Sandia National Laboratories

Matching algorithms with physics: exact sequences of finite element spaces

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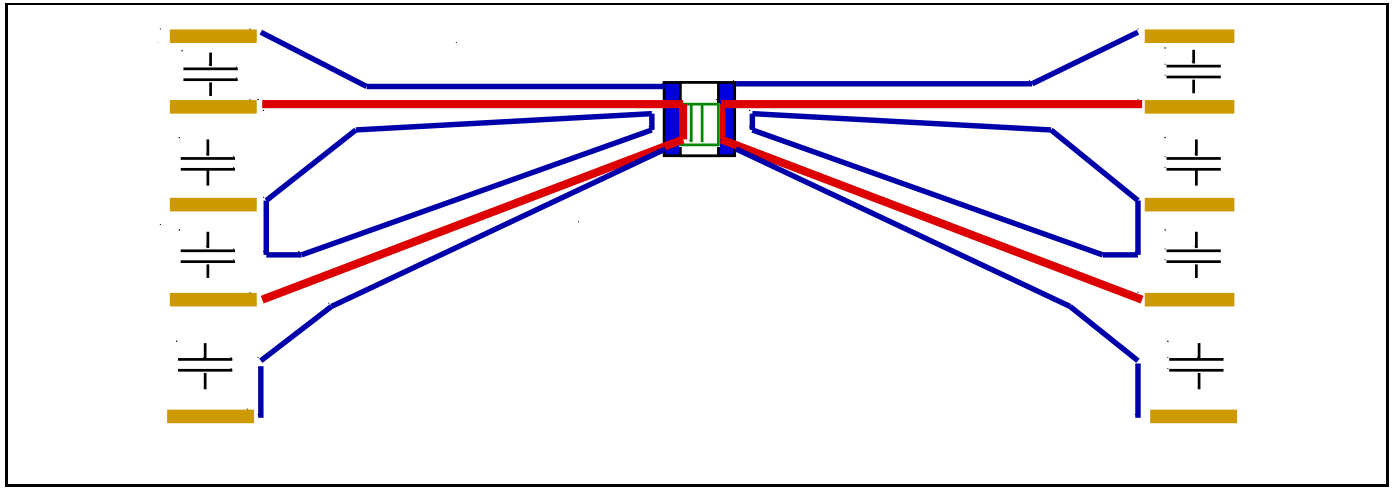
Outline

- The z-pinch: a simple idea with a complicated model
- Stability of multiphysics models: "the world is not enough"
- Magnetic Diffusion I: the rise and fall of potentials
  - Two or one potentials?
  - The art of gauging
  - So what went wrong (and why)??
- Magnetic Diffusion II: Matching algorithms with the physics:
  - De Rham complex and Tonti diagrams
  - Discrete De Rham complex
  - It works!!

Z-Pinch Physics on Z at Sandia



Z-pinch Components

- radiation transport
- electromechanics
- solid dynamics

→ **resistive MHD** → **magnetic diffusion**

Allegra

- A parallel ALE coupled physics code
- unstructured hexahedral grids

Hydro

mass	$\rightarrow$	$\dot{\rho} + \rho \nabla \cdot \mathbf{u}$	$=$	0
momentum	$\rightarrow$	$\rho \dot{\mathbf{u}} - \nabla \cdot \mathbf{T}$	$=$	0
energy	$\rightarrow$	$\dot{e} - \mathbf{T} : \nabla \mathbf{u}$	$=$	0
constitutive eq.	$\rightarrow$	$\mathbf{T} + p(\rho, e)\mathbf{I}$	$=$	0

Magnetics

Ampere	$\rightarrow$	$\nabla \times \mathbf{H} - \mathbf{J}$	$=$	0	$\Longrightarrow$	$\nabla \cdot \mathbf{J} = 0$
Faraday	$\rightarrow$	$\nabla \times \mathbf{E} + \partial \mathbf{B} / \partial t$	$=$	0	$\Longrightarrow$	$\nabla \cdot \mathbf{B} = 0$
Ohm's law	$\rightarrow$	$\mathbf{J} - \sigma \mathbf{E}$	$=$	0		
constitutive eq.	$\rightarrow$	$\mathbf{B} - \mu \mathbf{H}$	$=$	0		

Hydro

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momentum	$\rightarrow$	$\rho \dot{\mathbf{u}} - \nabla \cdot \mathbf{T}$	$=$	$\boxed{\rho_f \mathbf{E} + \mathbf{J} \times \mathbf{B}}$	$\leftarrow$	Lorentz force
energy	$\rightarrow$	$\dot{e} - \mathbf{T} : \nabla \mathbf{u}$	$=$	0		
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Magnetics

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constitutive eq.	$\rightarrow$	$\mathbf{T} + p(\rho, e)\mathbf{I}$	$=$	0		

<u>MHD:</u>		**Magnetics**				**coupling**
Ampere	$\rightarrow$	$\nabla \times \mathbf{H} - \mathbf{J}$	$=$	0		
Faraday	$\rightarrow$	$\nabla \times \mathbf{E} + \partial \mathbf{B} / \partial t$	$=$	$\boxed{-\nabla \times (\mathbf{u} \times \mathbf{B})}$	$\leftarrow$	Induction
Ohm's law	$\rightarrow$	$\mathbf{J} - \sigma \mathbf{E}$	$=$	0		
constitutive eq.	$\rightarrow$	$\mathbf{B} - \mu \mathbf{H}$	$=$	0		

A taxonomy of discretization defects

as stability threats

Strong threats

advection	+	symmetric stencil	=	oscillations
saddle point	+	equal order FE	=	unstable FEM

- A recipe for disaster: loss of stability almost surely will happen

Weak (subtle) threats

$\nabla \cdot \mathbf{B} \neq 0$	$\Longrightarrow$	magnetic monopoles
nonphysical modes	$\Longrightarrow$	tiny nonphysical effects

- May or may not lead to failure
- May be tolerated in simple, single component models

Stability and multiphysics models

In coupled multiphysics models

- <u>ALL discretization defects</u> are potentially dangerous

$\nabla \cdot \mathbf{B} \neq 0$	$\Longrightarrow$	innacurate Lorentz/Joule	$\Longrightarrow$	wrong kinematics/energy
nonphysical modes	$\Longrightarrow$	polluted transients	$\Longrightarrow$	wrong transient/static?

Stability and multiphysics models

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- Remedies that work in simple models are not enough anymore:

advection of $\mathbf{B}$ $\longrightarrow$ upwinding

$\downarrow$

CURRENT REVERSALS $\Longleftarrow$ tiny oscillations

Stability and multiphysics models

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- Remedies that work in simple models are not enough anymore:

$$\begin{array}{ccc} \boxed{\text{advection of } \mathbf{B}} & \longrightarrow & \boxed{\text{upwinding}} \\ & & \downarrow \\ \boxed{\text{CURRENT REVERSALS}} & \Longleftarrow & \boxed{\text{tiny oscillations}} \end{array}$$

Since many of these defects are caused by

inconsistencies between physics and discretizations

a sensible approach would be to

Match physics and discretization!

