Electromagnetic Simulations

CAS course on “RF for Accelerators“,
18 June – 01 July 2023, Berlin, Germany

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Berlin, 20.06.2023

Why do we need Electromagnetic Simulation and Numerical Methods?

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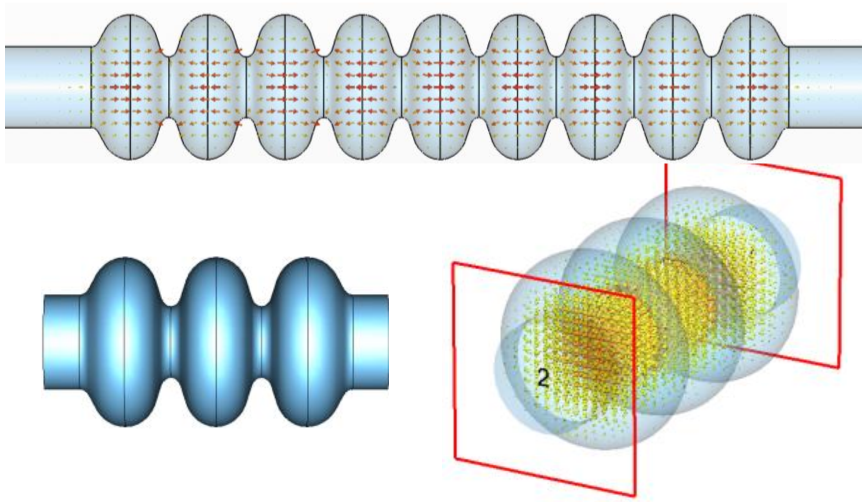
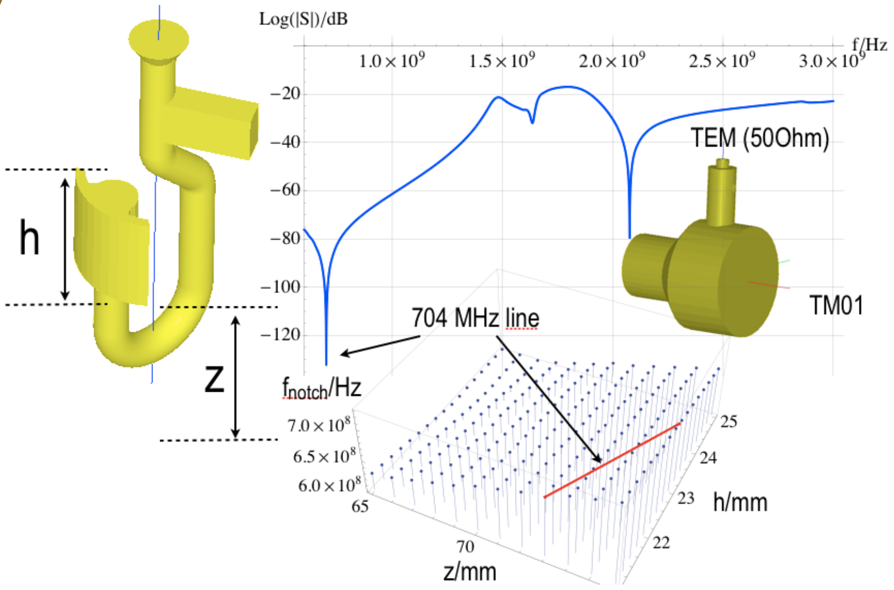
Field Problems in the Context of RF for Particle Accelerators

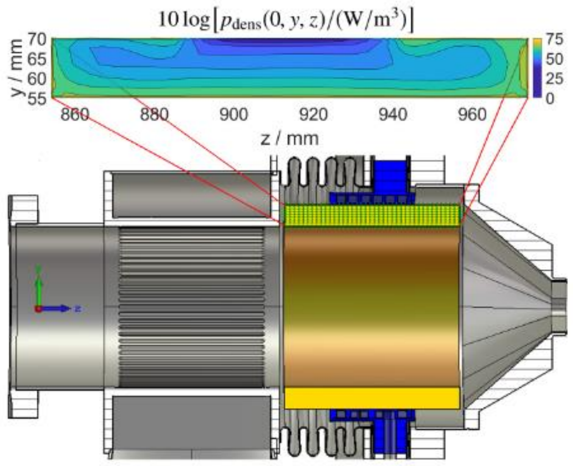
- Electromagnetic devices and systems are key components of particle accelerators:



Cavity geometry taken from T. Khabibouline, N. Solyak, and R. Wanzenberg, TESLA-FEL Report No. TESLA-FEL 2003-01, 2003



C. Potratz, H.-W. Glock and U. van Rienen, Time-Domain Field and Scattering Parameter Computation in Waveguide Structures by GPU-Accelerated Discontinuous-Galerkin Method, IEEE TMTT vol. 59, no. 11, pp. 2788-2797, Nov. 2011



T. Flisgen, H.-W. Glock, A. Tsakanian, Estimation of Dielectric Losses in the Bessy VSR Warm Beam Pipe Absorbers, IPAC2018, Vancouver, BC, Canada

- Electromagnetic phenomena are mathematically described by **Maxwell's equations** (system of coupled **P**artial **D**ifferential **E**quations), so they need to be solved for understanding and optimizing the devices and systems

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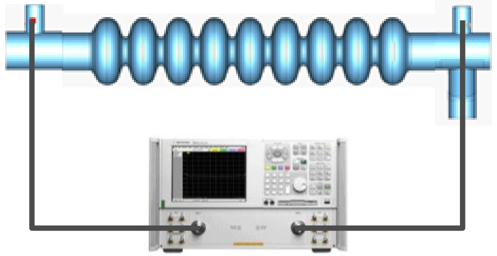
(Some) Important Derived Integral Quantities in Context of RF for Accelerators

$$\nabla \times \left[\mu^{-1}\nabla \times \mathbf{E}(\mathbf{r},t)\right] + \varepsilon\frac{\partial^2}{\partial t^2}\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t)$$ curl-curl equation

Network parameters

Cavity model courtesy of N. Eddy / FNAL

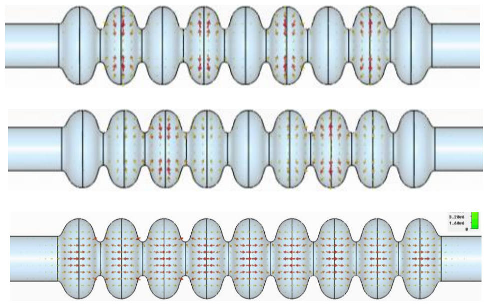


$$\underline{\mathbf{S}}(j\omega)\,\underline{\mathbf{a}}(j\omega) = \underline{\mathbf{b}}(j\omega)$$

$$\underline{\mathbf{Z}}(j\omega)\,\underline{\mathbf{i}}(j\omega) = \underline{\mathbf{v}}(j\omega)$$

$$\underline{\mathbf{Y}}(j\omega)\,\underline{\mathbf{v}}(j\omega) = \underline{\mathbf{i}}(j\omega)$$

Eigenmodes

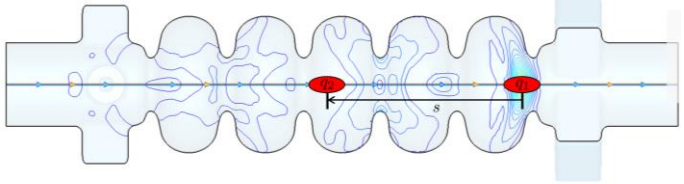


$$\mathbf{E}_n(\mathbf{r}),\ \omega_n$$

$$\frac{R_n}{Q_n} = \frac{|V_n|^2}{\omega_n W_n},\ Q_{0,n}$$

Wake potentials or beam coupling impedances

Cavity model courtesy of A. Vèlez / HZB



$$\Delta\mathbf{p}(s) = q_2 q_1 \mathbf{W}(s)$$

$$\underline{\mathbf{Z}}(j\omega) = \mathcal{F}\left[\mathbf{W}(s)\right]$$

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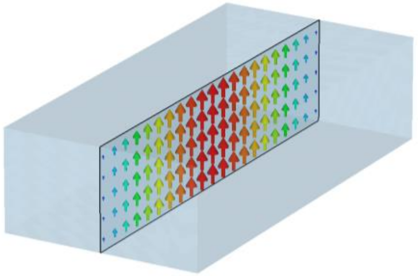
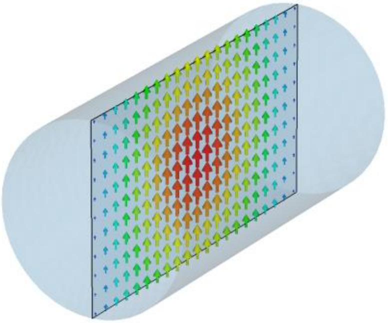
Analytical Solutions of Maxwell‘s Equations

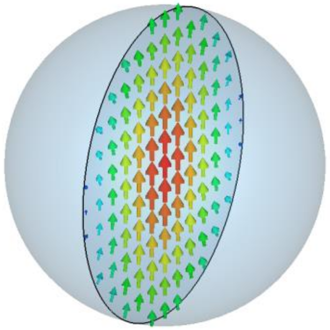
- Analytical solutions for Maxwell’s equations in general (and for curl-curl equation in particular) can only be derived for very simple geometries, e.g.



Rectangular Resonator



Cylindrical Resonator



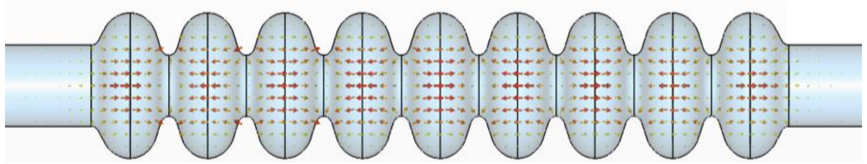
Spherical Resonator

- Typically, analytical solutions can solely be found if boundaries of the geometry coincide with coordinate planes of a suitable coordinate system (Cartesian, cylindrical, spherical etc. …)

- If there is an analytical solution **USE IT**, because
  - it is continuous, so its derivatives for optimization are available
  - parameter studies are readily performable …
  - no errors from numerical approximations
  - almost no computational costs

Numerical Solutions determined during EM Simulations

- Solutions of field distributions in real-life geometries generally require EM simulation, i.e. application of numerical methods, because it is difficult to find coordinate systems whose planes are parallel to e.g. following geometries



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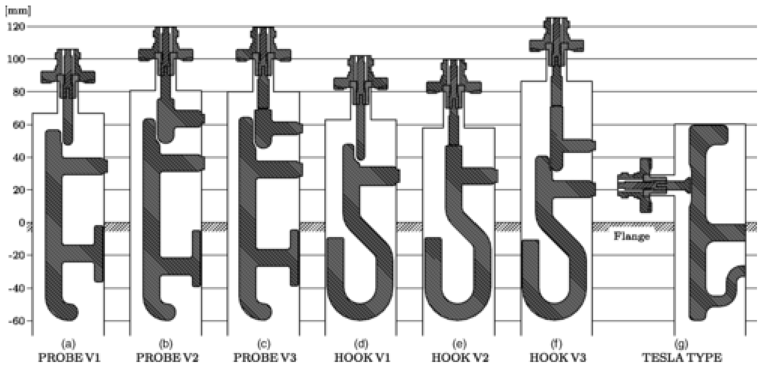
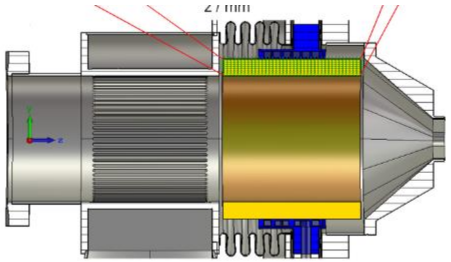


K. Papke, F. Gerigk, and U. van Rienen, Comparison of coaxial higher order mode couplers for the CERN Superconducting Proton Linac study, Phys. Rev. Accel. Beams 20, 060401, June 2017



T. Flisgen, H.-W. Glock, A. Tsakanian, Estimation of Dielectric Losses in the Bessy VSR Warm Beam Pipe Absorbers, IPAC2018, Vancouver, BC, Canada, 2018

- Numerical methods have the advantage to be much more flexible, i.e. applicable to sophisticated geometries

- Computational Electromagnetics / Computational Electromagnetism (CEM) deals with numerical methods to solve Maxwell’s equations

Workflow for (EM) Simulations

Initial engineering problem

↓

Idealization and simplification of the problem

↓

Preparation of the (partial) differential equations describing the problem (in our case curl-curl equation)

↓

Transfer the partial differential equations to matrix-vector equations using discretization techniques (Finite Integration Technique, Finite Element Methods, etc.)

↓

Determine field solutions and derived (scalar) quantities from the matrix-vector equations

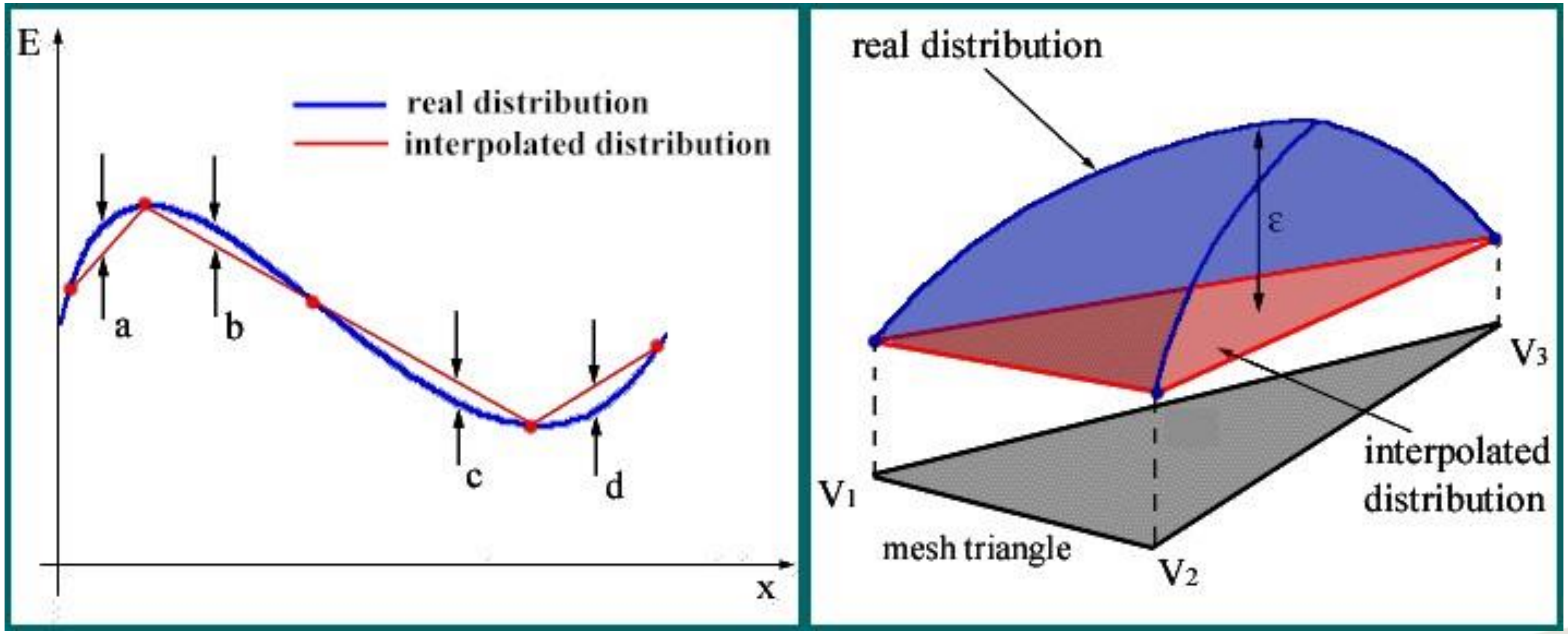
↓

Visualization, interpretation and validation (!!!) of the results

Spatial Discretization

Discretization

- Discretization is required to transfer partial differential equations into matrix-vector equations (i.e. algebraic equations)
- Modern digital computers are very powerful in handling matrix-vector multiplications



Discretization error; 1D and 2D

Image source: http://www.integra.co.jp/eng/whitepapers/inspirer/inspirer.htm

Spatial Discretization of Induction Law and Ampère's Law

- Induction law and Ampère's law

$$\mu \frac{\partial}{\partial t}\mathbf{H}(\mathbf{r},t) = -\nabla \times \mathbf{E}(\mathbf{r},t), \quad \varepsilon \frac{\partial}{\partial t}\mathbf{E}(\mathbf{r},t) = -\sigma\,\mathbf{E}(\mathbf{r},t) + \nabla \times \mathbf{H}(\mathbf{r},t) - \mathbf{J}(\mathbf{r},t)$$

can be written as a "pseudo" matrix-vector equation

$$\begin{pmatrix} \varepsilon & 0 \\ 0 & \mu \end{pmatrix} \frac{\partial}{\partial t} \begin{pmatrix} \mathbf{E}(\mathbf{r},t) \\ \mathbf{H}(\mathbf{r},t) \end{pmatrix} = \begin{pmatrix} -\sigma & \nabla\times \\ -\nabla\times & 0 \end{pmatrix} \begin{pmatrix} \mathbf{E}(\mathbf{r},t) \\ \mathbf{H}(\mathbf{r},t) \end{pmatrix} + \begin{pmatrix} -1 \\ 0 \end{pmatrix} \mathbf{J}(\mathbf{r},t)$$

- Spatial discretization allows for transferring this equation into a matrix-vector equation, where spatial derivatives vanished (time derivative still present)

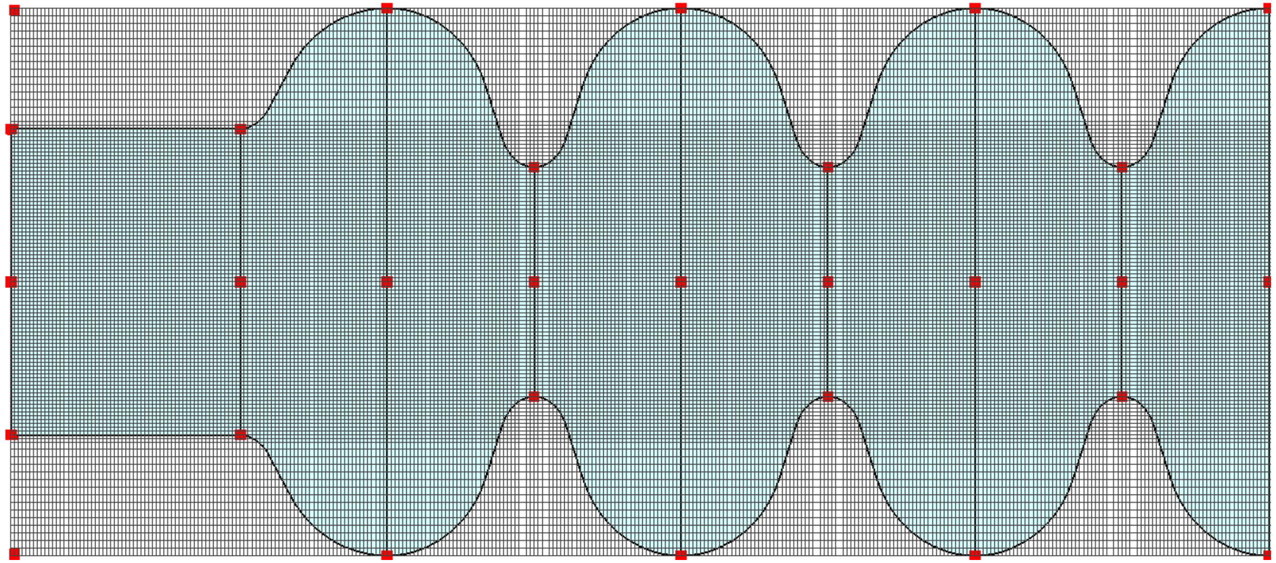
$$\mathbf{M}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathbf{A}\,\mathbf{x}(t) + \mathbf{B}\,\mathbf{i}(t)$$

- Matrices **M**, **A** result from discretization, vector **x**(t) contains discrete field distribution (typically electric and magnetic field), and matrix **B** contains field distribution of excitation current densities, and **i**(t) excitation currents

$$\mathbf{M} \in \mathbb{R}^{N\times N},\ \mathbf{x}(t) \in \mathbb{R}^{N},\ \mathbf{A} \in \mathbb{R}^{N\times N},\ \mathbf{B}(t) \in \mathbb{R}^{N\times N_s},\ \mathbf{i}(t) \in \mathbb{R}^{N_s},\ N = 10^3, \ldots, 10^8, \ldots$$

Spatial Discretization with the Finite Integration Technique (FIT)

Definition Primary Grid



- Points $P\,(i,j,k)$

- Elementary lines (edges):

$\Delta\, u(i) = \overline{u(i)\, u(i+1)}$ with $1 \le i \le I-1$

$\Delta\, v(j) = \overline{v(j)\, v(j+1)}$ with $1 \le j \le J-1$

$\Delta\, w(k) = \overline{w(k)\, w(k+1)}$ with $1 \le k \le K-1$

- Elementary areas (facets):

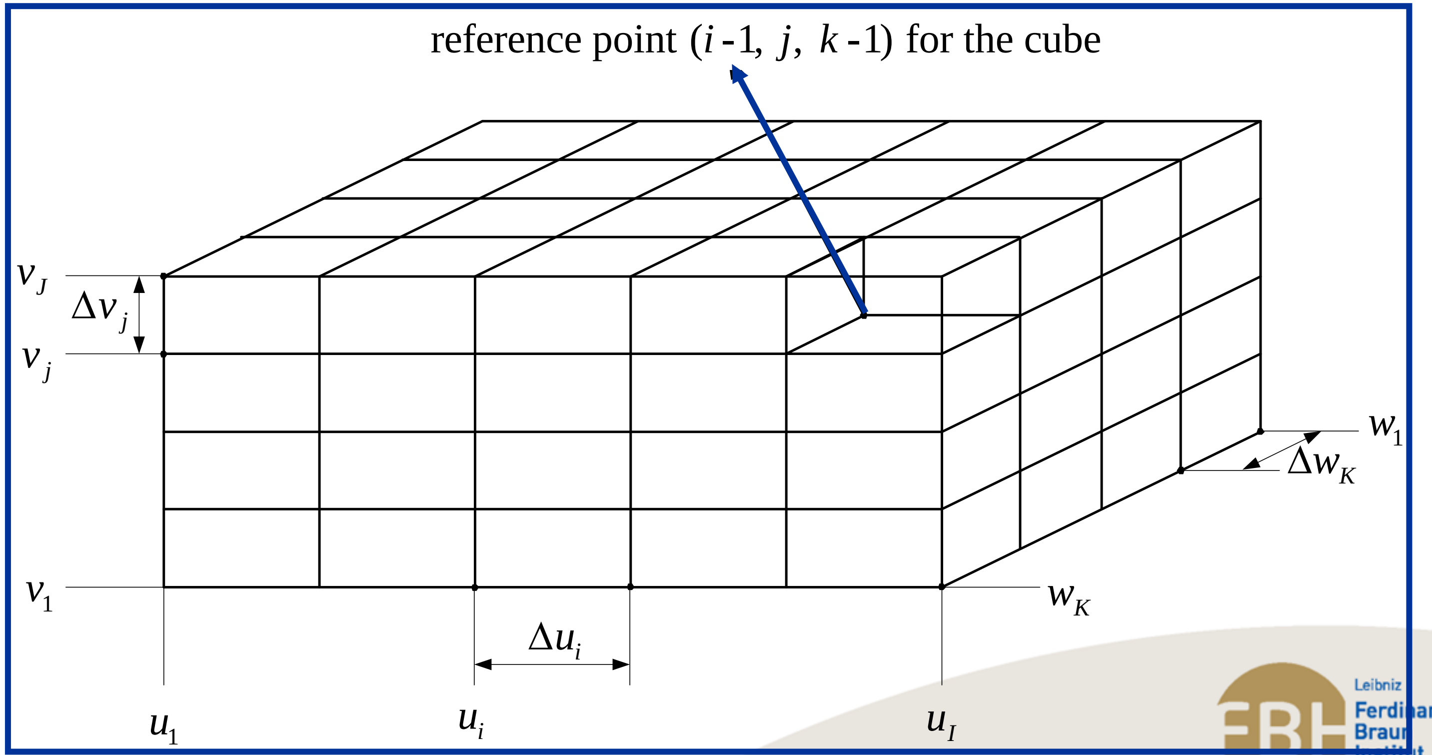
$A_u\,(j,k) = \Delta v(j)\, \Delta w(k)$ with $1 \le j \le J-1,$
$1 \le k \le K-1$

$A_v\,(i,k), A_w\,(i,j)$ analogously

- Elementary volume (cells):

$V\,(i,j,k) = \Delta\, u(i)\, \Delta v(j)\, \Delta w(k)$ with $1 \le i \le I-1,$
$1 \le j \le J-1,$
$1 \le k \le K-1,$

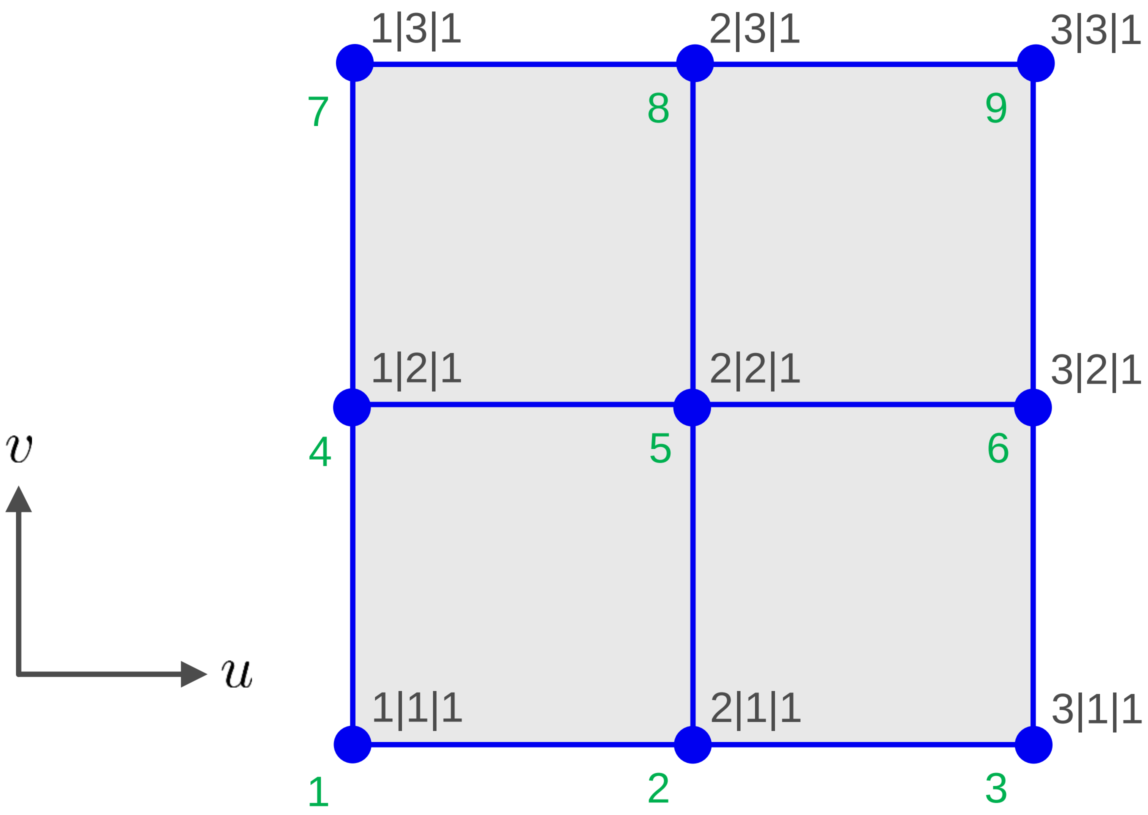
- $N_p = IJK$

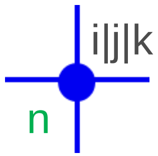


Slide courtesy of U. van Rienen / University of Rostock

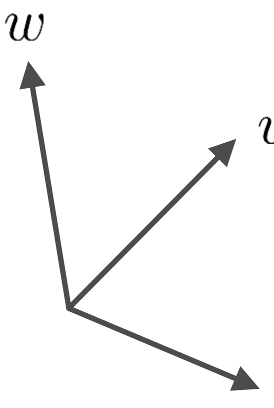
Lexicographic Index or Super Index

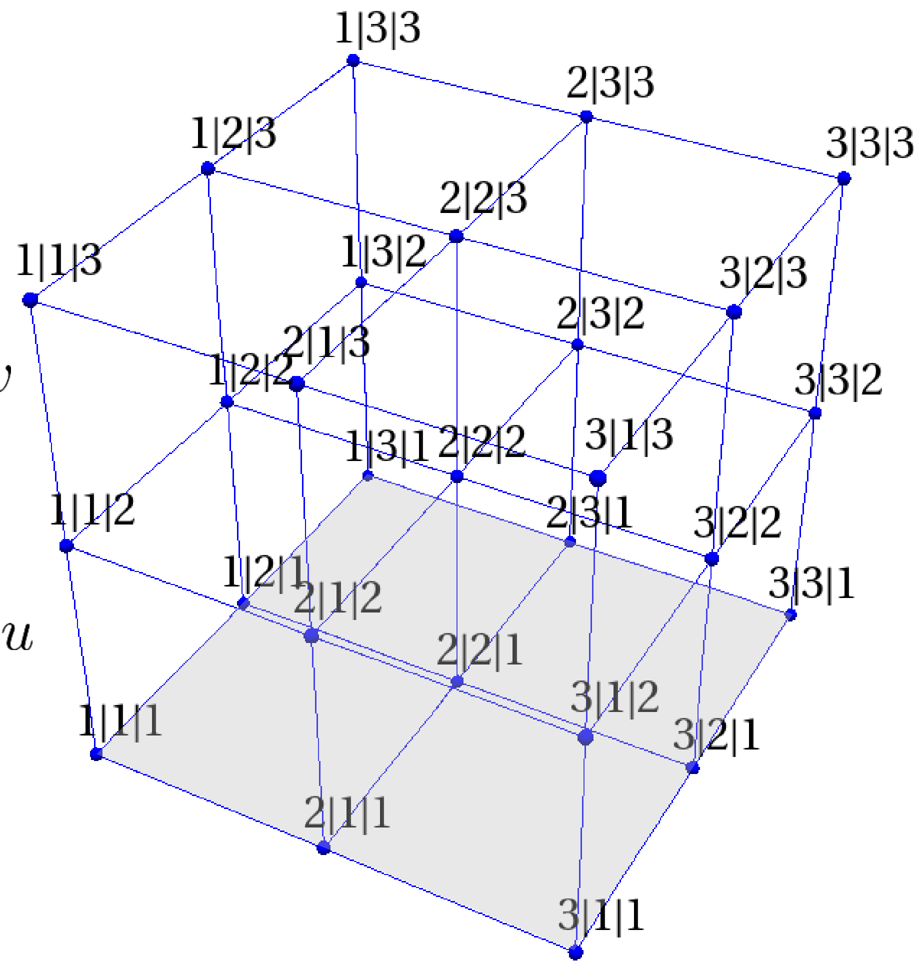
- Required to systematically sort field quantities allocated in 3D space and indexed by i|j||k in one vector with super index n





