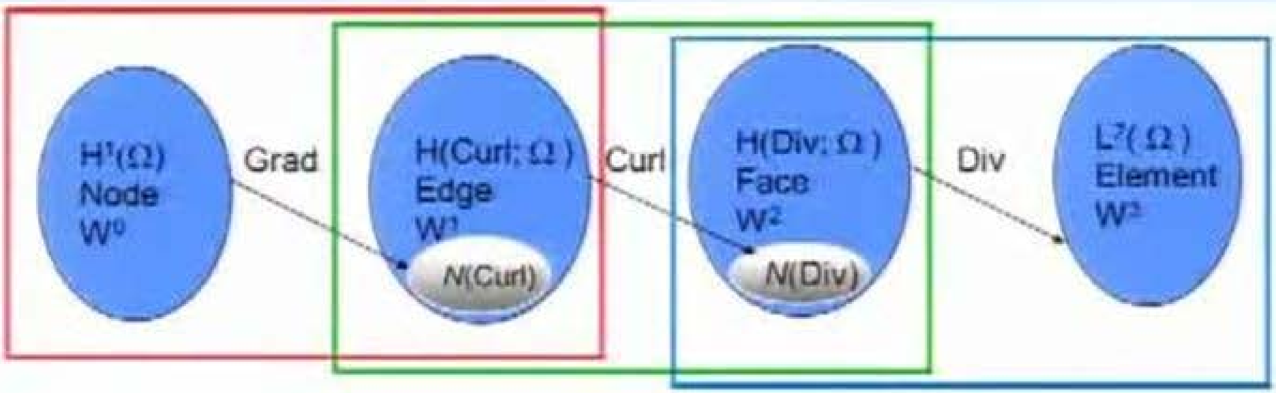

Multiphysics Lagrangian/Eulerian Modeling and De Rham Complex Based Algorithms

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Sandia National Laboratories

SIAM Conference on Computational Science and Engineering, Salt Lake City, Utah

Minisymposia on Physics-Compatible Numerical Methods

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Outline

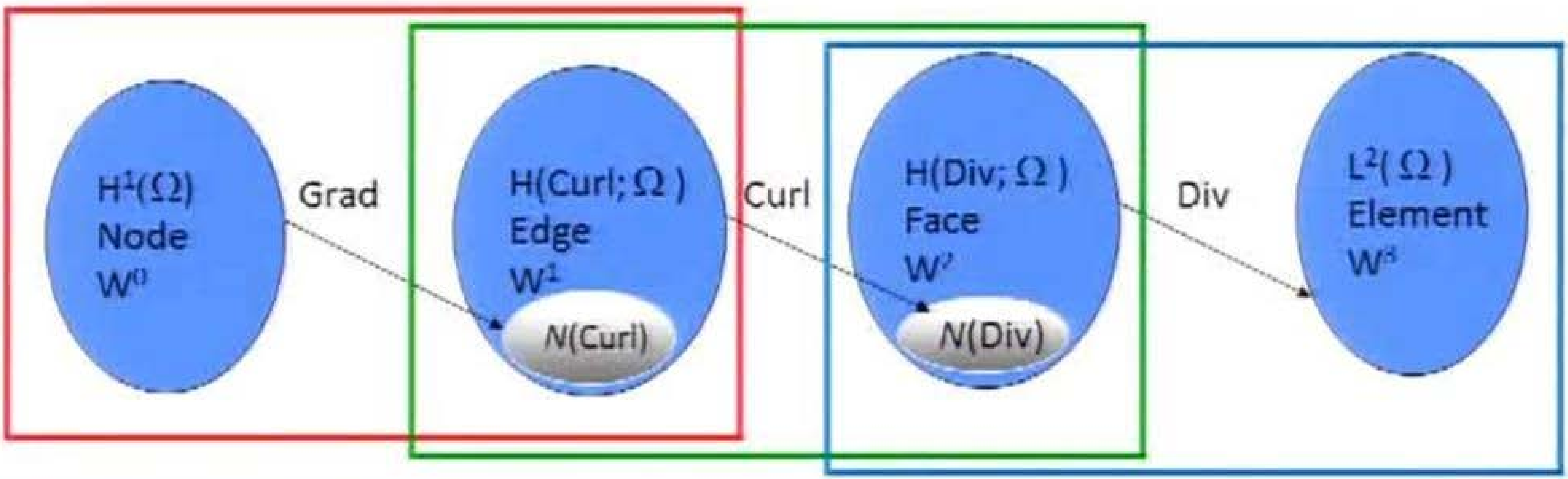
- Presentation Purpose: Expand physical and mathematical intuition and the basis for cross field communication and understanding.
- Lagrangian/Eulerian Numerical Methods
- De Rham Complex, Lie Derivative and Cartan's Magic Formula
- Physics and Remapping Examples
  - Inverse Deformation Gradient
  - Magnetic Flux Density
  - Mass
  - Electric Displacement
- Conclusion

Arbitrary Lagrangian/Eulerian (ALE)

- **Lagrangian:**
  - Mesh moves with material points.
  - Mesh-quality may deteriorate over time
- **REMESH**
  - Mesh-quality is adjusted to improve solution-quality or robustness or simply to move mesh back to original location (Eulerian).
- **REMAP**
  - Algorithm transfers dependent variables to the new mesh.

Geometric Structure and Numerical Methods

- The structure of physics equations is related to their geometric origins.
- The deRham structure shown below is used to discuss issues of "compatible discretizations." Stable discretizations depend on maintaining proper relationships of the discrete spaces.
- FEEC (Finite Element Exterior Calculus) – See recently published "Periodic Table of Finite Elements", Doug Arnold, et. al., femtable.org. FEEC includes discrete spaces for 0-forms, 1-forms, 2-forms and 3-forms in 3 space for example.
- Frankel, <u>Geometry of Physics</u>, 3rd Ed, Cambridge University Press
- Flanders, <u>Differential Forms with Application to Physical Sciences</u>, Dover.