Magnetic Diffusion: design specifications

Physics:

- state transitions: solid $\rightarrow$ melt $\rightarrow$ plasma
- highly heterogeneous media, especially σ:

  $\sigma_{\text{solid=high}} \quad \rightarrow \quad \sigma_{\text{melt=low}} \quad \rightarrow \quad \sigma_{\text{plasma=high}}$
- **non-static** void-material interface

Required:

- accurate $\mathbf{J} \times \mathbf{B}$ and $\mathbf{J} \cdot \mathbf{E}$
- correct time scale for $\mathbf{B}$ diffusion

Possible approaches:

- use potentials to ensure $\nabla \cdot \mathbf{B} = 0$

Magnetic Diffusion: the candidate model

Differential equations

$$
\begin{aligned}
\nabla \times \mathbf{H} &= \mathbf{J} \quad \text{in } \Omega \quad \leftarrow \quad \text{Ampere} \\
\nabla \cdot \mathbf{J} &= 0 \quad \text{in } \Omega \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \quad \text{in } \Omega \quad \leftarrow \quad \text{Faraday} \\
\nabla \cdot \mathbf{B} &= 0 \quad \text{in } \Omega
\end{aligned}
$$

Boundary conditions

$$
\begin{aligned}
\mathbf{n} \cdot \mathbf{B} &= \mathbf{n} \cdot \mathbf{B}_{\mathrm{b}} \quad \text{and} \quad \mathbf{n} \times \mathbf{E} = \mathbf{n} \times \mathbf{E}_{\mathrm{b}} \quad \text{on } \Gamma^* \text{ (Type } I) \\
\mathbf{n} \times \mathbf{H} &= \mathbf{n} \times \mathbf{H}_{\mathrm{b}} \quad \text{and} \quad \mathbf{n} \cdot \mathbf{J} = \mathbf{n} \cdot \mathbf{J}_{\mathrm{b}} \quad \text{on } \Gamma \text{ (Type } II)
\end{aligned}
$$

Constitutive equations

$$\mathbf{B} = \mu \mathbf{H} \quad \text{and} \quad \mathbf{J} = \sigma \mathbf{E}$$

The two magnetic potentials

In void: $\sigma = 0 \quad \Longrightarrow \quad \mathbf{J} = 0$

1. Faraday's law:

$$\textbf{no current} \quad \Longrightarrow \quad \text{skip!}$$

2. Ampere's Theorem:

$$\nabla \times \mathbf{H} = \mathbf{J} = 0 \qquad \Longrightarrow \qquad \mathbf{H} = \nabla\psi$$

Now substitute $\mathbf{B} = \mu\mathbf{H} = \mu\nabla\psi$:

$$\begin{aligned} \nabla \cdot \mathbf{B} &= 0 \\ \Downarrow & \\ \nabla \cdot \mu\nabla\psi &= 0 \end{aligned}$$

In conductors: $\nabla \cdot \mathbf{B} = 0 \quad \Longrightarrow \quad \mathbf{B} = \nabla \times \mathbf{A}$

1. Faraday's law:

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad \Longrightarrow \quad \nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t}\right) = 0 \quad \Longrightarrow \quad \mathbf{E} = -(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi)$$

2. Ampere's Theorem:

$$\begin{array}{ccc}
\nabla \times \mathbf{H} & = & \mathbf{J} \\
\downarrow & & \downarrow \\
\mathbf{H} = \frac{1}{\mu}\mathbf{B} = \frac{1}{\mu}\nabla \times \mathbf{A} & & \mathbf{J} = \sigma \mathbf{E} = -\sigma(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi) \\
\downarrow & & \downarrow \\
\nabla \times \frac{1}{\mu}\nabla \times \mathbf{A} & = & -\sigma(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi)
\end{array}$$

Add boundary and interface conditions...

Conductor

$$\begin{aligned} \nabla \times \tfrac{1}{\mu}\nabla \times \mathbf{A} + \sigma\left(\tfrac{\partial \mathbf{A}}{\partial t} + \nabla\phi\right) &= 0 && \text{in } \Omega_C \\ \tfrac{1}{\mu}\nabla \times \mathbf{A} \times \mathbf{n} &= \mathbf{H}_b \times \mathbf{n} && \text{on Type 2} \\ \mathbf{n} \times \mathbf{A} &= 0 && \text{on Type 1} \end{aligned}$$

Void

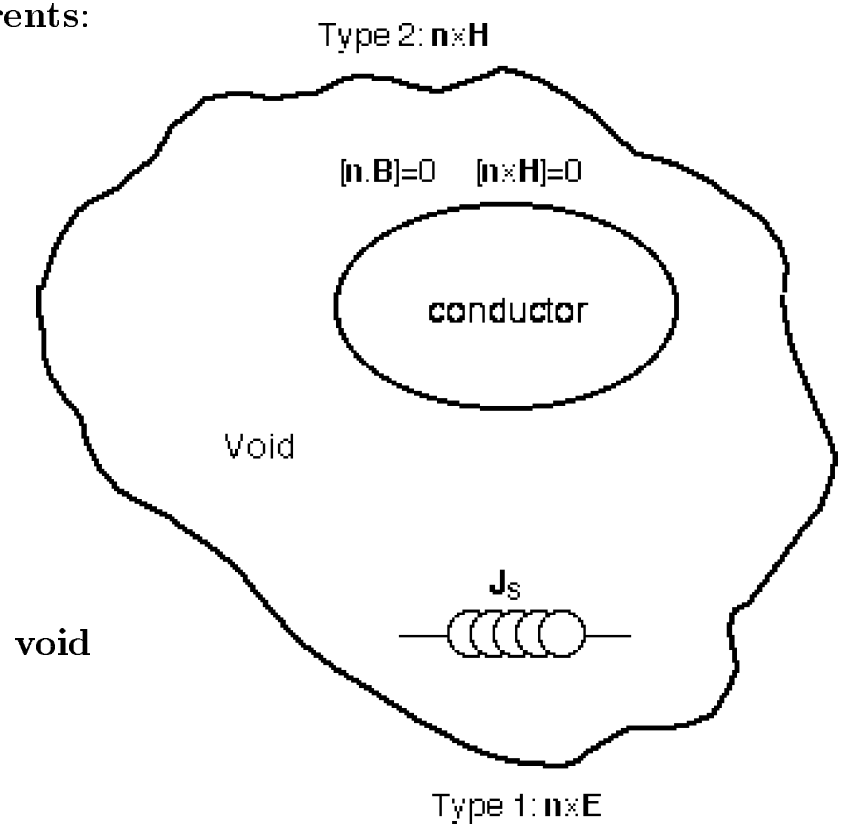
$$\begin{aligned} \nabla \cdot \mu\nabla\psi &= 0 && \text{in } \Omega_{NC} \\ \nabla\psi \times \mathbf{n} &= \mathbf{H}_b \times \mathbf{n} && \text{on Type 2} \end{aligned}$$

Interface Γ_{NC}

$$\begin{aligned} [\mathbf{B} \cdot \mathbf{n}] = 0 \quad &\rightarrow \quad \nabla \times \mathbf{A} \cdot \mathbf{n} = -\mu\nabla\psi \cdot \mathbf{n} \\ [\mathbf{n} \times \mathbf{H}] = 0 \quad &\rightarrow \quad \tfrac{1}{\mu}\nabla \times \mathbf{A} \times \mathbf{n} = -\nabla\psi \cdot \mathbf{n} \end{aligned}$$

The $(\mathbf{A}, \psi)$ approach works great for **eddy-currents**:

$$\sigma = \begin{cases} \sigma(\mathbf{x}) & \text{in conductors} \\ 0 & \text{in void (air)} \end{cases}$$



Interface conditions

$$[\mathbf{n} \cdot \mathbf{B}] = 0 \quad \text{and} \quad [\mathbf{n} \times \mathbf{H}] = 0 \quad \text{on } \Gamma_{NC}$$

The catch

- The static interface between **conductor** and **void**

A remedy

- introduce fudged "void conductivity" to transport $\mathbf{B}$ across void
- discard ψ and use $\mathbf{A}$ everywhere

The price: Must deal with a **single**, highly **heterogeneous** conductor:

$$0 < \sigma_{\min} \leq \sigma(\mathbf{x}, t) \leq \sigma_{\max} \quad \text{and} \quad \sigma_{min} << \sigma_{max}$$

Magnetic vector potential formulations

<u>**Ungauged $\mathbf{A} - \phi$ equations**</u>

$$\nabla \times \frac{1}{\mu} \nabla \times \mathbf{A} + \sigma\left(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi\right) \;=\; 0 \qquad \text{in } \Omega \;\leftarrow \qquad \text{Ampere}$$

$$\frac{1}{\mu} \nabla \times \mathbf{A} \times \mathbf{n} \;=\; \mathbf{H}_b \times \mathbf{n} \quad \text{on } \Gamma$$