Example Grid with I = J = K = 3





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Lexicographic Index or Super Index

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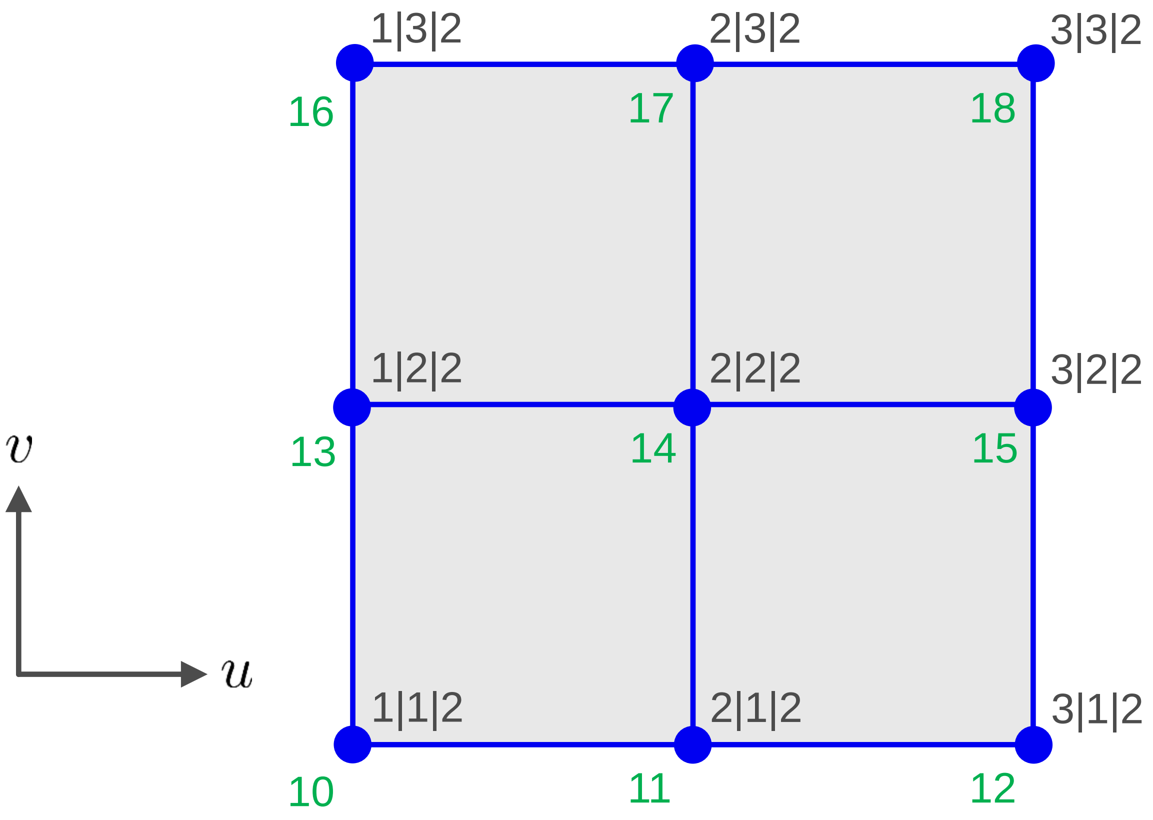

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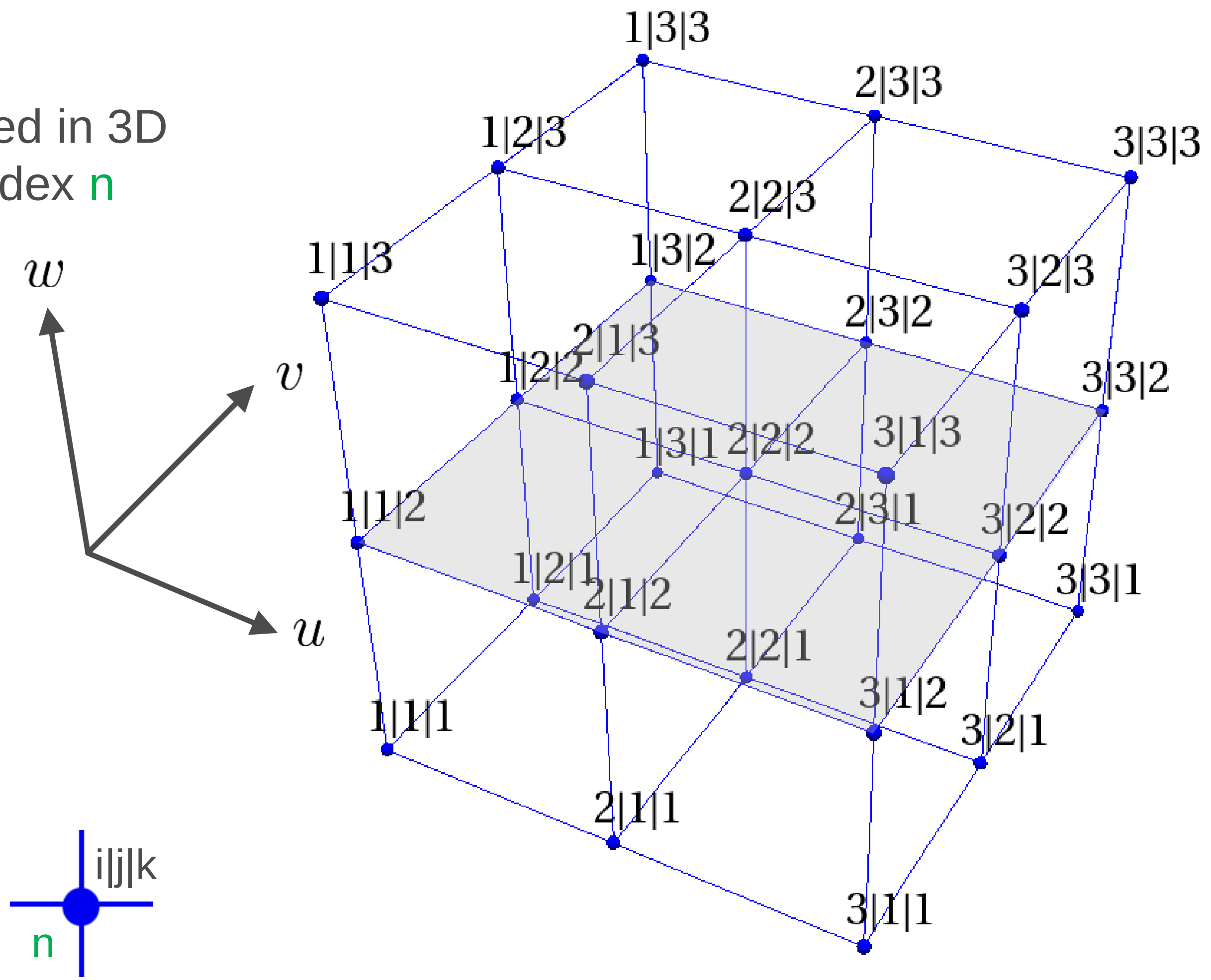

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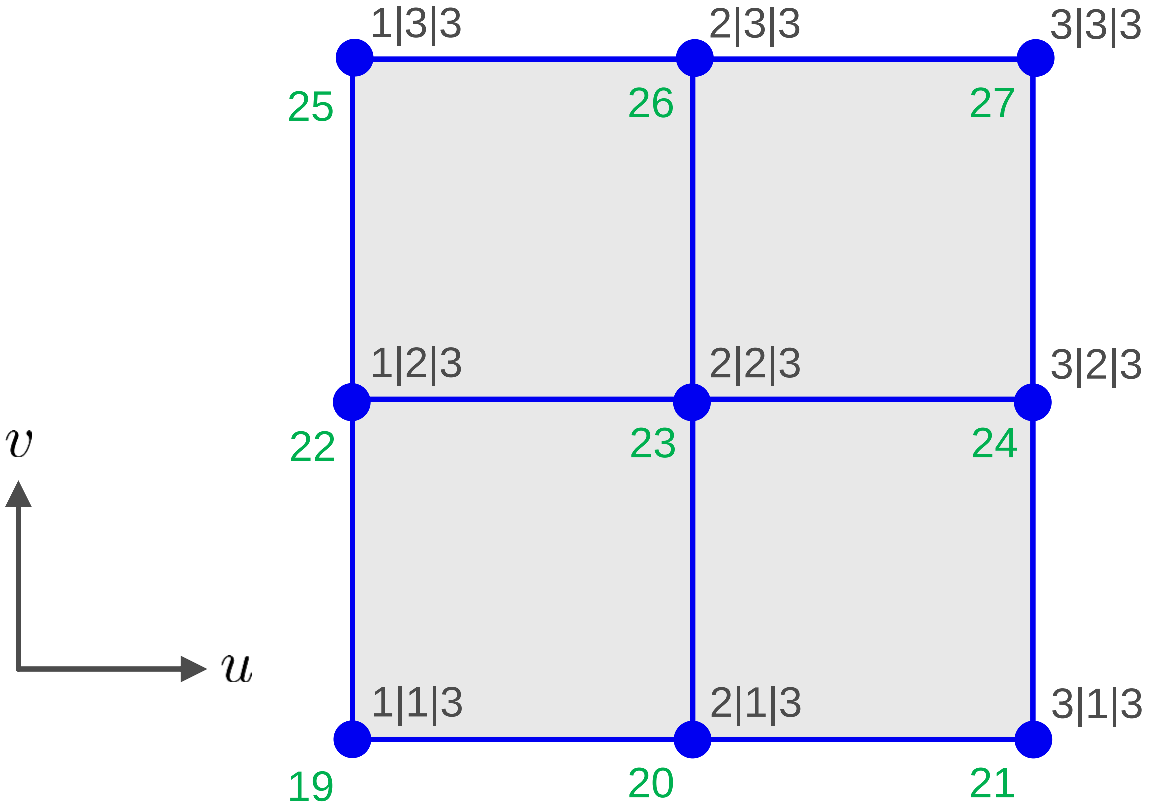

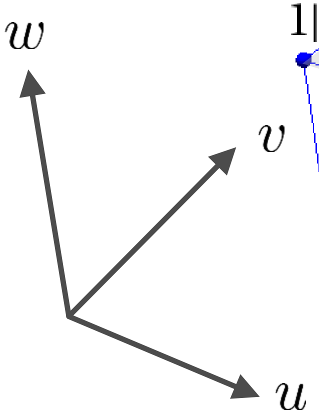

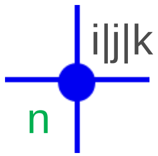

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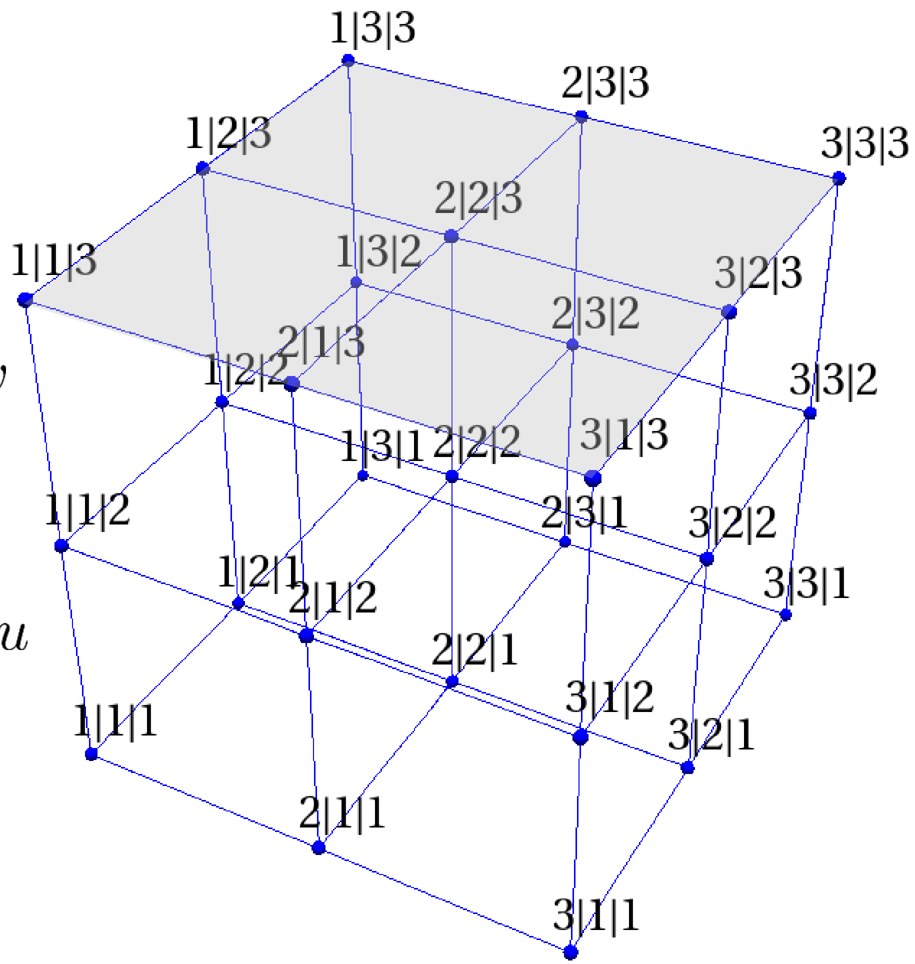

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Lexicographic Index or Super Index

- Required to systematically sort field quantities allocated in 3D space and indexed by i|j||k in one vector with super index n

- Relationship triple index and super index:

$$n = 1 + (i-1)M_u + (j-1)M_v + (k-1)M_w$$

- The constants are given by

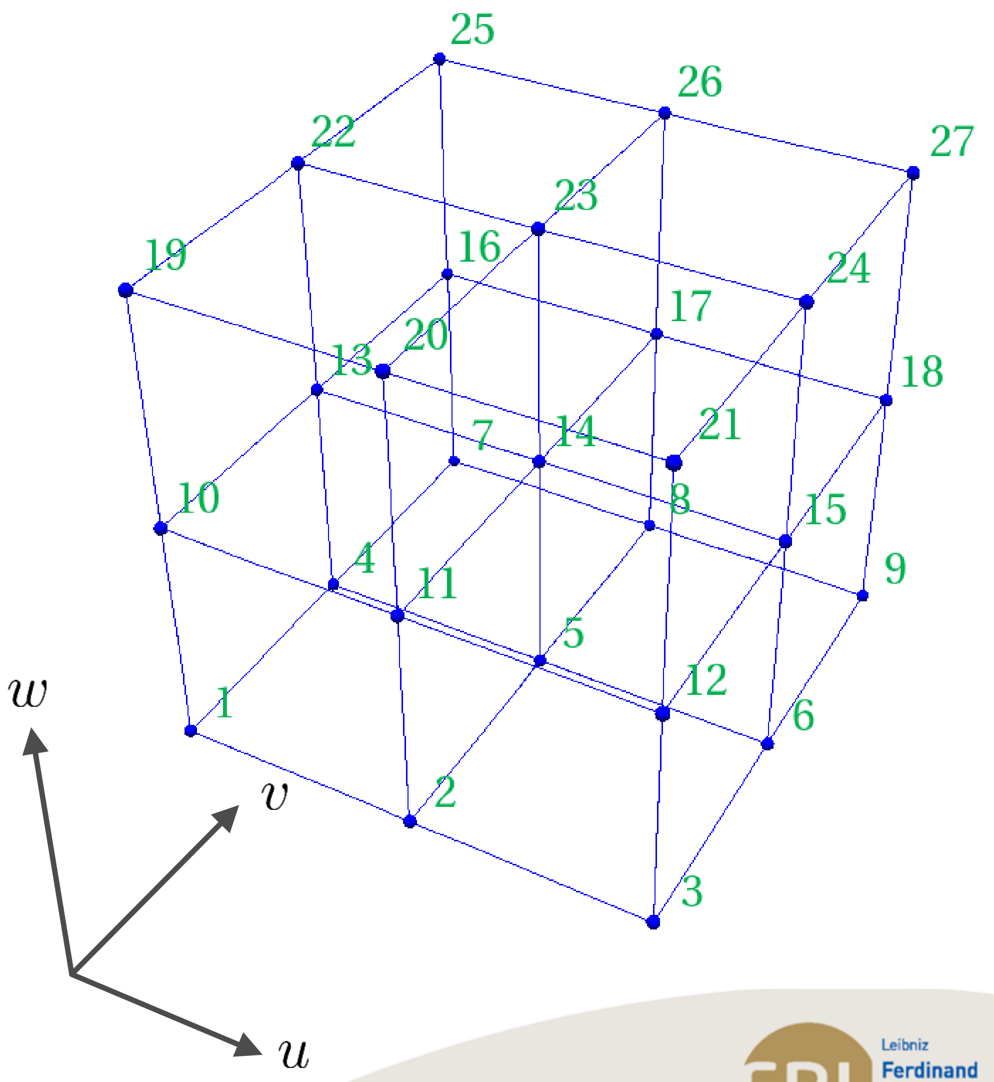
$$M_u = 1, \quad M_v = I, \quad M_w = IJ$$

and specify what to add to super index when moving in a respective direction in the grid

- For our example:

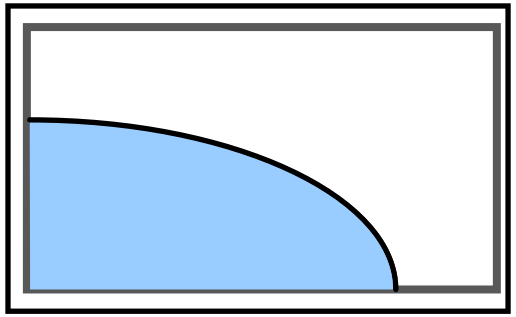
$$M_u = 1, \quad M_v = 3, \quad M_w = 9$$

Example Grid with I = J = K = 3

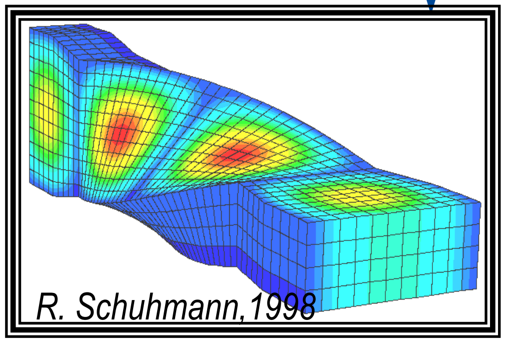


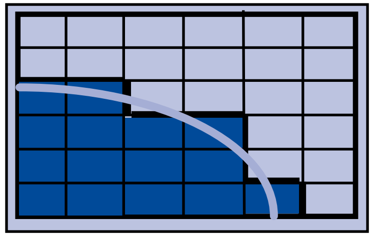
Boundary Discretization

Modelling Curved Boundaries

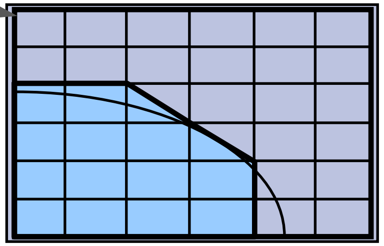


FIT on
non-orthogonal
grids

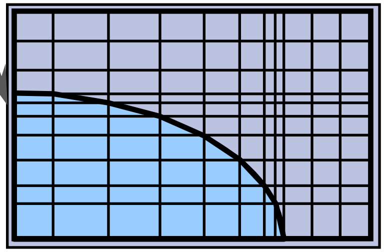




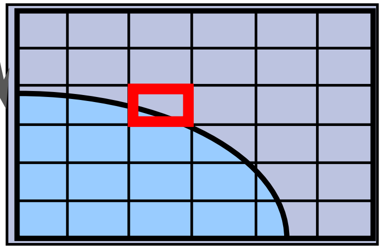
FIT with staircase
[Finite-difference time-domain (FDTD),
Finite-difference frequency-domain (FDFD)]
(standard): poor convergence



FIT with diagonal filling:
better convergence
Weiland 1977



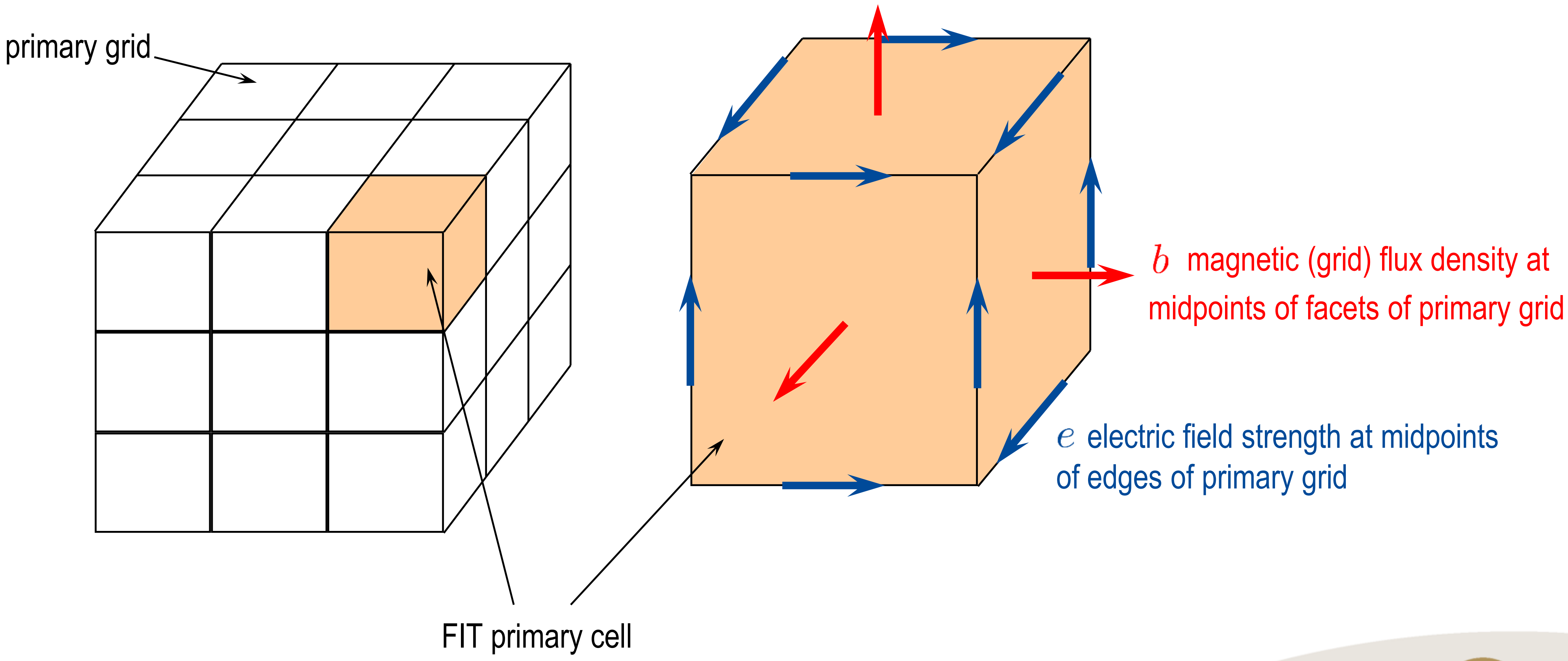
FIT with
non-equidistant step size



Conformal FIT / “Perfect Boundary Approximation” (PBA)®:
Krietenstein, Schuhmann, Thoma, Weiland 1998

Slide courtesy of U. van Rienen / University of Rostock

Quantities on Primary Grid



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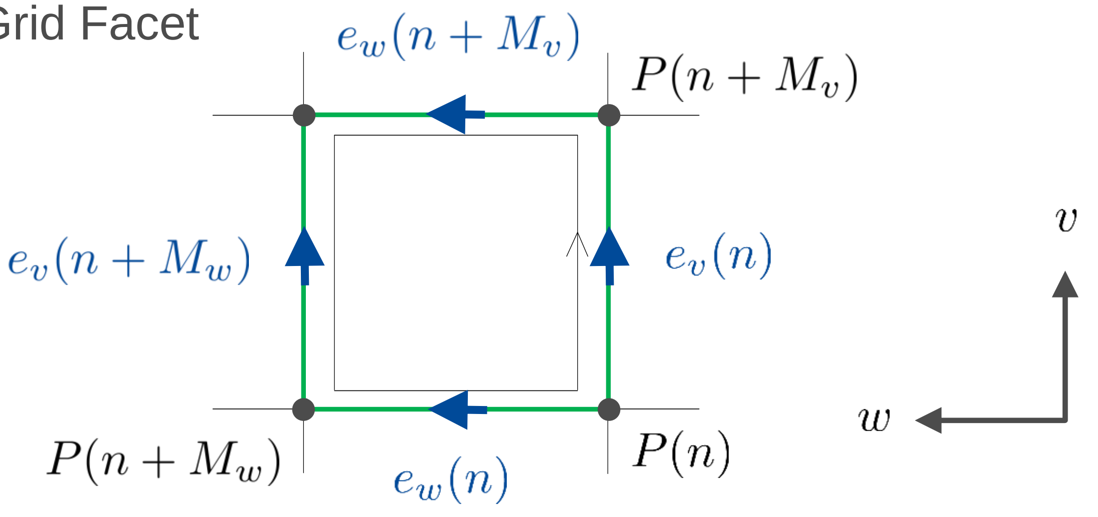
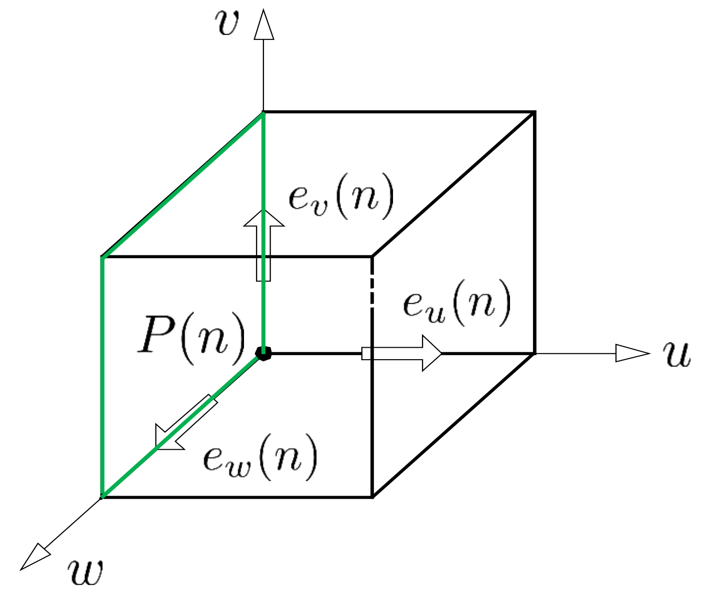
FIT Discretization of Induction Law (lhs)

