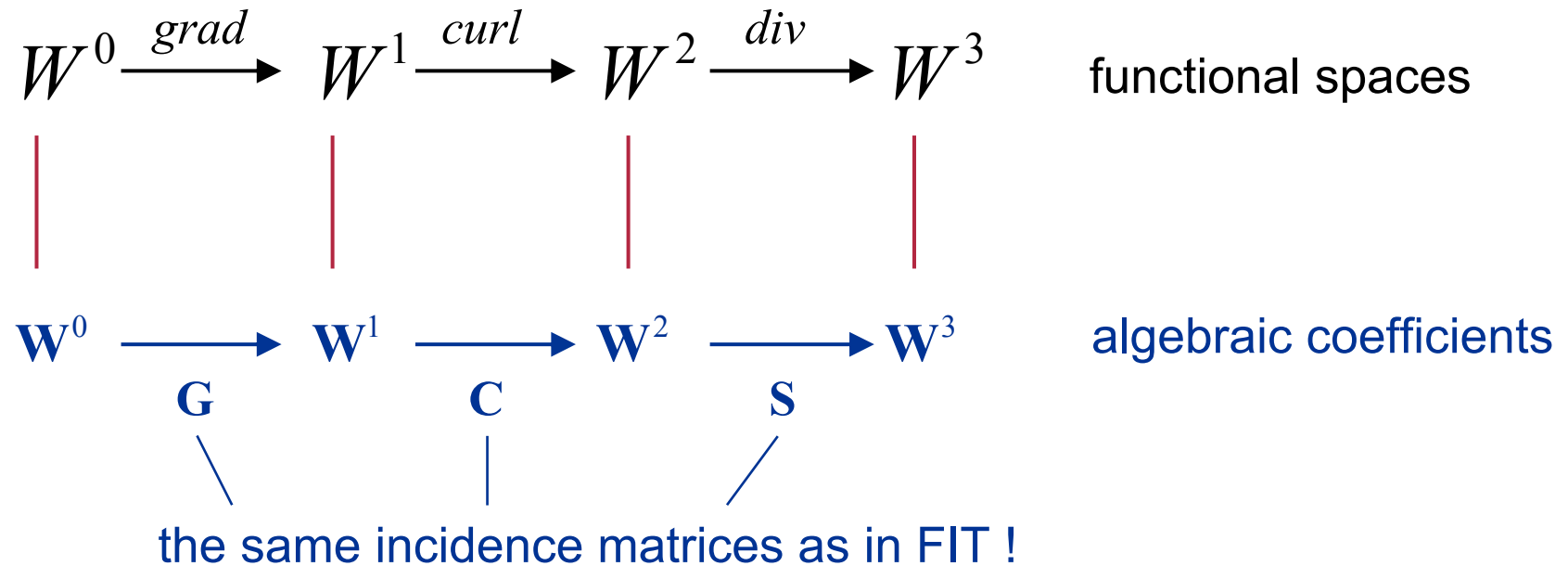
$$\int_{L_i} \vec{E} \cdot d\vec{s} = \int_{L_i} \sum_j E_j \vec{w}_j \cdot d\vec{s} = E_i = \hat{e}_i$$

state variables equivalent 😊



„Whitney Complex“

- defines nodal (W^0), edge (W^1), face (W^2), and volume (W^3) functions
- complete sequence property:



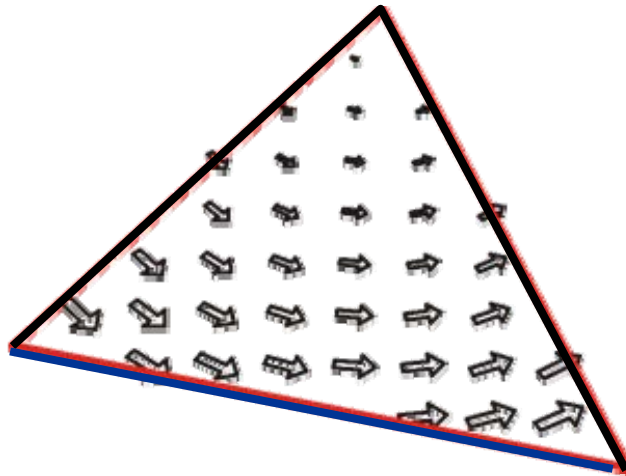
- consistent discretization, e.g. no ghost modes !

