SAND2008-3745C

Remap of solenoidal fields on unstructured quadrilateral grids

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ALE from ART to SCIENCE
June 10th - June 13th
LANL

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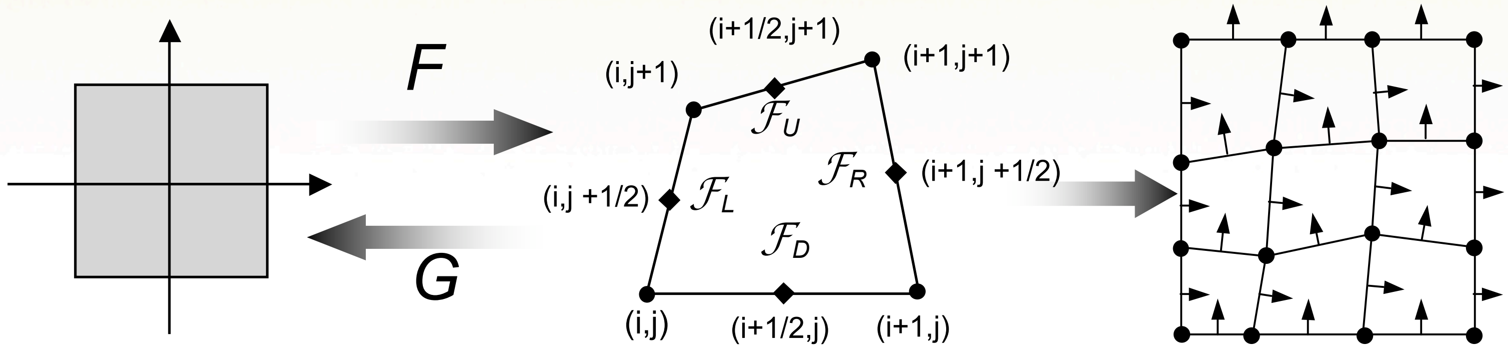
Summary

- Edge and face finite element spaces on quads
- Formal statement of the remap problem
- Constrained Interpolation (CI) remapper
  - Recovery
  - Optimization
  - Interpolation
- Numerical results
  - Optimization of potentials
  - Discontinuous B

Edge and Face Elements on Logically Rectangular Grids



Virtual edge functions W¹

$$W_{ij}(\mathbf{x}) = \frac{1}{4}\left(1 - G_1(\mathbf{x})\right)\left(1 - G_2(\mathbf{x})\right)\vec{\mathbf{k}}$$

$$W_{i+1,j}(\mathbf{x}) = \frac{1}{4}\left(1 + G_1(\mathbf{x})\right)\left(1 - G_2(\mathbf{x})\right)\vec{\mathbf{k}}$$

$$W_{i,j+1}(\mathbf{x}) = \frac{1}{4}\left(1 - G_1(\mathbf{x})\right)\left(1 + G_2(\mathbf{x})\right)\vec{\mathbf{k}}$$

$$W_{i+1,j+1}(\mathbf{x}) = \frac{1}{4}\left(1 + G_1(\mathbf{x})\right)\left(1 + G_2(\mathbf{x})\right)\vec{\mathbf{k}}$$

Local shape functions

Face functions W²

$$W_L(\mathbf{x}) = \frac{1}{4}\left(1 - G_1(\mathbf{x})\right)\nabla G_2(\mathbf{x}) \times \vec{\mathbf{k}}$$

$$W_R(\mathbf{x}) = \frac{1}{4}\left(1 + G_1(\mathbf{x})\right)\nabla G_2(\mathbf{x}) \times \vec{\mathbf{k}}$$

$$W_D(\mathbf{x}) = \frac{1}{4}\left(1 - G_2(\mathbf{x})\right)\vec{\mathbf{k}} \times \nabla G_1(\mathbf{x})$$

$$W_U(\mathbf{x}) = \frac{1}{4}\left(1 - G_2(\mathbf{x})\right)\vec{\mathbf{k}} \times \nabla G_1(\mathbf{x})$$

Piola transform is "hidden" in function definition

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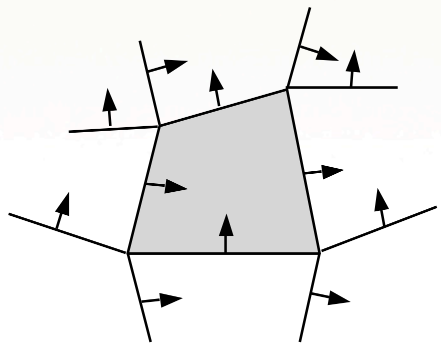
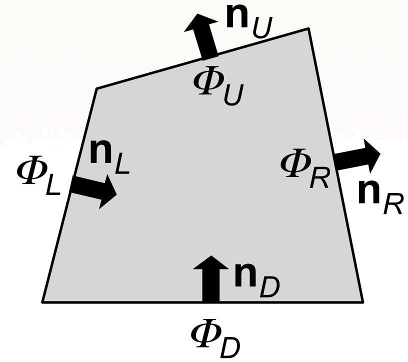
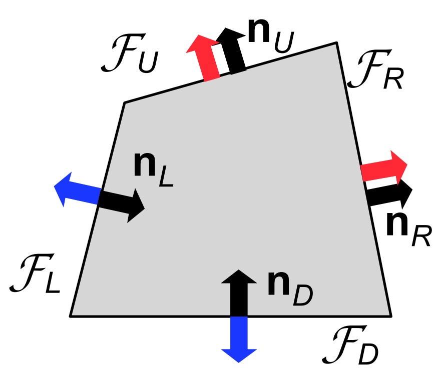
Definition of discrete derivative

Duality of ∂ and d







$$\mathbf{B} = \Phi_D W_D + \Phi_R W_R + \Phi_U W_U + \Phi_L W_L$$

$$\Phi_{\mathcal{F}} = \int_{\mathcal{F}} \mathbf{B} \bullet \mathbf{n}\, ds$$

$$\partial \mathcal{K} = -\mathcal{F}_D + \mathcal{F}_R + \mathcal{F}_U - \mathcal{F}_L = \sum \sigma_s \mathcal{F}_s$$

$$\mathbf{dB}V(K) = -\Phi_D + \Phi_R + \Phi_U - \Phi_L = \sum \sigma_s \Phi_s$$

d=div

Coordinate independent definitions of grad, curl, div

Exactness Relation

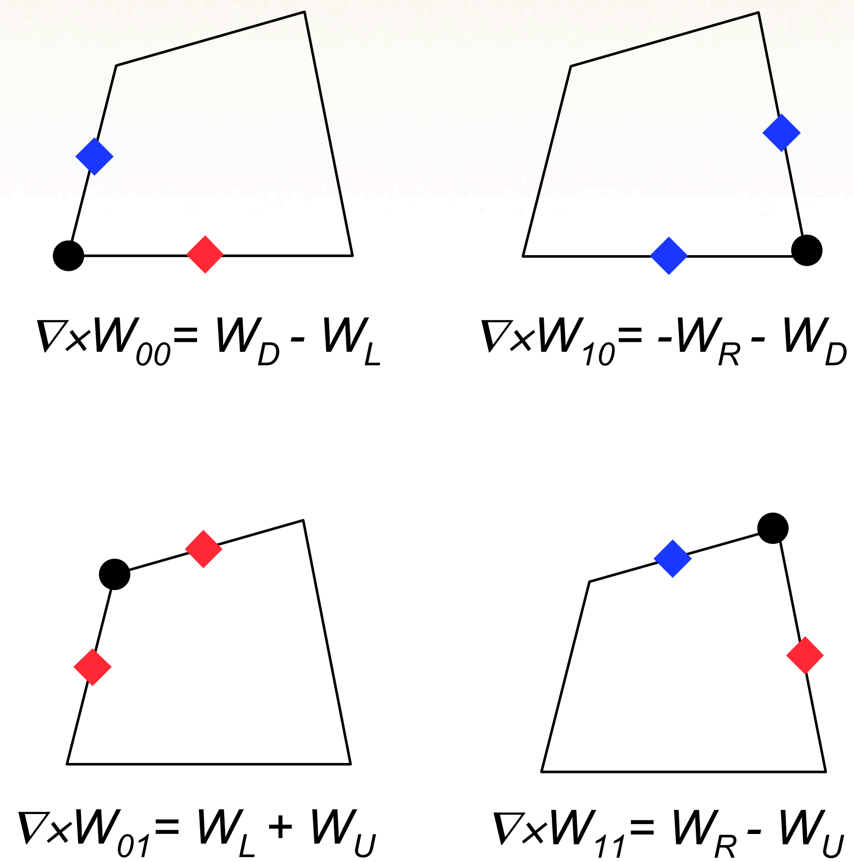
$$\mathbf{A} = \begin{pmatrix} 0 & 0 & \phi \end{pmatrix}^T$$