Primary Grid Facet



Primary Grid Cell

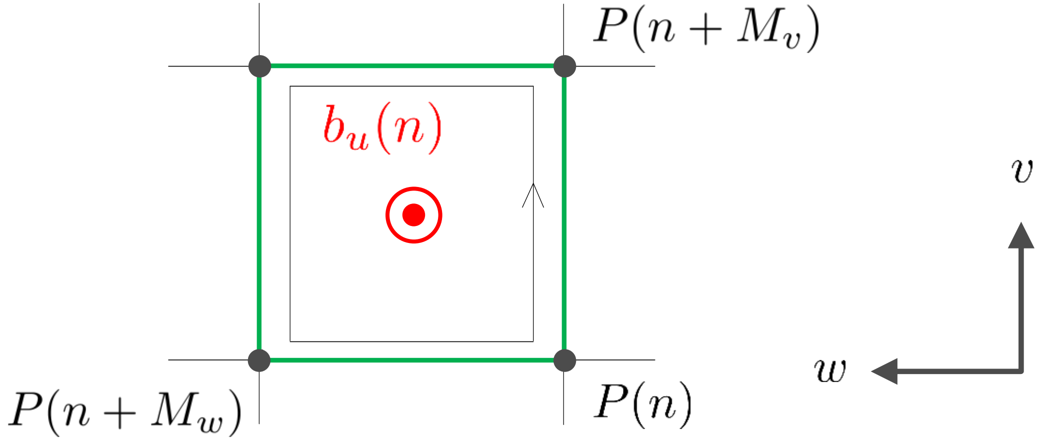


$$\oint_{\partial A_u(n)} \mathbf{E}(\mathbf{r},t)\cdot \mathrm{ds} \approx \Delta v(n) e_v(n) + \Delta w(n+M_v) e_w(n+M_v) - \Delta v(n+M_w) e_v(n+M_w) - \Delta w(n) e_w(n)$$

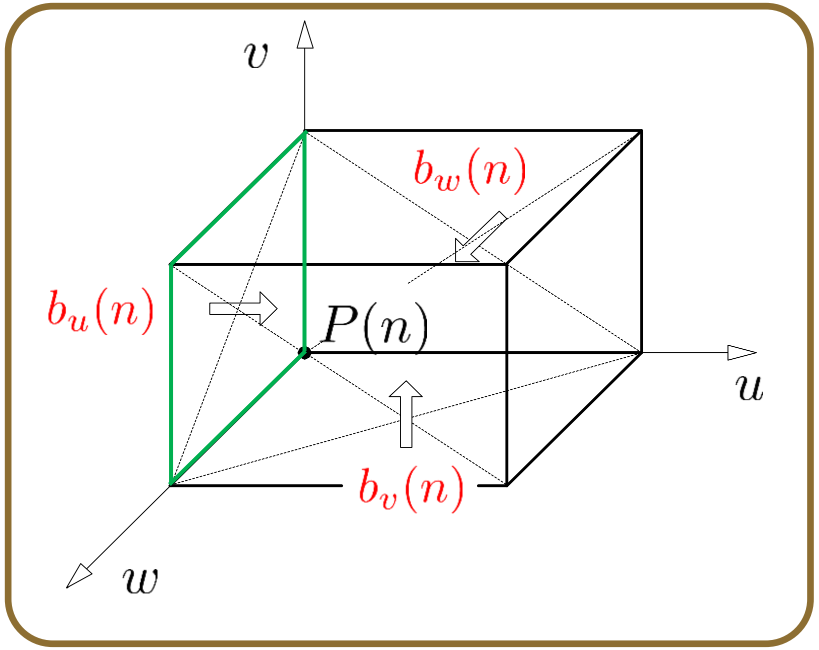
Slide closely following U. van Rienen / University of Rostock

FIT Discretization of Induction Law (rhs)

Primary Grid Facet



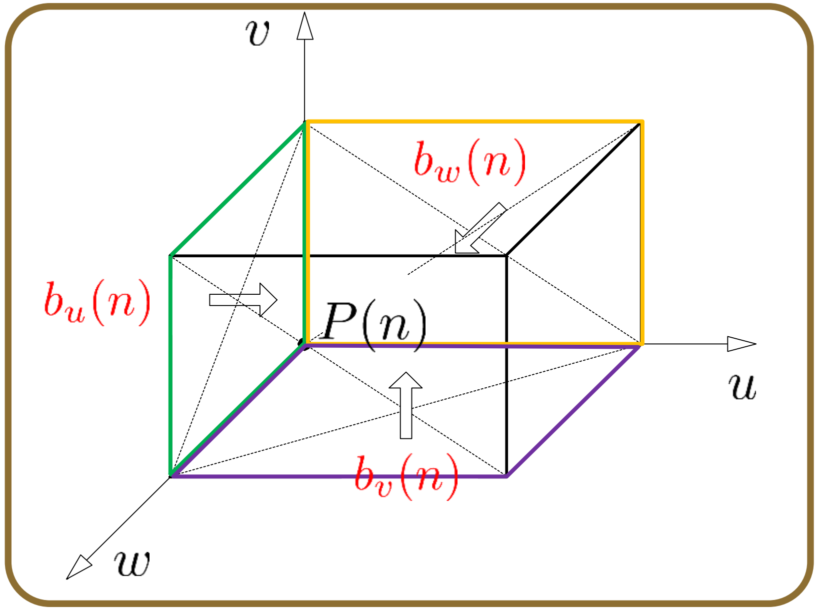
Primary Grid Cell



$$-\iint_{A_u(n)} \frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)\cdot \mathrm{d}\mathbf{A} \approx -A_u(n)\frac{\mathrm{d}}{\mathrm{d}t}b_u(n)$$

FIT Discretization of Induction Law for all Facets of Node n

Primary Grid Cell



$$\Delta v(n)e_v(n) + \Delta w(n+M_v)e_w(n+M_v) - \Delta v(n+M_w)e_v(n+M_w) - \Delta w(n)e_w(n) = -A_u(n)\frac{\mathrm{d}}{\mathrm{d}t}b_u(n)$$

$$-\Delta u(n)e_u(n) + \Delta u(n+M_w)e_u(n+M_w) + \Delta w(n)e_w(n) - \Delta w(n+M_u)e_w(n+M_u) = -A_v(n)\frac{\mathrm{d}}{\mathrm{d}t}b_v(n)$$

$$\Delta u(n)e_u(n) - \Delta u(n+M_v)e_u(n+M_v) - \Delta v(n)e_v(n) + \Delta v(n+M_u)e_v(n+M_u) = -A_w(n)\frac{\mathrm{d}}{\mathrm{d}t}b_w(n)$$

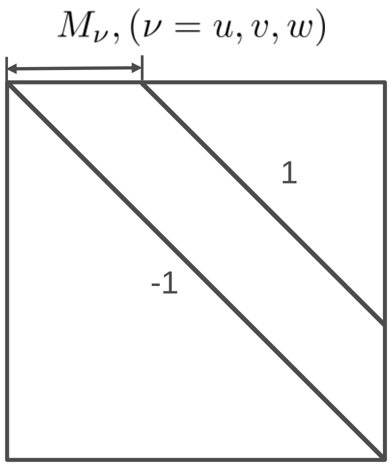
Collating Induction Law for all Facets and all Nodes → Discrete Induction Law

$$\mathbf{C}\mathbf{D}_s\mathbf{e} = -\mathbf{D}_A \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{b}$$

$$\begin{pmatrix} e_u(1) \\ \vdots \\ e_u(N_p) \\ e_v(1) \\ \vdots \\ e_v(N_p) \\ e_w(1) \\ \vdots \\ e_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

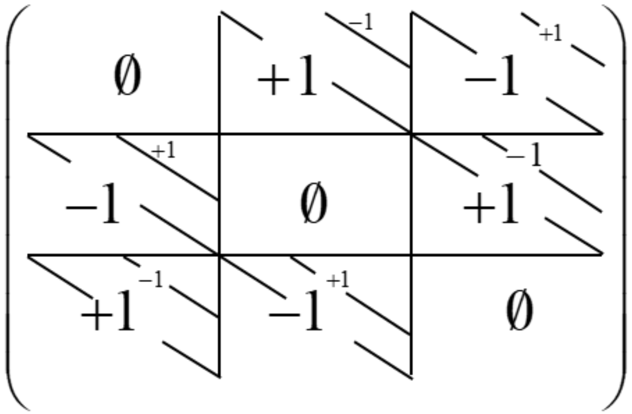
$$\begin{pmatrix} b_u(1) \\ \vdots \\ b_u(N_p) \\ b_v(1) \\ \vdots \\ b_v(N_p) \\ b_w(1) \\ \vdots \\ b_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

Collating Induction Law for all Facets and all Nodes → Discrete Induction Law



$$\mathbf{D}_A = \operatorname{diag}\left[A_u(1), \ldots, A_u(N_p), A_v(1), \ldots, A_v(N_p), A_w(1), \ldots, A_w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

$$\mathbf{C}\mathbf{D}_s\mathbf{e} = -\mathbf{D}_A \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{b}$$

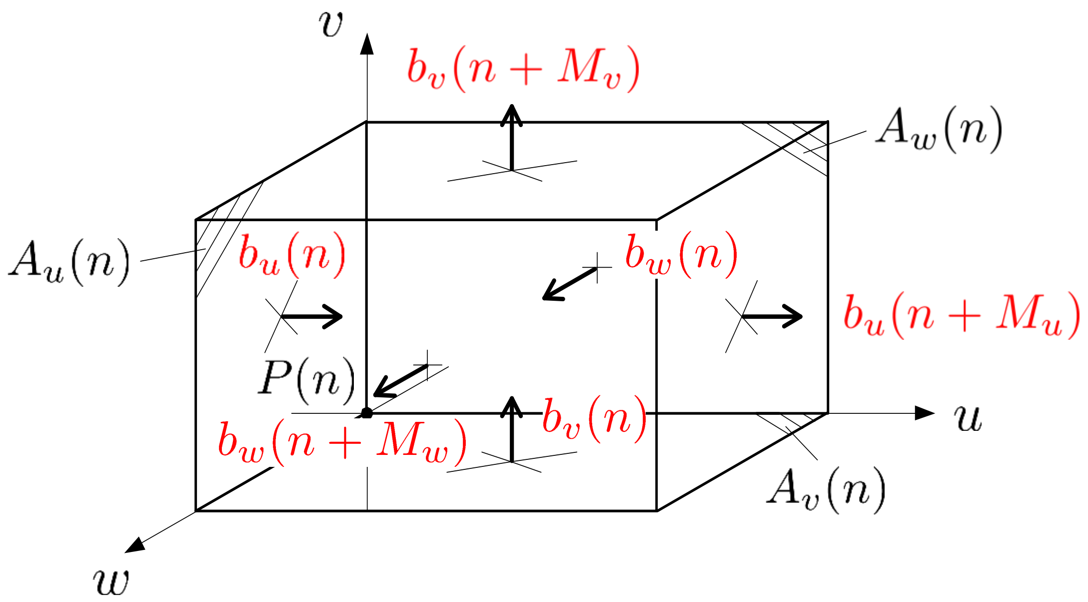


$\in \mathbb{R}^{3N_p \times 3N_p}$

$$\mathbf{D}_s = \operatorname{diag}\left[\Delta u(1), \ldots, \Delta u(N_p), \Delta v(1), \ldots, \Delta v(N_p), \Delta w(1), \ldots, \Delta w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

FIT Discretization of Gauss‘ Law for Magnetism

Primary Grid Cell



$$\oiint_{\partial V(n)} \mathbf{B}(\mathbf{r},t)\cdot \mathrm{d}\mathbf{A} \approx -A_u(n)b_u(n) + A_u(n+M_u)b_u(n+M_u) - A_v(n)b_v(n) + A_v(n+M_v)b_v(n+M_v)$$

$$-A_w(n)b_w(n) + A_w(n+M_w)b_w(n+M_w) = 0$$

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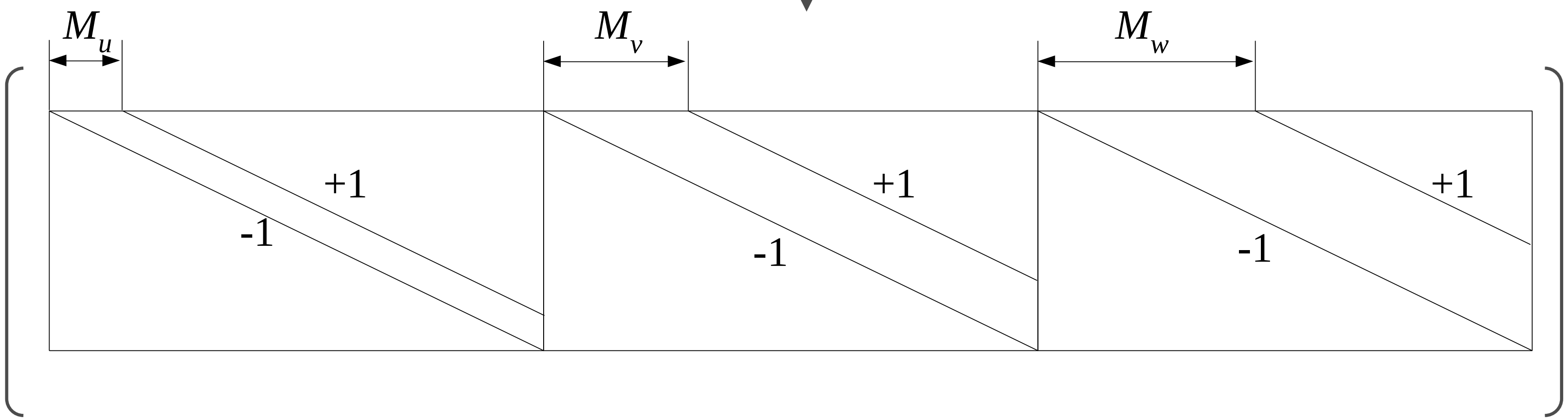
Collating Gauss' Law for all Volumes of Primary Grid → Discrete Gauss' Law

$$\mathbf{D}_A = \mathrm{diag}\left[A_u(1), \ldots, A_u(N_p), A_v(1), \ldots, A_v(N_p), A_w(1), \ldots, A_w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

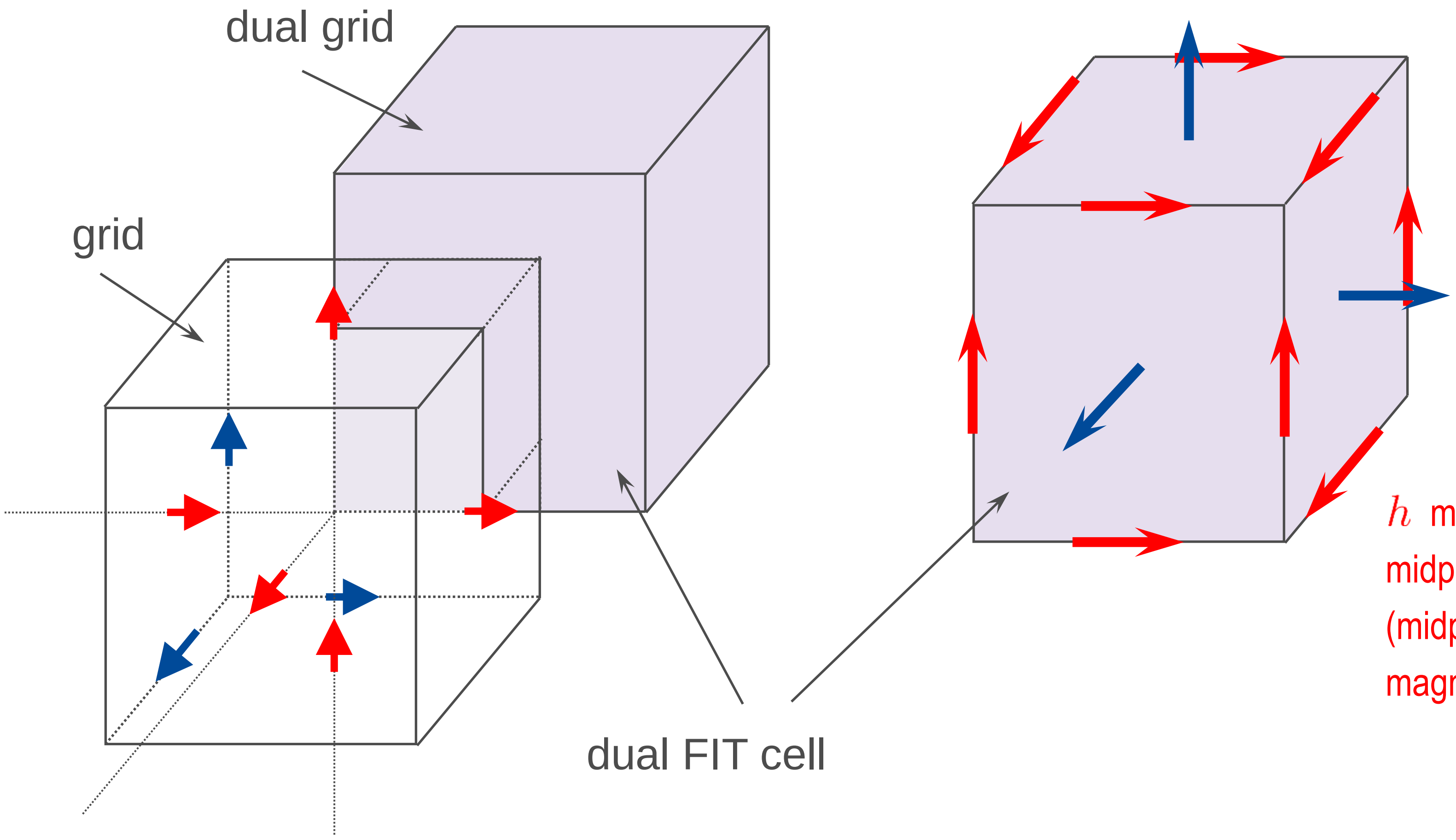
$$\mathbf{S}\mathbf{D}_A\mathbf{b} = \mathbf{0}$$



$\in \mathbb{R}^{N_p \times 3N_p}$

$$\begin{pmatrix} b_u(1) \\ \vdots \\ b_u(N_p) \\ b_v(1) \\ \vdots \\ b_v(N_p) \\ b_w(1) \\ \vdots \\ b_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

Quantities on Dual Grid



d electric displacement field at midpoints of facets of dual grid (midpoints of edges of primary grid, where electric field strengths e were defined)

h magnetic field strength at midpoints of edges of dual grid (midpoints of facets of primary grid, where magnetic flux densities b were defined)

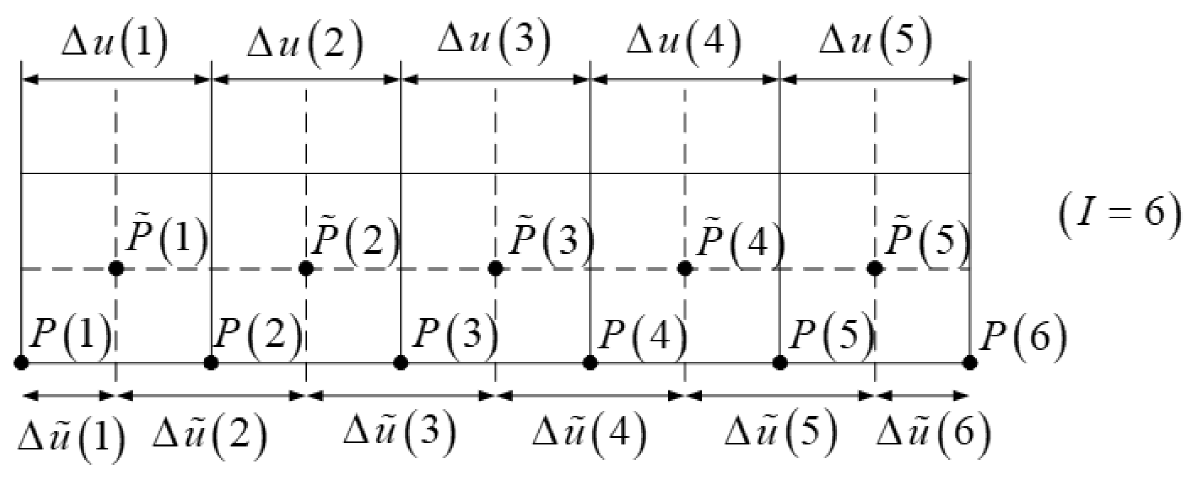
Slide courtesy of U. van Rienen / University of Rostock

Dual Grid Nodes

$$\tilde{G} = \left\{ \left(\tilde{u}(i), \tilde{v}(j), \tilde{w}(k)\right) \in R^3 \,\middle|\, \tilde{u}(i) = \frac{1}{2}\left(u(i) + u(i+1)\right) \qquad 1 \le i \le I-1, \right.$$

$$\tilde{v}(j) = \frac{1}{2}\left(v(j) + v(j+1)\right) \qquad 1 \le j \le J-1,$$

$$\left. \tilde{w}(k) = \frac{1}{2}\left(w(k) + w(k+1)\right) \qquad 1 \le k \le K-1 \right\}$$

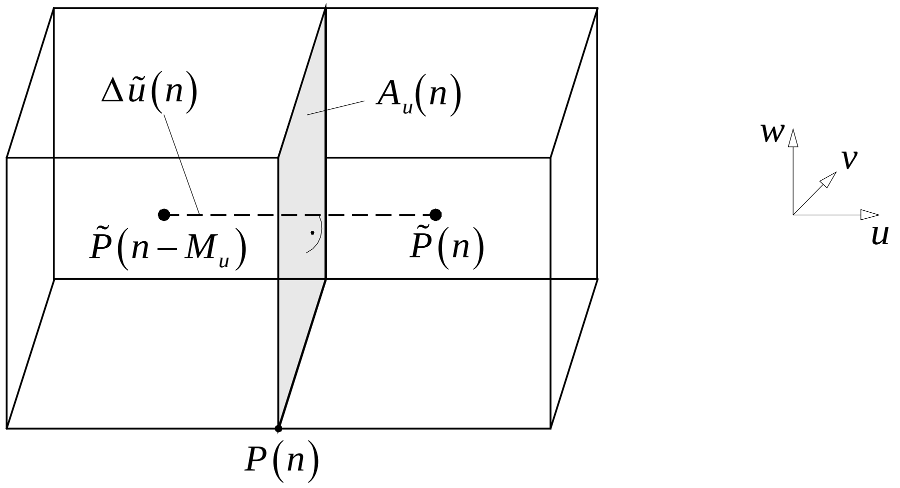


Slide courtesy of U. van Rienen / University of Rostock

Nodes, Edges, Areas and Volumes of Dual Grid

- dual points $\tilde{P}(i,\ j,k)$
- dual elementary lines:

$$\Delta\tilde{u}(i)=\overline{\tilde{u}(i-1)\,\tilde{u}(i)}\quad \text{with } 2\le i\le I-1,$$
$$\Delta\tilde{u}(1)=\Delta u(1)/2,$$
$$\Delta\tilde{u}(I)=\Delta u(I-1)/2,$$
$$\Delta\tilde{v}(j),\ \Delta\tilde{w}(k)\ \text{analogously.}$$

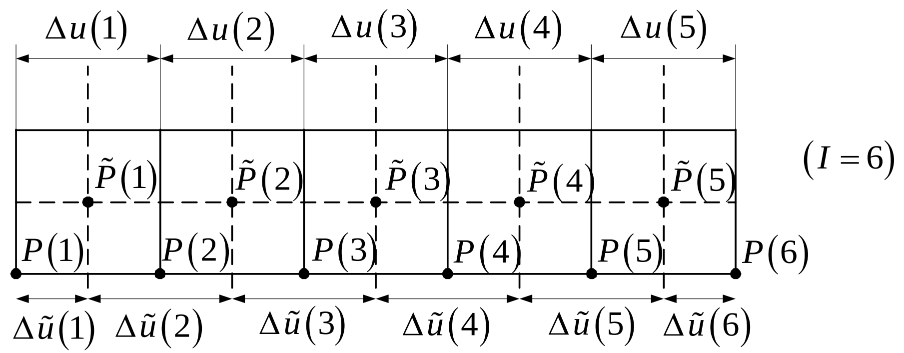


- dual elementary areas:

$$\tilde{A}_u(i,j,k)=\Delta\tilde{v}(j)\,\Delta\tilde{w}(k)\quad \text{with}\quad 1\le i\le I-1,$$
$$\tilde{A}_v(i,j,k),\ \tilde{A}_w(i,\ j,k)\ \text{analogously}$$

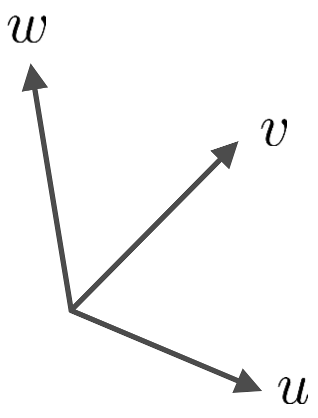
- dual elementary volumes:

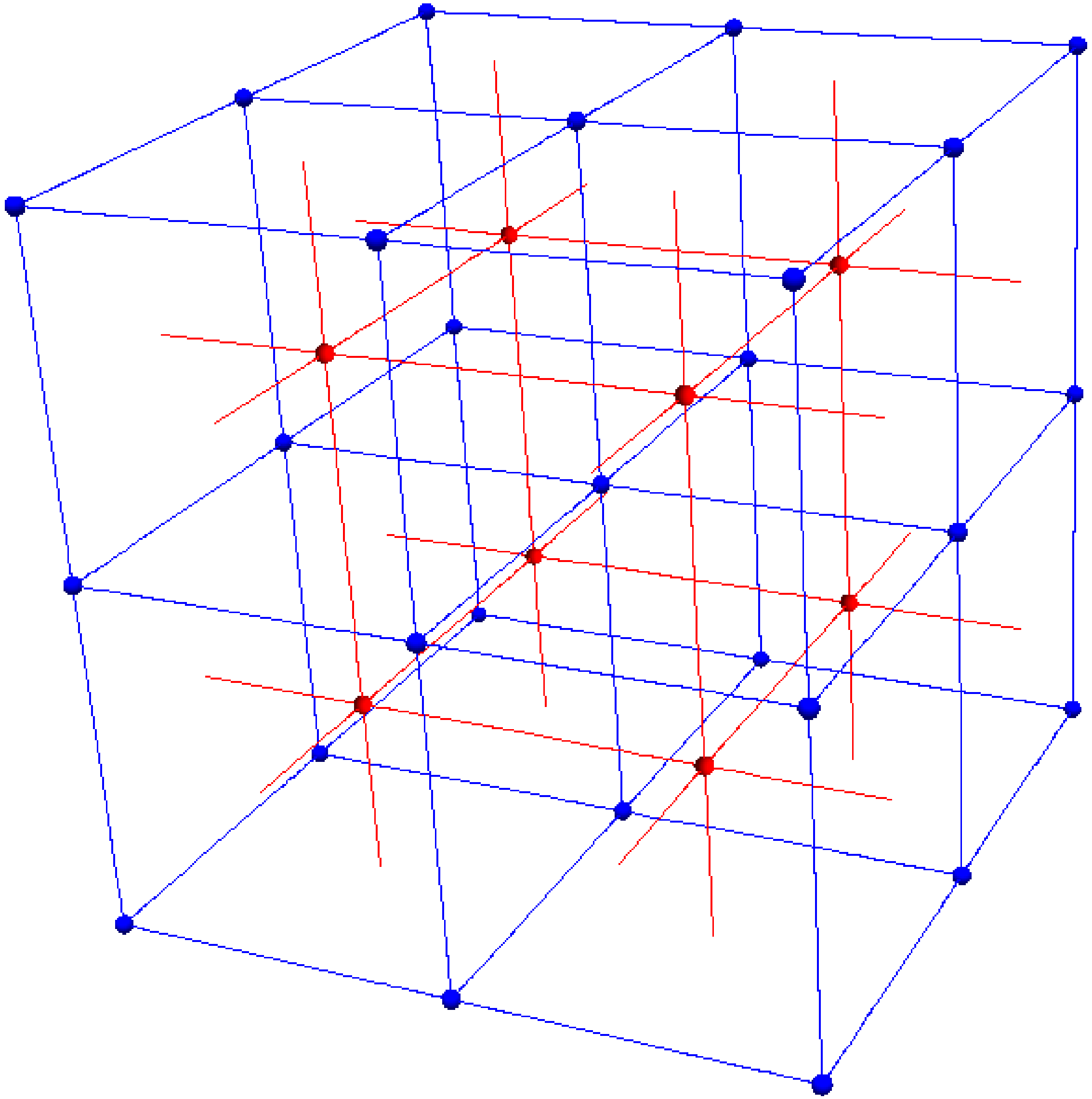
$$\tilde{V}(i,\ j,k)=\Delta\tilde{u}(i)\,\Delta\tilde{v}(j)\,\Delta\tilde{w}(k)$$



$$\text{with}\quad 1\le i\le I-1,\qquad 1\le j\le J-1,\qquad 1\le k\le K-1,$$

Primary Grid and Dual Grid for I = J = K = 3





Grid Properties

Duality:

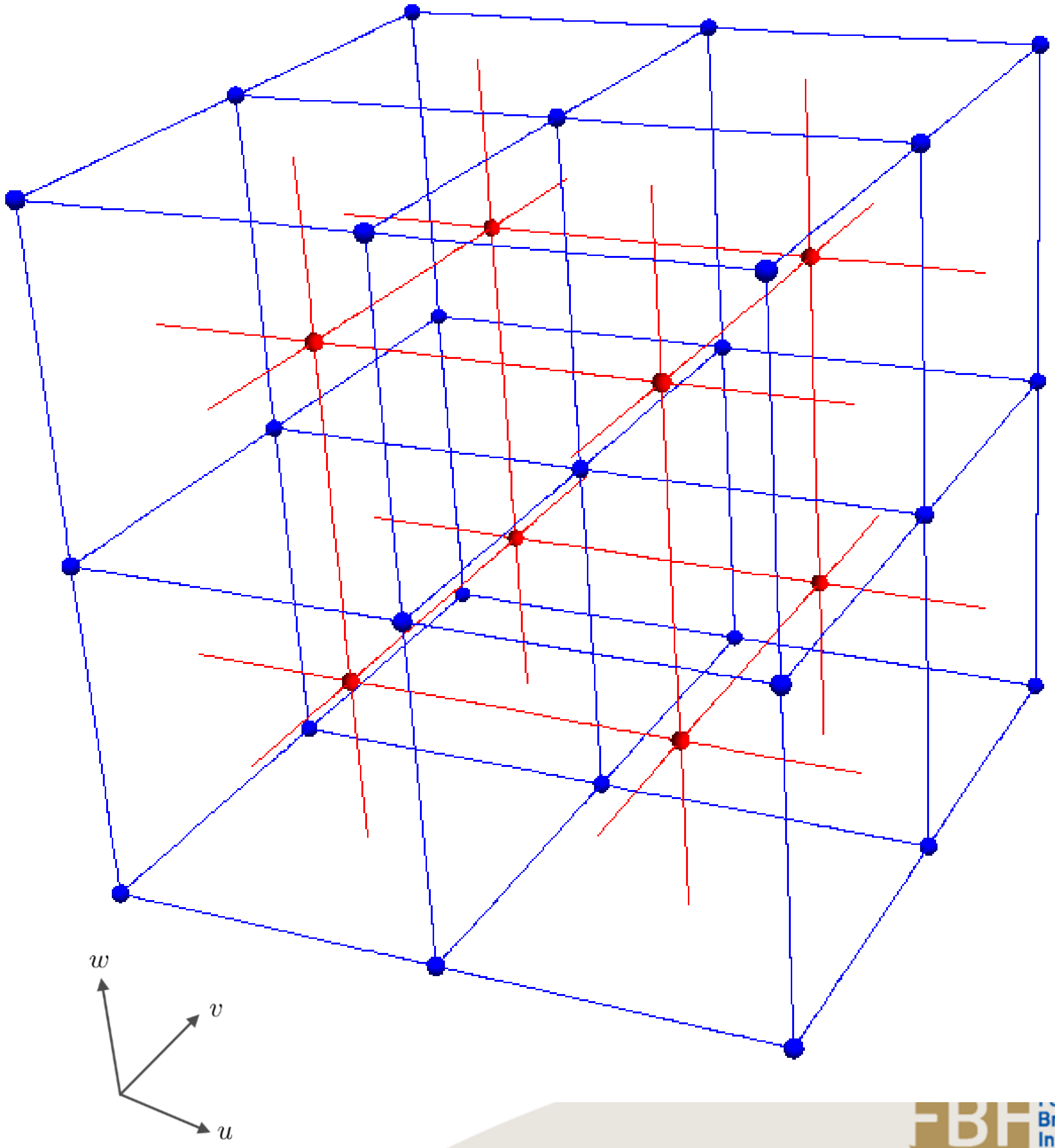
- For each facet of the primary grid there is only exactly one edge of the dual grid intersecting this area in just one point
- Each primary grid point lies inside of one dual volume and vice versa

Orthogonality:

- The primary facets and the dual edges (and vice versa) intersect with an angle of 90°

Midpoint of each facet of primary grid is also a midpoint of an edge of dual grid

Midpoint of each facet of dual grid is also a midpoint of each edge of primary grid



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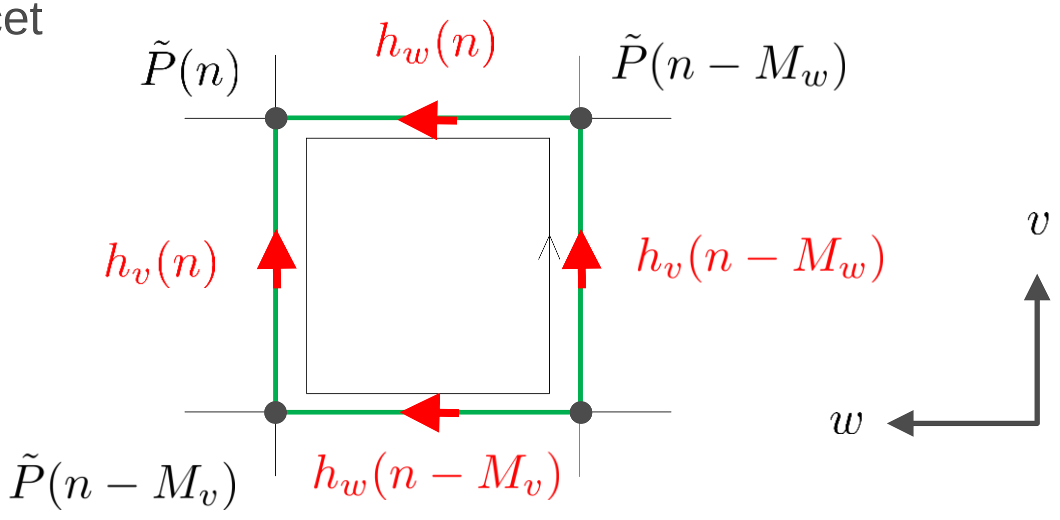
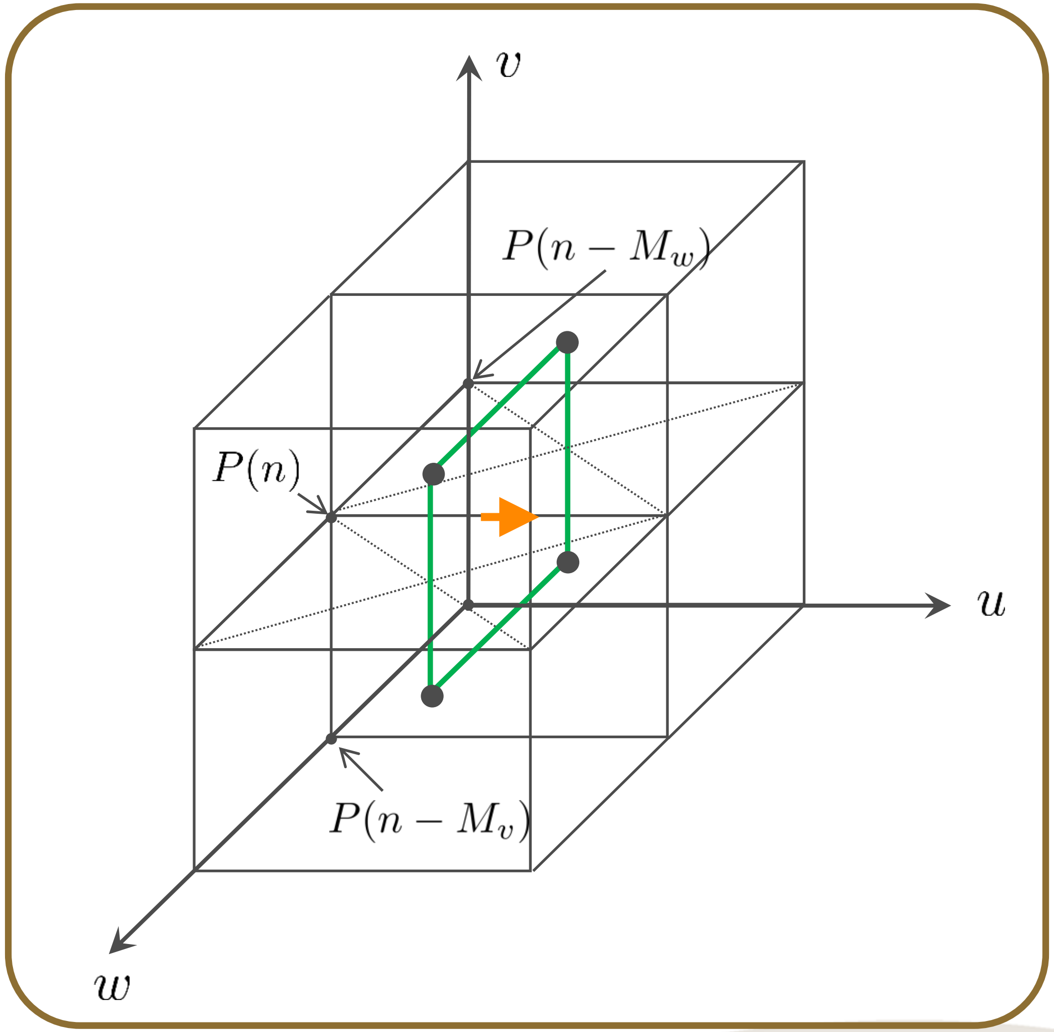
FIT Discretization of Ampère’s Law (lhs)

Dual grid facet



Primary Grid Cell



$$\oint_{\partial \tilde{A}_u(n)} \mathbf{H}(\mathbf{r},t)\cdot \mathrm{d}\mathbf{s} \approx -\Delta\tilde{v}(n)h_v(n) + \Delta\tilde{v}(n-M_w)h_v(n-M_w)$$

$$+\,\Delta\tilde{w}(n)h_w(n) - \Delta\tilde{w}(n-M_v)h_w(n-M_v)$$

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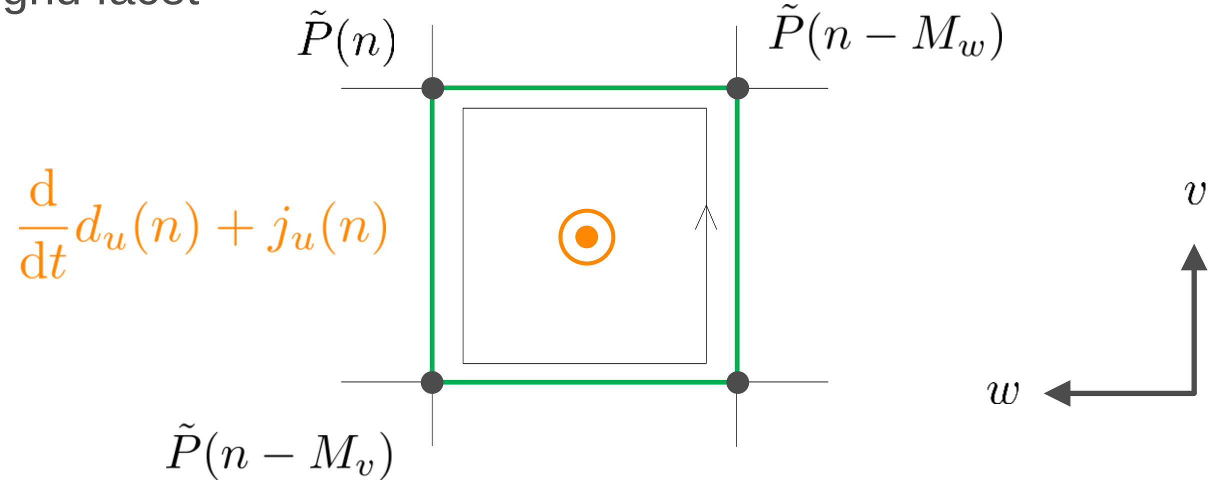
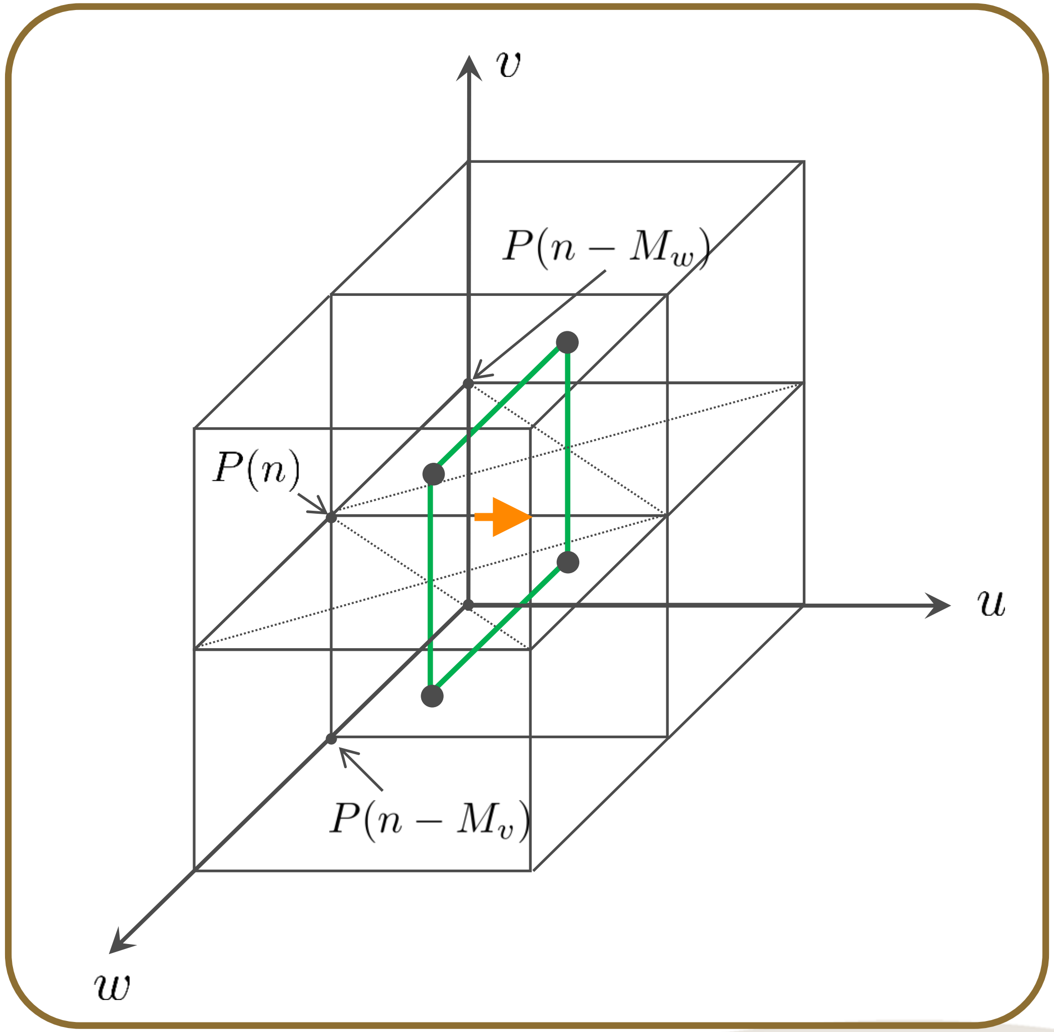
FIT Discretization of Ampère’s Law (rhs)

Dual grid facet

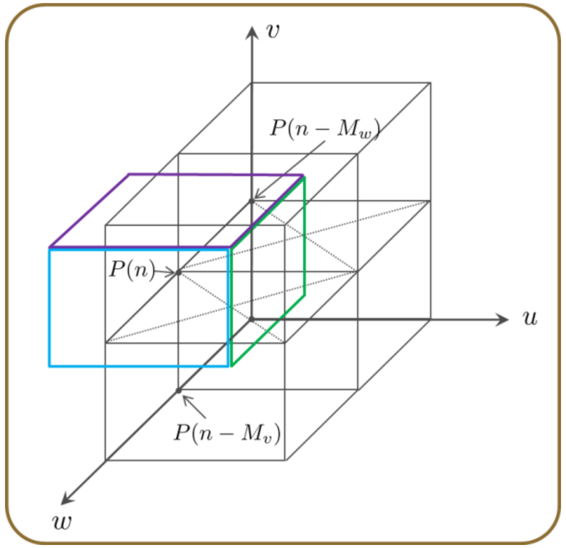


Primary Grid Cell



$$\iint_{\tilde{A}_u(n)} \left(\mathbf{J}(\mathbf{r},t)+\frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t)\right)\cdot \mathrm{d}\mathbf{A} \approx \tilde{A}_u(n)\left(\frac{\mathrm{d}}{\mathrm{d}t}d_u(n)+j_u(n)\right)$$

FIT Discretization of Ampère's Law for all Facets of Node n



$$-\Delta\tilde{v}(n)h_v(n)+\Delta\tilde{v}(n-M_w)h_v(n-M_w)+\Delta\tilde{w}(n)h_w(n)-\Delta\tilde{w}(n-M_v)h_w(n-M_v)=\tilde{A}_u(n)\left(\frac{\mathrm{d}}{\mathrm{d}t}d_u(n)+j_u(n)\right)$$

$$\Delta\tilde{u}(n)h_u(n)-\Delta\tilde{u}(n-M_w)h_u(n-M_w)-\Delta\tilde{w}(n)h_w(n)+\Delta\tilde{w}(n-M_u)h_w(n-M_u)=\tilde{A}_v(n)\left(\frac{\mathrm{d}}{\mathrm{d}t}d_v(n)+j_v(n)\right)$$

$$-\Delta\tilde{u}(n)h_u(n)+\Delta\tilde{u}(n-M_v)h_u(n-M_v)+\Delta\tilde{v}(n)h_v(n)-\Delta\tilde{v}(n-M_u)h_v(n-M_u)=\tilde{A}_w(n)\left(\frac{\mathrm{d}}{\mathrm{d}t}d_w(n)+j_w(n)\right)$$

Collating Ampère's Law for all Facets and all Nodes → Discrete Ampère's Law

$$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h} = \tilde{\mathbf{D}}_A\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{d} + \mathbf{j}\right)$$

$$\begin{pmatrix} h_u(1) \\ \vdots \\ h_u(N_p) \\ h_v(1) \\ \vdots \\ h_v(N_p) \\ h_w(1) \\ \vdots \\ h_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p} \quad \begin{pmatrix} d_u(1) \\ \vdots \\ d_u(N_p) \\ d_v(1) \\ \vdots \\ d_v(N_p) \\ d_w(1) \\ \vdots \\ d_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p} \quad \begin{pmatrix} j_u(1) \\ \vdots \\ j_u(N_p) \\ j_v(1) \\ \vdots \\ j_v(N_p) \\ j_w(1) \\ \vdots \\ j_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

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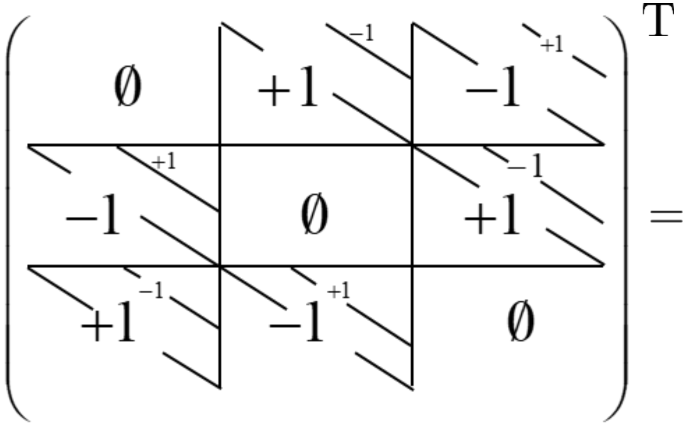
Collating Ampère's Law for all Facets and all Nodes → Discrete Ampère's Law

$$\tilde{\mathbf{D}}_A = \mathrm{diag}\left[\tilde{A}_u(1), \ldots, \tilde{A}_u(N_p), \tilde{A}_v(1), \ldots, \tilde{A}_v(N_p), \tilde{A}_w(1), \ldots, \tilde{A}_w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

$$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h} = \tilde{\mathbf{D}}_A\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{d} + \mathbf{j}\right)$$

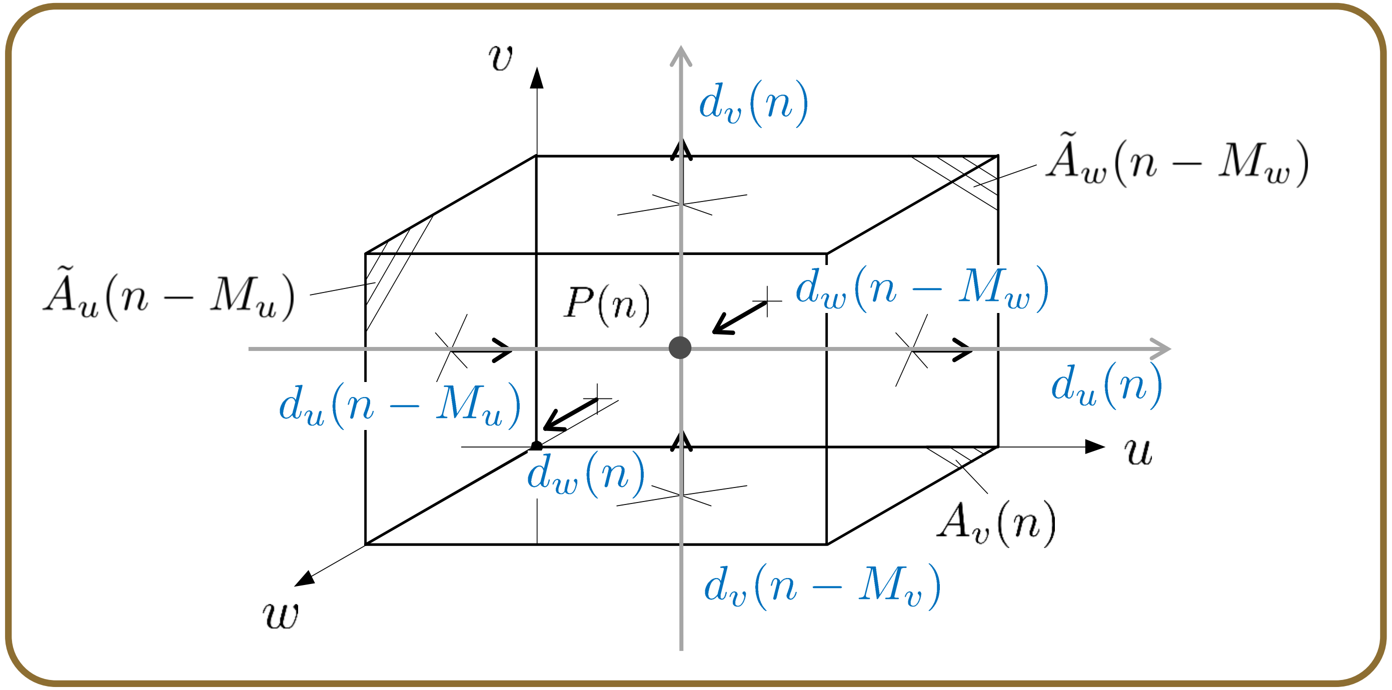


$$= \mathbf{C}^{\mathrm{T}} \in \mathbb{R}^{3N_p \times 3N_p}$$

$$\tilde{\mathbf{D}}_s = \mathrm{diag}\left[\Delta\tilde{u}(1), \ldots, \Delta\tilde{u}(N_p), \Delta\tilde{v}(1), \ldots, \Delta\tilde{v}(N_p), \Delta\tilde{w}(1), \ldots, \Delta\tilde{w}(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

FIT Discretization of Gauss' Law for Electricity (lhs)

Dual Grid Volume

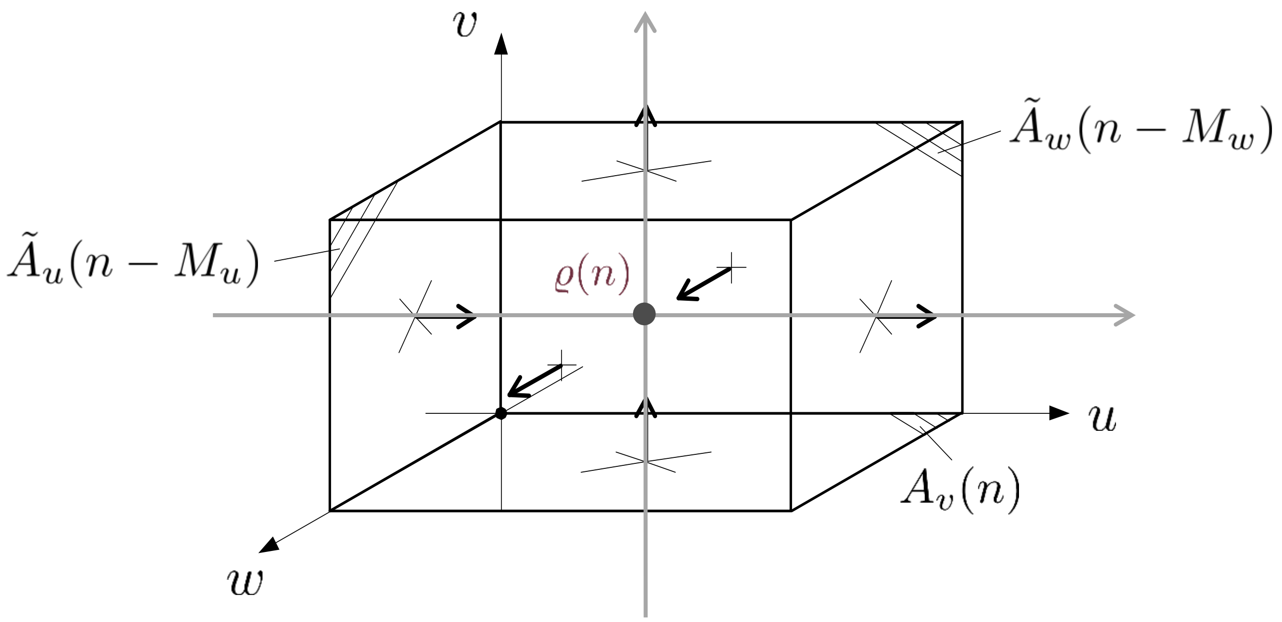


$$\oiint_{\partial\tilde{V}(n)} \mathbf{D}(\mathbf{r},t)\cdot \mathrm{d}\mathbf{A} \approx \tilde{A}_u(n)d_u(n) - \tilde{A}_u(n-M_u)d_u(n-M_u) + \tilde{A}_v(n)d_v(n) - \tilde{A}_v(n-M_v)d_v(n-M_v)$$

$$+\tilde{A}_w(n)d_w(n) - \tilde{A}_w(n-M_w)d_w(n-M_w)$$

FIT Discretization of Gauss‘ Law for Electricity (rhs)

Dual Grid Volume



$$\iiint_{\tilde{V}(n)} \rho(\mathbf{r}, t) \cdot \mathrm{d}\mathbf{A} = Q_{\tilde{V}}(n) \approx \tilde{V}(n)\varrho(n)$$

Collating Gauss‘ Law for Electricity for all Volumes → Discrete Gauss’ Law f. E.

$$\tilde{\mathbf{S}}\tilde{\mathbf{D}}_A \mathbf{d} = \tilde{\mathbf{D}}_V \varrho$$

$$\begin{pmatrix} d_u(1) \\ \vdots \\ d_u(N_p) \\ d_v(1) \\ \vdots \\ d_v(N_p) \\ d_w(1) \\ \vdots \\ d_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

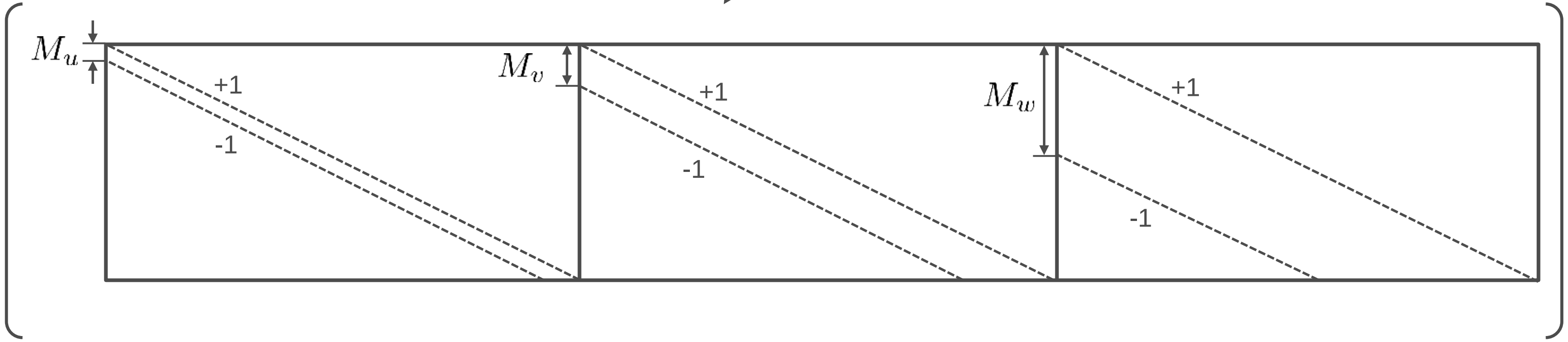
$$\begin{pmatrix} \varrho(1) \\ \vdots \\ \varrho(N_p) \end{pmatrix} \in \mathbb{R}^{N_p}$$

Collating Gauss' Law for Electricity for all Volumes → Discrete Gauss' Law f. E.

$$\tilde{\mathbf{D}}_A = \operatorname{diag}\left[\tilde{A}_u(1), \dots, \tilde{A}_u(N_p), \tilde{A}_v(1), \dots, \tilde{A}_v(N_p), \tilde{A}_w(1), \dots, \tilde{A}_w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

$$\tilde{\mathbf{S}}\tilde{\mathbf{D}}_A \mathbf{d} = \tilde{\mathbf{D}}_V \varrho$$

$$\tilde{\mathbf{D}}_V = \operatorname{diag}\left[\tilde{V}(1), \dots, \tilde{V}_u(N_p)\right] \in \mathbb{R}^{N_p \times N_p}$$