Stoke's Theorem and the Lie Derivative

Stoke's Theorem

$$\int_{\partial M^k} \alpha^{k-1} = \int_{M^k} d\alpha^{k-1}$$

$$\frac{d}{dt}\int_{M_t}\alpha = \int_{M_t}\frac{\partial\alpha}{\partial t} + \mathcal{L}_v\alpha = \int_{M_t}\frac{\partial\alpha}{\partial t} + \mathcal{I}_v d\alpha + d\mathcal{I}_v\alpha \quad \Leftrightarrow$$

Lie Derivative and Cartan's Magic Formula

Classical Transport Formulas in Vector Notation

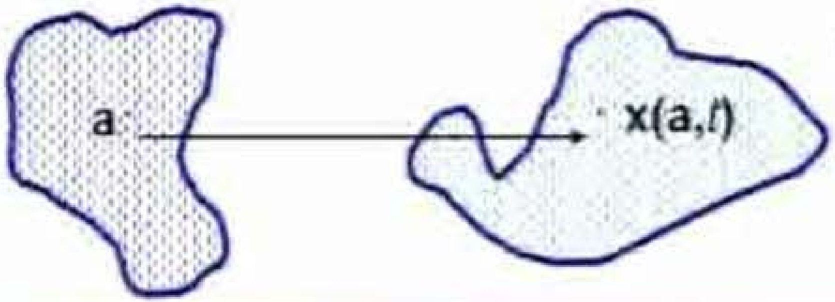
$$\frac{d}{dt} f = \frac{\partial f}{\partial t} + v\cdot\nabla f$$

$$\frac{d}{dt}\int_{M_t^1} A\cdot dx = \int_{M_t^1}\left[\frac{\partial A}{\partial t} - v\times(\nabla\times A) + \nabla(v\cdot A)\right]\cdot dx$$

$$\frac{d}{dt}\int_{M_t^2} B\cdot da = \int_{M_t^2}\left[\frac{\partial B}{\partial t} + v(\nabla\cdot B) - \nabla\times(v\times B)\right]\cdot da$$

$$\frac{d}{dt}\int_{M_t^3}\rho\, dV = \int_{M_t^3}\left[\frac{\partial\rho}{\partial t} + \nabla\cdot(v\rho)\right] dV$$

Solid Kinematics



(Reference) Material Coordinates

$\mathbf{x}(\mathbf{a},t)$

(Current) Spatial Coordinates

Deformation gradient and inverse:

$$\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{a}$$

$$\mathbf{G} = \mathbf{F}^{-1} = \partial \mathbf{a} / \partial \mathbf{x}$$

***Polar Decomposition*:** **F = VR**

Symmetric Positive Definite (Stretch) Tensor	Proper Orthogonal (Rotation) Tensor

Remap

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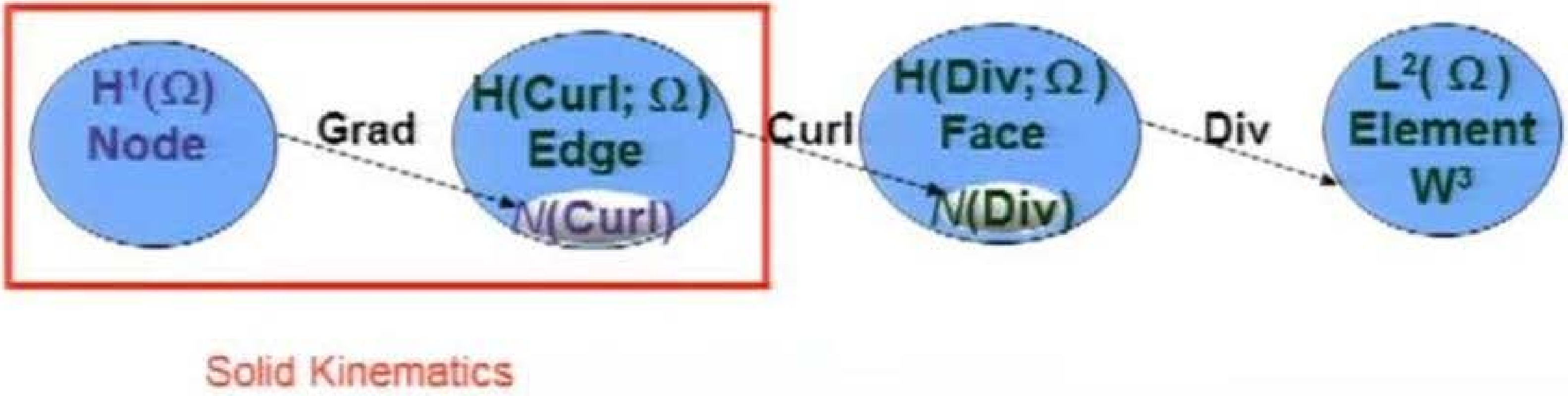
- Some material models require that the kinematic description (i.e. F) be available. The rotation tensor in particular is needed.
- Any method for tracking F on a discrete grid may fail eventually.
  - Det(F)>0
  - Positive definiteness of the stretch, V, can be lost.
  - R proper orthogonal: $RR^{t} = I$, Det(R)>0.
  - Rows of the inverse deformation tensor $G=F^{-1}$ should be gradients.
- These constraints may not hold due to truncation error in the remap step and finite accuracy discretizations.
- What is the best approach?
  - "fixes" will be required.
  - Storage, accuracy and speed should be considered.

Curl Free Remap

- Representation of G on edges allows for a discrete curl-free inverse deformation gradient.
- Remap algorithm should preserve this global property.
- Constrained transport (CT) approach pioneered by Evans and Hawley for divergence free MHD algorithm on Cartesian grid is the prototype algorithm.
- More generally we might say "Cartan" transport. $d\mathcal{I}_v\alpha$



Curl Free Remap Algorithm

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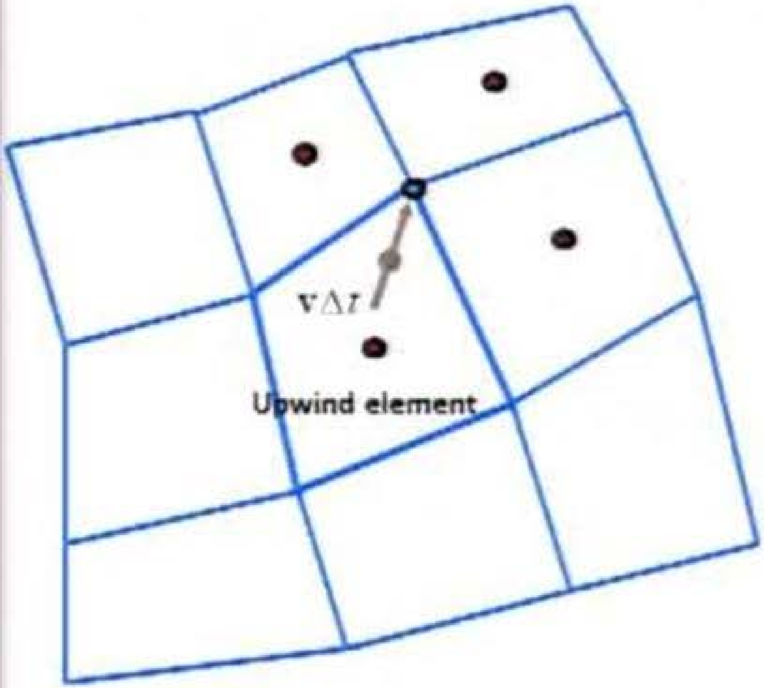