$$\Downarrow$$

$$\mathbf{A} = \phi_{00} W_{00} + \phi_{10} W_{10} + \phi_{01} W_{01} + \phi_{11} W_{11}$$

$$\nabla \times \mathbf{A} = \phi_{00}\left(W_D - W_L\right) + \phi_{10}\left(-W_L - W_R\right)$$
$$+\phi_{01}\left(W_L + W_U\right) + \phi_{11}\left(W_R - W_U\right)$$

$$\nabla \times \mathbf{A} = \left(\phi_{00} - \phi_{10}\right)W_D + \left(\phi_{01} - \phi_{11}\right)W_U$$
$$+\left(\phi_{11} - \phi_{10}\right)W_R + \left(\phi_{01} - \phi_{00}\right)W_L$$



Discrete Poincare Lemma: $\nabla \cdot \mathbf{B} = 0 \Leftrightarrow \mathbf{B} = \nabla \times \mathbf{A}$

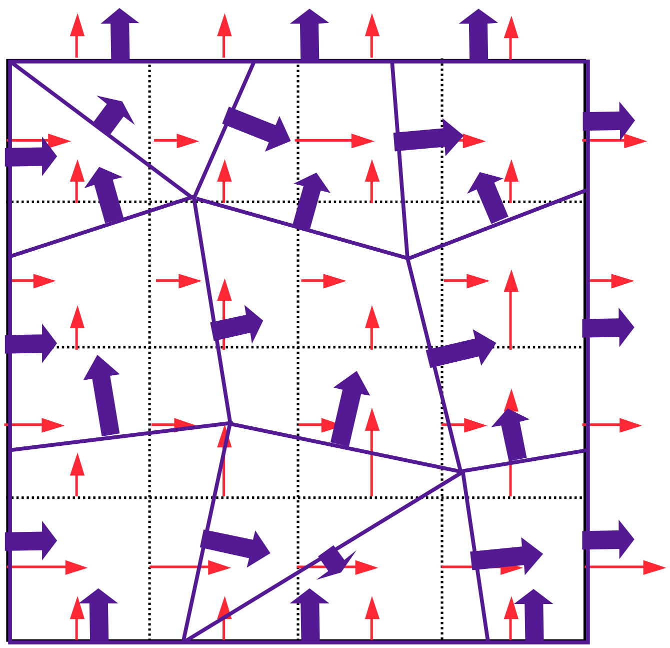
(Formal) Statement of the remap problem:

Given:

- **NEW** and **OLD** meshes with possibly **different** types and numbers of cells
- Discrete solenoidal field **B** on the **OLD** mesh, represented by its fluxes

Find:

- Discrete solenoidal field **B** on the **NEW** mesh such that $\mathbf{B} \approx \mathbf{B}$



A good remapper

- ✓ Is accurate
- ✓ Preserves energy
- ✓ Has good feature retention
- ✓ Does not “ring” at jumps
- ✓ Is efficient (EXPLICIT)!

Taxonomy of Remap Algorithms

Remap via Transport Algorithms: (*Robinson, Bochev, Rambo, SAND2001-2146P*)

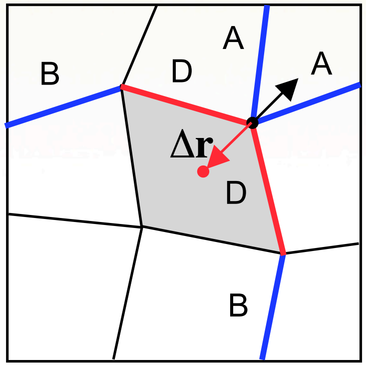
- ❑ Same connectivity required for grids
- ❑ Explicit
- ❑ Upwinding required.
- ❑ Equivalent to Taylor expansion:

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left(\mathbf{B} \times \mathbf{u}_{REL}\right)$$

$$\mathbf{B}^{n+1} = \mathbf{B}^{n} - \Delta t \nabla \times \left(\mathbf{B}^{n} \times \mathbf{u}_{REL}\right)$$

details

$$\mathbf{B}(\mathbf{r} + \Delta\mathbf{r}) = \mathbf{B}(\mathbf{r}) - \nabla \times \left(\Delta\mathbf{r} \times \mathbf{B}\right) + O\left(\left|\Delta\mathbf{r}\right|^{2}\right)$$



Remap via Constrained Optimization: (*Carey et al. IJNME 50, **2001**, Girault **2003***)

- ❑ Arbitrary grids
- ❑ Implicit: solution of a saddle-point “Darcy” problem **required**:

$$\min_{\mathbf{B}^{new} \in W^{new}(\Omega)} \int_{\Omega} \left|\mathbf{B}^{old} - \mathbf{B}^{new}\right|^{2} dx \quad \text{subject to } \nabla \cdot \mathbf{B}^{new} = 0 \quad \Rightarrow \quad \begin{pmatrix} A & C \\ C^{T} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{B}^{new} \\ \lambda \end{pmatrix} = \begin{pmatrix} \mathbf{B}^{old} \\ 0 \end{pmatrix}$$

Remap via Grid Structure:(*Balsara JCP 174, **2001**, Roe & Toth JCP 180, **2002***)

- ❑ Limited to Cartesian grids
- ❑ Additional restrictions required: factor-of-2 resolution change, etc.

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Constrained Interpolation (CI) Algorithm

Principal idea: exploit **existence** of discrete potentials in exact sequences
⇒ **divergence-free constraint automatically satisfied**

Key component: an **explicit** potential recovery algorithm

RECOVERY

$$W^1 \overset{C}{\mapsto} W^2 \overset{D}{\mapsto} W^3$$

$$D\mathbf{B} = \mathbf{0} \Leftrightarrow \mathbf{B} = C\mathbf{A}$$

$$\begin{array}{ccc}
\nabla \cdot \mathbf{B}^{old} = 0 & & \nabla \cdot \mathbf{B}^{new} = 0 \\
\downarrow & & \uparrow \\
\mathbf{B}^{old} = \nabla \times \mathbf{A}^{old} & & \mathbf{B}^{new} = \nabla \times \mathbf{A}^{new} \\
\downarrow & & \uparrow \\
\mathbf{A}^{old} & \longrightarrow & \mathbf{A}^{new}
\end{array}$$

REMAP

POSTPROCESSING

$$\mathcal{R}\left(\mathbf{A}^{old}\right) \mapsto$$

Patch recovery
PP operators
FV reconstruction

"reconstruction"