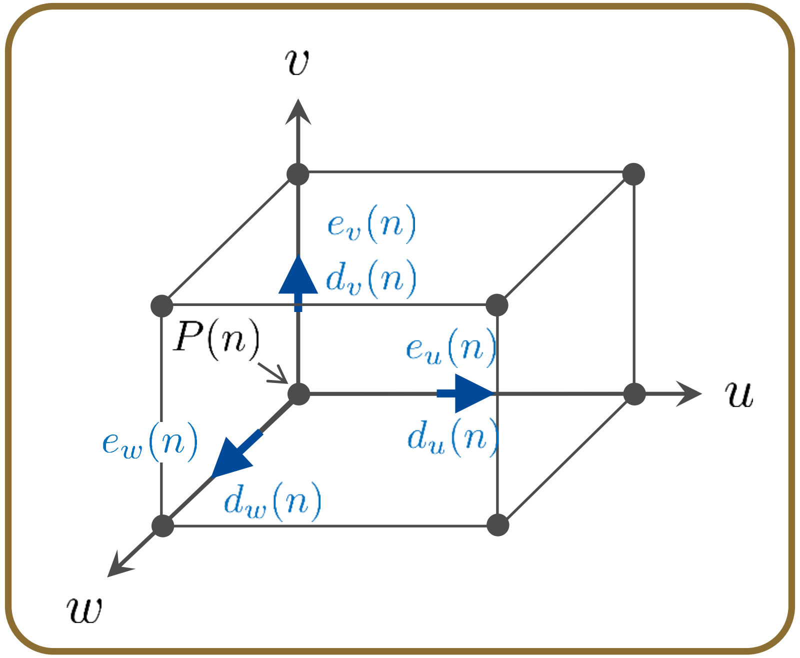


$\in \mathbb{R}^{3N_p \times N_p}$

Relationship Electric Field Strengths and Electric Flux Densities in Grid Space

$$\bar{\varepsilon}_u e_u(n) = d_u(n)$$
$$\bar{\varepsilon}_v e_v(n) = d_v(n)$$
$$\bar{\varepsilon}_w e_w(n) = d_w(n)$$

Primary Grid Cell



$$\mathbf{D}_\varepsilon = \operatorname{diag}\left[\bar{\varepsilon}_u(1), \ldots, \bar{\varepsilon}_u(N_p), \bar{\varepsilon}_v(1), \ldots, \bar{\varepsilon}_v(N_p), \bar{\varepsilon}_w(1), \ldots, \bar{\varepsilon}_w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

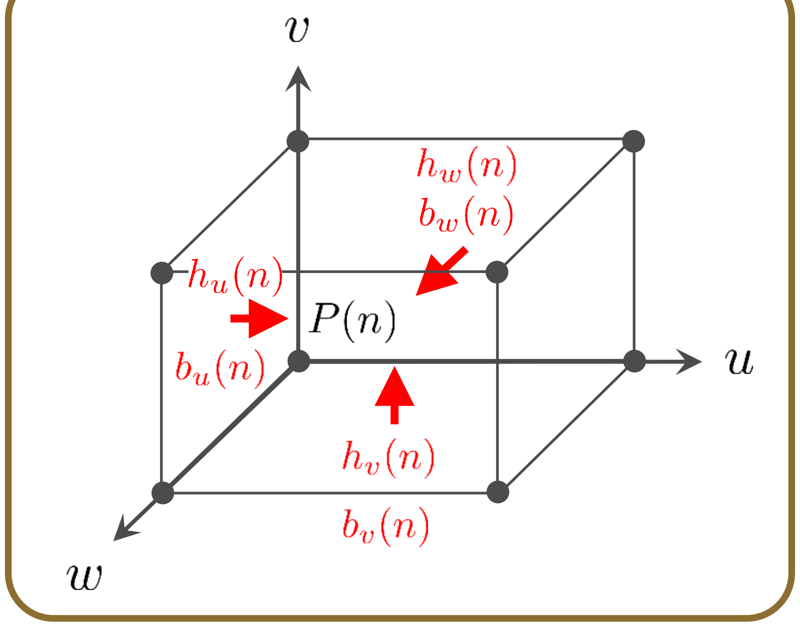
$$\mathbf{D}_\varepsilon \mathbf{e} = \mathbf{d}$$

$$\mathbf{e} = \begin{pmatrix} e_u(1) \\ \vdots \\ e_u(N_p) \\ e_v(1) \\ \vdots \\ e_v(N_p) \\ e_w(1) \\ \vdots \\ e_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p} \qquad \mathbf{d} = \begin{pmatrix} d_u(1) \\ \vdots \\ d_u(N_p) \\ d_v(1) \\ \vdots \\ d_v(N_p) \\ d_w(1) \\ \vdots \\ d_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

Relationship Magnetic Field Strengths and Magnetic Flux Densities in Grid Space

$$\bar{\mu}_u h_u(n) = b_u(n)$$
$$\bar{\mu}_v h_v(n) = b_v(n)$$
$$\bar{\mu}_w h_w(n) = b_w(n)$$

Primary Grid Cell



$$\mathbf{D}_\mu = \mathrm{diag}\left[\bar{\mu}_u(1), \ldots, \bar{\mu}_u(N_p), \bar{\mu}_v(1), \ldots, \bar{\mu}_v(N_p), \bar{\mu}_w(1), \ldots, \bar{\mu}_w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

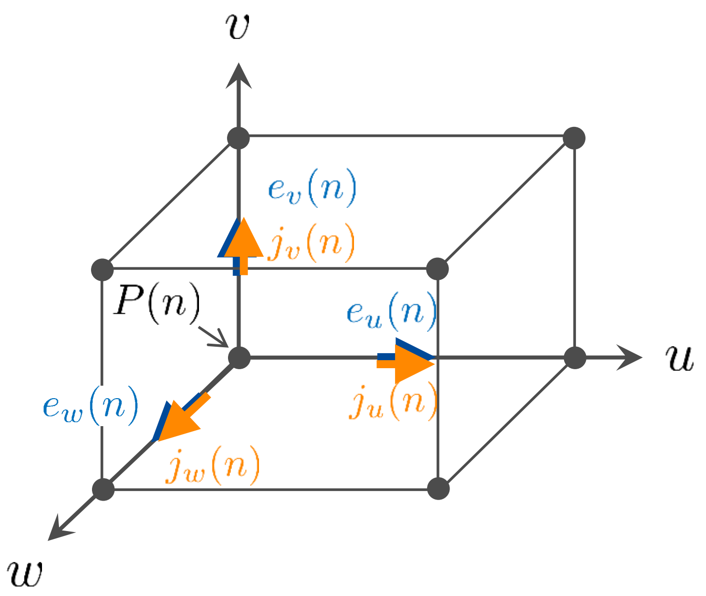
$$\mathbf{D}_\mu \mathbf{h} = \mathbf{b}$$

$$\begin{pmatrix} h_u(1) \\ \vdots \\ h_u(N_p) \\ h_v(1) \\ \vdots \\ h_v(N_p) \\ h_w(1) \\ \vdots \\ h_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p} \qquad \begin{pmatrix} b_u(1) \\ \vdots \\ b_u(N_p) \\ b_v(1) \\ \vdots \\ b_v(N_p) \\ b_w(1) \\ \vdots \\ b_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

Relationship Electric Currents and Electric Field Strength in Grid Space

$$\bar{\sigma}_u e_u(n) = j_u(n)$$
$$\bar{\sigma}_v e_v(n) = j_v(n)$$
$$\bar{\sigma}_w e_w(n) = j_w(n)$$

Primary Grid Cell



$$\mathbf{D}_\sigma = \mathrm{diag}\left[\bar{\sigma}_u(1), \ldots, \bar{\sigma}_u(N_p), \bar{\sigma}_v(1), \ldots, \bar{\sigma}_v(N_p), \bar{\sigma}_w(1), \ldots, \bar{\sigma}_w(N_p)\right] \in \mathbb{R}^{3N_p \times 3N_p}$$

$$\mathbf{D}_\sigma \mathbf{e} = \mathbf{j}$$

$$\begin{pmatrix} e_u(1) \\ \vdots \\ e_u(N_p) \\ e_v(1) \\ \vdots \\ e_v(N_p) \\ e_w(1) \\ \vdots \\ e_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p} \qquad \begin{pmatrix} j_u(1) \\ \vdots \\ j_u(N_p) \\ j_v(1) \\ \vdots \\ j_v(N_p) \\ j_w(1) \\ \vdots \\ j_w(N_p) \end{pmatrix} \in \mathbb{R}^{3N_p}$$

Maxwell‘s Equations and Maxwell’s Grid Equations (MGE)

Continuous Space	Grid Space
$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$	$\mathbf{C}\mathbf{D}_s\mathbf{e} = -\mathbf{D}_A\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{b}$
$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0$	$\mathbf{S}\mathbf{D}_A\mathbf{b} = \mathbf{0}$
$\nabla \times \mathbf{H}(\mathbf{r},t) = \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) + \mathbf{J}(\mathbf{r},t)$	$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h} = \tilde{\mathbf{D}}_A\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{d} + \tilde{\mathbf{D}}_A\mathbf{j}$
$\nabla \cdot \mathbf{D}(\mathbf{r},t) = \rho(\mathbf{r},t)$	$\tilde{\mathbf{S}}\tilde{\mathbf{D}}_A\mathbf{d} = \tilde{\mathbf{D}}_V\varrho$

$\varepsilon\,\mathbf{E}(\mathbf{r},t) = \mathbf{D}(\mathbf{r},t)$	$\mathbf{D}_\varepsilon\mathbf{e} = \mathbf{d}$
$\mu\,\mathbf{H}(\mathbf{r},t) = \mathbf{B}(\mathbf{r},t)$	$\mathbf{D}_\mu\mathbf{h} = \mathbf{b}$
$\sigma\,\mathbf{E}(\mathbf{r},t) = \mathbf{J}(\mathbf{r},t)$	$\mathbf{D}_\sigma\mathbf{e} = \mathbf{j}$

Summary – Maxwell's Grid Equations (MGE)

Continuous Space	Grid Space
$\nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$	$\mathbf{C}\mathbf{D}_s\mathbf{e} = -\mathbf{D}_A\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{b}$
$\nabla \cdot \mathbf{B}(\mathbf{r},t) = 0$	$\mathbf{S}\mathbf{D}_A\mathbf{b} = \mathbf{0}$
$\nabla \times \mathbf{H}(\mathbf{r},t) = \frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) + \mathbf{J}(\mathbf{r},t)$	$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h} = \tilde{\mathbf{D}}_A\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{d} + \tilde{\mathbf{D}}_A\mathbf{j}$
$\nabla \cdot \mathbf{D}(\mathbf{r},t) = \rho(\mathbf{r},t)$	$\tilde{\mathbf{S}}\tilde{\mathbf{D}}_A\mathbf{d} = \tilde{\mathbf{D}}_V\varrho$

$\varepsilon\,\mathbf{E}(\mathbf{r},t) = \mathbf{D}(\mathbf{r},t)$	$\mathbf{D}_\varepsilon\mathbf{e} = \mathbf{d}$
$\mu\,\mathbf{H}(\mathbf{r},t) = \mathbf{B}(\mathbf{r},t)$	$\mathbf{D}_\mu\mathbf{h} = \mathbf{b}$
$\sigma\,\mathbf{E}(\mathbf{r},t) = \mathbf{J}(\mathbf{r},t)$	$\mathbf{D}_\sigma\mathbf{e} = \mathbf{j}$

- Discretization method provides a one-to-one mapping for Maxwell's equations from continuous space onto the dual grid system in the grid space
- Since the integral form of Maxwell's equations was directly used on the grid cells, we also call this technique Finite-Integration Technique, briefly FIT
- The resulting linear matrix-vector equations are denoted as Maxwell-Grid-Equations, briefly MGE
- Special allocation (sampling of field components in space) allows for application of mid-point rule for integral approximation (second-order approximation of field quantities)

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Collating Discrete Induction Law and Discrete Ampère‘s Law

- Discrete induction law, discrete Ampère‘s law and discrete Ohm’s law

$$\mathbf{C}\mathbf{D}_s\mathbf{e} = -\mathbf{D}_A \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{b} \qquad \tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h} = \tilde{\mathbf{D}}_A \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{d} + \tilde{\mathbf{D}}_A\mathbf{D}_\sigma\,\mathbf{e} + \tilde{\mathbf{D}}_A\,\mathbf{j}$$

- Employing material relations yields

$$-\mathbf{C}\mathbf{D}_s\mathbf{e} = \mathbf{D}_A\mathbf{D}_\mu \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{h} \qquad \tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h} = \tilde{\mathbf{D}}_A\mathbf{D}_\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e} + \tilde{\mathbf{D}}_A\mathbf{D}_\sigma\,\mathbf{e} + \tilde{\mathbf{D}}_A\,\mathbf{j}$$

- Collating both equations allows for transferring this equation into a matrix-vector equation, where spatial derivatives vanished (time derivative still present)

$$\underbrace{\begin{pmatrix} \tilde{\mathbf{D}}_A\mathbf{D}_\varepsilon & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_A\mathbf{D}_\mu \end{pmatrix}}_{\mathbf{M}} \frac{\mathrm{d}}{\mathrm{d}t} \underbrace{\begin{pmatrix} \mathbf{e} \\ \mathbf{h} \end{pmatrix}}_{\mathbf{x}(t)} = \underbrace{\begin{pmatrix} -\tilde{\mathbf{D}}_A\mathbf{D}_\sigma & \tilde{\mathbf{C}}\tilde{\mathbf{D}}_s \\ -\mathbf{C}\mathbf{D}_s & \mathbf{0} \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} \mathbf{e} \\ \mathbf{h} \end{pmatrix}}_{\mathbf{x}(t)} + \underbrace{\begin{pmatrix} -\tilde{\mathbf{D}}_A \\ 0 \end{pmatrix} \mathbf{j}}_{\mathbf{B}\,\mathbf{i}(t)}$$

- Matrix **M** is a diagonal matrix (!) and

$$\mathbf{M} \in \mathbb{R}^{6N_\mathrm{p}\times 6N_\mathrm{p}},\ \mathbf{x}(t) \in \mathbb{R}^{6N_\mathrm{p}},\ \mathbf{A} \in \mathbb{R}^{6N_\mathrm{p}\times 6N_\mathrm{p}},\ \mathbf{B}(t) \in \mathbb{R}^{6N_\mathrm{p}\times N_s},\ \mathbf{i}(t) \in \mathbb{R}^{N_s}$$

Spatial Discretization with the Finite Element Method (FEM)

Transferring Curl-Curl Equation into its Weak Form (Weighted and Averaged)

$$\nabla \times \left[\mu^{-1}\nabla \times \mathbf{E}(\mathbf{r},t)\right] + \varepsilon \frac{\partial^2}{\partial t^2}\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) - \sigma \frac{\partial}{\partial t}\mathbf{E}(\mathbf{r},t) \qquad \Big| \mathbf{W}_i(\mathbf{r}) \cdot$$

$$\mathbf{W}_i(\mathbf{r})\cdot\nabla\times\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right] + \varepsilon\frac{\partial^2}{\partial t^2}\mathbf{W}_i(\mathbf{r})\cdot\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{W}_i(\mathbf{r})\cdot\mathbf{J}(\mathbf{r},t) - \sigma\frac{\partial}{\partial t}\mathbf{W}_i(\mathbf{r})\cdot\mathbf{E}(\mathbf{r},t)$$

Using the identity:

$$\mathbf{B}\cdot[\nabla\times\mathbf{A}] = -\nabla\cdot[\mathbf{B}\times\mathbf{A}] + \mathbf{A}\cdot[\nabla\times\mathbf{B}]$$

$$\mathbf{W}_i(\mathbf{r})\cdot\nabla\times\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right] = -\nabla\cdot\left(\mathbf{W}_i(\mathbf{r})\times\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\right) + \left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\cdot\left[\nabla\times\mathbf{W}_i(\mathbf{r})\right]$$

$$-\nabla\cdot\left(\mathbf{W}_i(\mathbf{r})\times\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\right) + \left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\cdot\left[\nabla\times\mathbf{W}_i(\mathbf{r})\right]$$
$$+\varepsilon\frac{\partial^2}{\partial t^2}\mathbf{W}_i(\mathbf{r})\cdot\mathbf{E}(\mathbf{r},t) = -\frac{\partial}{\partial t}\mathbf{W}_i(\mathbf{r})\cdot\mathbf{J}(\mathbf{r},t) - \sigma\frac{\partial}{\partial t}\mathbf{W}_i(\mathbf{r})\cdot\mathbf{E}(\mathbf{r},t) \qquad \Big| \iiint_{\Omega} \ldots \mathrm{d}V$$

Transferring Curl-Curl Equation into its Weak Form (Weighted and Averaged)

$$-\iiint_{\boldsymbol{\Omega}} \nabla\cdot\left(\mathbf{W}_i(\mathbf{r})\times\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\right)\mathrm{d}V+\iiint_{\boldsymbol{\Omega}}\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\cdot\left[\nabla\times\mathbf{W}_i(\mathbf{r})\right]\mathrm{d}V$$

$$+\frac{\partial^2}{\partial t^2}\iiint_{\boldsymbol{\Omega}}\varepsilon\mathbf{W}_i(\mathbf{r})\cdot\mathbf{E}(\mathbf{r},t)\mathrm{d}V=-\frac{\partial}{\partial t}\iiint_{\boldsymbol{\Omega}}\mathbf{W}_i(\mathbf{r})\cdot\mathbf{J}(\mathbf{r},t)\mathrm{d}V-\frac{\partial}{\partial t}\iiint_{\boldsymbol{\Omega}}\sigma\mathbf{W}_i(\mathbf{r})\cdot\mathbf{E}(\mathbf{r},t)\mathrm{d}V$$

Applying Gauss' theorem:

$$-\iiint_{\boldsymbol{\Omega}}\nabla\cdot\left(\mathbf{W}_i(\mathbf{r})\times\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\right)\mathrm{d}V=-\oiint_{\partial\boldsymbol{\Omega}}\left(\mathbf{W}_i(\mathbf{r})\times\left[\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]\right)\cdot\mathbf{n}\,\mathrm{d}A$$

$$=\oiint_{\partial\boldsymbol{\Omega}}\left(\mathbf{W}_i(\mathbf{r})\cdot\underbrace{\left[\mathbf{n}\times\mu^{-1}\nabla\times\mathbf{E}(\mathbf{r},t)\right]}_{\mathbf{Q}(\mathbf{r},t)}\right)\mathrm{d}A$$

function to be specified on the boundary

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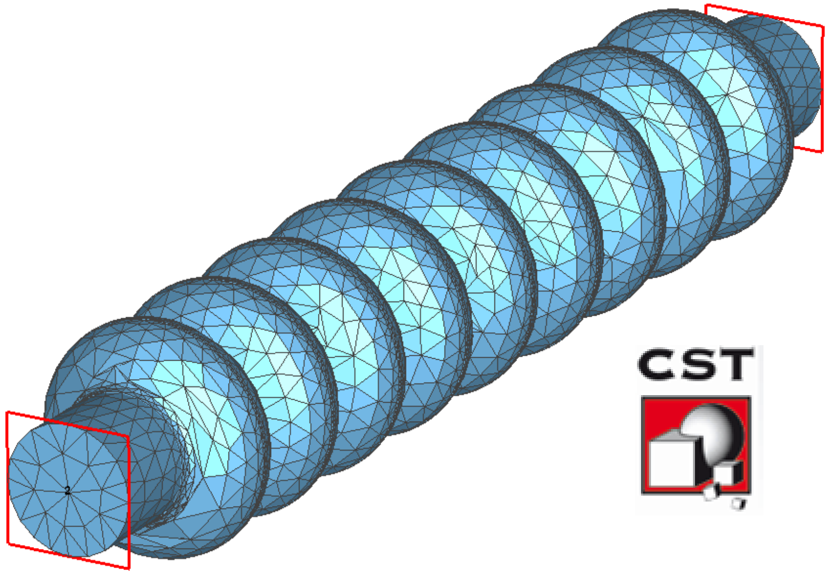
Transferring Curl-Curl Equation into its Weak Form (Weighted and Averaged)

$$\oiint_{\partial\mathbf{\Omega}} \left(\mathbf{W}_i(\mathbf{r}) \cdot \underbrace{\left[\mathbf{n} \times \mu^{-1} \nabla \times \mathbf{E}(\mathbf{r},t)\right]}_{\mathbf{Q}(\mathbf{r},t)} \right) \mathrm{d}A + \iiint_{\mathbf{\Omega}} \left[\mu^{-1} \nabla \times \mathbf{E}(\mathbf{r},t)\right] \cdot \left[\nabla \times \mathbf{W}_i(\mathbf{r})\right] \mathrm{d}V$$

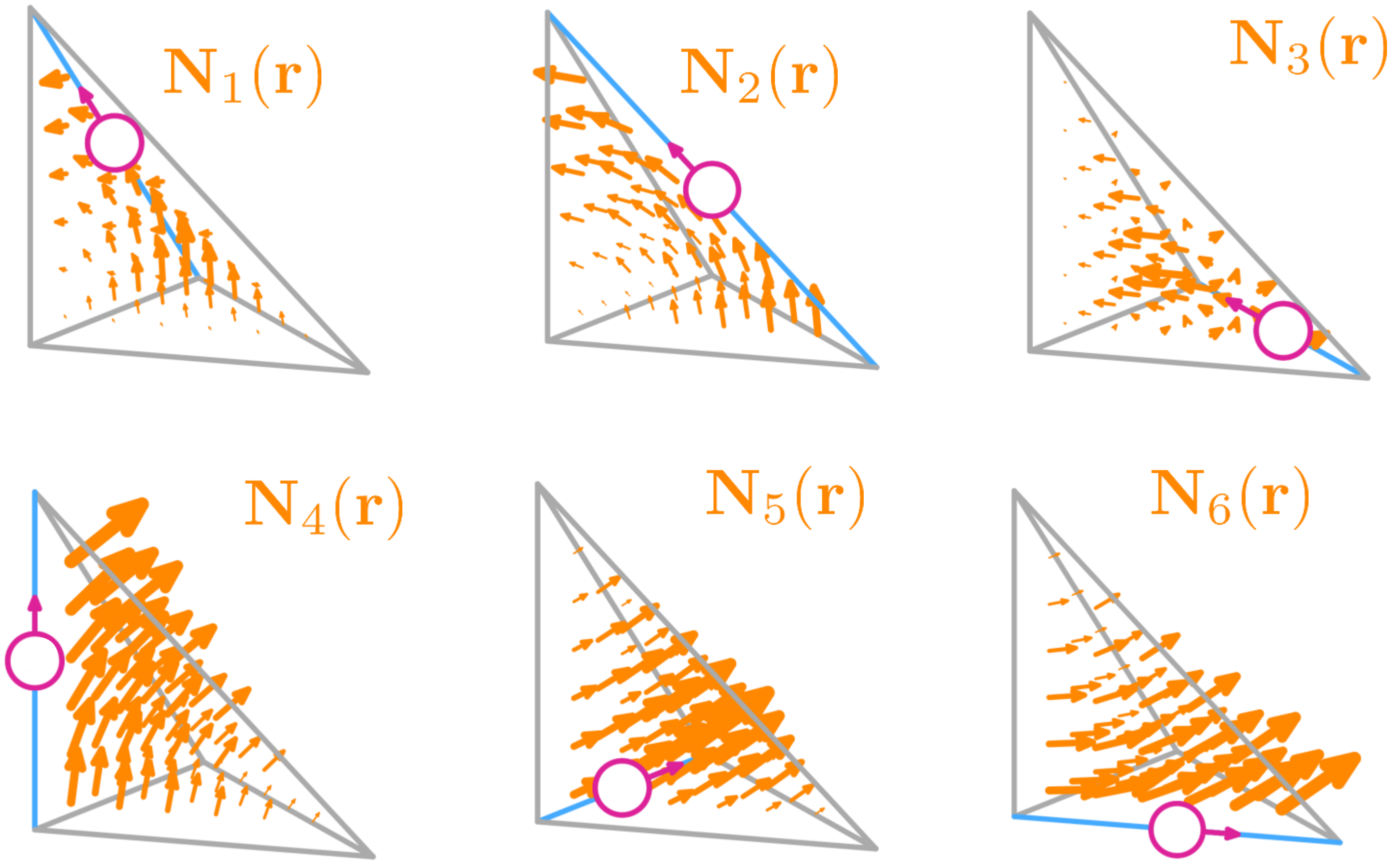
$$+ \frac{\partial^2}{\partial t^2} \iiint_{\mathbf{\Omega}} \varepsilon \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r},t) \mathrm{d}V = -\frac{\partial}{\partial t} \iiint_{\mathbf{\Omega}} \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r},t) \mathrm{d}V - \frac{\partial}{\partial t} \iiint_{\mathbf{\Omega}} \sigma \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r},t) \mathrm{d}V$$

Weak form of curl-curl equation, because curl-curl equation is not required to be fulfilled in each point, but fulfilled in an weighted averaged sense!

Field Expansion using Edge Elements on an e.g. Tetrahedral Mesh



$$\mathbf{E}(\mathbf{r},t) = \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t)$$



Source: The DefElement contributors. DefElement: an encyclopedia of finite element definitions, 2023, https://defelement.com [Online; accessed: 15-May-2023]

Expressing E-Field in Terms of Field Expansion

$$\oiint_{\partial\boldsymbol{\Omega}} \left(\mathbf{W}_i(\mathbf{r}) \cdot \mathbf{Q}(\mathbf{r},t)\right) \mathrm{d}A + \iiint_{\boldsymbol{\Omega}} \left[\mu^{-1}\nabla \times \mathbf{E}(\mathbf{r},t)\right] \cdot \left[\nabla \times \mathbf{W}_i(\mathbf{r})\right] \mathrm{d}V + \frac{\partial^2}{\partial t^2} \iiint_{\boldsymbol{\Omega}} \varepsilon \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r},t) \mathrm{d}V = -\frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r},t) \mathrm{d}V - \frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \sigma \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r},t) \mathrm{d}V$$

$$\oiint_{\partial\boldsymbol{\Omega}} \left(\mathbf{W}_i(\mathbf{r}) \cdot \mathbf{Q}(\mathbf{r},t)\right) \mathrm{d}A + \iiint_{\boldsymbol{\Omega}} \left[\mu^{-1}\nabla \times \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t)\right] \cdot \left[\nabla \times \mathbf{W}_i(\mathbf{r})\right] \mathrm{d}V + \frac{\partial^2}{\partial t^2} \iiint_{\boldsymbol{\Omega}} \varepsilon \mathbf{W}_i(\mathbf{r}) \cdot \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t) \mathrm{d}V = -\frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \mathbf{W}_i(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r},t) \mathrm{d}V - \frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \sigma \mathbf{W}_i(\mathbf{r}) \cdot \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t) \mathrm{d}V$$

Galerkin Approach - Weighting Functions are Expansion Functions: $\mathbf{W}_i(\mathbf{r}) = \mathbf{N}_i(\mathbf{r}), i = 1, \ldots, N$

$$\oint\!\!\!\oint_{\partial\boldsymbol{\Omega}} \Big(\mathbf{W}_i(\mathbf{r}) \cdot \mathbf{Q}(\mathbf{r},t)\Big)\,\mathrm{d}A + \iiint_{\boldsymbol{\Omega}} \left[\mu^{-1}\nabla \times \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t)\right] \cdot \Big[\nabla \times \mathbf{N}_i(\mathbf{r})\Big]\mathrm{d}V$$

$$+ \frac{\partial^2}{\partial t^2} \iiint_{\boldsymbol{\Omega}} \varepsilon \mathbf{N}_i(\mathbf{r}) \cdot \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t)\mathrm{d}V = -\frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r},t)\mathrm{d}V - \frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \sigma \mathbf{N}_i(\mathbf{r}) \cdot \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t)\mathrm{d}V$$

$$\Downarrow$$

$$\oint\!\!\!\oint_{\partial\boldsymbol{\Omega}} \Big(\mathbf{W}_i(\mathbf{r}) \cdot \mathbf{Q}(\mathbf{r},t)\Big)\,\mathrm{d}A + \sum_{j=1}^{N} \iiint_{\boldsymbol{\Omega}} \Big[\mu^{-1}\nabla \times \mathbf{N}_j(\mathbf{r})\Big] \cdot \Big[\nabla \times \mathbf{N}_i(\mathbf{r})\Big]\mathrm{d}V\, x_j(t)$$

$$+ \sum_{j=1}^{N} \iiint_{\boldsymbol{\Omega}} \varepsilon \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{N}_j(\mathbf{r})\mathrm{d}V\, \frac{\partial^2}{\partial t^2} x_j(t) = -\frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r},t)\mathrm{d}V - \sum_{j=1}^{N} \iiint_{\boldsymbol{\Omega}} \sigma \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{N}_j(\mathbf{r})\mathrm{d}V\, \frac{\partial}{\partial t} x_j(t)$$