Magnetic vector potential formulations

Ungauged $\mathbf{A} - \phi$ equations

$$\nabla \times \tfrac{1}{\mu} \nabla \times \mathbf{A} + \sigma\left(\tfrac{\partial \mathbf{A}}{\partial t} + \nabla \phi\right) = 0 \qquad \text{in } \Omega \quad \leftarrow \qquad \text{Ampere}$$

$$\nabla \cdot \left(\sigma\left(\tfrac{\partial \mathbf{A}}{\partial t} + \nabla \phi\right)\right) = 0 \qquad \text{in } \Omega \quad \leftarrow \qquad \nabla \cdot \mathbf{J} = 0$$

$$\tfrac{1}{\mu} \nabla \times \mathbf{A} \times \mathbf{n} = \mathbf{H}_b \times \mathbf{n} \quad \text{on } \Gamma$$

$$-\sigma\left(\tfrac{\partial \mathbf{A}}{\partial t} + \nabla \phi\right) \times \mathbf{n} = \mathbf{E}_b \times \mathbf{n} \quad \text{on } \Gamma^*$$

- In the static limit $\longrightarrow$ $\begin{cases} \nabla \times \frac{1}{\mu} \nabla \times \mathbf{A} + \sigma \nabla \phi = 0 \\ \nabla \cdot \sigma \nabla \phi = 0 \quad \Rightarrow \quad \phi = 0 \end{cases}$

- *field recovery* is not affected: $\nabla \times \mathbf{A} = \nabla \times (\mathbf{A} + \nabla q)$

- *numerical solution* may be affected:

$$\partial \mathbf{A} / \partial t \mapsto 0 \quad \Longrightarrow \quad \text{ill-conditioned (or singular) FEM linear system}$$

$$\Downarrow$$

reaching the static limit may be problematic

<u>A remedy:</u>

Impose a <u>gauge</u> = a set of conditions ensuring unique potential

Gauged formulations

<u>The Coulomb gauge</u> (Morisue, 82)

$$\begin{aligned} \nabla \cdot \mathbf{A} &= 0 \quad \text{in } \Omega \\ \phi &= 0 \quad \text{on } \Gamma, \text{ or} \\ \mathbf{A} \cdot \mathbf{n} &= 0 \quad \text{on } \Gamma \end{aligned}$$

- preferred for material discontinuities and multiply connected regions;
- hard to satisfy exactly numerically with **nodal** elements;
- enforced by adding **penalty** like terms

The Lorentz gauge (Bryant, Emson, Trowbridge 85-90)

$$\begin{aligned} \nabla \cdot \mathbf{A} &= -\mu\sigma\phi \quad \text{in } \Omega \\ \phi &= 0 \quad \text{on } \Gamma_1 \\ \mathbf{A} \cdot \mathbf{n} &= \kappa^2 \mu\sigma l \phi \quad \text{on } \Gamma_2 \end{aligned}$$

- leads to non-symmetric weak problems unless $\sigma = const$

$\Longrightarrow$ use is restricted to **homogeneous** conductors when it is equivalent to Coulomb gauge (Biro and Preiss 1990).

$$\Downarrow$$

Neither gauge works for us!

<u>Modified A-formulation:</u> Eliminate ϕ (Emson, Simkin 1983)

$$\mathbf{A}^* = \mathbf{A} + \int_0^t \nabla\phi dt \quad \longrightarrow \quad \begin{cases} \nabla \times \mathbf{A}^* = \nabla \times \mathbf{A} \\ \\ \frac{\partial \mathbf{A}^*}{\partial t} = \frac{\partial \mathbf{A}}{\partial t} + \nabla\phi \end{cases}$$

$$\boxed{\nabla \times \frac{1}{\mu} \nabla \times \mathbf{A}^* + \sigma \frac{\partial \mathbf{A}^*}{\partial t} = 0 \quad \text{in } \Omega.}$$

- *implied* gauge: $\nabla \cdot \sigma \mathbf{A}^* = 0 \quad \text{in } \Omega.$
- in the static limit: $\nabla \times \frac{1}{\mu} \nabla \times \mathbf{A}^* = 0$

$\Longrightarrow$ same difficulties arise as with the ungauged equations.

Modified Lorentz gauge (Bochev, Robinson 99, Bossavit 99)

$$\begin{aligned} \nabla \cdot \sigma \mathbf{A} &= -\mu\sigma^2\phi \quad \text{in } \Omega \\ \phi &= 0 \quad \text{on } \Gamma^* \\ \mathbf{A} \cdot \mathbf{n} &= \kappa^2 \mu\sigma l \phi \quad \text{on } \Gamma \end{aligned}$$

$$\boxed{\nabla \times \frac{1}{\mu} \nabla \times \mathbf{A} + \sigma \frac{\partial \mathbf{A}}{\partial t} - \sigma \nabla \left(\frac{1}{\mu\sigma^2} \nabla \cdot \sigma \mathbf{A} \right) = 0 \quad \text{in } \Omega.}$$

- gives symmetric formulations
- works for **smooth** σ but what about highly **heterogeneous** media?

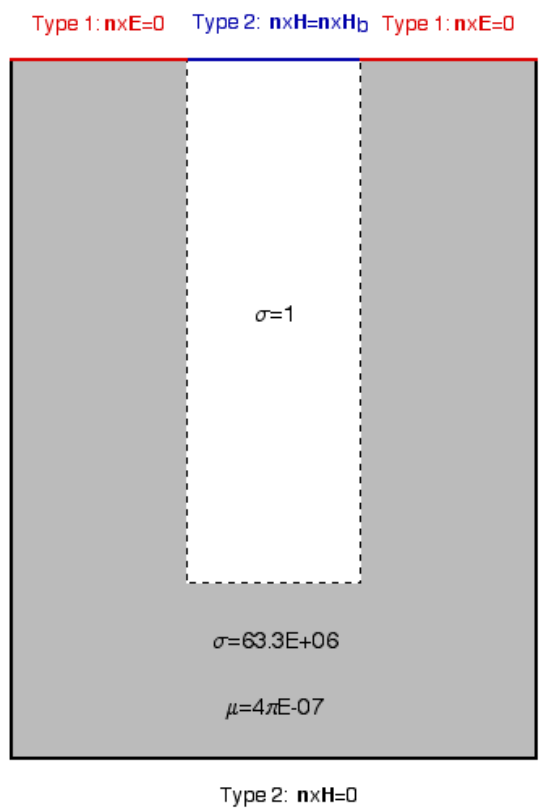
Model Problem in 2D

Setting

- $\mathbf{H} = H_z\mathbf{k}$ and $\mathbf{E} = E_x\mathbf{i} + E_y\mathbf{j}$
- $\mu \sim 4\pi \cdot 10^{-7}$
- $\sigma_{\text{conductor}} = 63.3 \times 10^6$
- $\sigma_{\text{void}} = 1$

What must happen

- $t_{\text{steady}} \approx 50 \times 10^{-6}$sec
- skin current
- "tent" solution at steady state



What happened?