OPTIMIZATION

$$\mathbf{A}\ (\lambda) = \lambda \mathbf{A}^{old} + (1-\lambda)\mathcal{R}\left(\mathbf{A}^{old}\right)$$

$$\lambda_{opt} = \arg\min J\left(\mathbf{A}^{old}, \mathbf{A}(\lambda)\right)$$

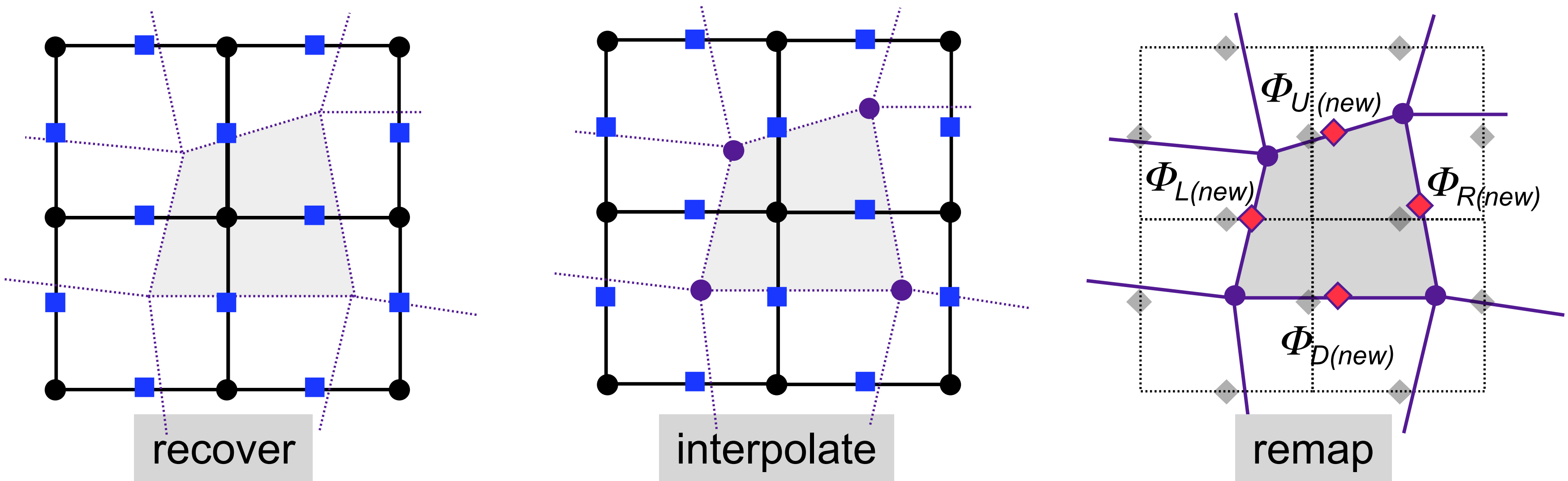
"limiting"

INTERPOLATION

$$\mathbf{A}^{new} = \mathcal{I}\mathbf{A}\left(\lambda_{opt}\right)$$

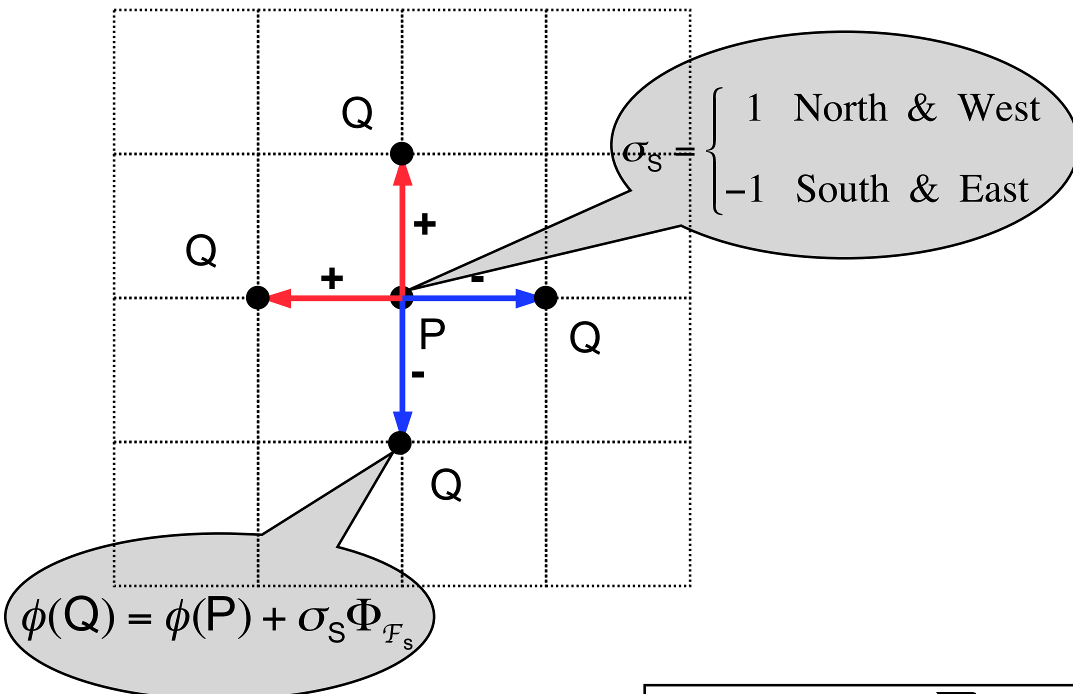
"upwinding"

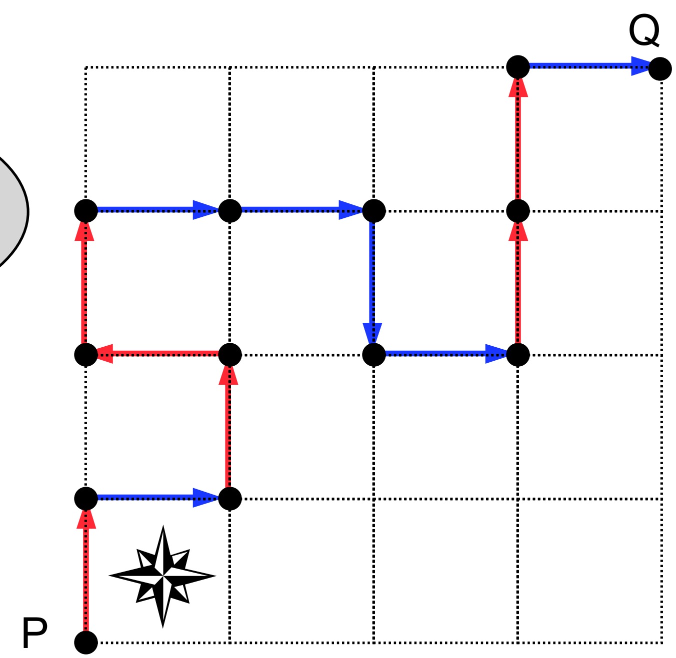
CI Remap in a Nutshell



Explicit Potential Recovery

$$\left.\begin{aligned}\nabla\times\mathbf{A}_{\mathbf{B}} &= (\phi_{00}-\phi_{10})W_D + (\phi_{01}-\phi_{11})W_U \\ &\quad + (\phi_{11}-\phi_{10})W_R + (\phi_{01}-\phi_{00})W_L \\ \mathbf{B} &= \Phi_D W_D + \Phi_U W_U + \Phi_R W_R + \Phi_L W_L\end{aligned}\right\} \Rightarrow \nabla\times\mathbf{A}_{\mathbf{B}} = \mathbf{B} \Leftrightarrow \begin{cases}\Phi_D = (\phi_{00}-\phi_{10}) & \Phi_L = (\phi_{01}-\phi_{00}) \\ \Phi_U = (\phi_{01}-\phi_{11}) & \Phi_R = (\phi_{11}-\phi_{10})\end{cases}$$





$$\boxed{\phi(Q) = \phi(P) + \sum_{\mathcal{F}_S} \sigma_S \Phi_{\mathcal{F}_S}}$$