- Edge element representation

$$\mathbf{g}(\xi_1,\xi_2,\xi_3) = \sum_{i\neq j\neq k,\alpha,\beta} \Gamma_{ij}^{\alpha\beta}(\xi_k) W_{ij}^{\alpha\beta}$$

- Use reconstructed nodal values of G to compute trial edge element gradient coefficients along each edge.

$$\Gamma_{ij}^{\alpha\beta}(\xi_k) = \Gamma_{ij}^{\alpha\beta} + s_{ij}^{\alpha\beta}\xi_k \qquad Nc_1^g \Rightarrow AA_1^g \text{ (PTFE)}$$

- Limit slopes along each edge (minmod,harmonic)
- Compute the node circulation contributions in the upwind element by a midpoint integration rule at the center of the node motion vector.

$$\int_\Gamma \mathbf{g}\cdot d\mathbf{s} \approx \sum_{i\neq j\neq k,\alpha,\beta} \Gamma_{ij}^{\alpha\beta}(\hat{\xi}_k)(1+\alpha\hat{\xi}_i)(1+\beta\hat{\xi}_j)\delta\xi_k/8$$

- Take gradient and add to edge element circulations.
- Robinson, Ketcheson, Ames, Farnsworth, "A comparison of Lagrangian/Eulerian approaches for tracking the kinematics of high deformation solid motion", SAND2009-5154.

Rows guaranteed to be curl free. ☺

No control on det(G). ☹

Speed ☹

One approach to det(G)>0 question

- Kamm, Love, Robinson, Young, Ridzal, "Edge Remap for Solids," SAND2013-10281.
- Solve global optimization problem for nodal increments using the standard CT algorithm increments as the target.

$$\min_{u} f(u) \quad \text{subject to} \quad g(u) = 0 \quad \text{and} \quad h(u) > 0.$$

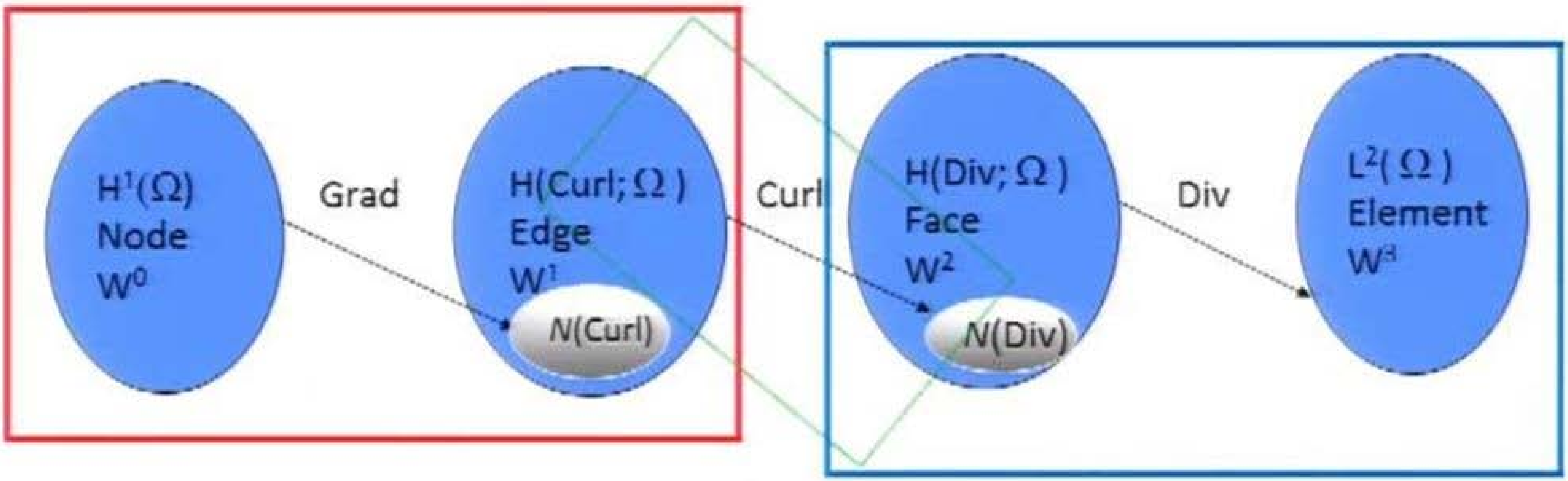
$$f(u) := \frac{1}{2}\sum_{i}(u_i - \tilde{u}_i)^2 \qquad h_j(u) := \det_j(u) - \varepsilon > 0 \quad \text{with} \quad \varepsilon := \min_{k \in \mathcal{K}}\{\det_k(u^L)\}$$

- Solve using slack variable formulation

$$\min_{u} f(u) \quad \text{subject to} \quad g(u) = 0,\ h(u) - s = 0 \quad \text{and} \quad s - \varepsilon > 0$$

- Not yet competitive.

Magnetohydrodynamics



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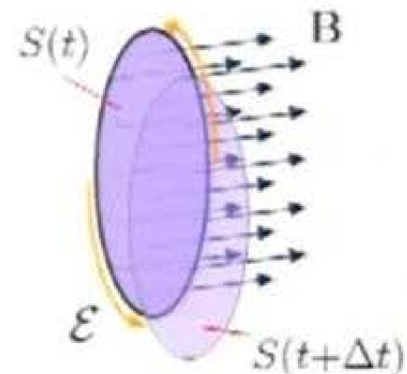
Faraday's Law (Natural operator splitting)

A straightforward **B**-field update is possible using Faraday's law.