[Bossavit 98]

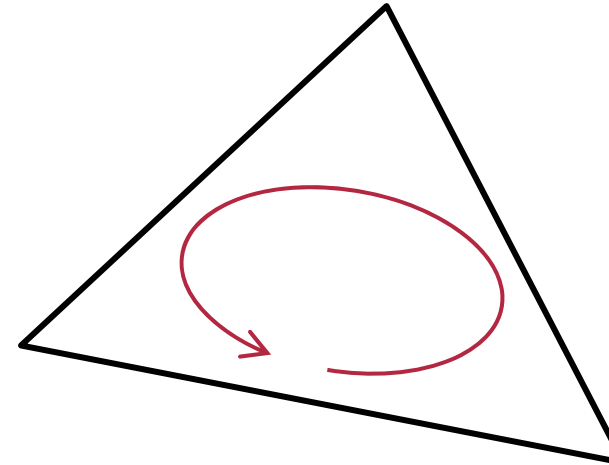


“Curl-Operation”: $\nabla \times \vec{A} = \vec{B}$

FE



FIT



$$\nabla \times \left(\sum A_j \vec{w}_j^{(1)} \right) = B_n \vec{w}_n^{(2)} \quad (\text{face function}) \quad \sum \pm \hat{a}_j = \hat{b}_n$$

use Curl-matrix in FE !





Finite Elements: Application to Wave Equation

$$\text{curl } \mu^{-1} \text{curl } \vec{E} - \omega^2 \varepsilon \vec{E} = -i\omega \vec{J} \quad \vec{E} = \sum_i E_i \vec{w}_i$$

– Weighted residuals: $\int \vec{w}_j \cdot \dots dV \quad \forall j$



$$\mathbf{A}(E_i) - \omega^2 \mathbf{B}(E_i) = \mathbf{r}$$

$$A_{ij} = \int \mu^{-1} (\text{curl } \vec{w}_i) \cdot (\text{curl } \vec{w}_j) dV$$

$$B_{ij} = \int \varepsilon \vec{w}_i \cdot \vec{w}_j dV$$

FIT: $\tilde{\mathbf{C}} \mathbf{M}_\mu^{-1} \mathbf{C} \hat{\mathbf{e}} - \omega^2 \mathbf{M}_\varepsilon \hat{\mathbf{e}} = \mathbf{r}$ analogy (for identical grids) ?



$\hat{\mathbf{e}}$ \leftrightarrow (E_i) degrees of freedom / state variables

$\tilde{\mathbf{C}} \mathbf{M}_\mu^{-1} \mathbf{C}$ \leftrightarrow \mathbf{A} stiffness matrix

\mathbf{M}_ε \leftrightarrow \mathbf{B} mass matrix



Finite Elements: Matrices

Stiffness Matrix:

$$A_{ij} = \int \mu^{-1} (\text{curl } \vec{w}_i) \cdot (\text{curl } \vec{w}_j) dV$$

– can be identified as

$$(A_{ij}) = \tilde{\mathbf{C}} \mathbf{M}_{\mu^{-1}}^{FE} \mathbf{C} \quad \text{with} \quad M_{\mu^{-1},ij}^{FE} = \int \mu^{-1} \vec{w}_i^{(2)} \cdot \vec{w}_j^{(2)} dV$$

(2nd FE mass matrix for face functions)

Mass Matrix:

- FIT: diagonal for dual-orthogonal grids
- FE: always non-diagonal
 - Cartesian grids: *mass lumping leads to FIT-equivalent matrix!*
[e.g. Rylander/Bondeson 2000]
 - Tetrahedral grids: mass lumping fails
[Bossavit / Kettunen 1999, 2001]
- (no explicit time domain scheme!)



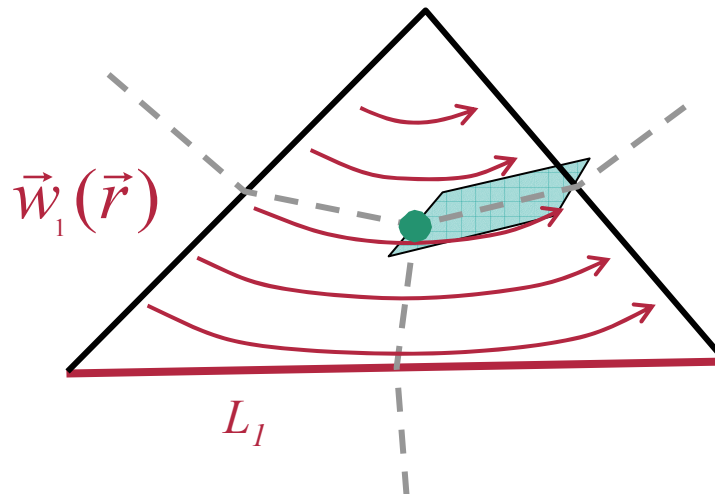
Finite Elements vs. Finite Integration

- (Lowest order) Whitney functions allow FIT framework in FE
 - topological matrices (incidence relations of grid)
 - material operators
- Hybridization:
 - both methods allow hybrid grids
 - analysis of properties by FE- and/or FIT-theory
- Example: Hybrid method (Rylander/Bondeson [2000] and Edelvik/Ledfelt [2002])
 - unstructured grids for complex geometries
 - structured (FDTD-) grids elsewhere
 - common stability analysis by re-interpretation of FDTD part as „FE with mass lumping“



Others...