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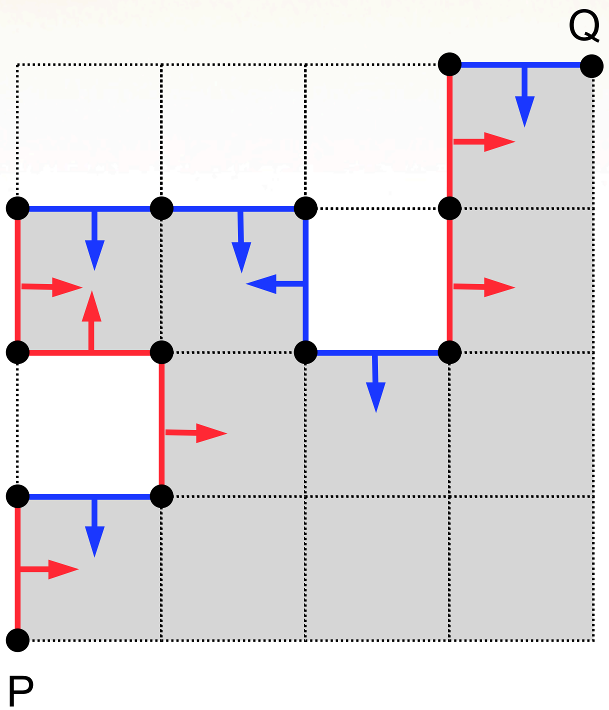
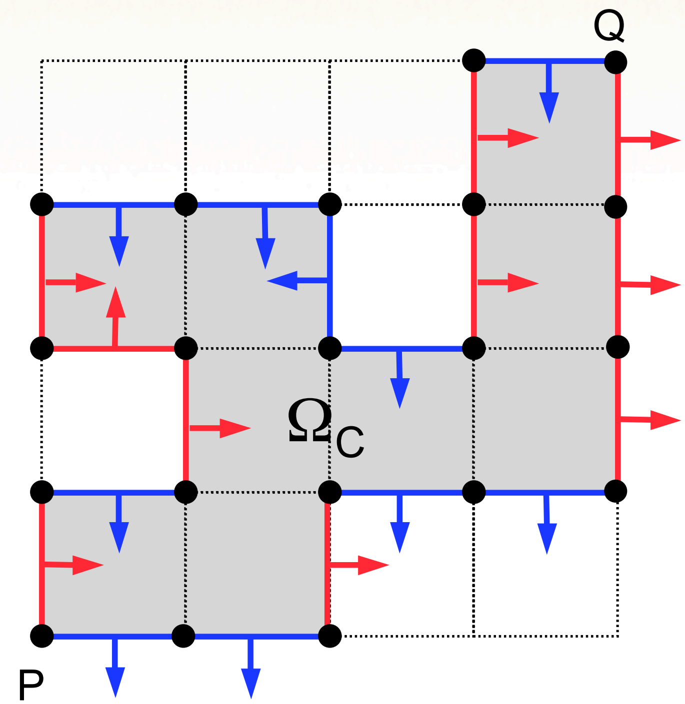
Path Independence



$$C_1 = \sum_{\mathcal{F}_{S_1}} \sigma_{S_1} \mathcal{F}_{S_1}$$

$$C_2 = \sum_{\mathcal{F}_{S_2}} \sigma_{S_2} \mathcal{F}_{S_2}$$



$$\left.\begin{array}{l} \partial\Omega_C = C_2 - C_1 \\ \nabla \cdot \mathbf{B} = 0 \end{array}\right\} \Rightarrow 0 = \int_{\Omega_C} \nabla \cdot \mathbf{B}\, dx = \int_{\partial\Omega_C} \mathbf{B} \cdot \mathbf{n}\, dx$$

$$\Rightarrow 0 = \int_{C_2} \mathbf{B} \cdot \mathbf{n}\, dx - \int_{C_1} \mathbf{B} \cdot \mathbf{n}\, dx \quad \Rightarrow \quad \boxed{\int_{C_2} \mathbf{B} \cdot \mathbf{n}\, dx = \int_{C_1} \mathbf{B} \cdot \mathbf{n}\, dx = \varphi(Q)}$$

Recovery on Logically Rectangular Grids

1. Choose a spanning tree

$$C_{sp} = \sum_{\mathcal{F}_{S_{sp}}} \sigma_{S_{sp}} \mathcal{F}_{S_{sp}}$$

2. Initialize the root

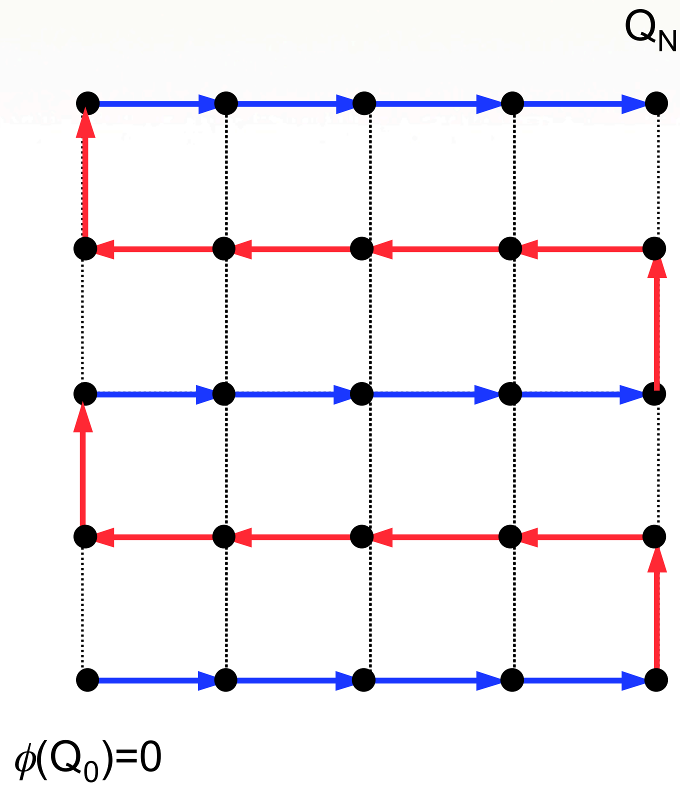
$$\phi(Q_0) = 0$$

3. Traverse the branches

for k=1:N

$$\phi(Q_k) = \phi(Q_{k-1}) + \sigma_k \Phi_{\mathcal{F}_k}$$

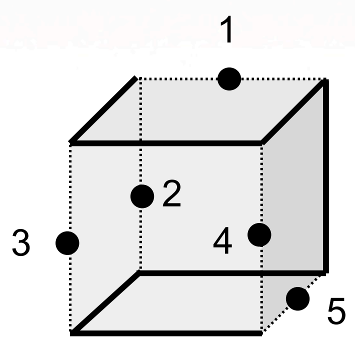
end



3D recovery on logically Cartesian grids similar

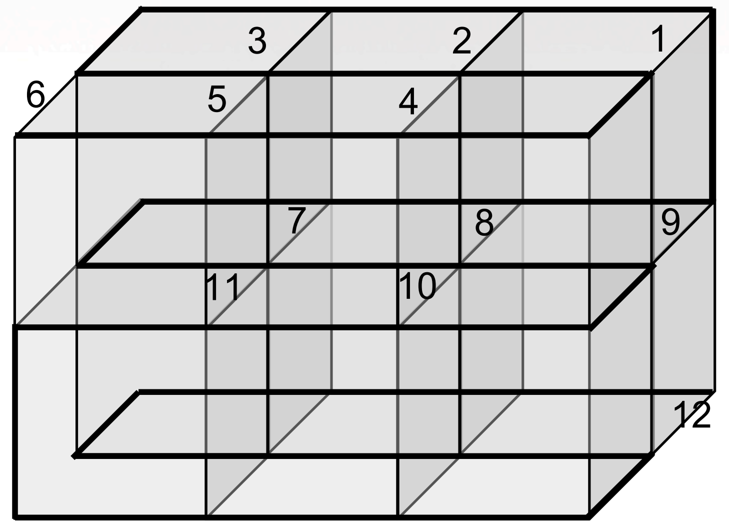
Base potential recovery in 3D

On one cell:



6 flux DOF - 1 constraint = 5
12 edges - 7SP edges = 5

On a logically rectangular mesh

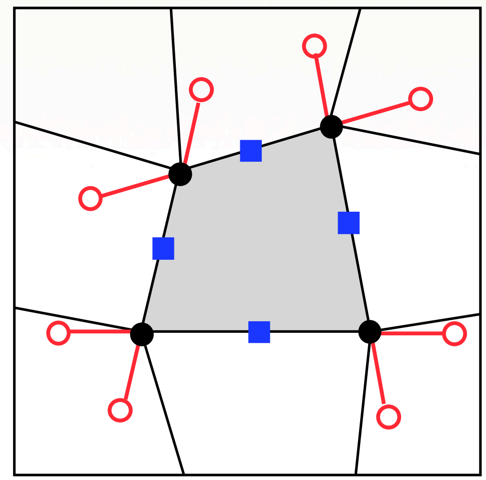


1. Choose a spanning tree and mark edges on co-spanning tree as **free**
2. Order faces with respect to the number of free edges
3. Recover $\mathbf{A}_B$ on all faces with 1 free edge; update number of free edges
4. If no faces with free edges left **then** stop, **else** proceed to step 3