Galerkin Approach: $\mathbf{W}_i(\mathbf{r}) = \mathbf{N}_i(\mathbf{r}), i = 1, \ldots, N$

$$\oiint_{\partial\boldsymbol{\Omega}} \Big(\mathbf{W}_i(\mathbf{r}) \cdot \mathbf{Q}(\mathbf{r},t)\Big)\, \mathrm{d}A + \iiint_{\boldsymbol{\Omega}} \left[\mu^{-1}\nabla \times \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t)\right] \cdot \Big[\nabla \times \mathbf{N}_i(\mathbf{r})\Big] \mathrm{d}V$$

$$+ \frac{\partial^2}{\partial t^2} \iiint_{\boldsymbol{\Omega}} \varepsilon \mathbf{N}_i(\mathbf{r}) \cdot \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t) \mathrm{d}V = -\frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r},t) \mathrm{d}V - \frac{\partial}{\partial t} \iiint_{\boldsymbol{\Omega}} \sigma \mathbf{N}_i(\mathbf{r}) \cdot \sum_{j=1}^{N} \mathbf{N}_j(\mathbf{r})\, x_j(t) \mathrm{d}V$$

$$\underbrace{\oiint_{\partial\boldsymbol{\Omega}} \left(\mathbf{W}_i(\mathbf{r}) \cdot \mathbf{Q}(\mathbf{r},t)\right) \mathrm{d}A}_{q_i(t)=0} + \sum_{j=1}^{N} \underbrace{\iiint_{\boldsymbol{\Omega}} \left[\mu^{-1}\nabla \times \mathbf{N}_j(\mathbf{r})\right] \cdot \Big[\nabla \times \mathbf{N}_i(\mathbf{r})\Big] \mathrm{d}V}_{s_{ij}}\, x_j(t)$$

$$+ \sum_{j=1}^{N} \underbrace{\iiint_{\boldsymbol{\Omega}} \varepsilon \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{N}_j(\mathbf{r}) \mathrm{d}V}_{m_{ij}}\, \frac{\partial^2}{\partial t^2} x_j(t) = -\frac{\partial}{\partial t} \underbrace{\iiint_{\boldsymbol{\Omega}} \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r},t) \mathrm{d}V}_{p_i(t)} - \sum_{j=1}^{N} \underbrace{\iiint_{\boldsymbol{\Omega}} \sigma \mathbf{N}_i(\mathbf{r}) \cdot \mathbf{N}_j(\mathbf{r}) \mathrm{d}V}_{k_{ij}}\, \frac{\partial}{\partial t} x_j(t)$$

Ordinary Differential Equations from Galerkin Approach

$$\sum_{j=1}^{N} s_{ij}\, x_j(t) + \sum_{j=1}^{N} m_{ij}\, \frac{\partial^2}{\partial t^2} x_j(t) = -\frac{\partial}{\partial t} p_i(t) - \sum_{j=1}^{N} k_{ij}\, \frac{\partial}{\partial t} x_j(t), \quad i = 1, \ldots, N \qquad \Big| \int \ldots \mathrm{d}t$$

$$\sum_{j=1}^{N} s_{ij}\, \hat{x}_j(t) + \sum_{j=1}^{N} m_{ij}\, \frac{\partial}{\partial t} x_j(t) = -p_i(t) - \sum_{j=1}^{N} k_{ij}\, x_j(t), \quad i = 1, \ldots, N$$

$$\frac{\partial}{\partial t} \hat{x}_j(t) = x_j(t)$$

Collating Differential Equations for All Weighting Functions

$$\sum_{j=1}^{N} s_{ij}\,\hat{x}_j(t) + \sum_{j=1}^{N} m_{ij}\,\frac{\partial}{\partial t} x_j(t) = -p_i(t) - \sum_{j=1}^{N} k_{ij}\,x_j(t), \quad i = 1,\dots,N$$

$$\frac{\partial}{\partial t}\hat{x}_j(t) = x_j(t)$$

$$\underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & m_{11} & 0 & m_{12} & \dots & 0 & m_{1N} \\ 0 & 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & m_{21} & 0 & m_{22} & \dots & 0 & m_{2N} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 & 0 \\ 0 & m_{N1} & 0 & m_{N2} & \dots & 0 & m_{NN} \end{pmatrix}}_{\mathbf{M}} \frac{\mathrm{d}}{\mathrm{d}t} \underbrace{\begin{pmatrix} \hat{x}_1(t) \\ x_1(t) \\ \hat{x}_2(t) \\ x_2(t) \\ \vdots \\ \hat{x}_N(t) \\ x_N(t) \end{pmatrix}}_{\mathbf{x}(t)} = \underbrace{\begin{pmatrix} 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ -s_{11} & -k_{11} & -s_{12} & -k_{12} & \dots & -s_{1N} & -k_{1N} \\ 0 & 0 & 0 & 1 & \dots & 0 & 0 \\ -s_{21} & -k_{21} & -s_{22} & -k_{22} & \dots & -s_{2N} & -k_{2N} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 \\ -s_{N1} & -k_{N1} & -s_{N2} & -k_{N2} & \dots & -s_{NN} & -k_{NN} \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} \hat{x}_1(t) \\ x_1(t) \\ \hat{x}_2(t) \\ x_2(t) \\ \vdots \\ \hat{x}_N(t) \\ x_N(t) \end{pmatrix}}_{\mathbf{x}(t)} + \underbrace{\begin{pmatrix} 0 \\ p_1(t) \\ 0 \\ p_2(t) \\ \vdots \\ 0 \\ p_N(t) \end{pmatrix}}_{\mathbf{B}\,\mathbf{i}(t)}$$

- Matrix-vector equation, where spatial derivatives vanished (time derivative still present)
- Coefficients are typically only unequal to zero for adjacent elements/edges!

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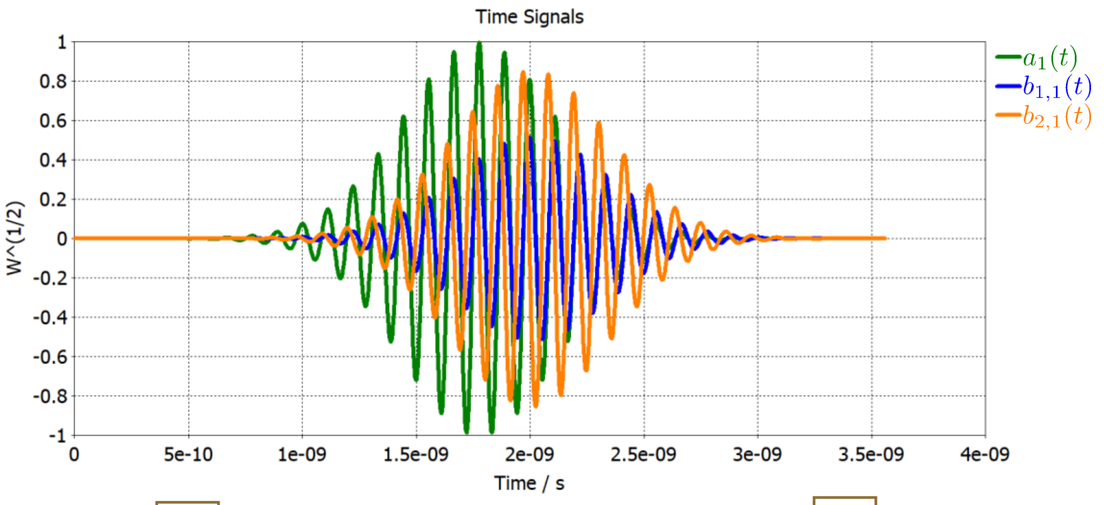
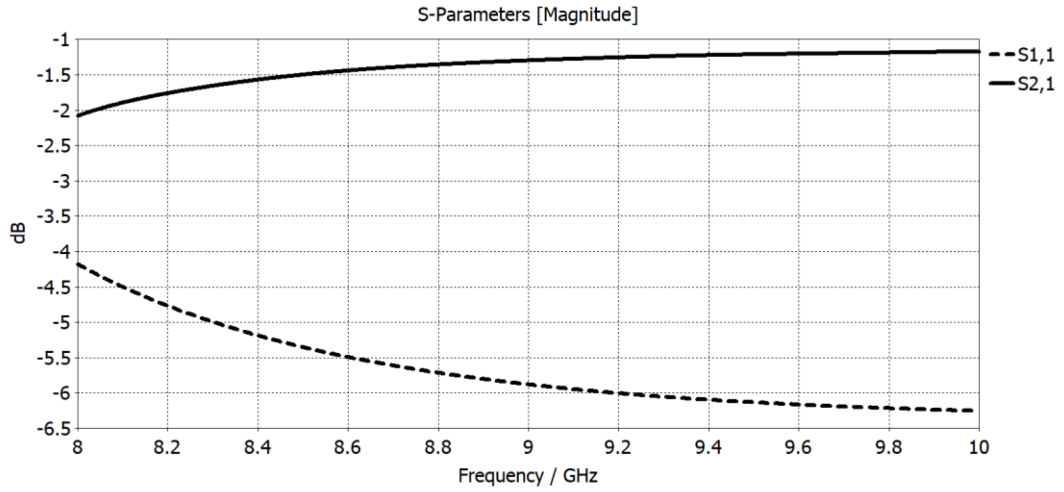
Time Domain Approaches

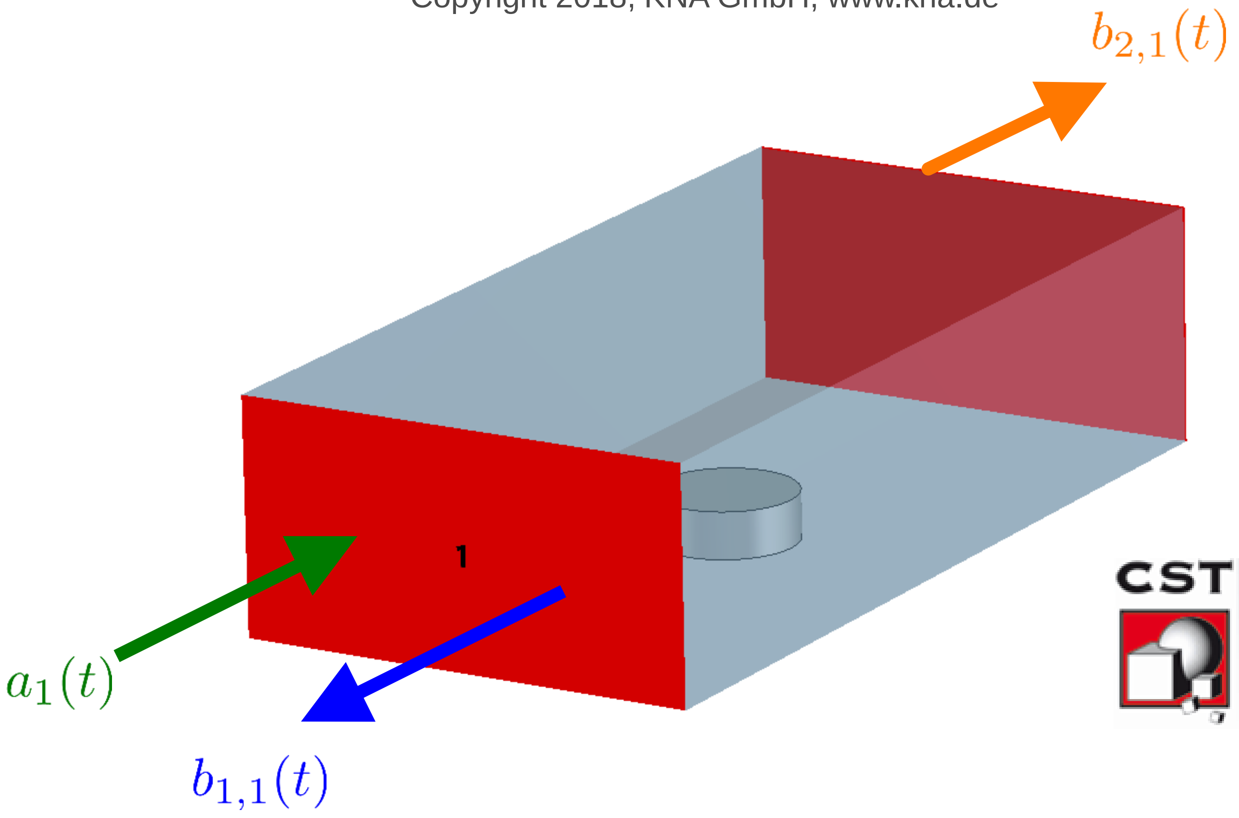
Transient Excitation of Ports with Gaussian Pulse



$$s_{i,1}(j\omega) = \frac{\mathrm{FFT}\left[b_{i,1}(t)\right]}{\mathrm{FFT}\left[a_1(t)\right]}$$



Picture courtesy of Harald Oppitz, Copyright 2018, KNA GmbH, www.kna.de



Determine Transient System Response

- Spatial discretization delivers: $\bar{\mathbf{M}}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \bar{\mathbf{A}}\,\mathbf{x}(t) + \bar{\mathbf{B}}\,\mathbf{a}(t)$

- Sorting for time derivative yields ***initial value problem*** or ***coupled first-order ordinary differential vector-equation*** (ODE)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \bar{\mathbf{M}}^{-1}\bar{\mathbf{A}}\,\mathbf{x}(t) + \bar{\mathbf{M}}^{-1}\bar{\mathbf{B}}\,\mathbf{a}(t)$$

- Formal integration gives

$$\mathbf{x}(t) = \int_{t_0}^{t} \bar{\mathbf{M}}^{-1}\bar{\mathbf{A}}\,\mathbf{x}(\tau) + \bar{\mathbf{M}}^{-1}\bar{\mathbf{B}}\,\mathbf{a}(\tau)\,\mathrm{d}\tau + \mathbf{x}(t_0)$$

- Vast amount of single- and multi-step methods (based on discretization in time) developed to solve problem, such as or ***Euler method***, ***Crank–Nicolson method*** or ***Runge–Kutta methods,*** **Adams–Bashforth methods** etc.

- Scattered wave amplitudes are available by an “output equation”:

$$\mathbf{b}(t) = \bar{\mathbf{C}}\,\mathbf{x}(t) + \bar{\mathbf{D}}\,\mathbf{a}(t)$$

Determine Transient System Response

- Spatial discretization delivers: $\bar{\mathbf{M}}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \bar{\mathbf{A}}\,\mathbf{x}(t) + \bar{\mathbf{B}}\,\mathbf{a}(t)$

- Sorting for time derivative yields ***initial value problem*** or ***coupled first-order ordinary differential vector-equation*** (ODE)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \bar{\mathbf{M}}^{-1}\bar{\mathbf{A}}\,\mathbf{x}(t) + \bar{\mathbf{M}}^{-1}\bar{\mathbf{B}}\,\mathbf{a}(t)$$

BUT:

BUT:

- Difficult to perform time-domain computations using standard Finite-Element approaches as inverse of mass matrix is not available (large)
- Solving a large system of linear equations would be required in each time step (which is expensive)
- Finite Integration Technique on hexahedral mesh does not suffer from the problem as mass matrix is of diagonal form, thus easy to invert
- Time-domain computation with FEM are nevertheless feasible with e.g. mass lumping or alternative formulations such as Discontinuous-Galerkin FEM

Famous Explicit Update Scheme for FIT: Leap Frog

- Starting point: discrete Faraday's and Ampere's law:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{h} = -\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{e}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e} = \mathbf{D}_\varepsilon^{-1}\tilde{\mathbf{D}}_A^{-1}\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h} - \mathbf{D}_\varepsilon^{-1}\mathbf{j}$$

i.e. a system of first order ordinary differential equations w.r.t. time

- Allocate one at full, the other at half time steps:

$$\mathbf{h}^{(m)} := \mathbf{h}(t_m = t_0 + m\Delta t), \quad \mathbf{j}^{(m)} := \mathbf{j}(t_m = t_0 + m\Delta t), \quad \mathbf{e}^{(m+\frac{1}{2})} := \mathbf{e}\left(t_m = t_0 + [m + 1/2]\,\Delta t\right)$$

- Approximation of derivatives using central differences

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{h}^{(m+\frac{1}{2})} \approx \frac{\mathbf{h}^{(m+1)} - \mathbf{h}^{(m)}}{\Delta t} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e}^{(m+1)} \approx \frac{\mathbf{e}^{(m+\frac{3}{2})} - \mathbf{e}^{(m+\frac{1}{2})}}{\Delta t}$$

- Resulting explicit update equations

$$\mathbf{h}^{(m+1)} = \mathbf{h}^{(m)} - \Delta t\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{e}^{(m+\frac{1}{2})}$$

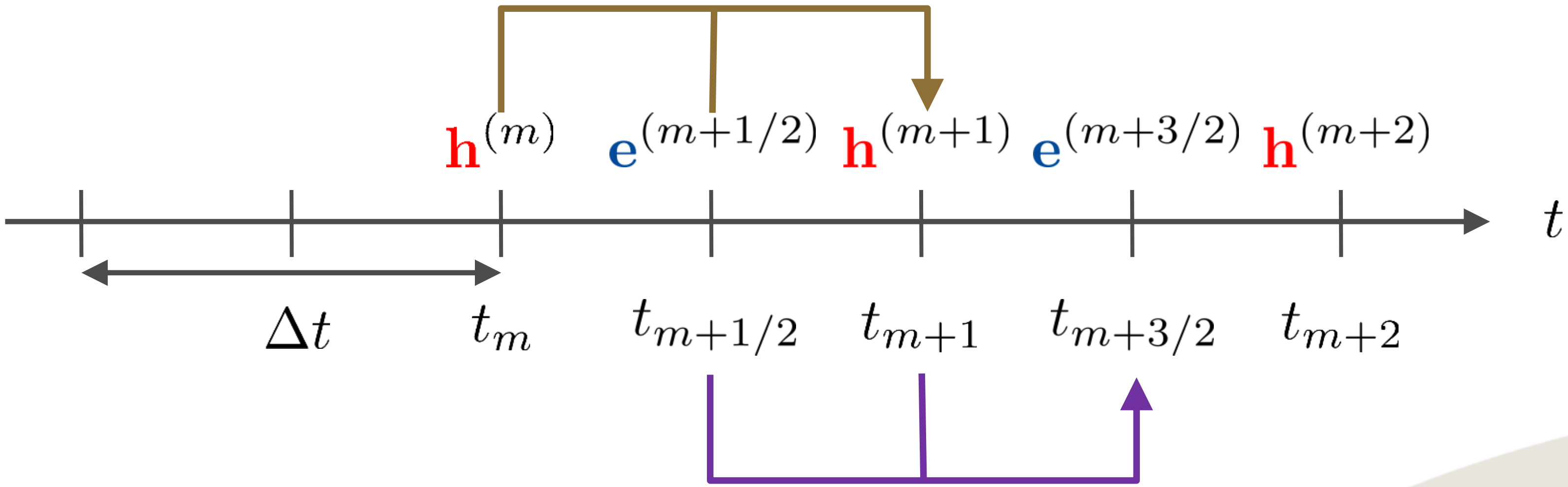
$$\mathbf{e}^{(m+\frac{3}{2})} = \mathbf{e}^{(m+\frac{1}{2})} + \Delta t\left(\mathbf{D}_\varepsilon^{-1}\tilde{\mathbf{D}}_A^{-1}\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h}^{(m+1)} - \mathbf{D}_\varepsilon^{-1}\mathbf{j}^{(m+1)}\right)$$

Leap Frog Update Scheme

$$\mathbf{h}^{(m+1)} = \mathbf{h}^{(m)} - \Delta t \mathbf{D}_{\mu}^{-1}\mathbf{D}_{A}^{-1}\mathbf{C}\mathbf{D}_{s}\mathbf{e}^{(m+\frac{1}{2})}$$

$$\mathbf{e}^{(m+\frac{3}{2})} = \mathbf{e}^{(m+\frac{1}{2})} + \Delta t \left(\mathbf{D}_{\varepsilon}^{-1}\tilde{\mathbf{D}}_{A}^{-1}\tilde{\mathbf{C}}\tilde{\mathbf{D}}_{s}\mathbf{h}^{(m+1)} - \mathbf{D}_{\varepsilon}^{-1}\mathbf{j}^{(m+1)}\right)$$

Explicit recursive scheme



Stability Condition for Leap Frog: Courant-Friedrichs-Levy Condition

- Maximal time step for stable (energy conservative) iteration with leap frog:

$$\Delta t \leq \min_i \left\{ \frac{\sqrt{\varepsilon_i \mu_i}}{\sqrt{\frac{1}{\Delta x_i^2} + \frac{1}{\Delta y_i^2} + \frac{1}{\Delta z_i^2}}} \right\} ,$$

where Δx_i , Δy_i , Δz_i are the edge lengths of the ith hexahedral mesh cell

- Smaller edge lengths (resulting in larger matrices and vectors) require smaller discrete time steps to maintain stability of the transient iteration
- In particular a problem for solving structures with tiny but not negligible details (such as higher-order mode couplers)

Frequency Domain Approaches

Transfer of State-Space Equation to Frequency Domain

- Formally transfer of spatially discretized equation (resulting from FIT or FEM)

$$\mathbf{M}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathbf{A}\,\mathbf{x}(t) + \mathbf{B}\,\mathbf{i}(t)$$

assuming frequency-domain excitation and field distributions

$$\mathbf{i}(t) = \Re\left[\underline{\mathbf{i}}(j\omega)\right], \quad \underline{\mathbf{i}}(j\omega) = \underline{\mathbf{i}}\exp\left(j\omega t\right)$$
$$\mathbf{x}(t) = \Re\left[\underline{\mathbf{x}}(j\omega)\right], \quad \underline{\mathbf{x}}(j\omega) = \underline{\mathbf{x}}\exp\left(j\omega t\right)$$

gives

$$\mathbf{M}j\omega\underline{\mathbf{x}}(j\omega) = \mathbf{A}\,\underline{\mathbf{x}}(j\omega) + \mathbf{B}\,\underline{\mathbf{i}}(j\omega)$$

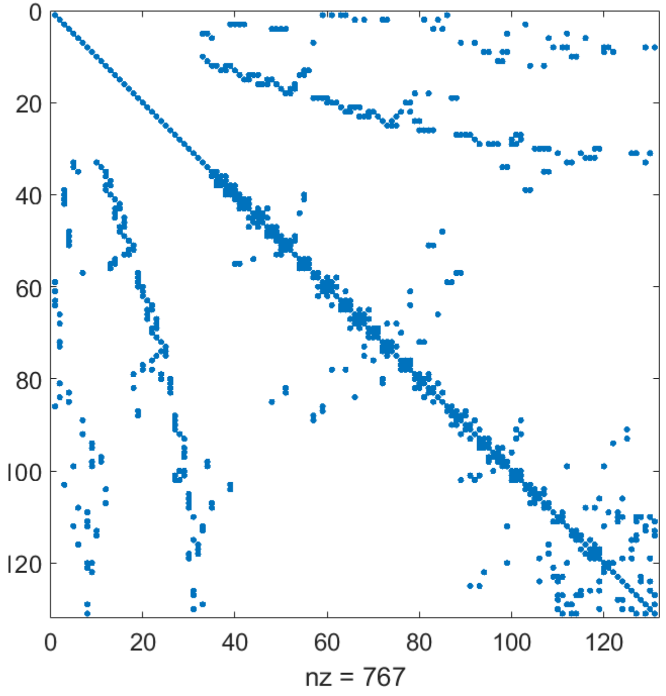
- Resorting yields complex-valued system of linear equations

$$\underbrace{\left[j\omega\mathbf{M} - \mathbf{A}\right]}_{\underline{\mathbf{G}}(j\omega)\in\mathbb{C}^{N\times N}}\ \underline{\mathbf{x}}(j\omega) = \underbrace{\mathbf{B}\,\underline{\mathbf{i}}(j\omega)}_{\underline{\mathbf{b}}(j\omega)\in\mathbb{C}^{N}}$$

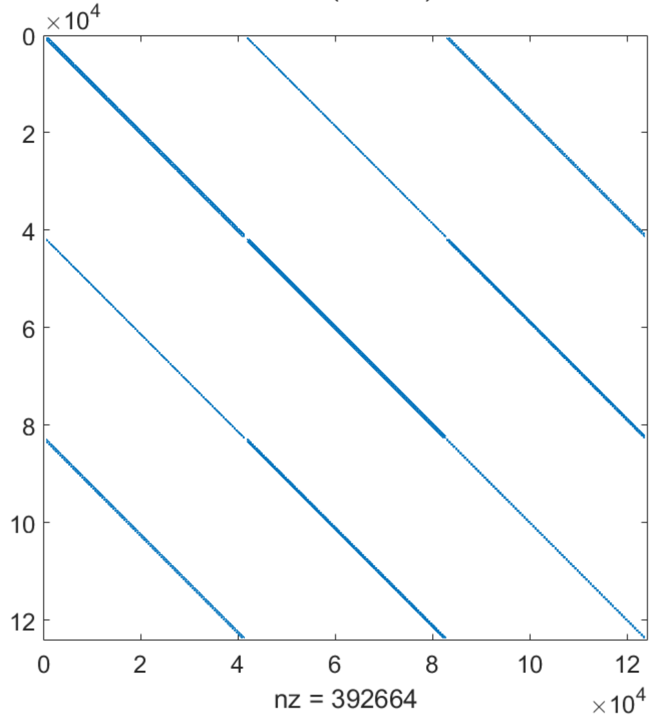
Properties of System Linear of Equations $\underline{\mathbf{G}}(j\omega)\,\underline{\mathbf{x}}(j\omega) = \underline{\mathbf{b}}(j\omega)$

- Large, sparse, frequency-dependent, complex-valued and full-rank system matrix

$\underline{\mathbf{G}}^{\mathrm{FEM}}(j\omega_0)$



$\underline{\mathbf{G}}^{\mathrm{FIT}}(j\omega_0)$



- Dedicated sparsity formats for matrix storage used, accounting solely for non-zero elements and the location where they occur

Solving Large Sparse Systems of Linear Equations

Methods to Solve Large Sparse Linear Systems of Equations

Direct methods such as *Gaussian elimination* or *matrix inversion* often not suitable for solving large, sparse linear systems of equation, since they

- scale with N^3 (doubling number of unknowns leads to eight times larger solver time)
- are not robust against round-off error, i.e. it comes to accumulation of round-off errors
- it can come to fill-in, i.e. the inverse of a sparse matrix is not required to be sparse as well

Iterative methods such as *Conjugate gradient method*, *Biconjugate gradient method*, *Jacobi method*, *Gauss–Seidel method*, *Successive over-relaxation method* etc. often much for suitable for solving large, sparse linear systems of equation, since they

- do not suffer from above mentioned drawbacks!