- Basis functions (Whitney or others), but matrices not from FE Galerkin approach
- Example: „FIT with Whitney“ (2D) [2001]

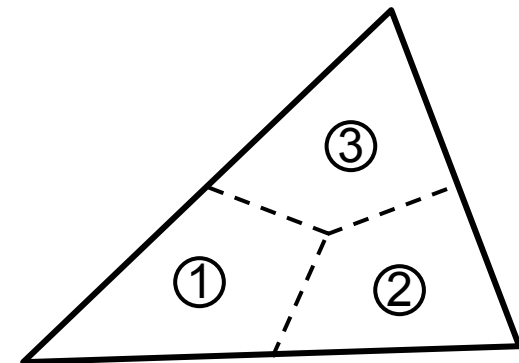


derive material operator from exact integration of basis function on dual face

needs modified dual grid for stability

- Example: „Microcell Method“ (2D) [Tonti 1975, Marrone 2001]

barycentric dual grid, piecewise constant fields in „micro cells“





Others...

– Hybrid: FIT + Microcell Method [Cinalli et al., Darmstadt, 2004]

– **FE: higher order**

- „higher order Whitney forms“: more DoF per edge / facet
- hierarchical functional spaces

– **FIT: higher order**

- no additional DoF
- larger stencils in material operators

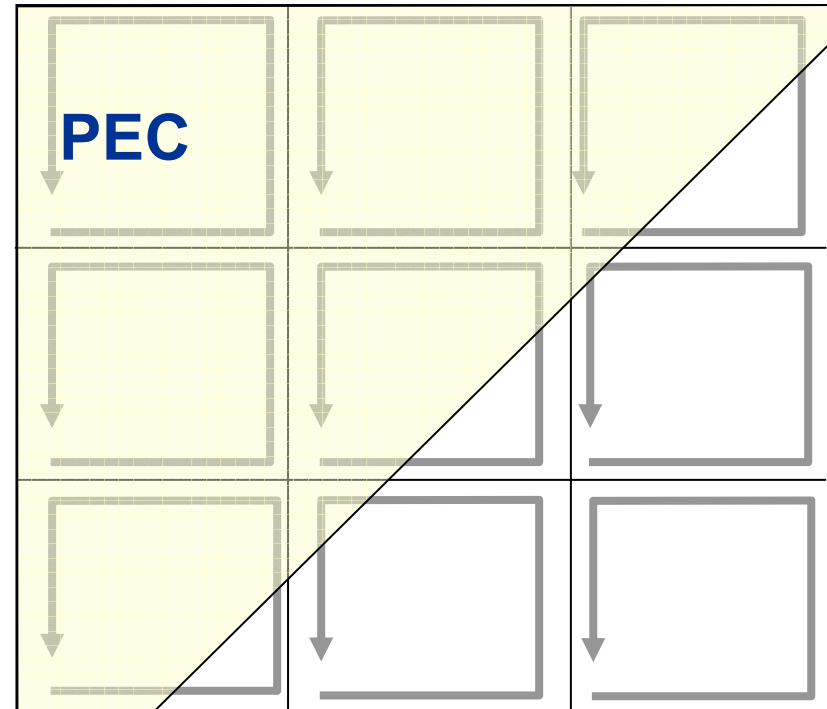
no FE-FIT correspondence; geometric interpretations?

– **Finite Volumes, Discontinuous Galerkin, Generalized FE, ...**



Conformal Modeling in a Cartesian Yee-Grid

- allow PEC-interfaces within cells



[Thoma 1997] („FIT + *Partially Filled Cells*“), [Dey, Mittra 1997] („*Conformal FDTD*“)



Conformal Modeling in a Cartesian Yee-Grid

- allow PEC-interfaces within cells
- omit PEC parts ($\int \vec{E} \cdot d\vec{s} = 0$)