Post-processing and Optimization

Post-processing

- A_B → **base** Q1 (bilinear interpolant)
- A_E → **extended** 8 node serendipity



Optimization

$$\mathbf{A}(\lambda) = \lambda \mathbf{A}^{old} + (1-\lambda)\mathcal{R}(\mathbf{A}^{old})$$

$$\lambda_{opt} = \arg\min J(\mathbf{A}^{old}, \mathbf{A}(\lambda))$$

A. Feedback

$$\lambda_{new} = \begin{cases} \max(0, \lambda_{old} + \varepsilon) & \varepsilon < 0 \\ \min(1, \lambda_{old} + \varepsilon) & \varepsilon > 0 \end{cases}; \qquad \varepsilon = \theta\left(1 - \frac{\|\mathbf{B}_{old}\|_\Omega}{\|\mathbf{B}_{new}\|_\Omega}\right)$$

B. l-parameter control

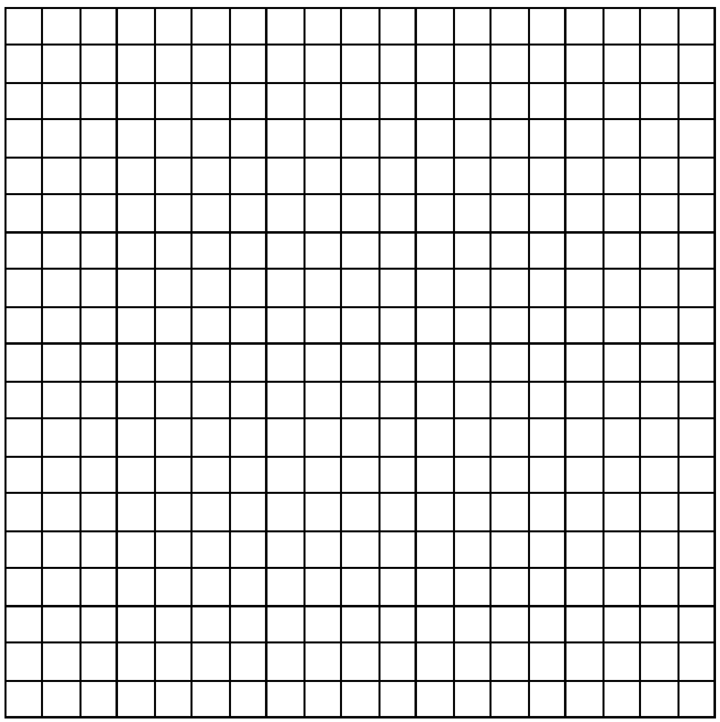
$$\lambda(\Omega) \rightarrow \arg\min\left(\|\mathbf{B}_{old}\|_\Omega^2 - \|\mathbf{B}_{new}(\lambda(\Omega))\|_\Omega^2\right)^2$$

C. Cell-by-cell control

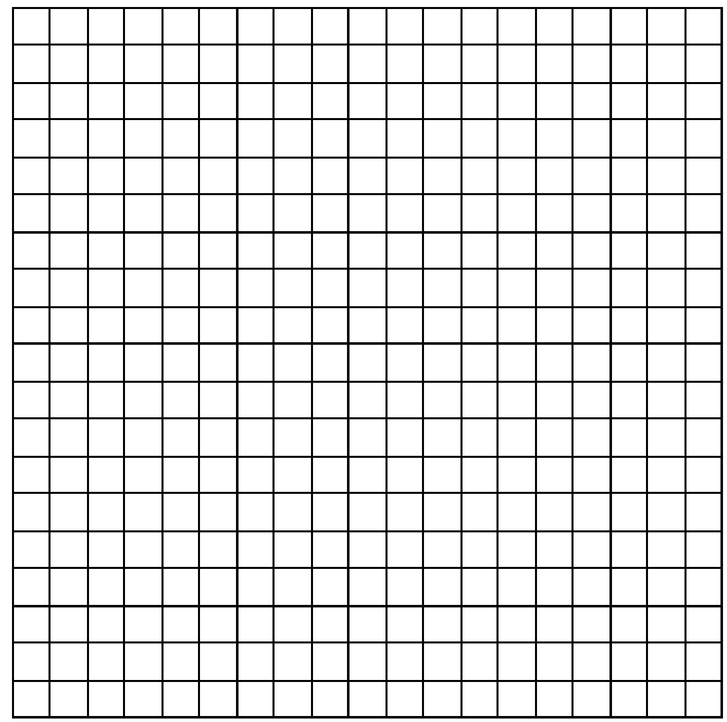
Requires conservative remap of magnetic energy (see *Shashkov and Margolin, LANL LAUR-2002*)