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \qquad \mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$



Integrate over time-dependent surface $S(t)$, apply Stokes theorem, and discretize in time:

$$\frac{d}{dt}\int_{S(t)} \mathbf{B}\cdot d\mathbf{a} + \oint_{\partial S(t)} \mathcal{E}\cdot d\mathbf{x} = 0$$

$$\frac{1}{\Delta t}\int_{S(t+\Delta t)} (\mathbf{B}^{n+1} - \tilde{\mathbf{B}}^{n+1})\cdot d\mathbf{a}^{n+1} + \oint_{\partial S(t+\Delta t)} \mathcal{E}^{n+1}\cdot d\mathbf{x}^{n+1}$$

$$+ \frac{1}{\Delta t}\left[\int_{S(t+\Delta t)} \tilde{\mathbf{B}}^{n+1}\cdot d\mathbf{a}^{n+1} - \int_{S(t)} \mathbf{B}^{n}\cdot d\mathbf{a}^{n}\right] = 0$$

Zero for **ideal MHD** by frozen-in flux theorem:

$$\frac{d}{dt}\int_{S_t} \mathbf{B}\cdot d\mathbf{a} = \int_{S_t} \mathring{\mathbf{B}}\cdot d\mathbf{a} = 0$$

Terms in red are zero for ideal MHD so nothing needs to be done if fluxes are degrees of freedom.

Solve magnetic diffusion using edge/face elements which preserve discrete divergence free property

Ω = a single conducting region in $\Re^3$.

weakly enforced

$$\nabla \times \mathbf{H} = \mathbf{J} \qquad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

Exact relationship

$$\nabla \bullet \mathbf{J} = 0 \qquad \nabla \bullet \mathbf{B} = 0$$

$$\mathbf{B} = \mu \mathbf{H} \qquad \mathbf{J} = \sigma \mathbf{E}$$

$$\text{boundary conditions} \begin{cases} \mathbf{E} \times \mathbf{n} = \mathbf{E}_b \times \mathbf{n} \text{ on } \Gamma_1 \,(Dirichlet), \\ \mathbf{H} \times \mathbf{n} = \mathbf{H}_b \times \mathbf{n} \text{ on } \Gamma_2 \,(Neumann) \end{cases}$$

Edge element

$$\int \sigma \mathbf{E}^{n+1} \bullet \hat{\mathbf{E}} dV + \Delta t \int \frac{\text{curl}\,\mathbf{E}^{n+1} \bullet \text{curl}\,\hat{\mathbf{E}}}{\mu} dV = \int \frac{\mathbf{B}^n \bullet \text{curl}\,\hat{\mathbf{E}}}{\mu} dV - \int \mathbf{H}_b \times \mathbf{n} \bullet \hat{\mathbf{E}} dA$$

B = magnetic flux density E = electric field H = magnetic field

μ = permeability σ = conductivity J = current density

μ and σ positive and finite everywhere in W

Magnetic Flux Density Remap

- The Lagrangian step maintains the discrete divergence free property via flux density updates given only in term of discrete curls of edge circulation variables.

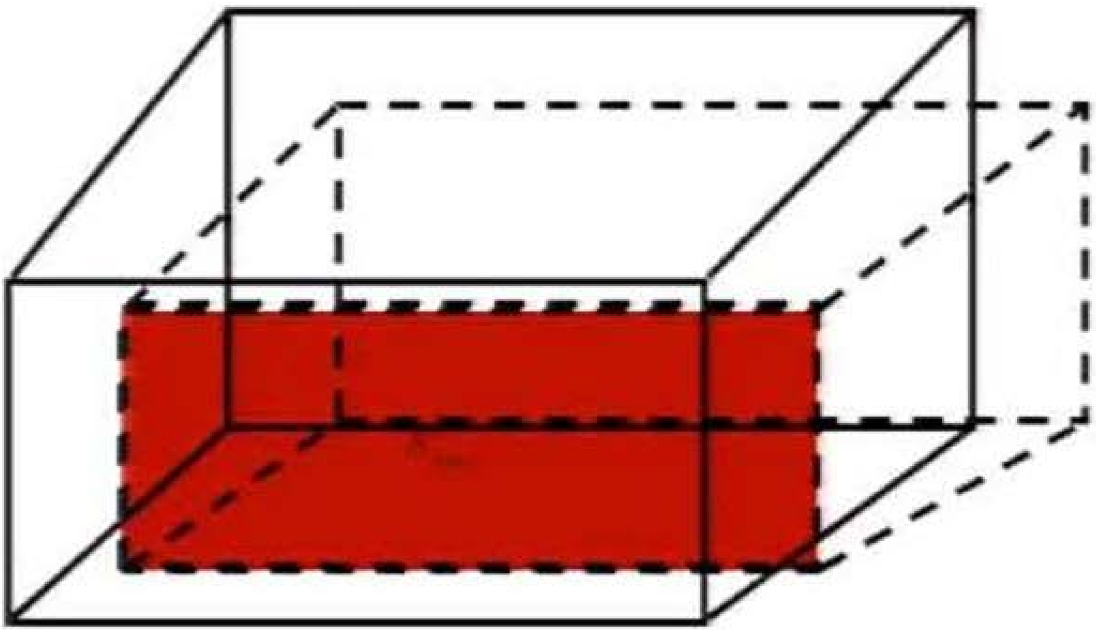
- The remap should not destroy this property.

- As in the curl free case, the $d\mathcal{I}_v\alpha$ part of the remap algorithm is fundamentally unsplit because it ensures that the global divergence free property is maintained.