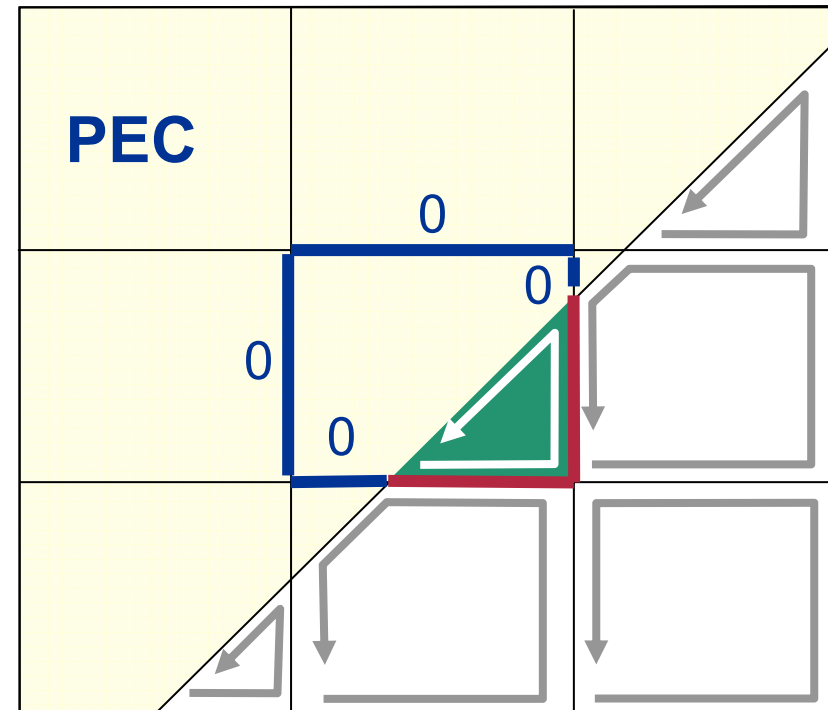
→ reduced edge lengths

$$L_{ijk} \rightarrow l_{ijk}$$

→ reduced facets

$$S_{ijk} \rightarrow s_{ijk}$$

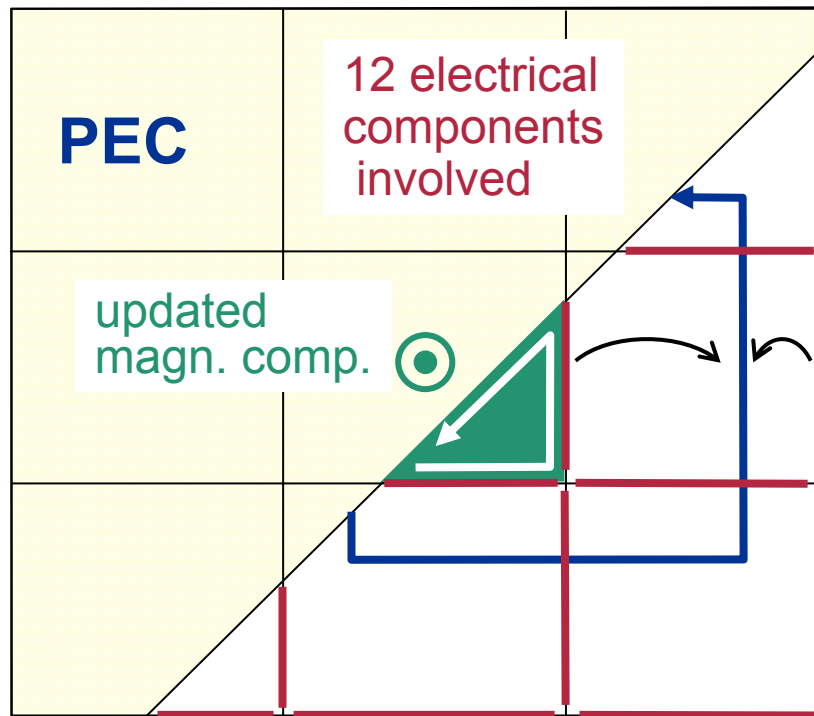
- 2nd order accurate (PEC)
- still diagonal matrices!
- needs smaller time step



[Thoma 1997] („FIT + *Partially Filled Cells*“), [Dey, Mittra 1997] („*Conformal FDTD*“)



To keep full time step (numerical dispersion...)



Uniform Stable Conformal scheme
(**USC**, 2003)

virtually enlarged cells
(off-diagonal entries)

FE analogon ??
(would need new basis
functions)