The semi-discrete problem

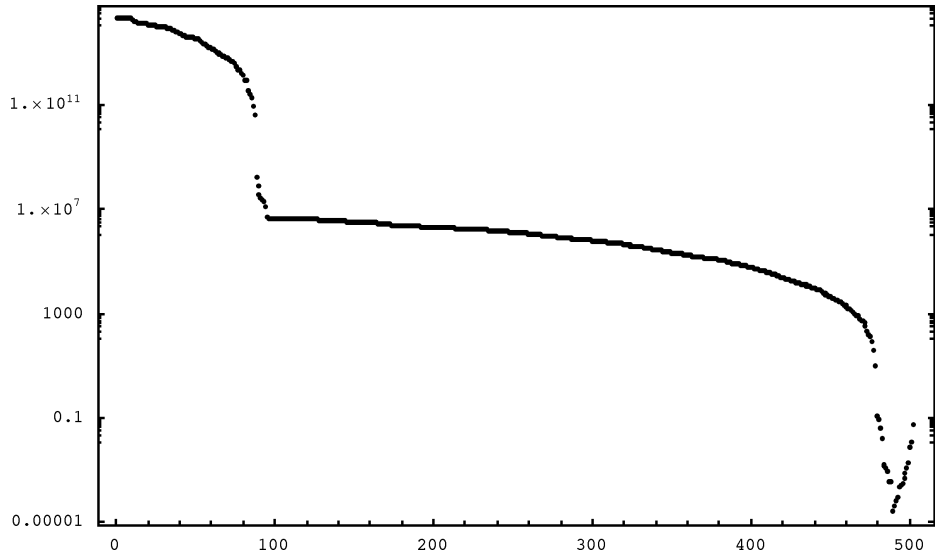
$$\mathbf{M}_\sigma \dot{\mathbf{A}} + \mathbf{C}_\mu \mathbf{A} = \mathbf{f}$$

$$\mathbf{M}_\sigma = (\mathbf{A}, \hat{\mathbf{A}}) \quad \text{and} \quad \mathbf{C}_\mu = (\frac{1}{\mu}\nabla \times \mathbf{A}, \nabla \times \hat{\mathbf{A}}) + \left\{ \begin{array}{c} (\nabla \cdot \mathbf{A}, \nabla \cdot \hat{\mathbf{A}}) \\ (\nabla \cdot \sigma \mathbf{A}, \nabla \cdot \sigma \hat{\mathbf{A}}) \\ \underbrace{\cdots\cdots\cdots\cdots\cdots\cdots}_{\text{gauge contribution}} \end{array} \right.$$

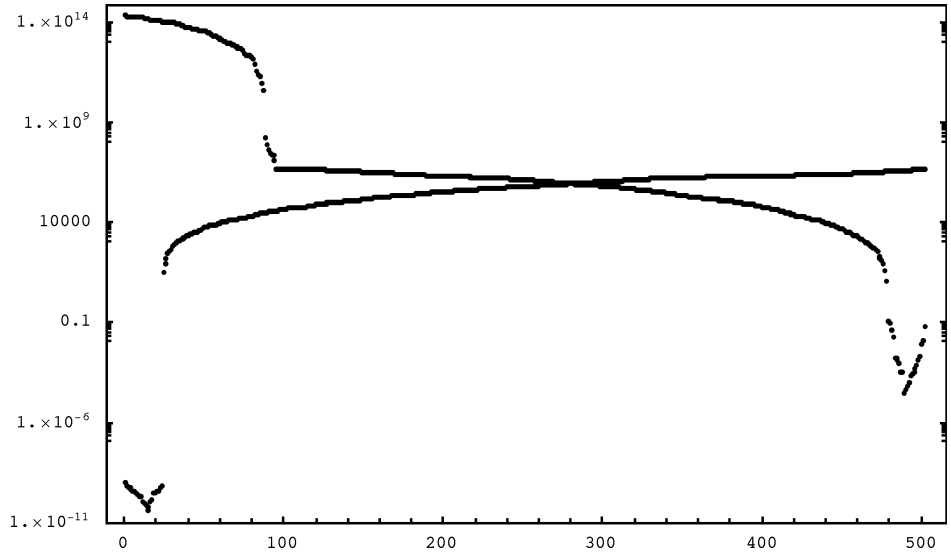
- stability
- transient time scales $\longrightarrow$ depend upon the eigenmodes $(\lambda, \mathbf{x}_\lambda)$:
- the steady state

$$(\lambda \mathbf{M}_\sigma + \mathbf{C}_\mu)\mathbf{x} = 0$$

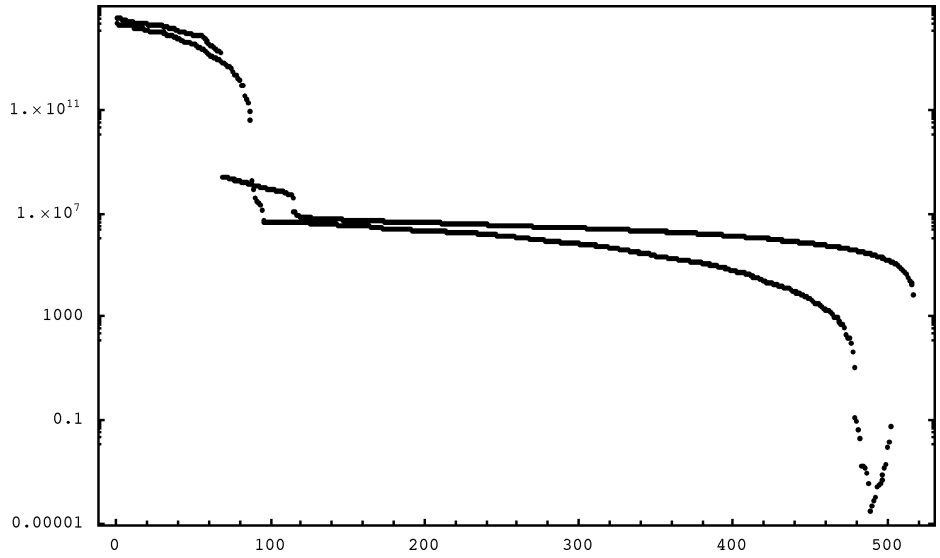
The spectrum: ungauged problem



The spectrum: ungauged + curl

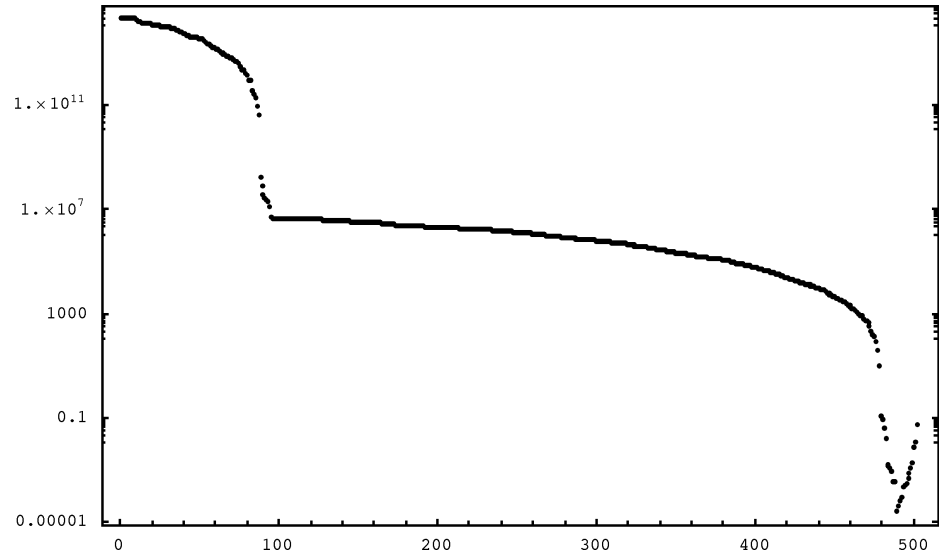


The spectrum: ungauged + Coulomb



Try a poor man's RPM:

- <u>guess</u> the "bad" modes
- at each time step
  project solution on ("bad")$^{\perp}$