Iterative Methods to Solve Linear Systems of Equations

- Start with an initial guess $\underline{\mathbf{x}}^{(0)}$

- Obtain improved guess being closer to exact solution $\underline{\mathbf{x}}^*$ in each iteration step:

$$\underbrace{\|\underline{\mathbf{x}}^* - \underline{\mathbf{x}}^{(k)}\|}_{e^{(k)}} > \underbrace{\|\underline{\mathbf{x}}^* - \underline{\mathbf{x}}^{(k+1)}\|}_{e^{(k+1)}}$$

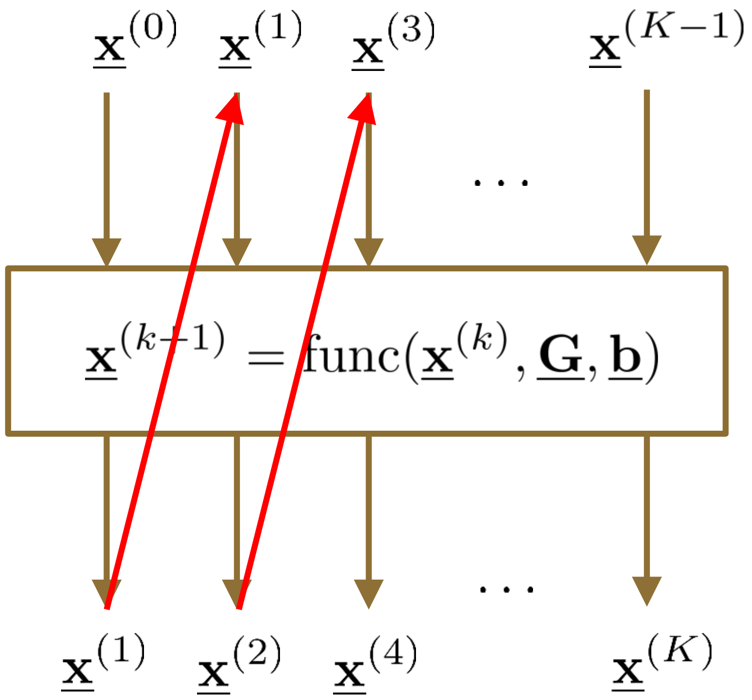
- Convergence after enough iterations

$$\lim_{k\to\infty} \underbrace{\|\underline{\mathbf{x}}^* - \underline{\mathbf{x}}^{(k)}\|}_{e^{(k)}} = 0$$

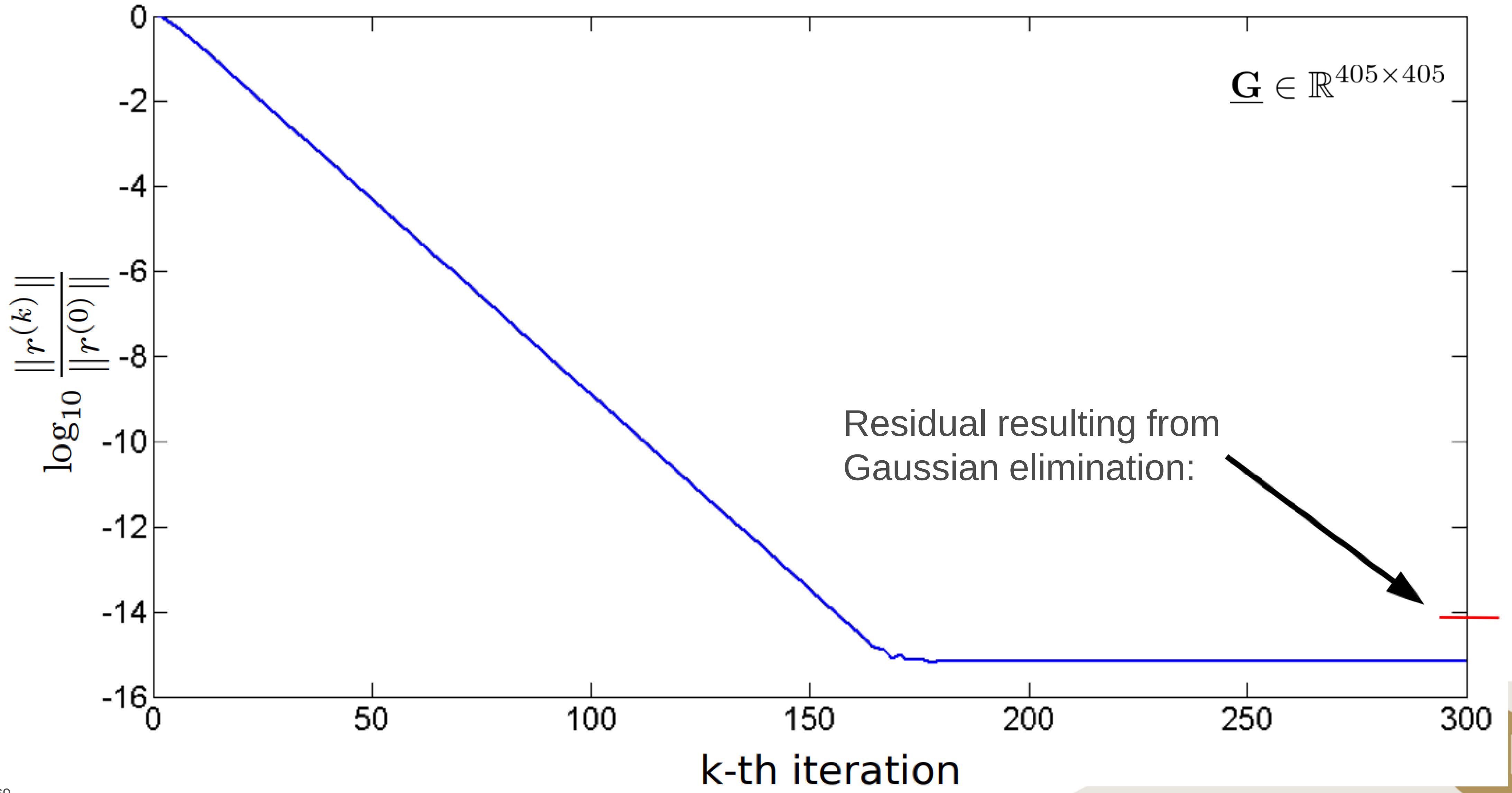
- Convergence not always guaranteed, each iterative method has convergence criteria depending on system matrix properties

- Error based stopping criterions not feasible, thus residuals are considered:

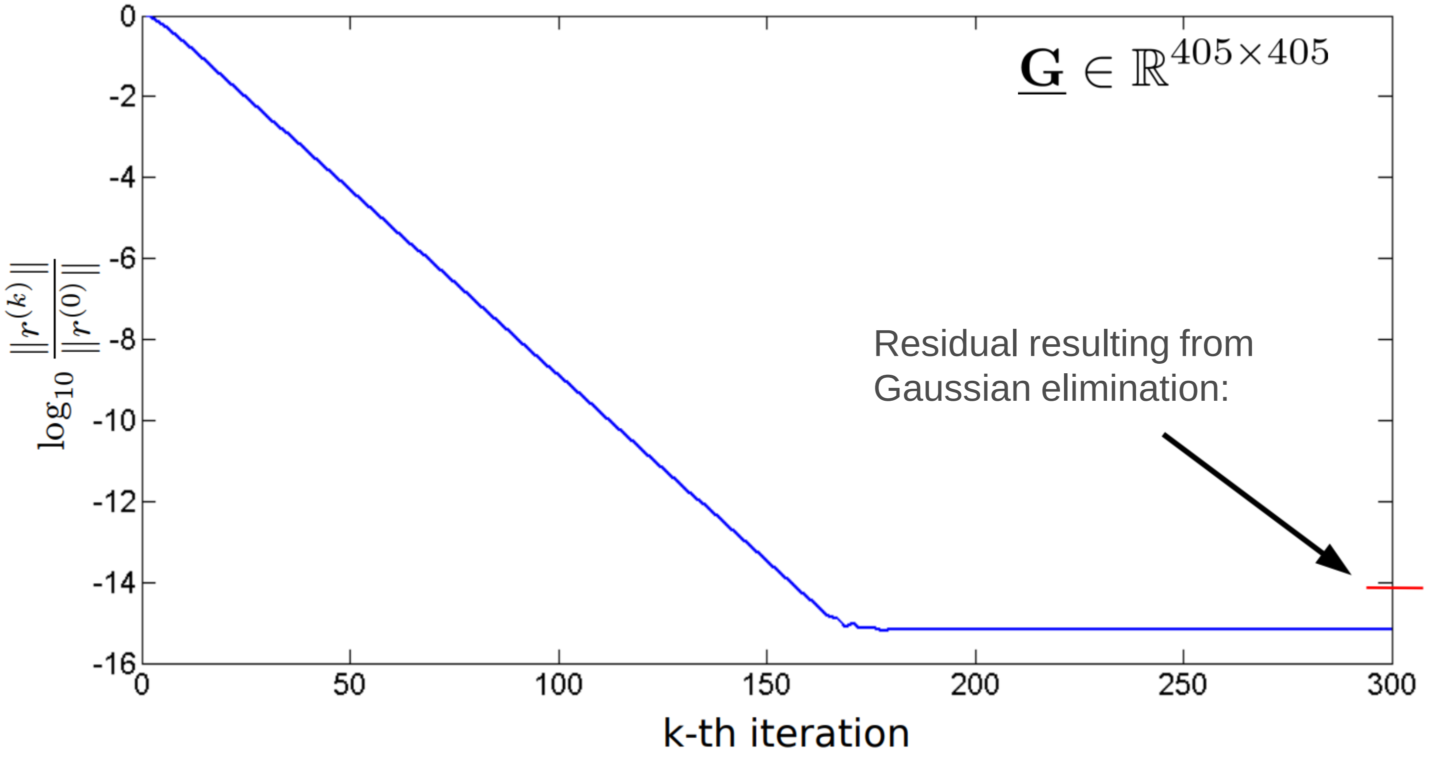
$$\underline{\mathbf{r}}^{(k)} = \underline{\mathbf{b}} - \underline{\mathbf{G}}\,\underline{\mathbf{x}}^{(k)}$$



Example Relative Residual after using Gauss-Seidel



Example Relative Residual after using Gauss-Seidel (cont.)



- After a certain number of iterations, relative residual stays constant, due to finite machine precision
- Gauss-Seidel (iterative method) gives a better approximation to exact solution than Gaussian elimination (direct method)

Condition Number of Matrix

- From theory:

$$\underbrace{\frac{\|\underline{\mathbf{x}}^* - \underline{\mathbf{x}}^{(k)}\|}{\|\underline{\mathbf{x}}^*\|}}_{\text{relative error}} \leq \underbrace{\|\underline{\mathbf{A}}\| \cdot \|\underline{\mathbf{A}}^{-1}\|}_{\text{condition number}} \cdot \underbrace{\frac{\|\underline{\mathbf{r}}^{(k)}\|}{\|\underline{\mathbf{b}}\|}}_{\text{relative residual}}$$

- Difficult to ensure small relative error, if matrix is ill-conditioned, because relative residual can only be minimised up to a certain level due to finite numerical accuracy!

- Relative error may be still large, if (in general unknown) condition number is large

- Ill-conditioned problems arise e.g. for large mesh aspect ratios

Challenges in Simulation of Scattering Parameters of Resonant Structures with Large Quality Factors

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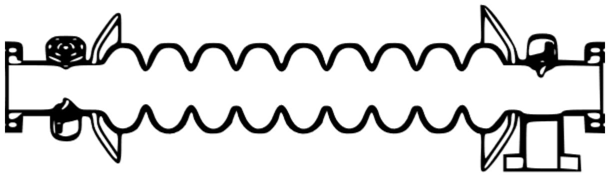
Large Quality Factors in Time Domain



E. Vogel et al., in Proceedings of the International Particle Accelerator Conference, Kyoto, Japan (ICR, Kyoto, 2010), pp. 4281–4283

- Structures with resonances having large quality factors

$$Q_n = \frac{\omega_n W_{\mathrm{stored},n}}{P_{\mathrm{loss},n}}$$

(filters or resonators), do have long rise times and decay times of field energy

- Modes in resonators with copper walls may have Q ≈ $7 \cdot 10^4$, in case of superconducting walls even Q ≈ 10^{10}!

- After Q / 2 π periods the stored energy decayed to about 37% of its initial value, i.e. ≈ 10^4 and ≈ 10^9 periods respectively, $P_n(t) \propto \exp\left(-\omega_n t / Q_n\right)$

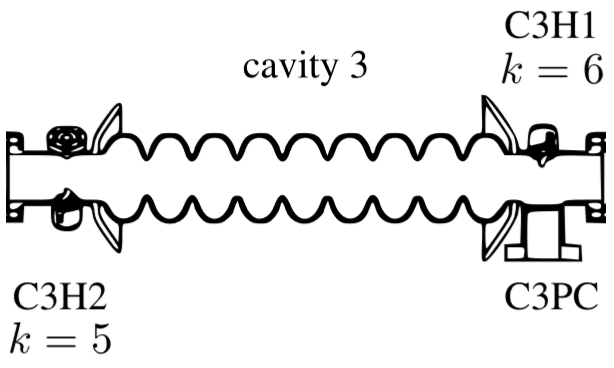
- A typical discretization in time domain with 20 time steps per period, results in 10^5 and 10^{10} discrete time steps ☹

Time domain approaches not well-suited for computing scattering matrices of structures with large quality factors!

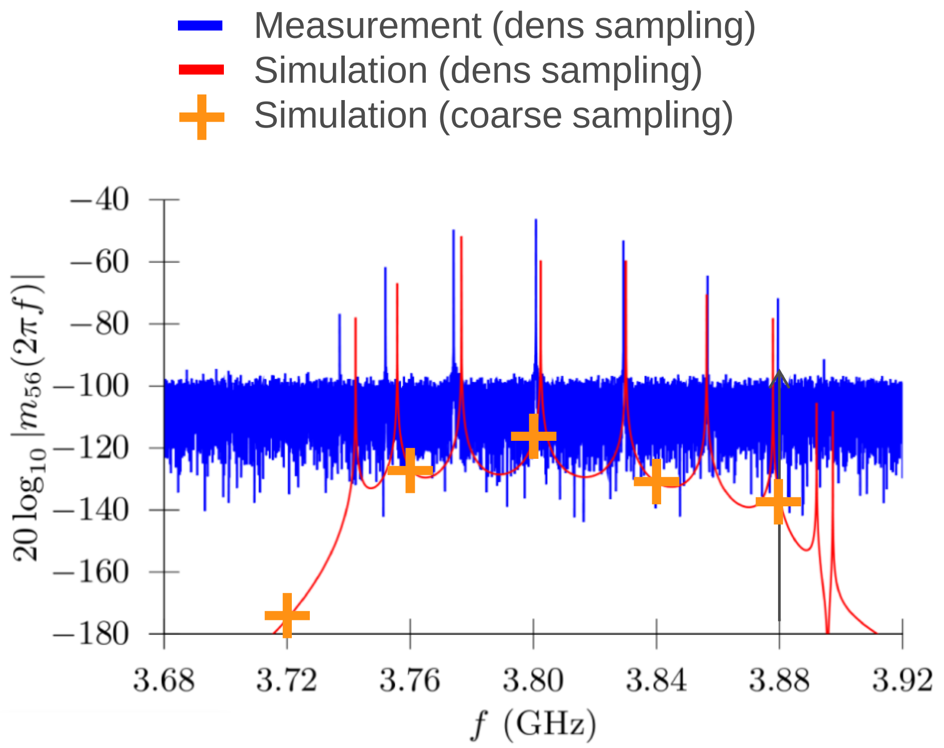
Large Quality Factors in Frequency Domain

- Frequency approaches assume steady state, i.e. no issues with long transients resulting from large quality factors ☺
- However, large quality factors result in sharp resonance peaks in spectra ($\Delta f = f_0/Q$), requiring a sufficient number of samples in frequency domain
- Each sample of scattering matrix requires solution of a large, sparse and complex-valued system of linear equations ☹
- Eigenmode computations deliver resonant frequencies (of non-excited closed structure), but do not (directly) provide network matrices

Straightforward frequency domain approaches not so well-suited to compute scattering matrices of structures with large quality factors!



E. Vogel et al., in Proceedings of the International Particle Accelerator Conference, Kyoto, Japan (ICR, Kyoto, 2010), pp. 4281–4283

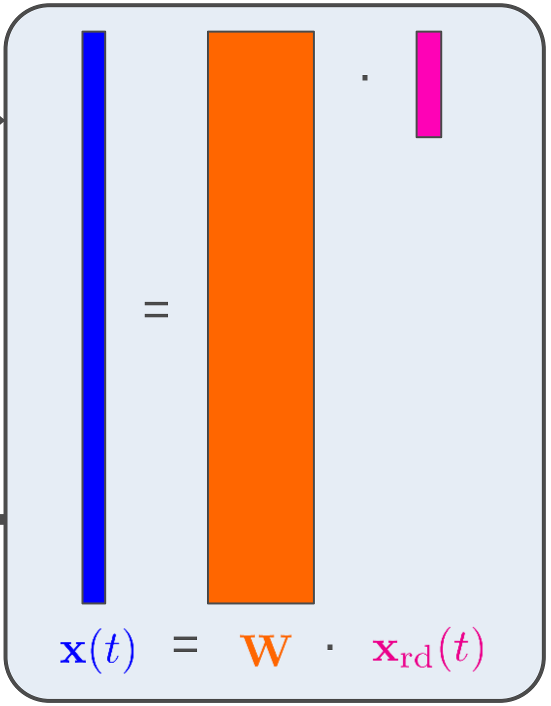


T. Flisgen, H.-W. Glock, P. Zhang, I. R.R. Shinton, N. Baboi, R. M. Jones, and U. van Rienen, Scattering parameters of the 3.9 GHz accelerating module in a free-electron laser linac: A rigorous comparison between simulations and measurements, Phys. Rev. ST Accel. Beams 17, 2014

Model-Order Reduction

Reduction of State-Space Model resulting from Spatial Discretization

$$\mathbf{M}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}(t) = \mathbf{A}\mathbf{x}(t)+\mathbf{B}\mathbf{i}(t)$$
$$\mathbf{v}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{D}\mathbf{i}(t)$$



$$\underbrace{\mathbf{W}^{\mathrm{T}}\mathbf{M}\mathbf{W}}_{\mathbf{M}_{\mathrm{rd}}}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{x}_{\mathrm{rd}}(t) = \underbrace{\mathbf{W}^{\mathrm{T}}\mathbf{A}\mathbf{W}}_{\mathbf{A}_{\mathrm{rd}}}\mathbf{x}_{\mathrm{rd}}(t)+\underbrace{\mathbf{W}_{r}^{\mathrm{T}}\mathbf{B}}_{\mathbf{B}_{\mathrm{rd}}}\mathbf{i}(t)$$
$$\mathbf{v}(t) = \underbrace{\mathbf{C}\mathbf{W}}_{\mathbf{C}_{\mathrm{rd}}}\mathbf{x}_{\mathrm{rd}}(t) + \mathbf{D}\mathbf{i}(t)$$

State-vector: $\mathbf{x}(t) \in \mathbb{R}^{N}, N \approx 10^5 \ldots 10^8$

Reduced state-vector: $\mathbf{x}_{\mathrm{rd}}(t) \in \mathbb{R}^{N_{\mathrm{rd}}}, N_{\mathrm{rd}} \approx 10^2$

Orthogonal projection*: $\mathbf{W} \in \mathbb{R}^{N \times N_{\mathrm{rd}}}, \mathbf{W}^{\mathrm{T}}\mathbf{W} = \mathbf{I}$, e.g. obtained by incomplete eigendecomposition, singular-value decomposition etc.

Peter Benner, Mario Ohlberger, Albert Cohen, and Karen Willcox, Model Reduction and Approximation, Society for Industrial and Applied Mathematics, 2017

Transfer of Reduced State-Space Equation to Frequency Domain

- Transfer of reduced-order equation (resulting from FEM or FIT)

$$\mathbf{M}_{\mathrm{rd}} \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{x}_{\mathrm{rd}}(t) = \mathbf{A}_{\mathrm{rd}}\, \mathbf{x}_{\mathrm{rd}}(t) + \mathbf{B}_{\mathrm{rd}}\, \mathbf{i}(t)$$

to frequency domain gives

$$\mathbf{M}_{\mathrm{rd}} j\omega \underline{\mathbf{x}}_{\mathrm{rd}}(j\omega) = \mathbf{A}_{\mathrm{rd}}\, \underline{\mathbf{x}}_{\mathrm{rd}}(j\omega) + \mathbf{B}_{\mathrm{rd}}\, \underline{\mathbf{i}}(j\omega)$$

- Resorting yields complex-valued (comparably small) system of linear equations

$$\underbrace{[j\omega \mathbf{M}_{\mathrm{rd}} - \mathbf{A}_{\mathrm{rd}}]}_{\underline{\mathbf{G}}(j\omega) \in \mathbb{C}^{N_{\mathrm{rd}} \times N_{\mathrm{rd}}}} \underline{\mathbf{x}}_{\mathrm{rd}}(j\omega) = \underbrace{\mathbf{B}_{\mathrm{rd}}\, \underline{\mathbf{i}}(j\omega)}_{\underline{\mathbf{b}}(j\omega) \in \mathbb{C}^{N_{\mathrm{rd}}}}, \qquad N_{\mathrm{rd}} \approx 10^2$$

- Formally sorting for state-vector gives:

$$\underline{\mathbf{x}}_{\mathrm{rd}}(j\omega) = [j\omega \mathbf{M}_{\mathrm{rd}} - \mathbf{A}_{\mathrm{rd}}]^{-1}\, \mathbf{B}_{\mathrm{rd}}\, \underline{\mathbf{i}}(j\omega)$$

- Combining with output equation allows for *fast frequency sweeps* of (in this case) impedance matrix:

$$\mathbf{v}(t) = \underbrace{\left(\mathbf{C}_{\mathrm{rd}}\, [j\omega \mathbf{M}_{\mathrm{rd}} - \mathbf{A}_{\mathrm{rd}}]^{-1}\, \mathbf{B}_{\mathrm{rd}} + \mathbf{D}\right)}_{\underline{\mathbf{Z}}(j\omega)} \mathbf{i}(t)$$

Some Remarks

Finite Integration Technique (FIT)

- Directly discretize Maxwell’s equations in integral form
- Use field components and fluxes, respectively, on a structured grid
- Requiring low storage due to simple band structures of arising matrices
- Sometimes still with staircase approximation on Cartesian grids [CST Studio Suite® using FIT with “perfect boundary approximation” (PBA)®]
- Explicit formulations naturally arise for time-domain problems, since matrix acting on the vector with time-derivates is diagonal and thus easy to invert

Slide courtesy of U. van Rienen / University of Rostock

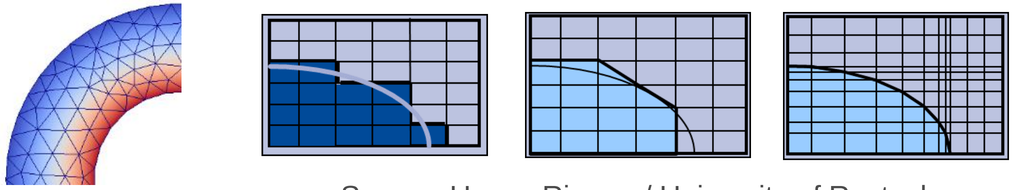
Finite Element Method (FEM)

- Approach based on the weak formulation of the partial differential equation
- Computational domain is divided into unstructured mesh (very flexible)
- Intrinsically easier to approximate curved boundaries due to unstructured mesh
- May be considerably slower than FIT for time-domain problems caused by the implicit problems arising
- Very often used for eddy-current problems and time-harmonic problems
- Several further developments like the Discontinuous Galerkin FEM (DG-FEM)
- Higher order approximations intrinsically easier to achieve than in FIT

Slide courtesy of U. van Rienen / University of Rostock

Errors Sources in Numerical Simulations

- **Modell Errors:**
  - Errors arising during creation of mathematical model such as linearization and homogenization of material properties, surface loss models or neglecting losses for good conductors etc.
- **Errors in Solving the Mathematical Problem:**
  - Geometry error introduced by mapping geometry to discrete mesh

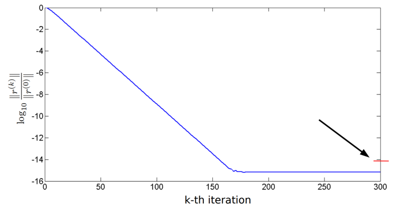


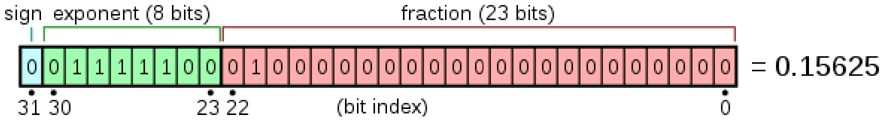
Source: U. van Rienen / University of Rostock

  - Error from discretization of derivations or from approximation continuous quantities by discrete ones, e.g. error using central differences

$$\frac{\mathrm{d}}{\mathrm{d}x} f(x) = \frac{f(x+h/2) - f(x-h/2)}{h} + \mathcal{O}(h^2)$$

  - Numerical errors resulting from finite accuracy of floating point operations as well as errors resulting from stopping criteria of iterative solvers for systems of linear equations





Source: https://en.wikipedia.org/wiki/File:Float_example.svg

Setting up Simulation of a New Problem

- Setting up simulations for problems one is (not yet) used to is sometimes not straightforward
- Nowadays packages such as CST Studio Suite® (refer to talk by Frank Demming-Janssen in the evening) are very flexible and support various methods **Finite Integration Technique**, **Finite Element method**, **Methods of Moments** etc., various meshes such as **hexahedral** or **tetrahedral**, **time domain** and **frequency domain** methods
- For each solver, for each mesh type, for frequency and time domain methods, there is a large number of options, whereas the default option is not always the best
- Sometimes (or often?) the meaning and the effect of the respective options is not fully clear, since the software is a kind of black box and help files are not always informative/conclusive
- Typically and naturally, various attempts are required to figure out a reasonable setup for the simulation for a specific problem
- BUT: How to decide whether a solution is reasonable? We do not know the solution, if we would know, there is no need for simulation?!

Validation and Critical Assessment of Results

- Never ever blindly believe in the solutions provided by numerical codes, since inappropriate assumptions, and/or inappropriate methods and/or wrong settings for the problem under study can lead to unreasonable results
- Use as much as possible knowledge from theory related to your problem! Despite the fact that closed-analytical formulas are often not available, theory knowledge is very helpful to assess validity of results (e.g. conservation of energy, reciprocity, causality etc.) → sanity check
- Use models with different accuracy (e.g. simple analytical models from theory and numerical models with different settings) in parallel and see whether they deliver similar/comparable results
- Always read the solver log file! It provides valuable information! Carefully account for warnings, not just for errors!
- If waveguide ports are used to excite domain with rectangular, circular or coaxial waveguides, do compare cutoff frequencies and propagation constants with analytical values
- Use all possibilities to compare simulations with measurements (future simulations can benefit from these comparisons)
- If it is not possible to obtain a reasonable agreement, problem is not well understood, carefully evaluate how simulations and/or measurements might be improved

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- Peter Benner, Mario Ohlberger, Albert Cohen, and Karen Willcox, Model Reduction and Approximation, Society for Industrial and Applied Mathematics, 2017

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Backup

Frequency Domain Solutions with FIT

$$\mathbf{C}\mathbf{D}_s\mathbf{e} = -\mathbf{D}_A\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{b}$$

$$\mathbf{C}\mathbf{D}_s\mathbf{e} = -\mathbf{D}_A\mathbf{D}_\mu\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{h} \qquad \Big|\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\cdot$$

$$\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{e} = -\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{h} \qquad \Big|\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\cdot$$

$$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{e} = -\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{h}$$

$$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{e} = -\tilde{\mathbf{D}}_A\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathbf{d} - \tilde{\mathbf{D}}_A\mathbf{D}_\sigma\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e} - \tilde{\mathbf{D}}_A\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{j}$$

$$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\mathbf{e} = -\tilde{\mathbf{D}}_A\mathbf{D}_\varepsilon\frac{\mathrm{d}^2}{\mathrm{d}t^2}\mathbf{e} - \tilde{\mathbf{D}}_A\mathbf{D}_\sigma\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{e} - \tilde{\mathbf{D}}_A\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{j}$$

$$\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s\underline{\mathbf{e}} = \omega^2\tilde{\mathbf{D}}_A\mathbf{D}_\varepsilon\underline{\mathbf{e}} - j\omega\tilde{\mathbf{D}}_A\mathbf{D}_\sigma\underline{\mathbf{e}} - j\omega\tilde{\mathbf{D}}_A\underline{\mathbf{j}}$$

$$\underbrace{\left[\tilde{\mathbf{C}}\tilde{\mathbf{D}}_s\mathbf{D}_\mu^{-1}\mathbf{D}_A^{-1}\mathbf{C}\mathbf{D}_s - \omega^2\tilde{\mathbf{D}}_A\mathbf{D}_\varepsilon + j\omega\tilde{\mathbf{D}}_A\mathbf{D}_\sigma\right]}_{\underline{\mathbf{G}}(\omega)\in\mathbb{C}^{3N_\mathrm{P}\times 3N_\mathrm{P}}}\underline{\mathbf{e}} = \underbrace{-j\omega\tilde{\mathbf{D}}_A\underline{\mathbf{j}}}_{\underline{b}(\omega)\in\mathbb{C}^{3N_\mathrm{P}}}$$

Frequency Domain Solutions with FEM

$$\sum_{j=1}^{N} s_{ij}\, x_j(t) + \sum_{j=1}^{N} m_{ij} \frac{\partial^2}{\partial t^2} x_j(t) = -\frac{\partial}{\partial t} p_i(t) - \sum_{j=1}^{N} k_{ij} \frac{\partial}{\partial t} x_j(t), \quad i = 1, \ldots, N$$

$$\sum_{j=1}^{N} s_{ij}\, \underline{x}_j - \omega^2 \sum_{j=1}^{N} m_{ij}\, \underline{x}_j = -j\omega \underline{p}_i - j\omega \sum_{j=1}^{N} k_{ij}\, \underline{x}_j, \quad i = 1, \ldots, N$$

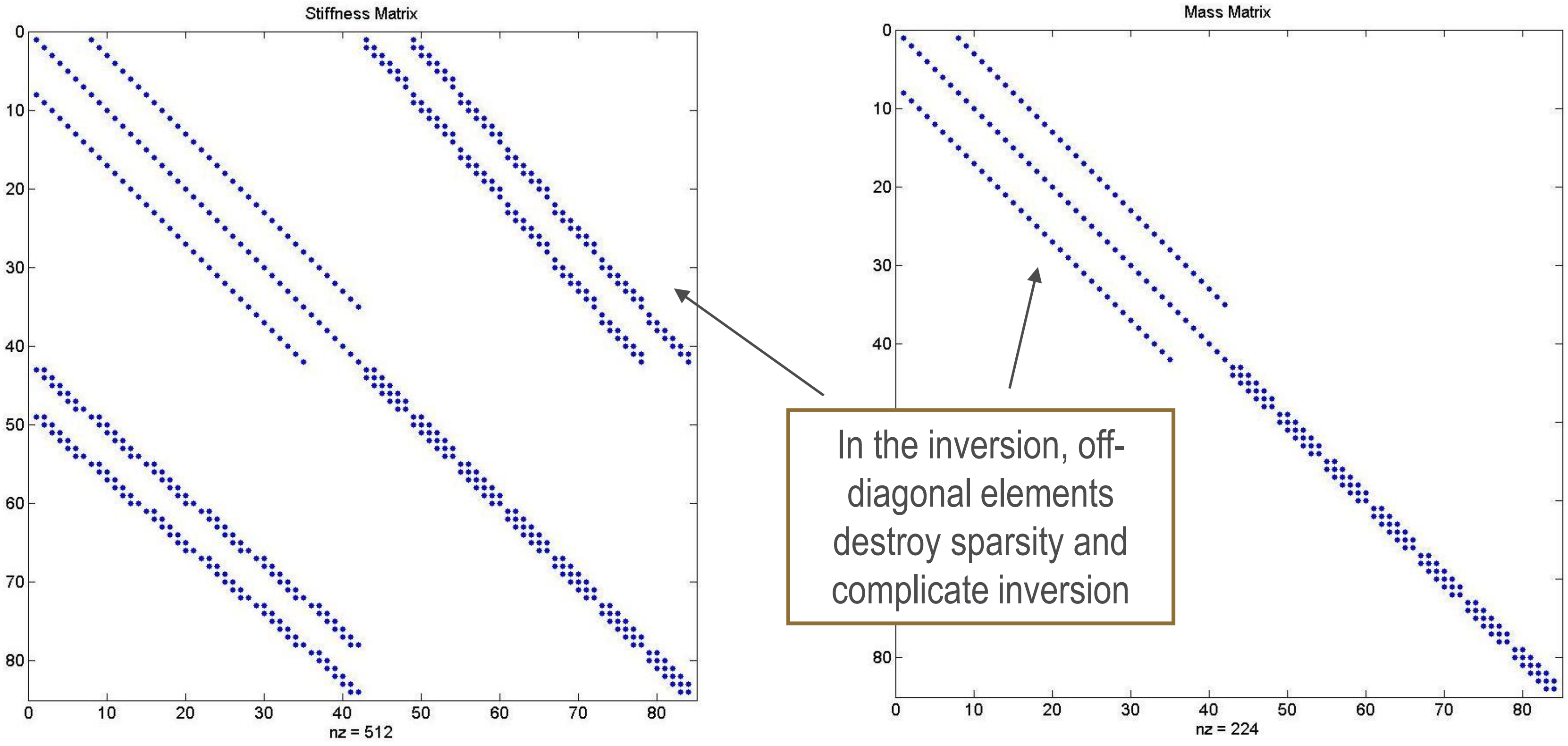
$$\sum_{j=1}^{N} \underbrace{\left(s_{ij} - \omega^2 m_{ij} + j\omega k_{ij}\right)}_{\underline{g}_{ij}(\omega)} \underline{x}_j = \underbrace{-j\omega \underline{p}_i}_{\underline{b}_i(\omega)}, \quad i = 1, \ldots, N$$

$$\underbrace{\begin{pmatrix} \underline{g}_{11}(\omega) & \underline{g}_{12}(\omega) & \underline{g}_{13}(\omega) & \cdots & \underline{g}_{1N}(\omega) \\ \underline{g}_{21}(\omega) & \underline{g}_{22}(\omega) & \underline{g}_{23}(\omega) & \cdots & \underline{g}_{2N}(\omega) \\ \underline{g}_{31}(\omega) & \underline{g}_{32}(\omega) & \underline{g}_{33}(\omega) & \cdots & \underline{g}_{3N}(\omega) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \underline{g}_{N1}(\omega) & \underline{g}_{N2}(\omega) & \underline{g}_{N3}(\omega) & \cdots & \underline{g}_{NN}(\omega) \end{pmatrix}}_{\underline{\mathbf{G}}(\omega) \in \mathbb{C}^{N \times N}} \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \underline{x}_3 \\ \vdots \\ \underline{x}_N \end{pmatrix} = \underbrace{\begin{pmatrix} \underline{b}_1(\omega) \\ \underline{b}_2(\omega) \\ \underline{b}_3(\omega) \\ \vdots \\ \underline{b}_N(\omega) \end{pmatrix}}_{\underline{\mathbf{b}}(\omega) \in \mathbb{C}^{N}}$$