Flux remap step

$$\int_{S} \mathbf{B} \bullet d\mathbf{a} = 0$$

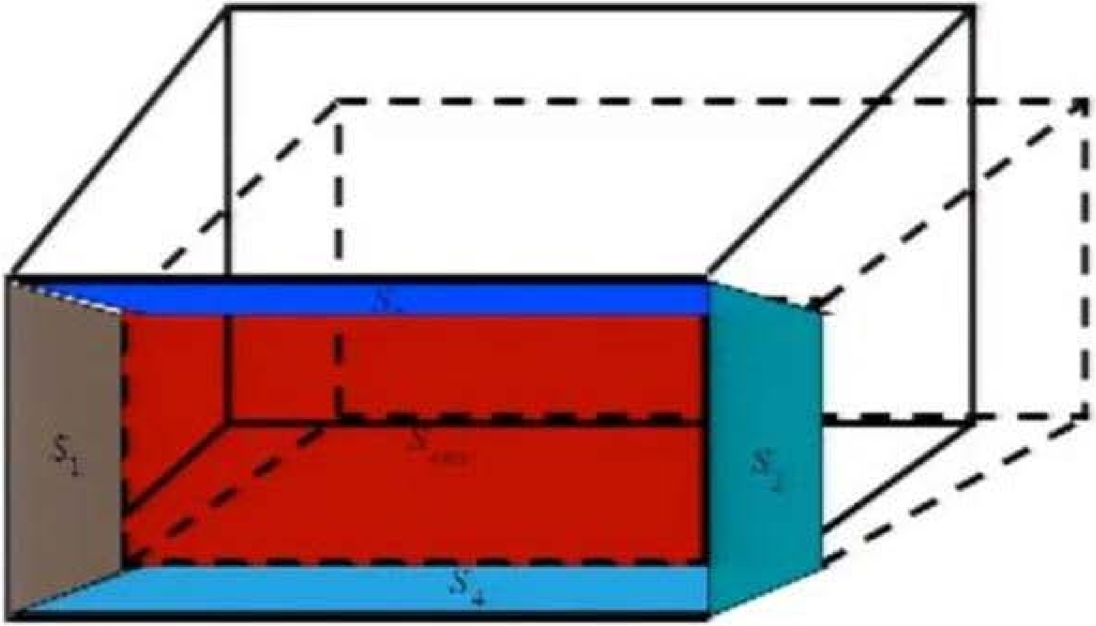
$$\int_{S_{old}} \mathbf{B} \bullet d\mathbf{a} + \int_{S_{new}} \mathbf{B} \bullet d\mathbf{a} + \sum_{i=1}^{4} \int_{S_i} \mathbf{B} \bullet (\mathbf{v}_g \Delta t \times \mathbf{dl}) = 0$$



$$\int_{S_{old}} \mathbf{B} \bullet d\mathbf{a} + \int_{S_{new}} \mathbf{B} \bullet d\mathbf{a} + \sum_{i=1}^{4} \int_{S_i} \mathbf{dl} \bullet (\mathbf{B} \times \mathbf{v}_g \Delta t) = 0$$

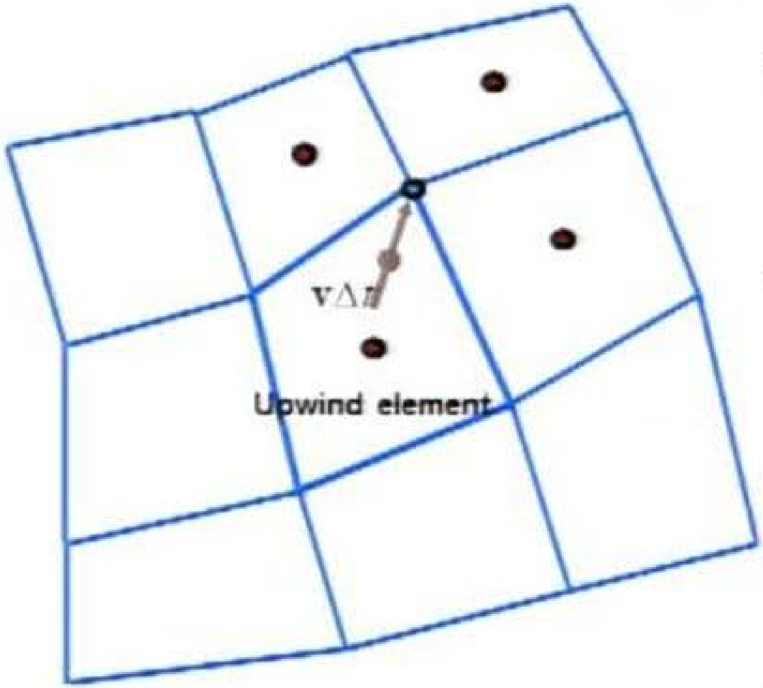
Flux remap step

$$\int_S \mathbf{B} \bullet d\mathbf{a} = 0 \qquad \int_{S_{old}} \mathbf{B} \bullet d\mathbf{a} + \int_{S_{new}} \mathbf{B} \bullet d\mathbf{a} + \sum_{i=1}^{4} \int_{S_i} \mathbf{B} \bullet (\mathbf{v}_g \Delta t \times \mathbf{dl}) = 0$$



$$\int_{S_{old}} \mathbf{B} \bullet d\mathbf{a} + \int_{S_{new}} \mathbf{B} \bullet d\mathbf{a} + \sum_{i=1}^{4} \int_{S_i} \mathbf{dl} \bullet (\mathbf{B} \times \mathbf{v}_g \Delta t) = 0$$

Constrained Transport Type Algorithm



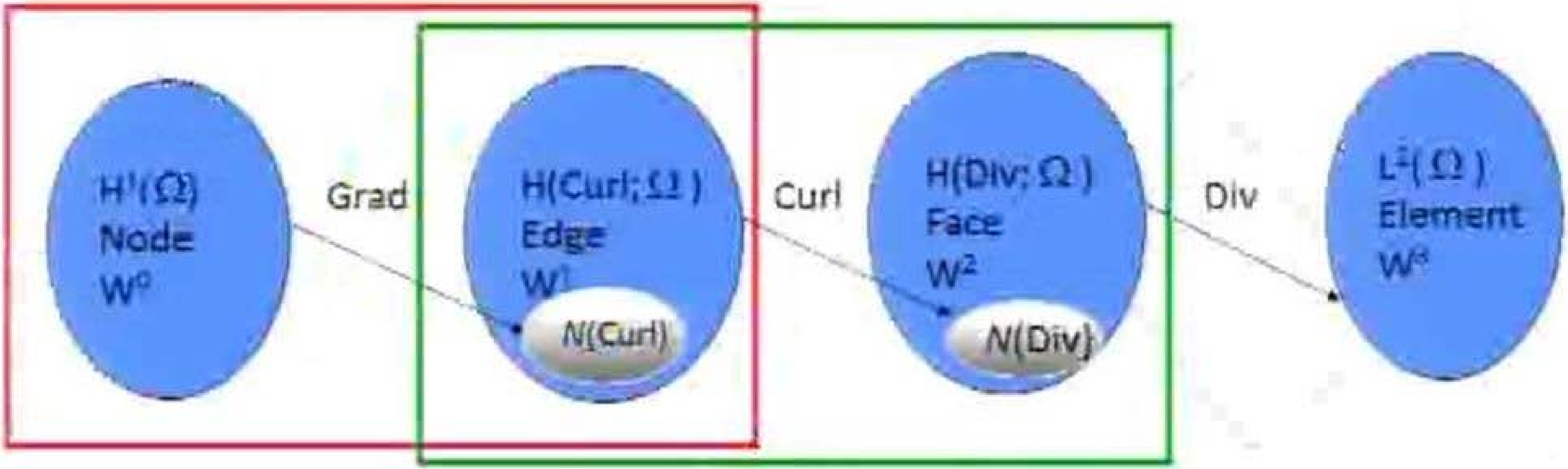
- Compute B at nodes from the face element representation at element centers. This must be second order accurate.
- Compute trial cross face element flux coefficients on each face using these nodal B.