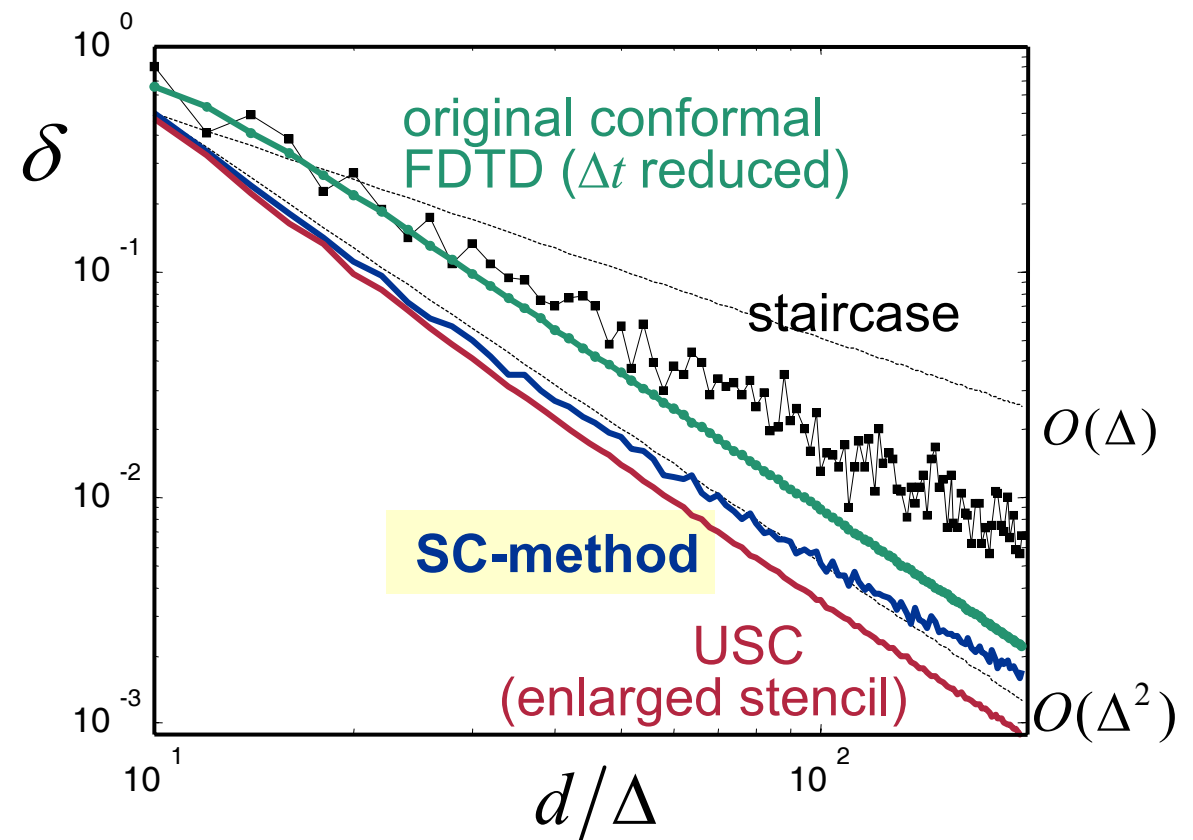
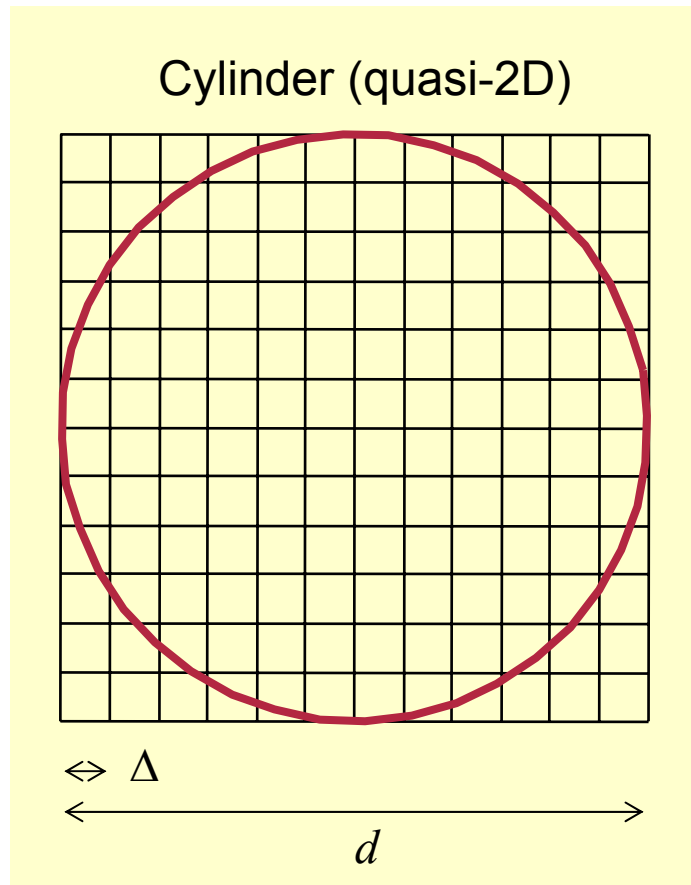
- simplified conformal scheme (SC 2006):
 - diagonal matrix with modified components
 - small loss of accuracy, still 2nd order

[I. Zagorodnov]



Convergence Analysis: Academic example

impress analytical field \rightarrow iterate N time steps $\rightarrow \delta = L_2$ -norm of field deviation



[I. Zagorodnov 2006]












Concepts of Finite Methods

	continuous	discrete	approximation
FD	Derivatives $\lim_{h \rightarrow 0} \frac{f(x + \frac{h}{2}) - f(x - \frac{h}{2})}{h}$	Differences $\frac{f(x + \frac{\Delta}{2}) - f(x - \frac{\Delta}{2})}{\Delta}$	locally in difference formulas (Taylor series)
FIT	Circulations $\int_{\partial A} \vec{E} \cdot d\vec{s} \quad \forall A \subset \Omega$	Discrete Circulations $\sum_{i \in \partial_k} \hat{e}_i \quad \forall A_k \subset G$	locally in material relations (Taylor series)
FE	Solutions space $H(\text{curl}), \dim = \infty$	Functional Space $H_h^p(\text{curl}), \dim = N$	globally (min. resid.): „optimal“ solution for chosen space and w.r.t. chosen inner product