Frequency Domain Solutions with FEM

Example: Eigenfrequencies of a rectangular cavity

Assembly of the stiffness matrix **S** and mass matrix **M**

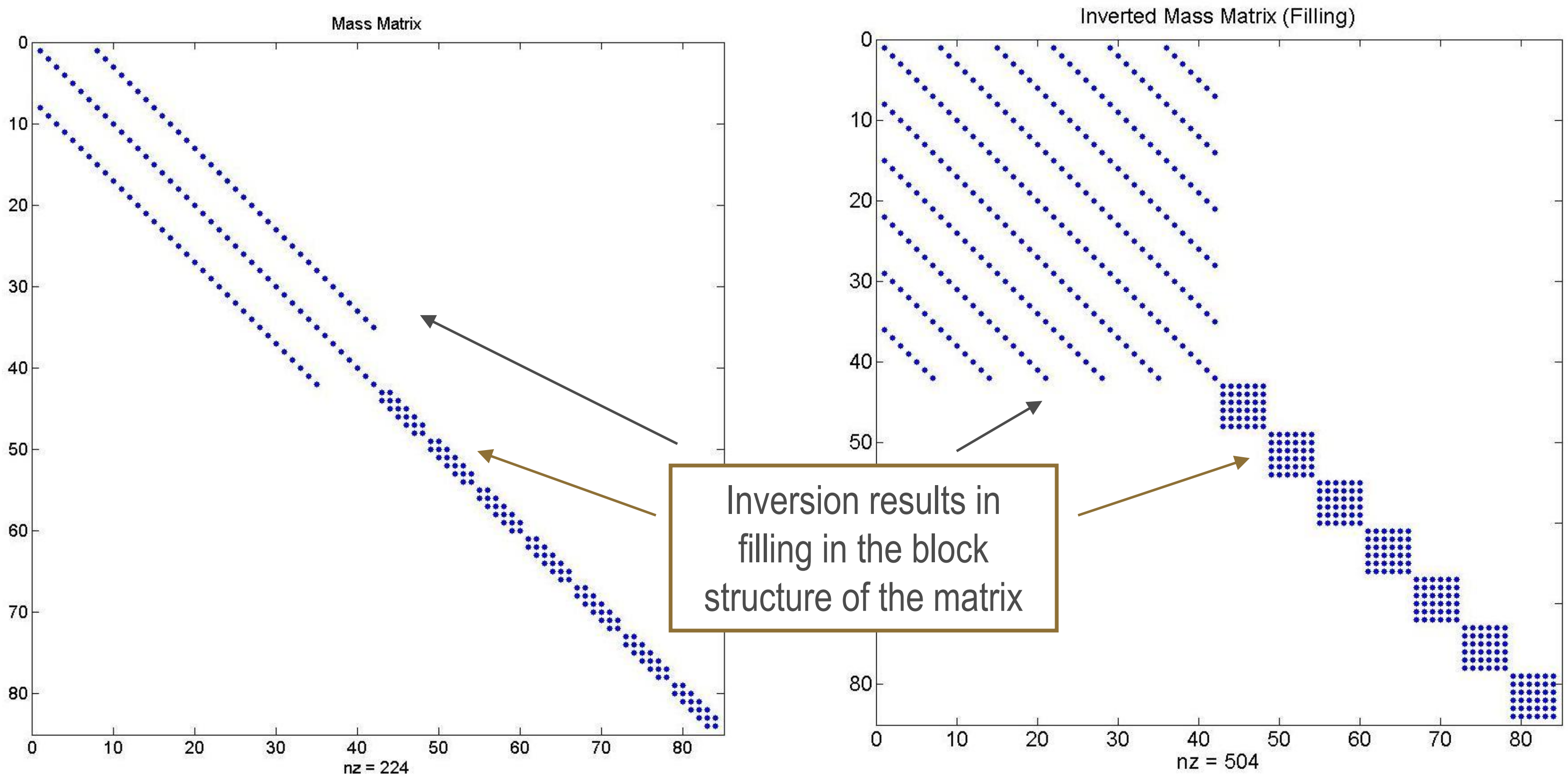


Simulation and pictures: Johann Heller

Frequency Domain Solutions with FEM

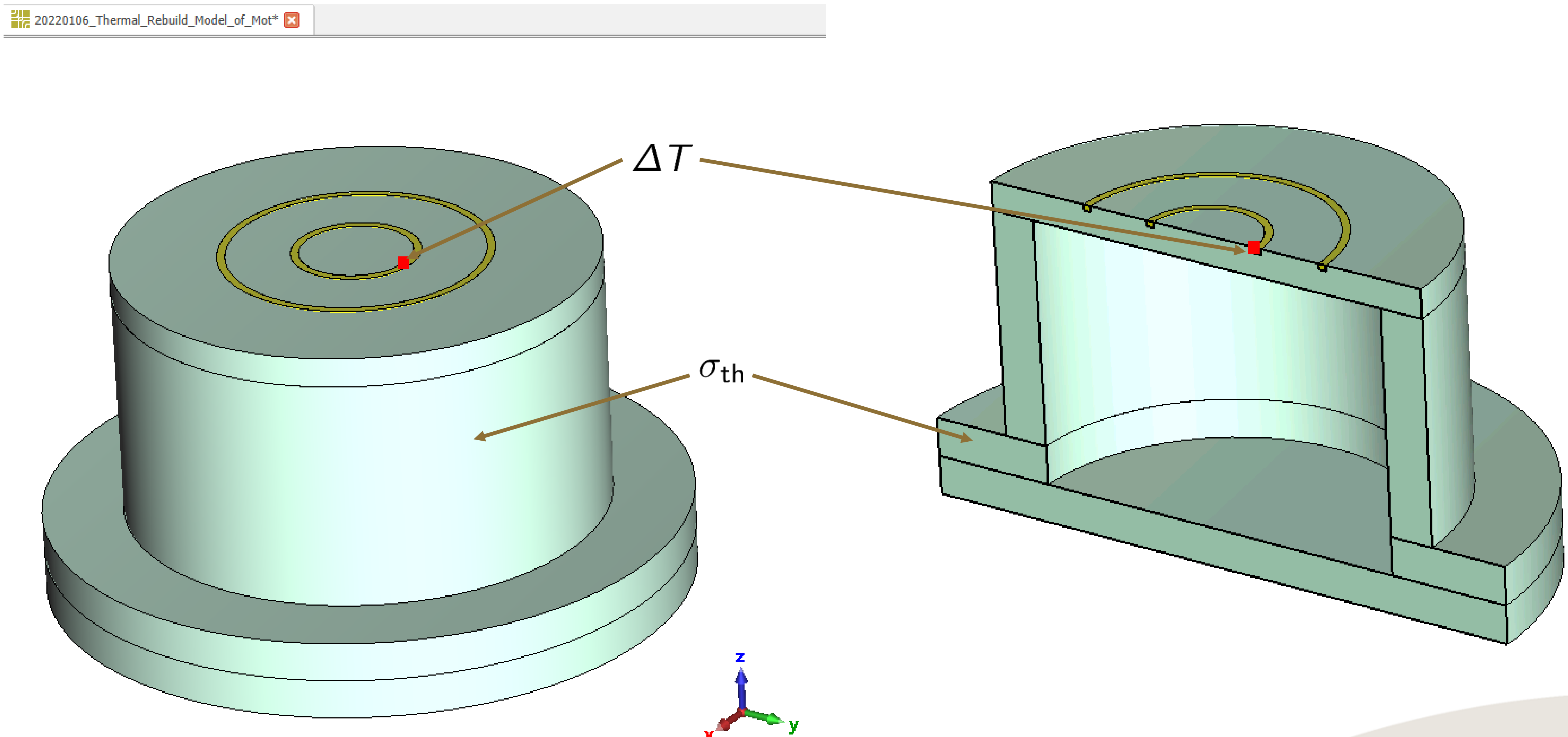
Example: Eigenfrequencies of a rectangular cavity

- Inversion of the mass matrix **M** is slow due to off-diagonal elements
- Inversion also leads to „filling“ of the matrix (destroying its sparse property)



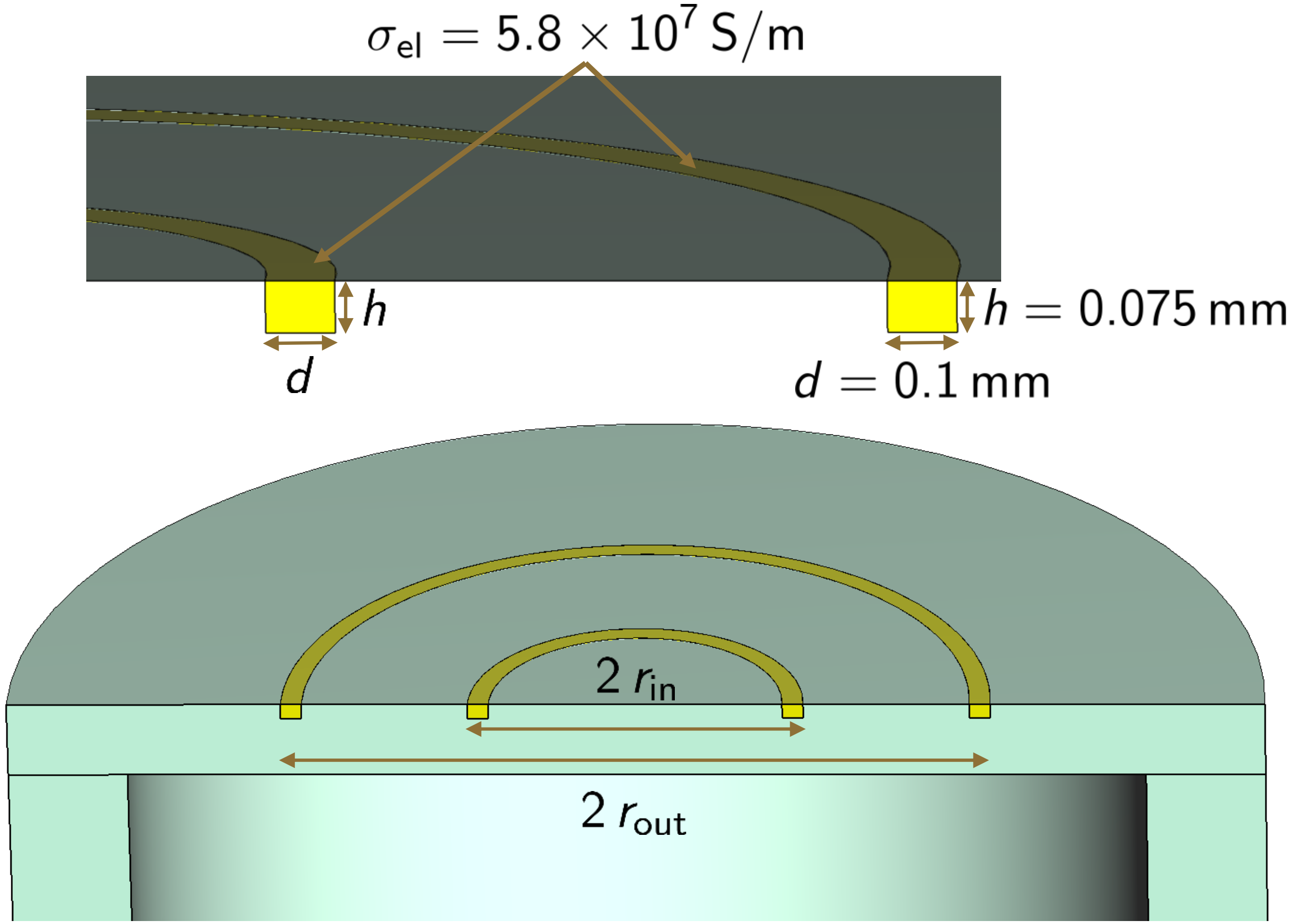
Simulation and pictures: Johann Heller

Thermal Model of Miniaturized MOT



Thermal Ground

Heat Sources of Thermal Model of Miniaturized MOT



Power density in loops:

$$p = EJ = \frac{1}{\sigma_{el}} J^2 = \frac{1}{\sigma_{el}} \left(\frac{I}{hd} \right)^2 = \frac{1}{\sigma_{el} h^2 d^2} I^2$$

Loop volumes:

$$V = \pi \left[r^2 - (r-d)^2 \right] h = \pi (2r - d) hd$$

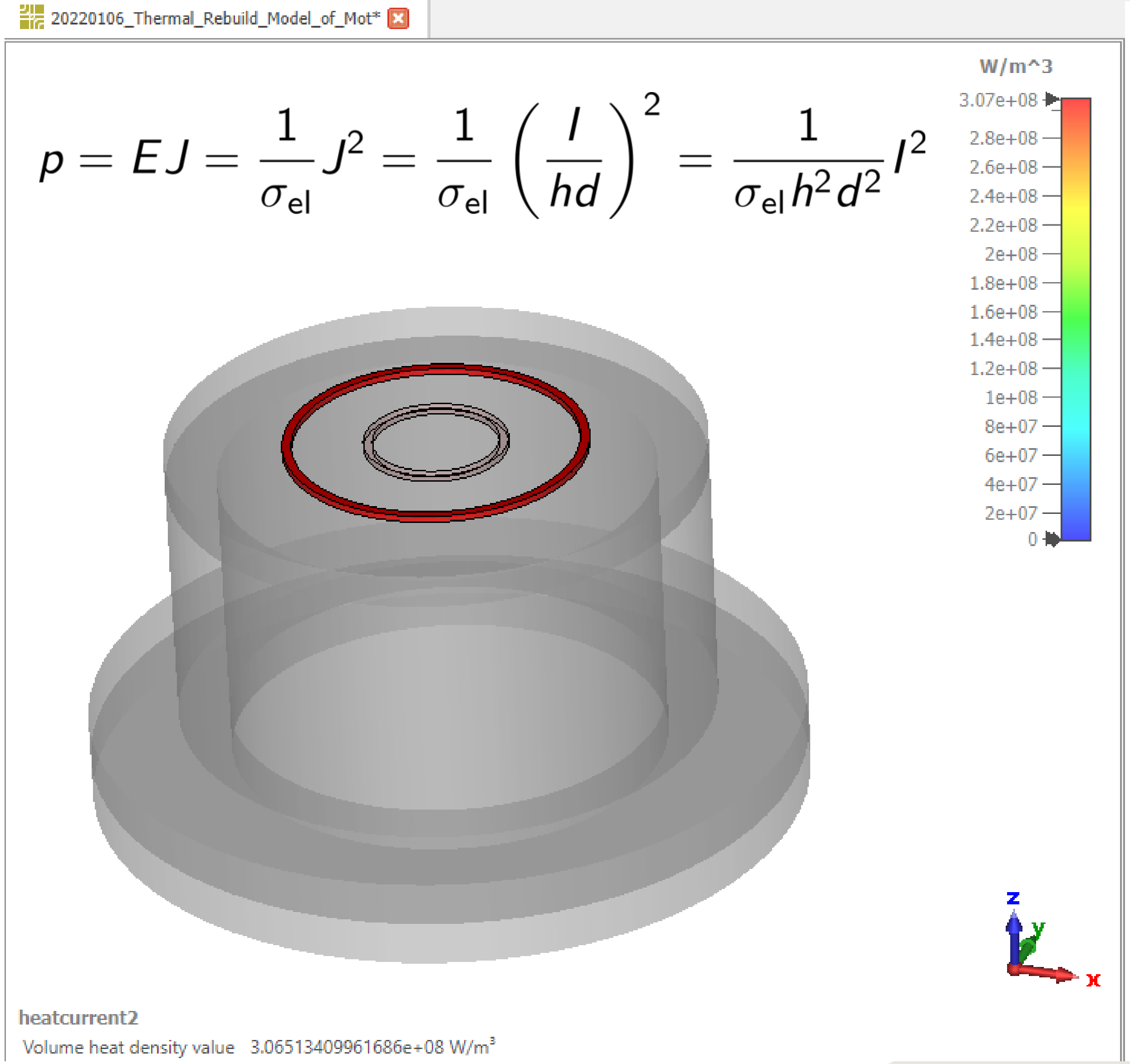
Total heat power inner and outer loop

$$P_{in} = pV_{in} = \frac{\pi(2r_{in} - d)}{\sigma_{el} hd} I^2 = 10.83\,\mathrm{m}\Omega I^2$$

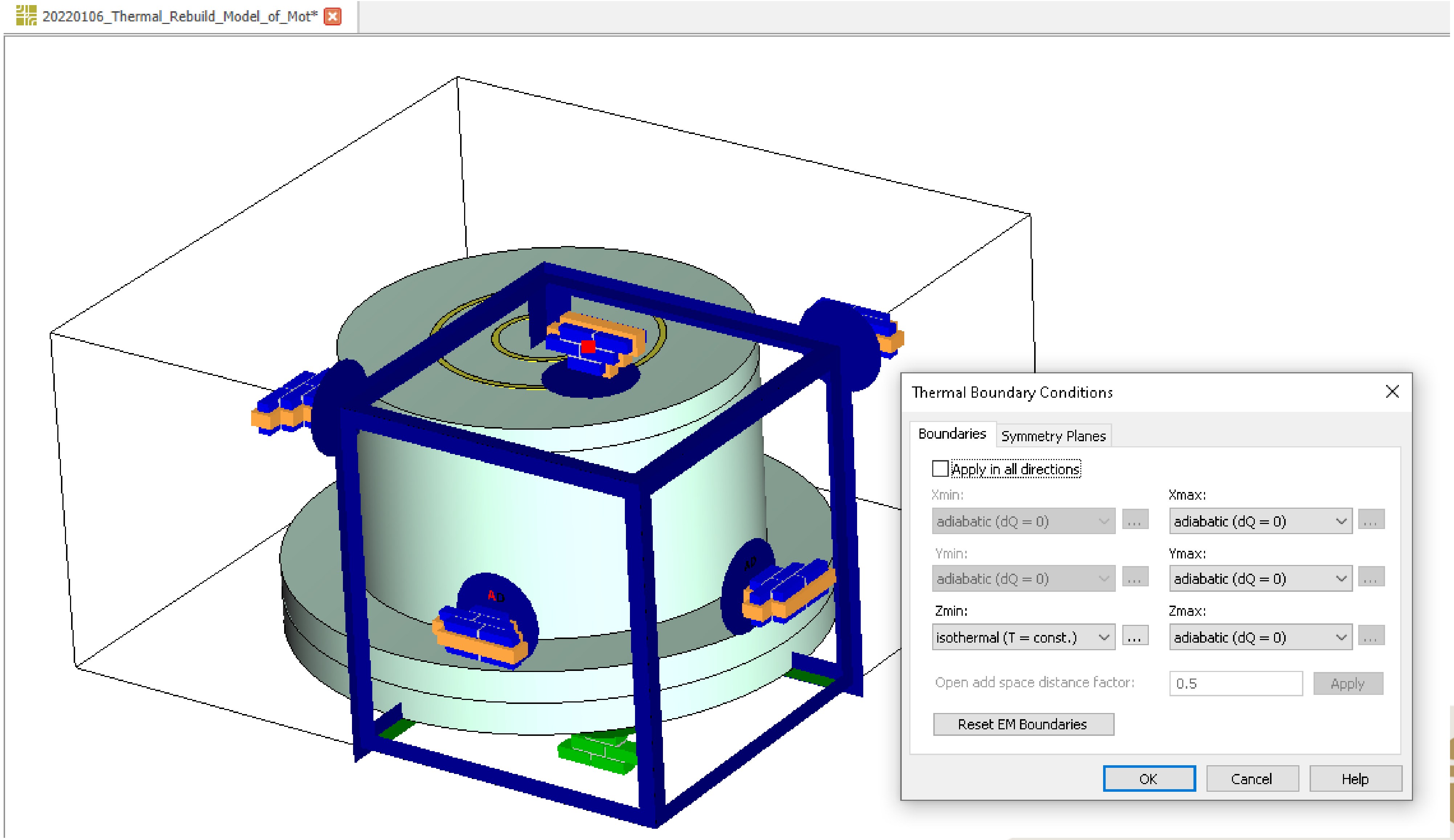
$$P_{out} = pV_{out} = \frac{\pi(2r_{out} - d)}{\sigma_{el} hd} I^2 = 23.72\,\mathrm{m}\Omega I^2$$

Heat Sources of Thermal Model of Miniaturized MOT for I = 1 A

$$p = EJ = \frac{1}{\sigma_{\mathrm{el}}} J^2 = \frac{1}{\sigma_{\mathrm{el}}} \left(\frac{I}{hd} \right)^2 = \frac{1}{\sigma_{\mathrm{el}} h^2 d^2} I^2$$



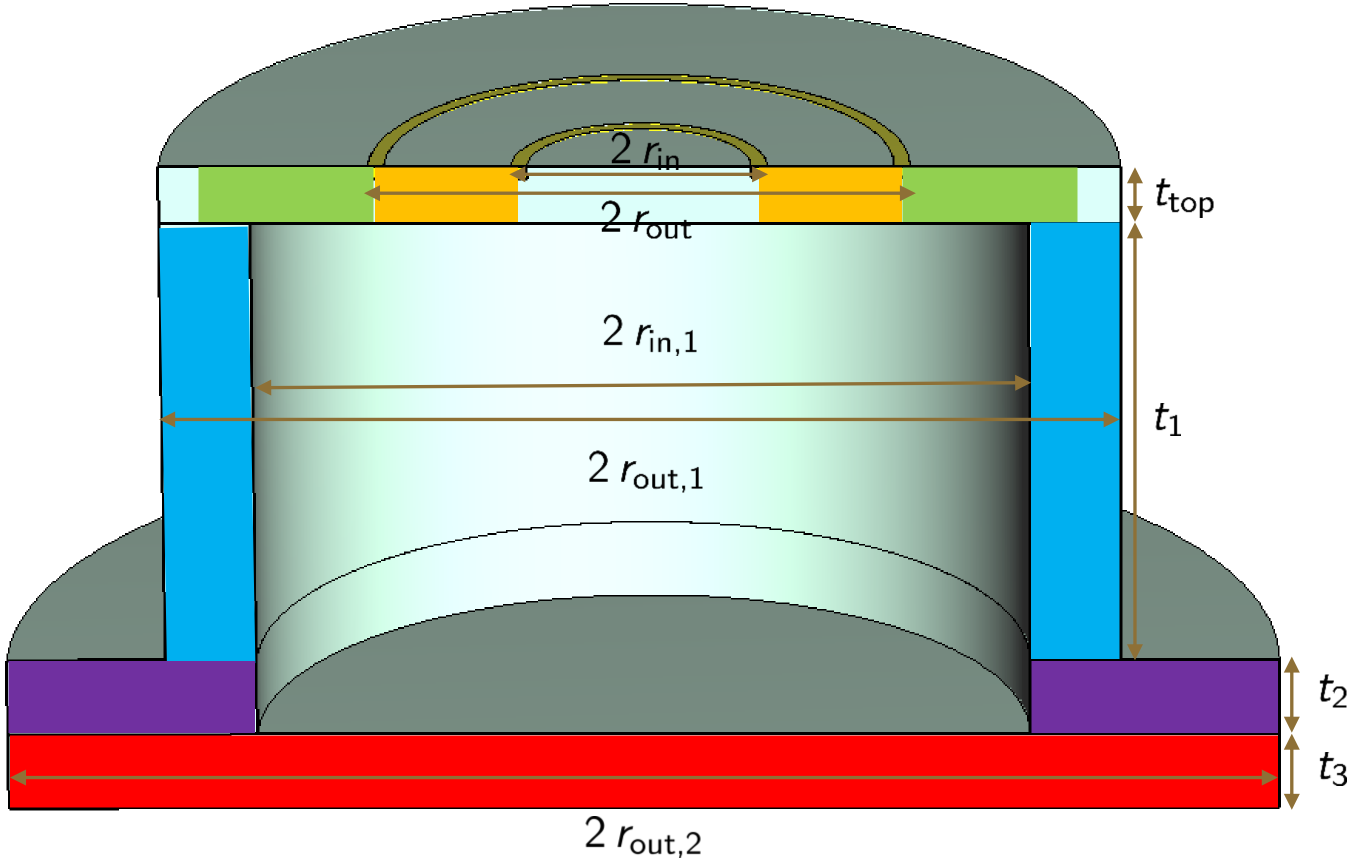
Thermal Model of Miniaturized MOT – Boundary and Symmetry Conditions

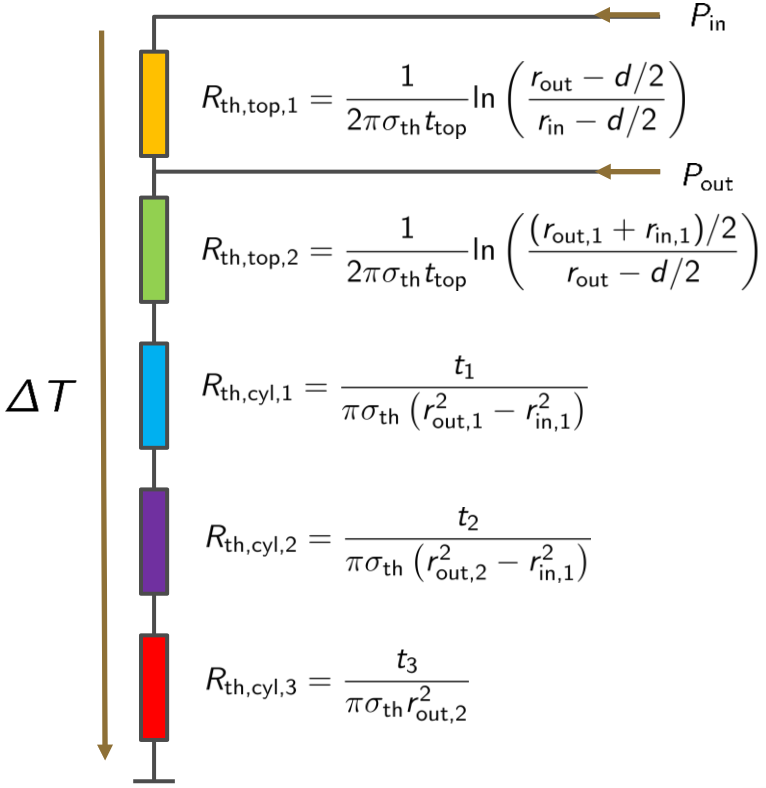


Analytical Thermal Model of Miniaturized MOT

$$\Delta T = (R_{th,top,2} + R_{th,cyl,1} + R_{th,cyl,2} + R_{th,cyl,3})(P_{in} + P_{out}) + R_{th,top,1}\, P_{in}$$

$$\Delta T = \frac{1}{\sigma_{th}} 19.82\, \frac{\mathrm{W}}{\mathrm{mA}^2}\, I^2$$





Temperature in Inner Loop in Dependency on Current

Material	σ_{th} [W/K/m]	g_{CST} [K/A^2]	g_{ana} [K/A^2]
Silicon	148	0.14155	0.13393
AlNi	321	0.06553	0.06175
Al_2O_3	30	0.69066	0.66070
Sapphire	42	0.49413	0.47193