$$Nc_1^f \Rightarrow AA_1^f \text{ (Periodic Table FE)}$$

- Limit on each face to obtain cross face flux coefficients which contribute zero total flux.
- Compute the edge flux contributions in the upwind element by a midpoint integration rule at the center of the edge centered motion vector.

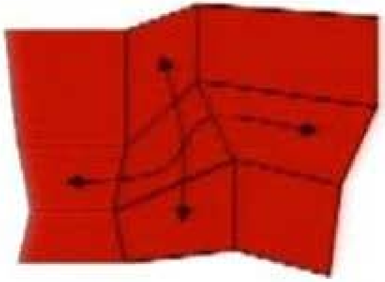
- ``Arbitrary Lagrangian-Eulerian 3D Ideal MHD Algorithms,'' Int. Journal Numerical Methods in Fluids, 2011;65:1438-1450. (remap and deBar energy conservation discussed)

Mass

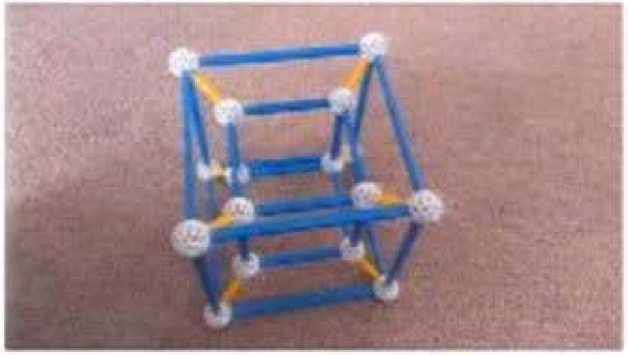

$H^1(\Omega)$
Node
W^0
Grad
$H(Curl;\Omega)$
Edge
W^1
N(Curl)
Curl
$H(Div;\Omega)$
Face
W^2
N(Div)
Div
$L^2(\Omega)$
Element
W^3

Mass

- Lagrangian Step
  - Mass is conserved in the Lagrangian frame.
  - Discrete Lagrangian continuity equation is trivial.



- Remap Step
  - Integration of reconstructed densities over swept surfaces or intersecting grids yield conservative mass changes.
  - These concepts are likely to be very familiar to many.



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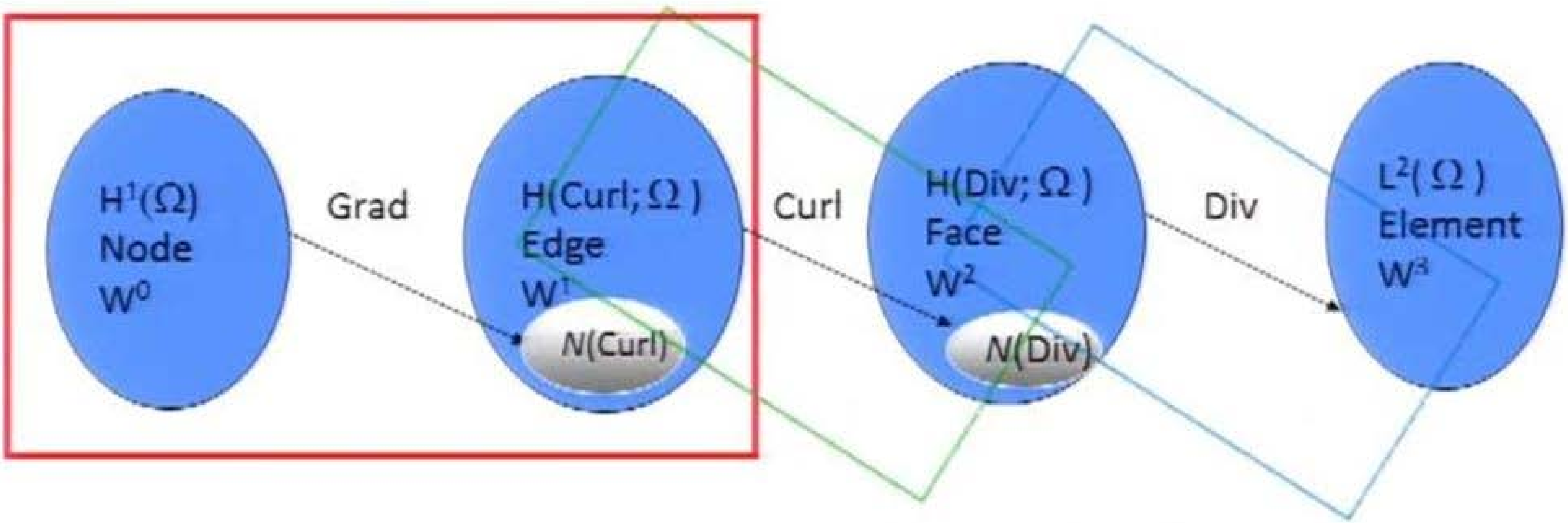
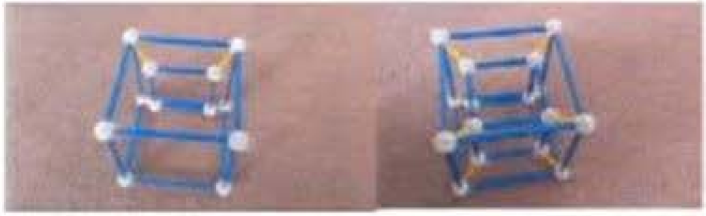
Cartan Magic Formula has Two Parts: When might one need both parts?