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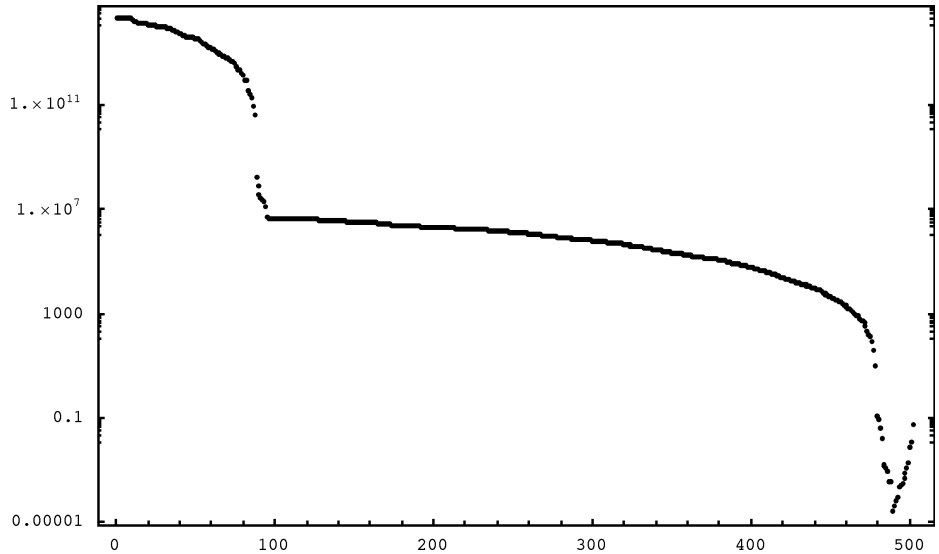

The catch:

- "Bad" modes may appear just at zero frequency
- But they may also pollute the whole numerical spectrum!! (see Boffi et. al. 1999)

$$\Downarrow$$

Extremely hard to distinguish physical from non-physical modes

The Maxwell's "house"

De Rham complex relative to Γ

$$
\begin{aligned}
H_0(\Omega, \mathbf{grad}) &= \{\phi \in H(\Omega, \mathbf{grad}) \mid \phi = 0 \quad \text{on } \Gamma\} \\
H_0(\Omega, \mathbf{curl}) &= \{\mathbf{H} \in H(\Omega, \mathbf{curl}) \mid \mathbf{n} \times \mathbf{H} = 0 \quad \text{on } \Gamma\} \\
H_0(\Omega, \mathrm{div}) &= \{\mathbf{B} \in H(\Omega, \mathrm{div}) \mid \mathbf{n} \cdot \mathbf{B} = 0 \quad \text{on } \Gamma\}
\end{aligned}
$$

The dual complex relative to Γ^*

$$
\begin{aligned}
H_0^*(\Omega, \mathrm{div}) &= \{\mathbf{B} \in H(\Omega, \mathrm{div}) \mid \mathbf{n} \cdot \mathbf{B} = 0 \quad \text{on } \Gamma^*\} \\
H_0^*(\Omega, \mathbf{curl}) &= \{\mathbf{H} \in H(\Omega, \mathbf{curl}) \mid \mathbf{n} \times \mathbf{H} = 0 \quad \text{on } \Gamma^*\} \\
H_0^*(\Omega, \mathbf{grad}) &= \{\phi \in H(\Omega, \mathbf{grad}) \mid \phi = 0 \quad \text{on } \Gamma^*\}
\end{aligned}
$$

Tonti diagram

	Ampere			*Faraday*	
$H_0(\Omega, \mathbf{grad})$	ψ			0	$L_0^2(\Omega)$
∇	$\downarrow$			$\Uparrow$	$\nabla\cdot$
$H_0(\Omega, \mathbf{curl})$	$\mathbf{H}$	$\Rightarrow$	$\mu\mathbf{H} = \mathbf{B}$ $\Rightarrow$	$\mathbf{B}$	$H_0^*(\Omega, \mathrm{div})$
$\nabla\times$	$\Downarrow$			$\Uparrow$	$\nabla\times$
$H_0(\Omega, \mathrm{div})$	$\mathbf{J}$	$\Leftarrow$	$\mathbf{J} = \sigma\mathbf{E}$ $\Leftarrow$	$\mathbf{E}$	$H_0^*(\Omega, \mathbf{curl})$
$\nabla\cdot$	$\Downarrow$			$\uparrow$	∇
$L_0^2(\Omega)$	0			ϕ	$H_0^*(\Omega, \mathbf{grad})$

The exactness property

$$\nabla \times (\nabla *) \quad = \quad \nabla \cdot (\nabla \times *) \quad = \quad \nabla(const) = 0$$

$$\boxed{H(\Omega, \mathbf{grad}\,) \xmapsto{\nabla} H(\Omega, \mathbf{curl}\,) \xmapsto{\nabla\times} H(\Omega, \mathrm{div}\,) \xmapsto{\nabla\cdot} L^2(\Omega)}$$

The exactness property

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$$\boxed{H(\Omega, \mathbf{grad}\,) \xmapsto{\nabla} H(\Omega, \mathbf{curl}\,) \xmapsto{\nabla\times} H(\Omega, \mathrm{div}\,) \xmapsto{\nabla\cdot} L^2(\Omega)}$$

What if we can find...

$$\boxed{\mathcal{W}^0 \xmapsto{\nabla} \mathcal{W}^1 \xmapsto{\nabla\times} \mathcal{W}^2 \xmapsto{\nabla\cdot} \mathcal{W}^3}$$

Discrete Tonti diagram

	Ampere		*Faraday*	
W^0	ψ		0	$\mathcal{W}^3$
∇	$\downarrow$		$\Uparrow$	$\nabla\cdot$
$\mathcal{W}^1$	$\mathbf{H}$	$\ldots\ \mu\mathbf{H} = \mathbf{B}\ \ldots$	$\mathbf{B}$	$\mathcal{W}^2$
$\nabla\times$	$\Downarrow$		$\Uparrow$	$\nabla\times$
$\mathcal{W}^2$	$\mathbf{J}$	$\ldots\ \mathbf{J} = \sigma\mathbf{E}\ \ldots$	$\mathbf{E}$	$\mathcal{W}^1$
$\nabla\cdot$	$\Downarrow$		$\uparrow$	∇
$\mathcal{W}^3$	0		ϕ	$\mathcal{W}^0$

Discrete approximations of De Rham complex

Individual components of a discrete De Rham complex have been developed in different contexts and for different elements:

<u>Raviart-Thomas elements:</u> (Raviart, Thomas, 1977)

- context = mixed methods ($H(\Omega, \mathrm{div})$ conforming)
- element = n-simplex

<u>Nedelec elements:</u> (Nedelec, 1980-85)

- context = mixed methods ($H(\Omega, \mathrm{div})$, $H(\Omega, \mathbf{curl})$ conforming)
- element = brick, prism, rectangle

<u>BDM elements:</u> (Brezzi, Douglas, Marini, late 80s)

- context = mixed methods ($H(\Omega, \mathrm{div})$, $H(\Omega, \mathbf{curl})$ conforming)
- element = brick, rectangle

Bossavit was first to recognize the importance of discrete analogues of De Rham's complex and to exploit *exactness* in computational electromagnetics.

The Whitney complex: (Bossavit, 1979-1985)

- context = electromagnetics (De Rham conforming)
- element = n-simplex

Our approach extends the construction of

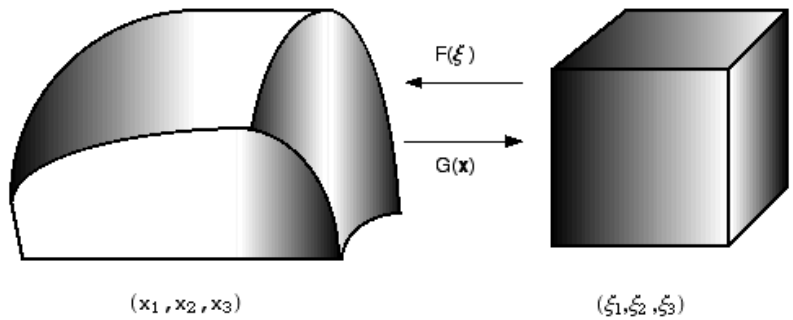
van Welij elements: (van Welij, 1985)

- context = eddy currents ($H(\Omega, \mathbf{curl})$ conforming)
- element = hexahedron (isoparametric brick)

to an exact sequence on arbitrary hexahedral grids.