Properties of Finite Methods

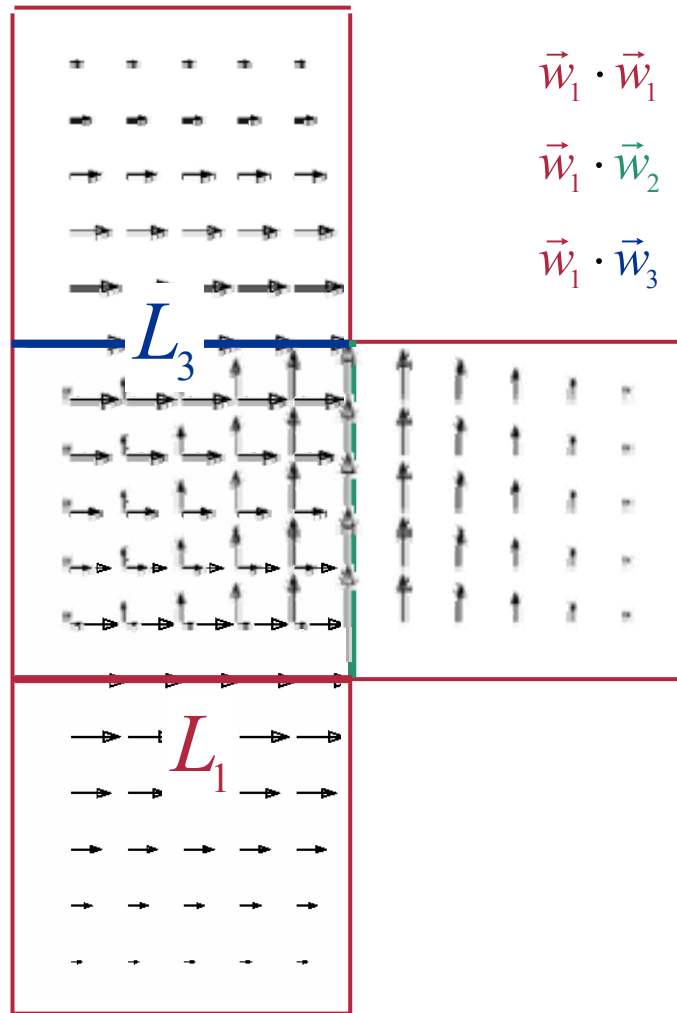
	FD / FIT	(Whitney-) FE
Basis functions	possible by re-interpretation	 main idea
Dual grid	 main idea	possible by re-interpretation
Topological Operators S, C	 main idea	possible by re-interpretation
Diagonal Material Matrix (explicit in Time Domain)		
General Computational Grid		
Higher Order Modeling		
Subcell Methods		



Finite Elements: Cartesian

Mass Matrix: 1) Cartesian grids

$$B_{ij} = \int \epsilon \vec{w}_i \cdot \vec{w}_j dV$$



$$\vec{w}_1 \cdot \vec{w}_1 \neq 0 \quad (\text{main diagonal})$$

$$\vec{w}_1 \cdot \vec{w}_2 \equiv 0$$

$$\vec{w}_1 \cdot \vec{w}_3 \neq 0$$



no diagonal matrix !

$$\mathbf{B} \neq \mathbf{M}_\epsilon$$



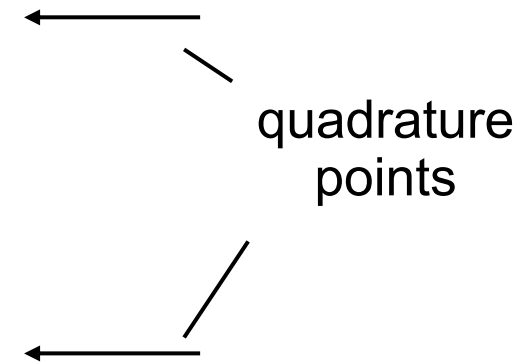
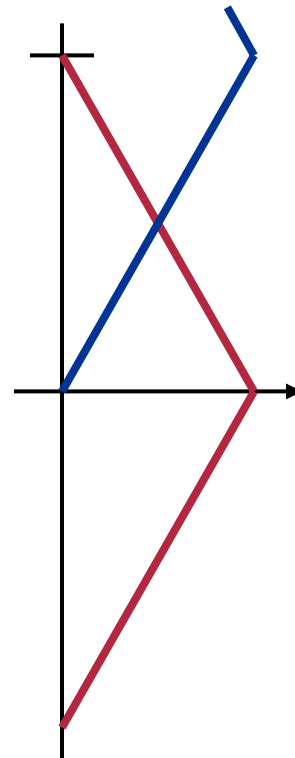
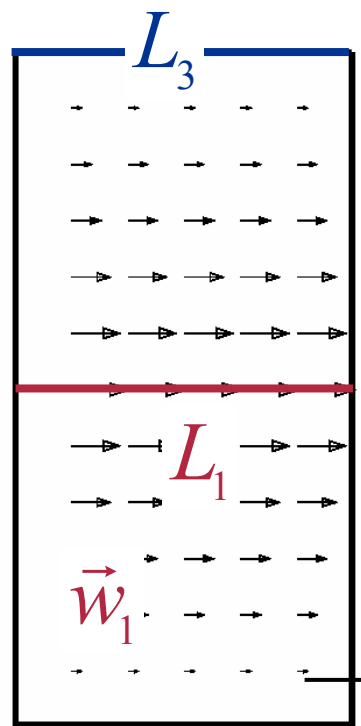
- ◆ eliminate off-diagonal entries by „mass lumping“
- ◆ idea: approximative evaluation of integrals (quadrature)