Maxwell Equations and Continuum Mechanics

- Kovetz

$$
\begin{aligned}
\nabla \times \mathcal{H} &= \mathcal{J} + \overset{*}{\mathbf{D}}. \\
\nabla \cdot \mathbf{D} &= q. \\
\nabla \times \mathcal{E} &= -\overset{*}{\mathbf{B}}. \\
\nabla \cdot \mathbf{B} &= 0. \\
\mathbf{D} &= \epsilon_0 \mathbf{E} + \mathbf{P}. \\
\mathcal{H} &= \mu_0^{-1}\mathbf{B} - \mathbf{v} \times \epsilon_0 \mathbf{E} - \mathcal{M}
\end{aligned}
$$

- Constitutive theory provides $\mathcal{M}$, $\mathbf{P}$ and $\mathcal{J}$ with $\mathcal{E} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$
- Flux derivatives

$$
\begin{aligned}
\overset{*}{\mathbf{B}} &= \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{B}) = \frac{\partial \mathbf{B}}{\partial t} + \nabla \times (\mathbf{B} \times \mathbf{v}) \\
\overset{*}{\mathbf{D}} &= \frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{D}) = \frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + q\mathbf{v}
\end{aligned}
$$

Physically, D and B are two-forms

- Take a page from 3D ALE MHD and place D and B as fundamental variables (fluxes) on faces using face elements.
- Operator split the Lagrangian step.
- Mesh motion occurs with constant D and B fluxes. This conserves both the zero magnetic flux divergence property and charge.
- Update the fluxes and electric displacements using a mimetic method perhaps following along ideas similar to Bochev and Gerritsma, "A spectral mimetic least-squares method," 2014.
- Magnetic flux remap is unchanged.
- Electric displacement remap needs both parts of Cartan's formula.

All terms will contribute

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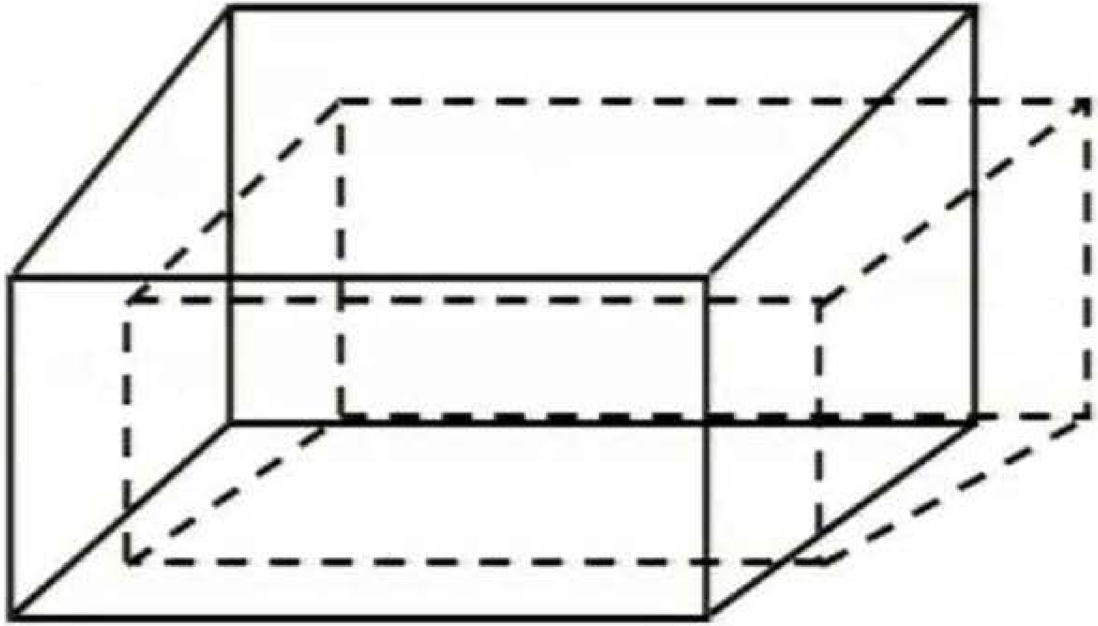
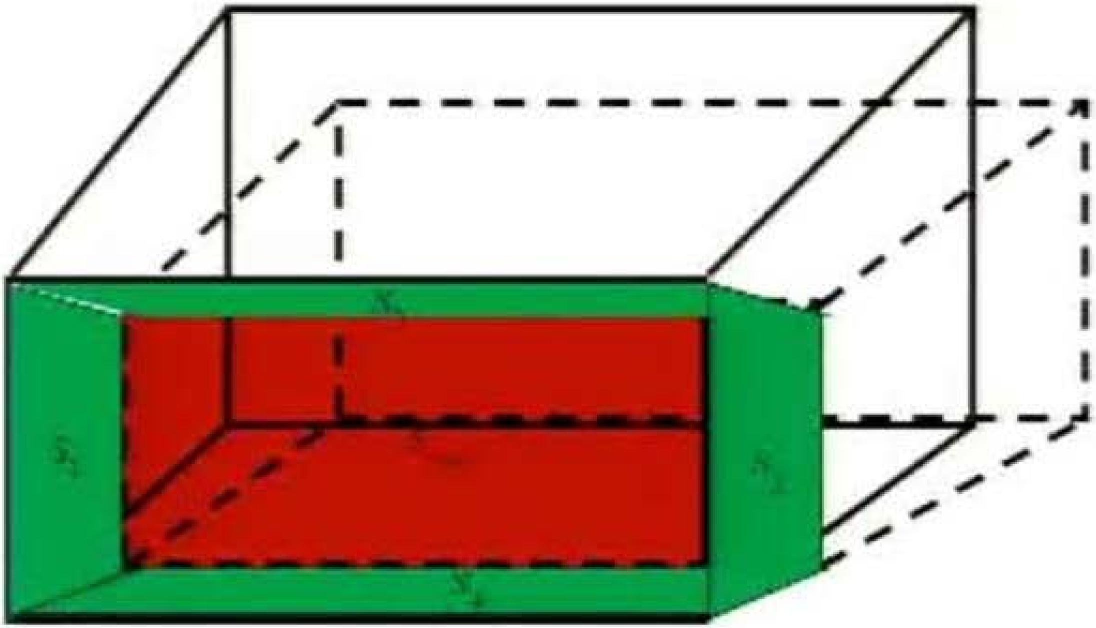
$$\frac{\partial \mathbf{D}}{\partial t} + \boxed{\nabla \times (\mathbf{D} \times \mathbf{v})} + \boxed{\mathbf{v}(\nabla \cdot \mathbf{D})}$$



New electric displacement flux is the oriented sum of swept edge contributions which do not change the charge plus swept volume contributions which do. This is really nothing more than Stokes theorem.