Exact sequences on hexahedral grids

Generalized hexahedrals



$\mathbb{R}^3 = \{(x_1, x_2, x_3) \equiv \mathbf{x}\}$ $\qquad$ $\hat{\mathbb{R}}^3 = \{(\xi_1, \xi_2, \xi_3) \equiv \boldsymbol{\xi}\}$

Physical space $\qquad$ Parameter space

$$F : \hat{\mathbb{R}}^3 \mapsto \mathbb{R}^3 \;\rightarrow\; \text{smooth deformation of } \hat{\mathbb{R}}^3$$

$$K = F(\hat{K}) \;\rightarrow\; \text{image of } \hat{K} = [-1, 1] \in \hat{\mathbb{R}}^3$$

Assume:

- $F = (F_1, F_2, F_3)$ is invertible when restricted to $\hat{K}$
- $G = (G_1, G_2, G_3) = F^{-1}$ is such that $G(K) = \hat{K}$

Base and reciprocal vectors

$$J_F = (V_1, V_2, V_3) \qquad J_G = (\nabla G_1, \nabla G_2, \nabla G_3)^T$$

$$\det J_F = V_i \cdot (V_j \times V_k) \qquad \det J_G = \nabla G_i \cdot (\nabla G_j \times \nabla G_k)$$

$$V_i = (\nabla G_j \times \nabla G_k) \det J_F \qquad \nabla G_i = (V_j \times V_k) \det J_G$$

$$\boxed{V_i \cdot \nabla G_j = \delta_{ij}}$$

Nodes, edges, faces and a hex:

$$\boldsymbol{\xi}^{\alpha\beta\gamma} = \{\boldsymbol{\xi} = (\pm 1, \pm 1, \pm 1)\} \;\rightarrow\; \mathbf{x}^{\alpha\beta\gamma} = F(\boldsymbol{\xi}^{\alpha\beta\gamma}) \qquad \text{“nodes”}$$

$$\boldsymbol{\xi}_{ij}^{\alpha\beta} = \{\xi_i = \pm 1; \xi_j = \pm 1\} \;\rightarrow\; \mathbf{x}_{ij}^{\alpha\beta} = F(\boldsymbol{\xi}_{ij}^{\alpha\beta}) \qquad \text{“edges”}$$

$$\boldsymbol{\xi}_i^{\alpha} = \{\xi_i = \pm 1\} \;\rightarrow\; \mathbf{x}_i^{\alpha} = F(\boldsymbol{\xi}_i^{\alpha}) \qquad \text{“faces”}$$

$$\boldsymbol{\xi} = \{\boldsymbol{\xi} \in \hat{K}\} \;\rightarrow\; \mathbf{x} = F(\boldsymbol{\xi}) \qquad \text{“hex”}$$

Note: $\mathbf{x}_i^{\alpha} \cap \mathbf{x}_j^{\beta} = \mathbf{x}_{ij}^{\alpha\beta}$ and $\mathbf{x}_i^{\alpha} \cap \mathbf{x}_j^{\beta} \cap \mathbf{x}_k^{\gamma} = \mathbf{x}^{\alpha\beta\gamma}$

Unit normal to face $\mathbf{x}_i^\alpha$

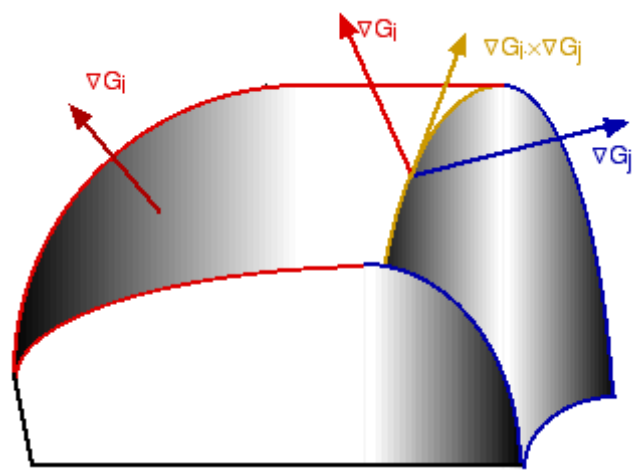
$$\mathbf{n} = \frac{\nabla G_i}{\|\nabla G_i\|}$$

$$(\mathbf{n} \circ F) = \frac{V_j \times V_k}{\|(V_j \times V_k)\|}$$

Unit tangent to edge $\mathbf{x}_{ij}^{\alpha\beta}$

$$\mathbf{t} = \frac{(\nabla G_i \times \nabla G_j)}{\|\nabla G_i \times \nabla G_j\|}$$

$$(\mathbf{t} \circ F) = \frac{V_k}{\|V_k\|}$$



"Basis" functions and spaces on K

$$
\begin{array}{lll}
\mathcal{W}^0 \text{ - nodal} & W_{ijk}^{\alpha\beta\gamma} & = \frac{1}{8}(1 \pm G_i)(1 \pm G_j)(1 \pm G_k) \\
\mathcal{W}^1 \text{ - edge} & W_{ij}^{\alpha\beta} & = \frac{1}{8}(1 \pm G_i)(1 \pm G_j)(\nabla G_k) \\
\mathcal{W}^2 \text{ - face} & W_i^{\alpha} & = \frac{1}{8}(1 \pm G_i)(\nabla G_j \times \nabla G_k) \\
\mathcal{W}^3 \text{ - volume} & W & = \frac{1}{8}\nabla G_i \cdot (\nabla G_j \times \nabla G_k)
\end{array}
$$

"Basis" functions and spaces on $\hat{K}$

$$
\begin{array}{lll}
\hat{\mathcal{W}}^0 \text{ - nodal} & \hat{W}_{ijk}^{\alpha\beta\gamma} & = \frac{1}{8}(1 \pm \xi_i)(1 \pm \xi_j)(1 \pm \xi_k) \\
\hat{\mathcal{W}}^1 \text{ - edge} & \hat{W}_{ij}^{\alpha\beta} & = \frac{1}{8}(1 \pm \xi_i)(1 \pm \xi_j)(V_i \times V_j)/\det J_F \\
\hat{\mathcal{W}}^2 \text{ - face} & \hat{W}_i^{\alpha} & = \frac{1}{8}(1 \pm \xi_i)V_i/\det J_F \\
\hat{\mathcal{W}}^3 \text{ - volume} & \hat{W} & = \frac{1}{8}V_i \cdot (V_j \times V_k)/\det J_F
\end{array}
$$

The exactness property

$$\nabla W_{ijk}^{\alpha\beta\gamma} = c_1 W_{ij}^{\alpha\beta} + c_2 W_{jk}^{\beta\gamma} + c_3 W_{ki}^{\gamma\alpha}$$

$$\nabla \times W_{ij}^{\alpha\beta} = c_1 W_i^{\alpha} + c_2 W_j^{\beta}$$

$$\nabla \cdot W_i^{\alpha} = c_1 W$$

$$\boxed{\mathcal{W}^0 \xmapsto{\nabla} \mathcal{W}^1 \xmapsto{\nabla\times} \mathcal{W}^2 \xmapsto{\nabla\cdot} \mathcal{W}^3}$$

Degrees of freedom

node $\longrightarrow$ point mass

$$\int_K W_{ijk}^{\alpha\beta\gamma}(\mathbf{x}) \cdot \delta(\mathbf{x}^{\kappa\mu\nu}) d\mathbf{x} = \begin{cases} 1 & \text{if } \mathbf{x}^{\kappa\mu\nu} = \mathbf{x}^{\alpha\beta\gamma} \\ 0 & \text{all other nodes} \end{cases}$$

edge $\longrightarrow$ circulation

$$\int_{\mathbf{x}_{st}^{\kappa\mu}} W_{ij}^{\alpha\beta}(\mathbf{x}) \cdot \mathbf{t} dl = \begin{cases} 1 & \text{if } \mathbf{x}_{st}^{\kappa\mu} = \mathbf{x}_{ij}^{\alpha\beta} \\ 0 & \text{all other edges} \end{cases}$$