Finite Elements: Cartesian

Mass Matrix: 1) Cartesian grids

$$B_{ij} = \int \epsilon \vec{w}_i \cdot \vec{w}_j dV$$



(...)

$$\mathbf{B} = \mathbf{M}_\epsilon$$

(...)

$$\mathbf{A} = \tilde{\mathbf{C}} \mathbf{M}_\mu^{-1} \mathbf{C}$$

FE with mass lumping leads to FIT-equivalent equations! 😊

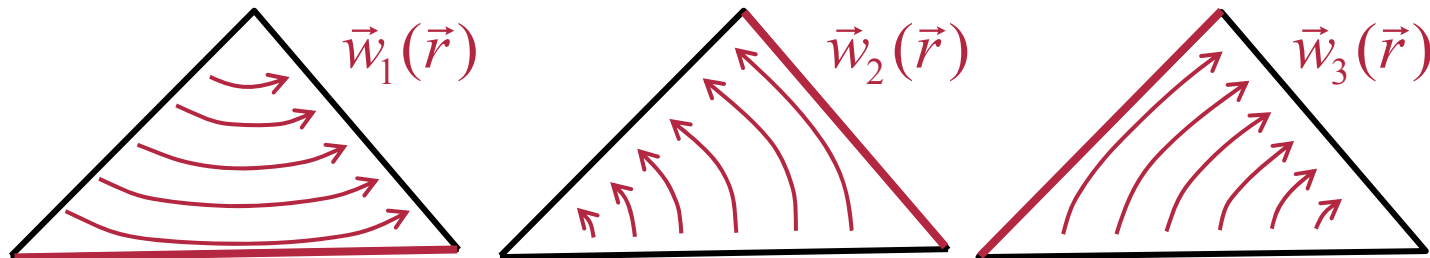
[e.g. Rylander/Bondeson 2000]




Finite Elements: Tetrahedral

Mass Matrix: 2) Tetrahedral grids

$$B_{ij} = \int \varepsilon \vec{w}_i \cdot \vec{w}_j dV$$



- Dot products $\vec{w}_i \cdot \vec{w}_j$ always $\neq 0$, **no diagonal matrix** (neither in systems with orthogonal dual grid)
- Mass lumping?  can lead to **indefinite matrices (in-stable !)** [Bossavit / Kettunen 1999, 2001]



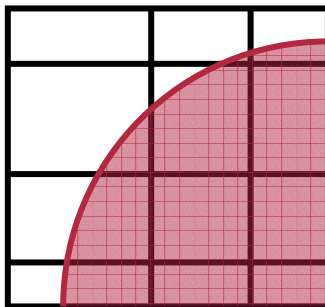
For tetrahedral / triangular grids no explicit time domain scheme with FE-matrices is available



FIT: Conformal Modeling

FIT: Conformal Modeling

- Another way to gain flexibility in geometric modeling:
„Conformal modeling“ with Cartesian grids



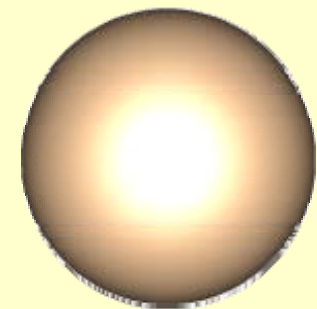
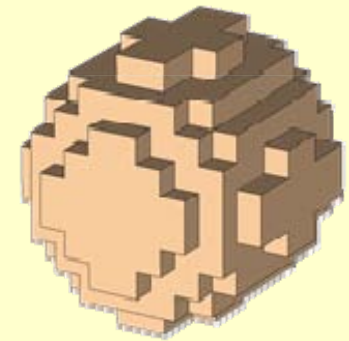
allow „**partially filled cells**“

= interfaces to perfect conductors (PEC) within cells



task of grid: only allocation of components
material distribution practically independent of grid!

- main advantage: **still Cartesian grids + diagonal material matrices**





Analyze Stability Situation

- effective material parameters in reduced cells:

$$\varepsilon_{eff} = \varepsilon \frac{L_{ijk}}{l_{ijk}} \nearrow$$

(edge reduction)

$$\mu_{eff} = \mu \frac{S_{ijk}}{S_{ijk}} \searrow$$

(area reduction)

$$\Delta t_{max} = \frac{\sqrt{\mu_{eff} \varepsilon_{eff}}}{\sqrt{\Delta x^{-2} + \Delta y^{-2} + \Delta z^{-2}}}$$