All terms will contribute

$$\frac{\partial \mathbf{D}}{\partial t} + \boxed{\nabla \times (\mathbf{D} \times \mathbf{v})} + \boxed{\mathbf{v}(\nabla \cdot \mathbf{D})}$$



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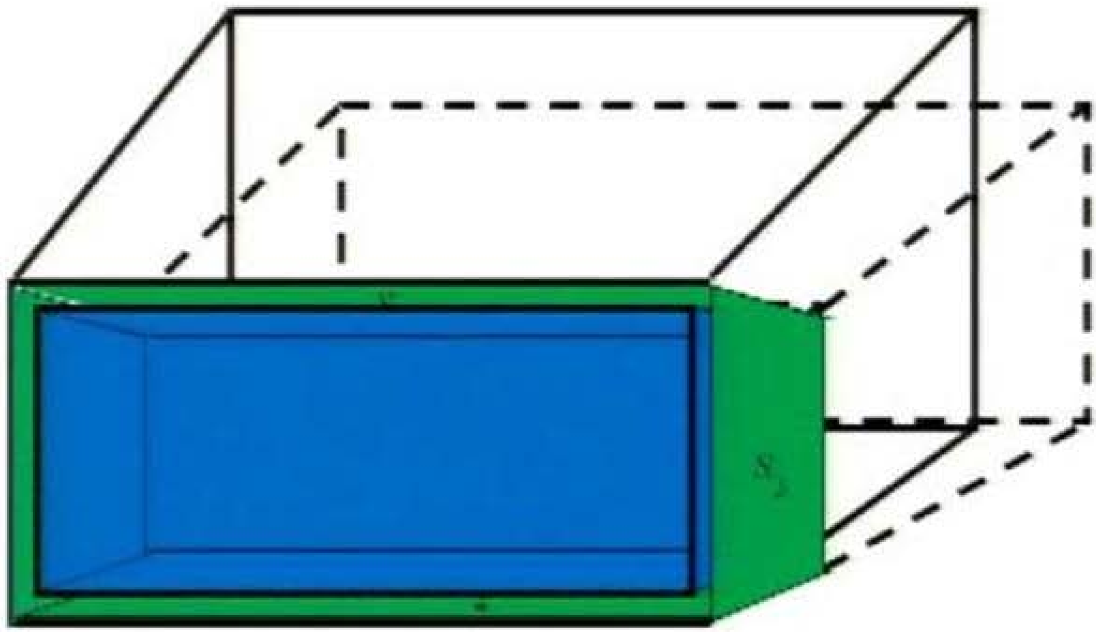
$$\frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{D})$$



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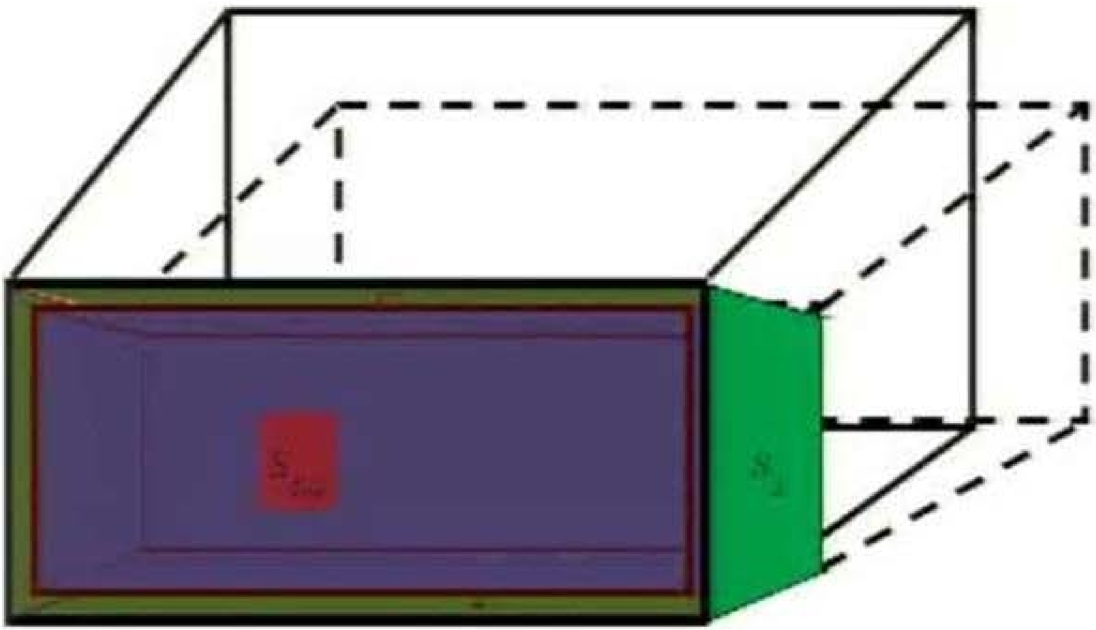
All terms will contribute

$$\frac{\partial \mathbf{D}}{\partial t} + \nabla \times (\mathbf{D} \times \mathbf{v}) + \mathbf{v}(\nabla \cdot \mathbf{D})$$



New electric displacement flux is the oriented sum of swept edge contributions which do not change the charge plus swept volume contributions which do.
This is really nothing more than Stokes theorem.

Conclusion

- Understanding at an intuitive level the de Rham complex, Stoke's theorem, the Lie Derivative, Cartan's magic formula, and classical transport theorems is fundamental to developing structure preserving Lagrangian/Eulerian algorithms for multiphysics.
- This presentation gives a small taste of why the general field of structure preserving discretizations (which uses differential forms as the fundamental descriptive language) may be important.
- Several researchers have developed advection algorithms for differential forms. (e.g. McKenzie, Heumann, Hiptmair, Xu)
- Ideas for high quality remap (e.g. optimization, WENO,...) can and should be applied in this general framework.
- Software remap libraries are not commonly built for general differential forms/FEEC at this time. Having such fundamental tools readily available would open up new avenues for utilization and testing of next-generation multi-physics modeling approaches.
- Many opportunities are available for additional advances at the geometrical intersection between physics and mathematics.