Numerical Results: Cyclic Remap

Wave Mesh



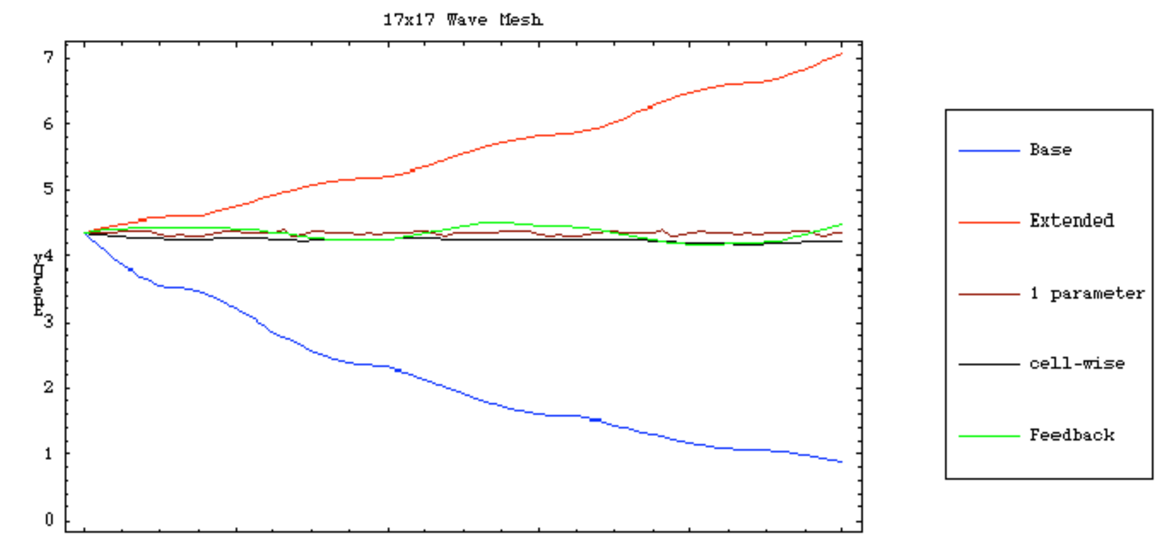
Random Mesh

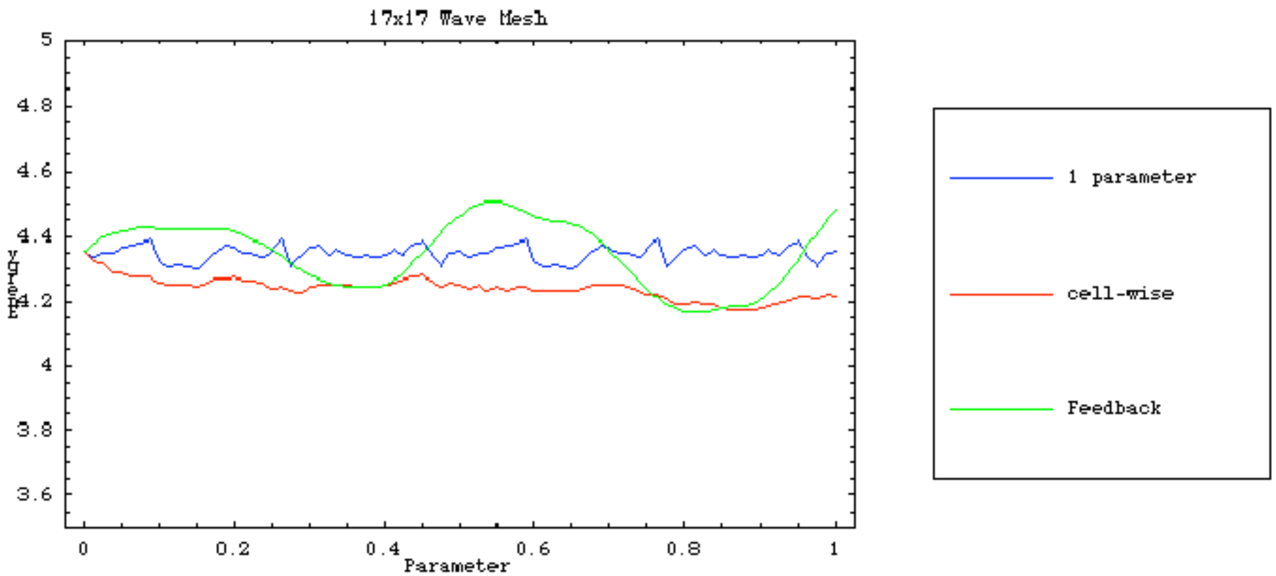


100 cycles

Shashkov and Margolin, LANL LAUR-2002

Potential Optimization: Wave Mesh



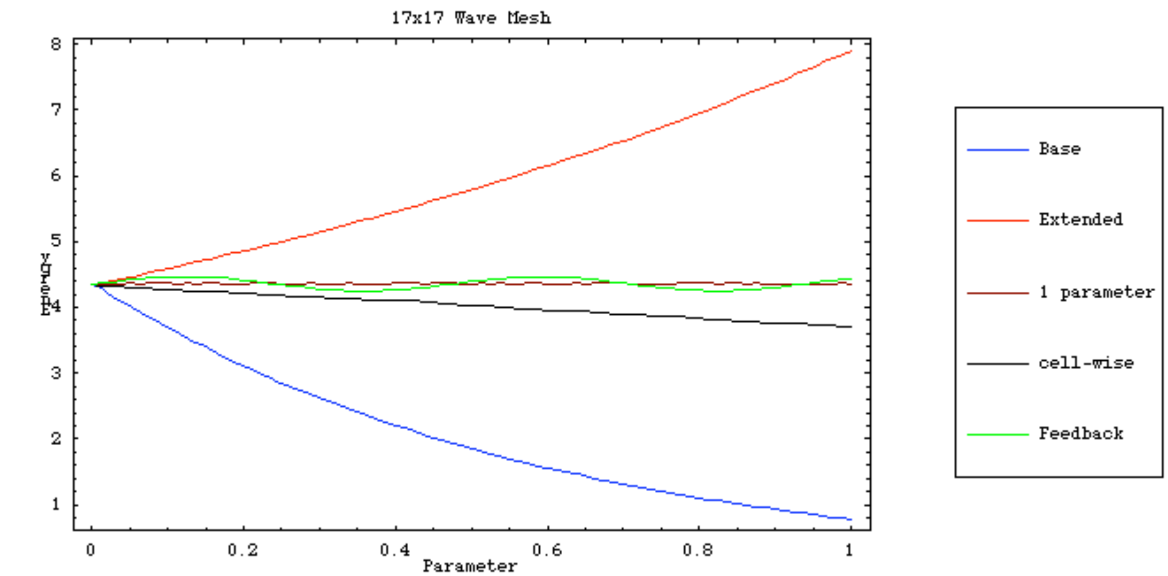


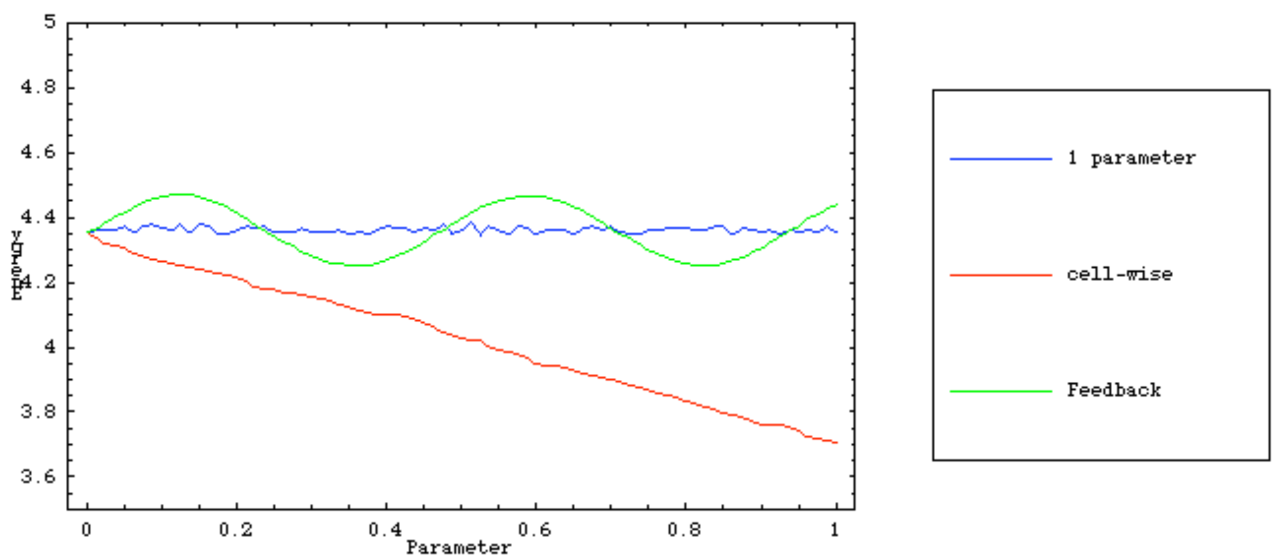
17x17 Wave Mesh:
80 cycles

$$\mathbf{B} = \nabla \times \mathbf{A};$$

$$\mathbf{A} = \sin(2\pi x)\sin(2\pi y)$$

Potential Optimization: Random Mesh





17x17 Random Mesh: 80 cycles

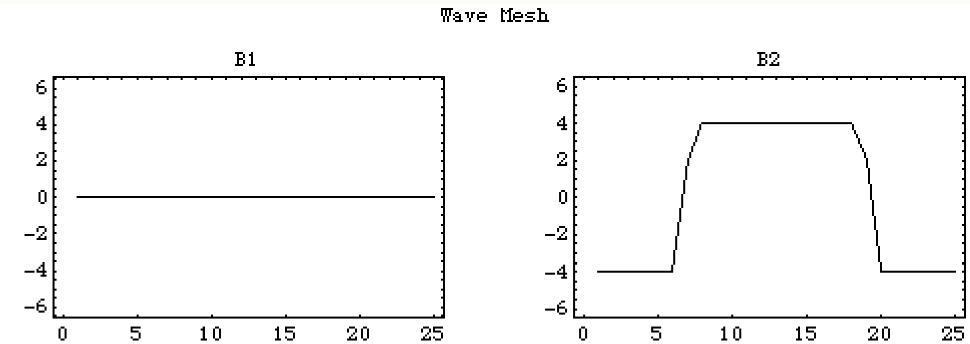
$$\mathbf{B} = \nabla \times \mathbf{A};$$

$$\mathbf{A} = \sin(2\pi x)\sin(2\pi y)$$

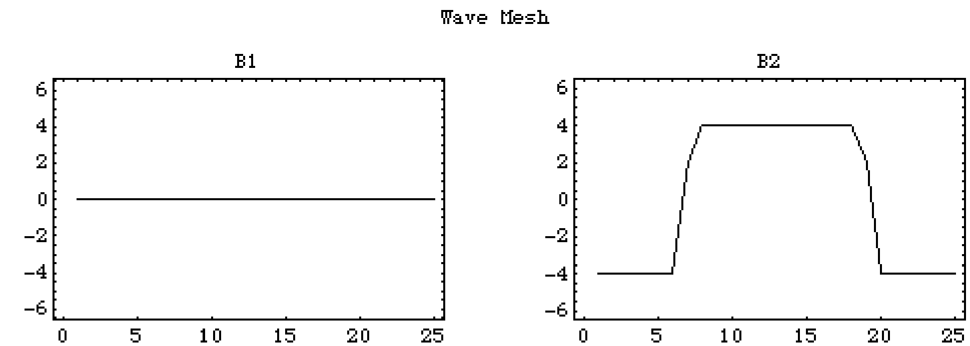
Potential Optimization:
Discontinuous Field