Degrees of freedom

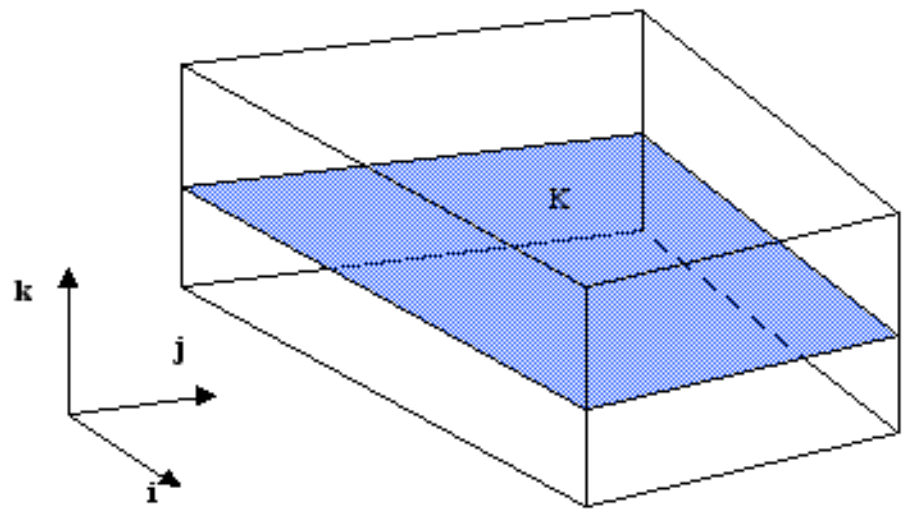
face $\longrightarrow$ flux

$$\int_{\mathbf{x}_s^\kappa} W_i^\alpha(\mathbf{x}) \cdot \mathbf{n} dS = \begin{cases} 1 & \text{if } \mathbf{x}_s^\kappa = \mathbf{x}_i^\alpha \\ \\ 0 & \text{all other faces} \end{cases}$$

hex $\longrightarrow$ total mass

$$\int_K W(\mathbf{x}) d\mathbf{x} = 1$$

Exact sequences on quadrilaterals



Set $F_3(\boldsymbol{\xi}) = \xi_3 \qquad \Longrightarrow \qquad V_3 = \mathbf{k} \quad \text{and} \quad \nabla G_3 = \mathbf{k}$

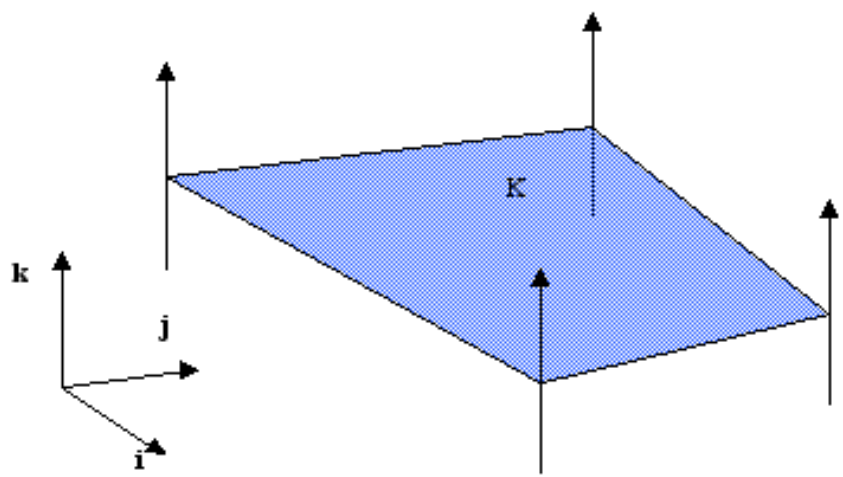
$$\begin{aligned} \nabla G_1 &= (V_2 \times \mathbf{k})/\det J_F \\ \nabla G_2 &= (\mathbf{k} \times V_1)/\det J_F \end{aligned} \qquad \begin{aligned} \nabla G_2 \times \nabla G_3 &= V_1/\det J_F \\ \nabla G_3 \times \nabla G_1 &= V_2/\det J_F \end{aligned}$$

	Basis on K			**Basis on $\hat{K}$**		
$\mathcal{W}^0$	$W_{ij*}^{\alpha\beta*}$	$=$	$\frac{1}{4}(1 \pm G_i)(1 \pm G_j)$	$\hat{W}_{ij*}^{\alpha\beta*}$	$=$	$\frac{1}{4}(1 \pm \xi_i)(1 \pm \xi_j)$
$\mathcal{W}^1$	$W_{ij}^{\alpha*}$	$=$	$\frac{1}{4}(1 \pm G_i)(\nabla G_j)$	$\hat{W}_{ij}^{\alpha*}$	$=$	$\frac{1}{4}(1 \pm \xi_i)(V_j \times \mathbf{k})/\det J_F$
$\mathcal{W}^2$	W_i^{α}	$=$	$\frac{1}{4}(1 \pm G_i)(\nabla G_j \times \mathbf{k})$	$\hat{W}_i^{\alpha}$	$=$	$\frac{1}{4}(1 \pm \xi_i)V_i/\det J_F$
$\mathcal{W}^3$	W	$=$	$\frac{1}{4}\nabla G_i \cdot (\nabla G_j \times \mathbf{k})$	$\hat{W}$	$=$	$\frac{1}{4}V_i \cdot (V_j \times V_k)/\det J_F = 1$

Exactness in two-dimensions

$$\nabla \mathcal{W}^0 \subset \mathcal{W}^1 \quad \text{and} \quad \nabla \cdot \mathcal{W}^2 \subset \mathcal{W}^3 \quad \text{but} \quad \nabla \times ? \quad \mapsto \quad ?$$

<u>The virtual edge functions</u>



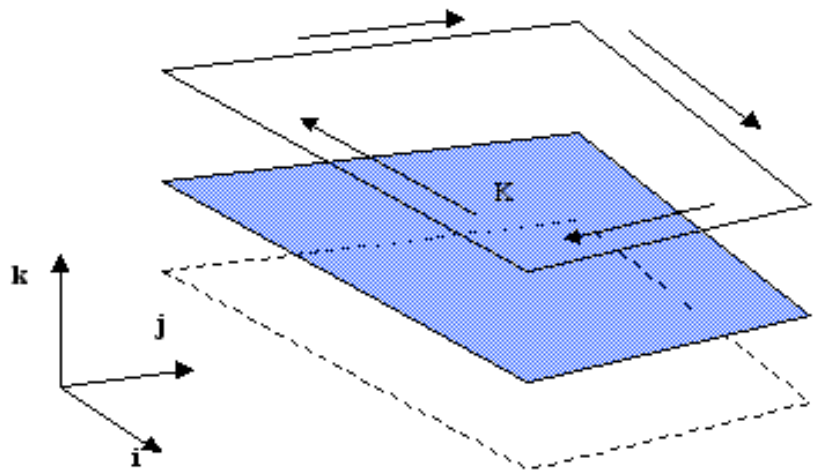
$$W_{ij}^{\alpha\beta} = \underbrace{\frac{1}{2}(1 \pm G_i)(1 \pm G_j)\nabla G_3}_{\text{3D edge BF}} = \underbrace{\frac{1}{2}(1 \pm G_i)(1 \pm G_j)}_{\text{2D node BF}}\,\mathbf{k} = W^{\alpha\beta *}\mathbf{k}$$

$$\nabla \times W_{ij}^{\alpha\beta} = \underbrace{\frac{1}{2}((1 \pm G_i)(\nabla G_j \times \mathbf{k}) - (1 \pm G_j)(\nabla G_i \times \mathbf{k}))}_{W_i^{\alpha} - W_j^{\beta} \in \mathcal{W}^2} = \nabla \times W_{ij}^{\alpha\beta *}$$