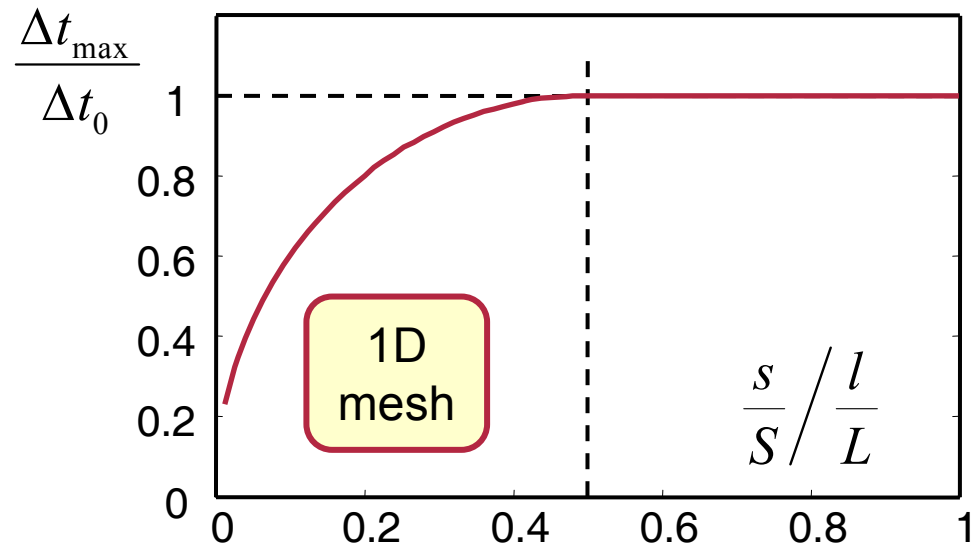
- formula for *critical cells*:

Δt has to be reduced, if

$$\frac{S_{ijk}}{S_{ijk}} < \frac{1}{2} \frac{l_{ijk}}{L_{ijk}}$$

relation between
facet- and edge reduction

(1D proof simple, 2D/3D empirical)



[I. Zagorodnov 2006]



Avoid Small “Effective” Cells

Uniform Stable Conformal scheme (USC, 2003)

- *virtually enlarge critical cells:* enlarged local curl-operation
 (“between” cells)
- unknown fields by interpolation (...)

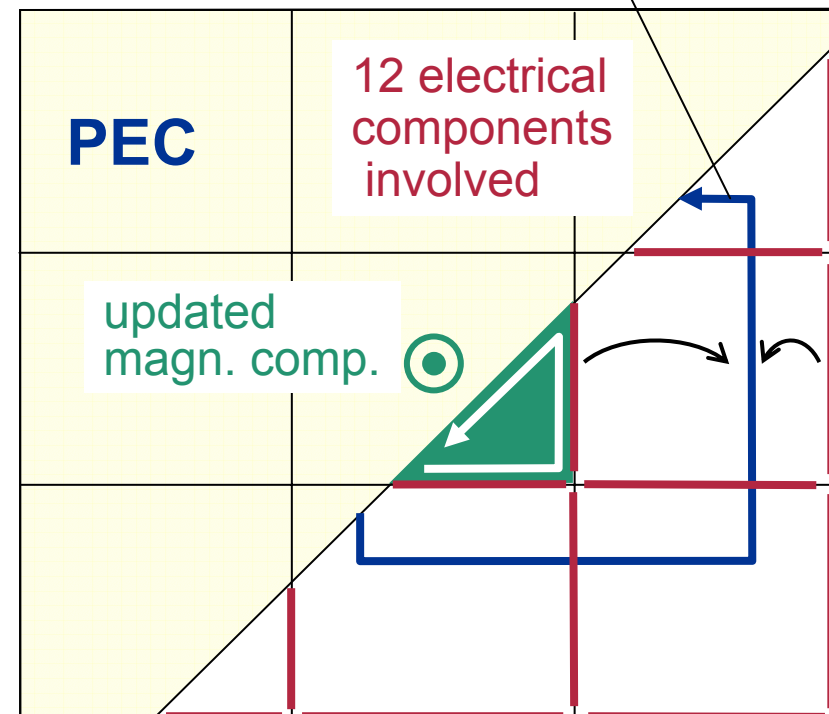
- enlarged stencil, but only for a small number of critical cells

(non-diagonal $\frac{1}{\mu}$ -matrix)

- still explicit (efficient),
but complicated formulas

→ **no time step reduction !**

→ **full 2nd order accuracy of
standard conformal FIT**



[with I. Zagorodnov]



Simplified Conformal (SC) Method

SC-Scheme = Simpler Approach without Enlarged Stencil

- idea: directly enforce stability constraint
 (“stability correction” of conformal FIT-coefficients)

for critical cells only: $\frac{s_{ijk}}{S_{ijk}} < \frac{1}{2} \frac{l_{ijk}}{L_{ijk}} \xrightarrow{\text{enforce}} \frac{s_{ijk}}{S_{ijk}} = \frac{1}{2} \frac{l_{ijk}}{L_{ijk}}$

„s-method“: enlarge s_{ijk} (reduced area) in all coefficients concerned

„SC“-method“: reduce l_{ijk} (reduced edge) in all coefficients concerned

- some accuracy is lost, *but only as much as necessary*:

→ small number of cells: $N_{corr} \ll N_{PFC} \ll N_{tot}$

→ small amount of correction

[with I. Zagorodnov]