The first curl exactness relation:

$$\boxed{\begin{array}{ccccccc} \mathcal{W}^1 & \xleftarrow{\nabla} & \mathcal{W}^0 & \xmapsto{\nabla\times} & \mathcal{W}^2 & \xmapsto{\nabla\cdot} & \mathcal{W}^3 \\ \\ \mathcal{W}^1 & & & \ldots & & & \mathcal{W}^3 \end{array}}$$

The parallel edge functions



$$W_{i3}^{\alpha+} = \underbrace{\frac{1}{4}(1 \pm G_i)\overbrace{(1+G_3)}^{2 \text{ on top face}}\nabla G_j}_{\text{3D Edge function}} = \underbrace{\frac{1}{2}(1 \pm G_i)\nabla G_j}_{\text{2D Edge function}} = W_{ij}^{\alpha *}$$

$$\nabla \times [W_{i3}^{\alpha+}]_{G_3=1} = \underbrace{\pm \nabla G_i \times \nabla G_j}_{\pm W \in \mathcal{W}^3} = \nabla \times W_{ij}^{\alpha *}.$$

<u>The two flavors of curl exactness</u>

$$\boxed{\begin{array}{ccccccc} \mathcal{W}^1 & \xleftarrow{\nabla} & \mathcal{W}^0 & \xmapsto{\nabla\times} & \mathcal{W}^2 & \xmapsto{\nabla\cdot} & \mathcal{W}^3 \\ \\ \mathcal{W}^1 & & & \xmapsto{\nabla\times} & & & \mathcal{W}^3 \end{array}}$$

Solution of the eddy current equations

1. Choose *Ampere's* or <u>*Faraday's*</u> side in Tonti diagram:

2. Eliminate $(\mathbf{H}, \mathbf{J})$ from *Ampere's* using constitutive laws:

	Ampere				<u>*Faraday*</u>	
$H_0(\Omega, \mathbf{curl})$	$1/\mu\mathbf{B}$	$\Leftarrow$	$\mu\mathbf{H} = \mathbf{B}$	$\Leftarrow$	$\mathbf{B}$	$H_0^*(\Omega, \mathrm{div})$
$\nabla\times$	$\vdots$				$\Uparrow$	$\nabla\times$
$H_0(\Omega, \mathrm{div})$	$\sigma\mathbf{E}$	$\Leftarrow$	$\mathbf{J} = \sigma\mathbf{E}$	$\Leftarrow$	$\mathbf{E}$	$H_0^*(\Omega, \mathbf{curl})$

3. Substitute with discrete De Rham structure:

	Ampere		*Faraday*	
$\mathcal{W}^2$	$1/\mu \mathbf{B}_h$	$\ldots$	$\mathbf{B}_h$	$\mathcal{W}^2$
$\nabla\times$	$\vdots$		$\Uparrow$	$\nabla\times$
$\mathcal{W}^1$	$\sigma \mathbf{E}_h$	$\ldots$	$\mathbf{E}_h$	$\mathcal{W}^1$

$$\boxed{\begin{aligned} \nabla \times \tfrac{1}{\mu}\mathbf{B}_h &= \sigma \mathbf{E}_h \quad \text{in } \mathcal{W}^2 \qquad \textit{weakly} \\ \nabla \times \mathbf{E}_h &= -\frac{\partial \mathbf{B}_h}{\partial t} \quad \text{in } \mathcal{W}^2 \qquad \textit{exactly} \end{aligned}}$$

$$\int_\Omega \frac{1}{\mu}\mathbf{B}\cdot\nabla\times\hat{\mathbf{E}}d\Omega - \int_\Gamma (\mathbf{H}_\mathrm{b}\times\mathbf{n})\cdot\hat{\mathbf{E}}d\Gamma = \int_\Omega \sigma\mathbf{E}\cdot\hat{\mathbf{E}}d\Omega \quad \forall\hat{\mathbf{E}}\in\mathcal{W}^1,$$

Fully discrete equations

$$\int_\Omega \frac{1}{\mu}\mathbf{B}_h^{n+1}\cdot\nabla\times\hat{\mathbf{E}}_h d\Omega - \int_\Gamma(\mathbf{H}_\mathrm{b}\times\mathbf{n})\cdot\hat{\mathbf{E}}_h d\Gamma \;=\; \int_\Omega \sigma\mathbf{E}_h^{n+1}\cdot\hat{\mathbf{E}}d\Omega \quad \forall\hat{\mathbf{E}}_h\in\mathcal{W}^1$$

$$-\frac{\mathbf{B}_h^{n+1}-\mathbf{B}_h^n}{\Delta t} \;=\; \nabla\times\mathbf{E}_h^{n+1}$$

Solution

1. solve Faraday's law *exactly* for $\mathbf{B}_h^{n+1}$:

$$\mathbf{B}_h^{n+1} = \mathbf{B}_h^n - \Delta t\nabla\times\mathbf{E}_h^{n+1}.$$

- $\nabla\cdot\mathbf{B}_h^0 = 0 \quad\Longrightarrow\quad \nabla\cdot\mathbf{B}_h^n = 0$ for all n!

2. insert in *weak* Ampere's Theorem to get equation for $\mathbf{E}_h^{n+1}$:

$$\int_\Omega \sigma \mathbf{E}_h^{n+1} \cdot \hat{\mathbf{E}}_h + \frac{\Delta t}{\mu}(\nabla \times \mathbf{E}_h^{n+1}) \cdot (\nabla \times \hat{\mathbf{E}}_h) d\Omega$$

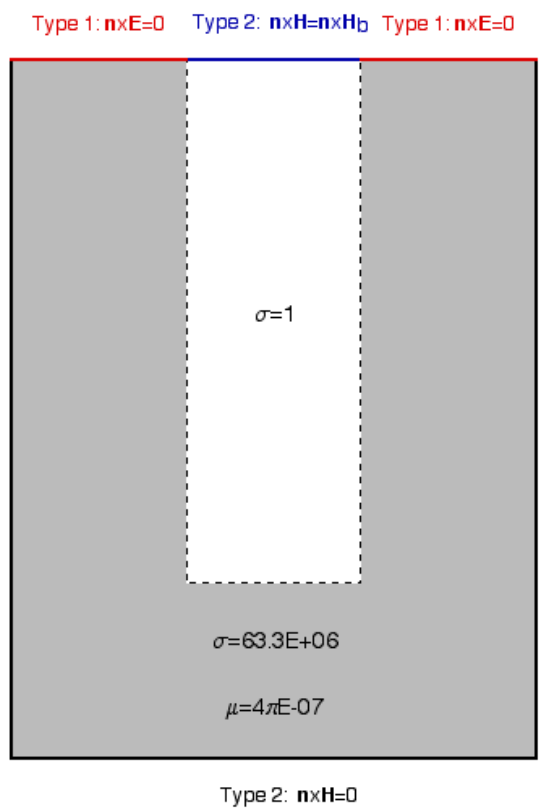
$$= \int_\Omega \frac{1}{\mu} \mathbf{B}_h^n \cdot (\nabla \times \hat{\mathbf{E}}_h) d\Omega - \int_\Gamma (\mathbf{H}_\mathrm{b} \times \mathbf{n}) \cdot \hat{\mathbf{E}}_h d\Gamma \quad \forall \hat{\mathbf{E}}_h \in \mathcal{W}^1.$$

- This scheme resembles:
  - Yee's FDTD method (on bricks)
  - CT FV method of Evans and Howley
  - Mimetic schemes of Misha Shaskov
- It is not a <u>mixed</u> FEM, rather a "hybrid" between FEM and FV

Model Problem in 2D

Setting

- $\mathbf{H} = H_z\mathbf{k}$ and $\mathbf{E} = E_x\mathbf{i} + E_y\mathbf{j}$
- $\mu \sim 4\pi \cdot 10^{-7}$
- $\sigma_{\text{conductor}} = 63.3 \times 10^6$
- $\sigma_{\text{void}} = 1$

What must happen

- $t_{\text{steady}} \approx 50 \times 10^{-6}$sec
- skin current
- "tent" solution at steady state