30x30 Wave Mesh:
100 cycles

1-parameter control

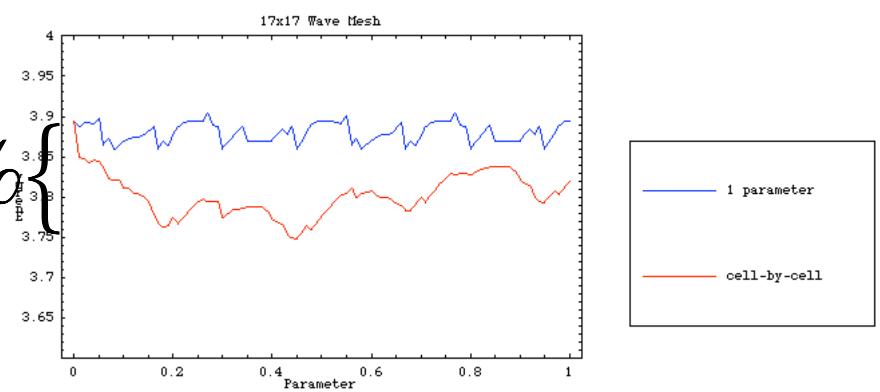


Cell-by-cell control



Energy

$< 4\%$

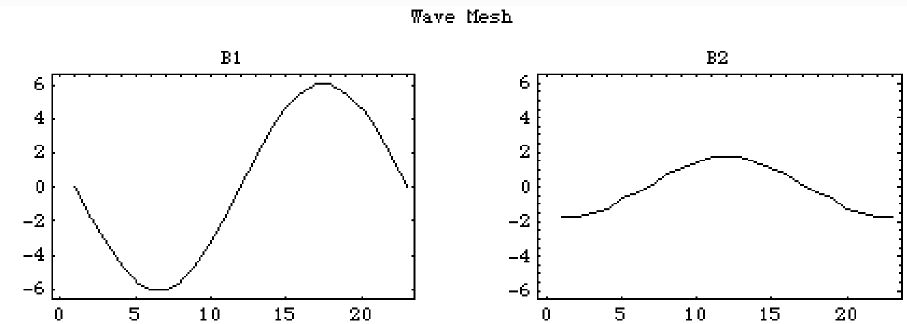


CI Base vs. CT Donor:
Smooth Field

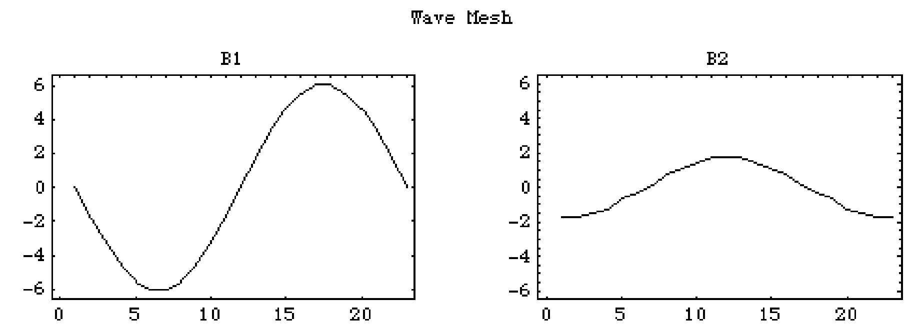
**30x30 Wave Mesh:
100 cycles**

$$\mathbf{B} = \nabla \times \mathbf{A}; \quad \mathbf{A} = \sin(2\pi x)\sin(2\pi y)$$

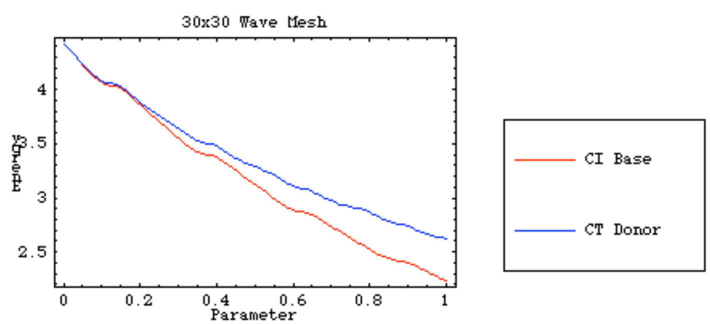
CI Base:



CT Donor:



Energy:

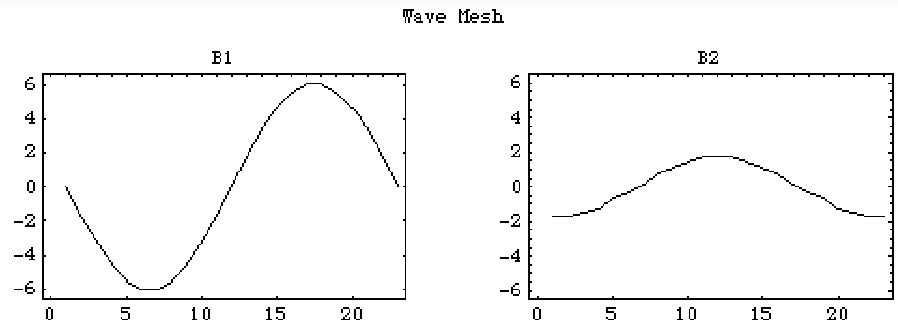


CI Base vs. CT Donor:
Smooth Field

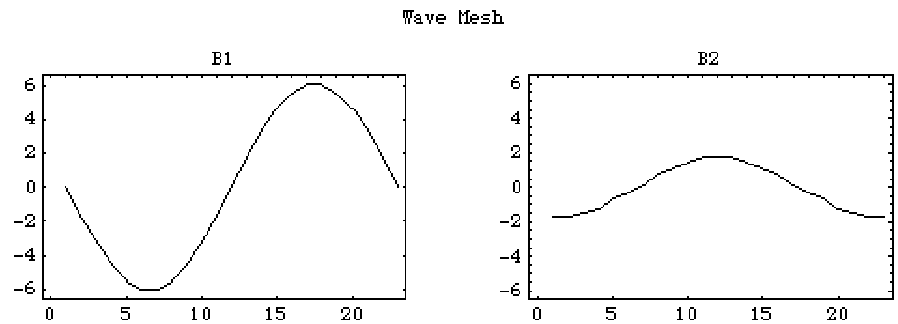
30x30 Random Mesh:
100 cycles

$$\mathbf{B} = \nabla \times \mathbf{A}; \quad \mathbf{A} = \sin(2\pi x)\sin(2\pi y)$$

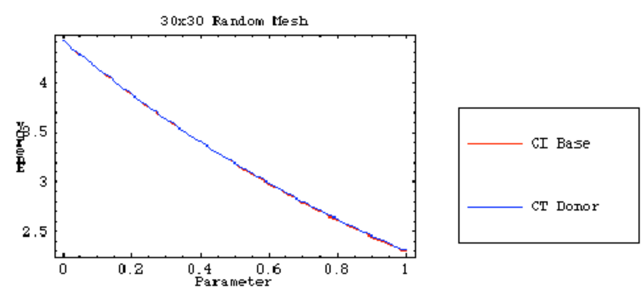
CI Base:



CT Donor:



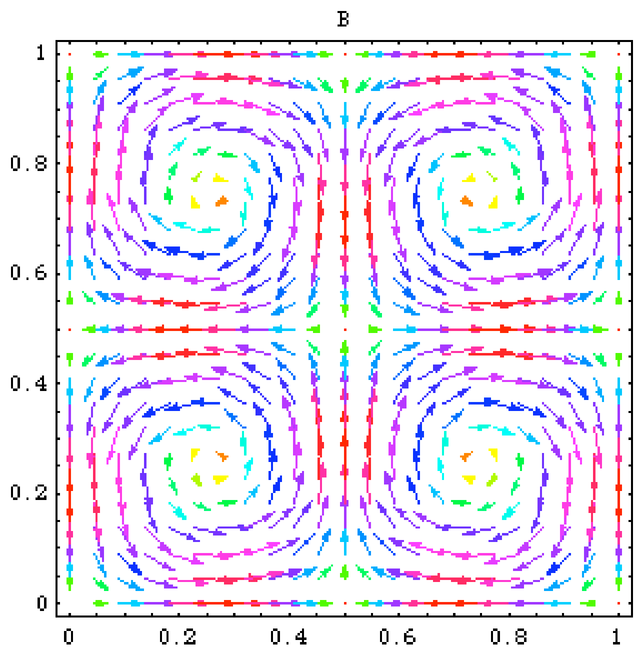
Energy:



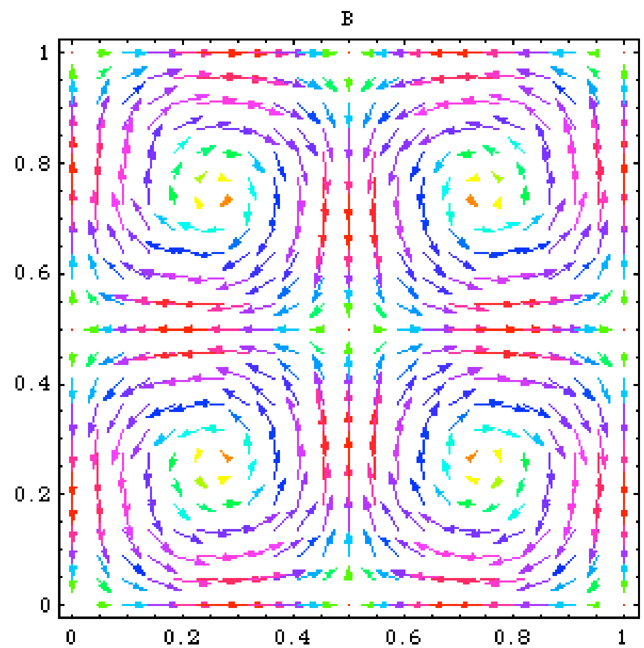
CI Base vs. CT Donor:
Smooth Field

Feature retention $\mathbf{B} = \nabla \times \mathbf{A}; \quad \mathbf{A} = \sin(2\pi x)\sin(2\pi y)$

CI Base



Constrained Transport Donor



30x30 Wave mesh:
100 cycles

Conclusions

Constrained Interpolation Remap:

- Algorithm applicable to arbitrary pairs of grids:

  1. Old and new grid can have different topologies (refinement)
  2. New grid is not necessarily a small perturbation of the old one (no CFL condition required for stability)
  3. High accuracy retained for unstructured grids
  4. Explicit!

- Modular: can be extended to different discretizations (FE, FV, FD)

Constrained Transport (CT) Remapper

Based on CT scheme of Evans, Hawley, The Astrophysical Journal 332, 1988

Advection equation

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left(\mathbf{B} \times \mathbf{u}_{REL}\right)$$

$$\mathbf{E} = \mathbf{B} \times \mathbf{u}_{REL}$$

Discretization

$$\mathbf{B}^{old} = \sum_{\mathcal{F}} \Phi_{\mathcal{F}}^{old} W_{\mathcal{F}}^{old}$$

$$\mathbf{E}^{old} = \sum_{\mathcal{N}} C_{\mathcal{N}}^{old} W_{\mathcal{N}}^{old}$$

CT Update

$$\mathbf{B}^{new} = \mathbf{B}^{old} - \Delta t \nabla \times \mathbf{E}^{old}$$

Flux update

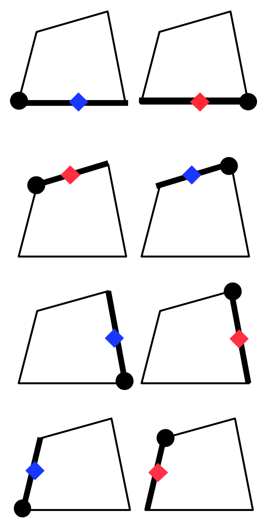
Exactness

$$\Phi_D^{new} = \Phi_D^{old} + \Delta t\left(C_{00}^{old} - C_{10}^{old}\right)$$

$$\Phi_U^{new} = \Phi_U^{old} + \Delta t\left(C_{01}^{old} - C_{11}^{old}\right)$$

$$\Phi_R^{new} = \Phi_R^{old} + \Delta t\left(C_{11}^{old} - C_{10}^{old}\right)$$

$$\Phi_L^{new} = \Phi_L^{old} + \Delta t\left(C_{01}^{old} - C_{00}^{old}\right)$$



$$\nabla \times \mathbf{E}^{old} = \left(C_{00}^{old} - C_{10}^{old}\right)W_D^{old} + \left(C_{01}^{old} - C_{11}^{old}\right)W_U^{old} + \left(C_{11}^{old} - C_{10}^{old}\right)W_R^{old} + \left(C_{01}^{old} - C_{00}^{old}\right)W_L^{old}$$

$$\nabla \cdot \mathbf{B}^{old} = 0 \quad \Rightarrow \quad \nabla \cdot \mathbf{B}^{new} = 0$$

Computation of EMF in CT

E is required at virtual edges **P** → $C^{old}_{\mathcal{N}} = \left(\mathbf{u}_2\mathbf{B}^{old}_1 - \mathbf{u}_1\mathbf{B}^{old}_2\right)(\mathrm{P})$

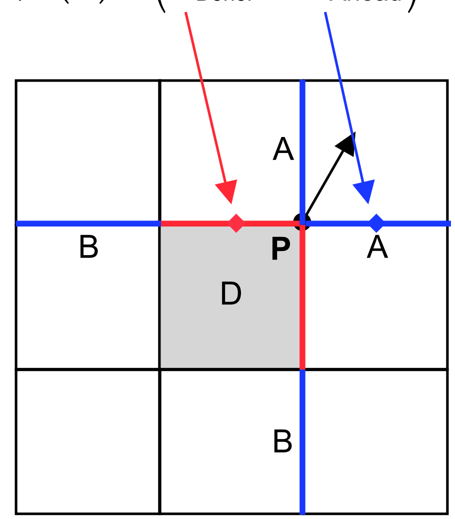
B is discontinuous at **P**

⇒ **B** must be (upwind) averaged at **P** → $\mathbf{B}^{old}_i(\mathrm{P}) = \left(\mathbf{B}^{old}_{\text{Donor}} + \hat{\mathbf{B}}^{old}_{\text{Ahead}}\right)/2$

Upwind interpolation at **P**:

$$\hat{\mathbf{B}}^{old}_{\text{Ahead}} = \mathbf{B}^{old}_{\text{Donor}} + S\left(\frac{|\mathcal{F}_{\text{Donor}}| + |\mathcal{F}_{\text{Ahead}}|}{2} - \Delta t\mathbf{u}_i\right)$$

$$\mathbf{B}^{old}_i(\mathrm{P}) = \mathbf{B}^{old}_{i,\text{Donor}}(\mathrm{P}) + \frac{S}{2}\left(\pm\frac{|\mathcal{F}_{\text{Donor}}| + |\mathcal{F}_{\text{Ahead}}|}{2} - \Delta t\mathbf{u}_i\right)$$



$$S = \begin{cases} \min\left(|S_1|,|S_2|\right)\operatorname{sgn}(S_i) & \text{monotone} \\ 2S_1S_2/\left(S_1 + S_2\right) & \text{harmonic} \\ \min\left(|S_3|,|S_4|,\left(|S_1| + |S_2|\right)/2\right)\operatorname{sgn}(S_i) & \text{Van Leer} \\ 0 \quad \text{if } S_1S_2 < 0 \quad \text{or} & \text{donor} \end{cases}$$

$S_1 = (\mathbf{B}_{\mathrm{A}} - \mathbf{B}_{\mathrm{D}})/\left(\left(|\mathcal{F}_{\mathrm{D}}| + |\mathcal{F}_{\mathrm{A}}|\right)/2\right)$; $S_3 = (\mathbf{B}_{\mathrm{A}} - \mathbf{B}_{\mathrm{D}})/\left(|\mathcal{F}_{\mathrm{D}}|/2\right)$

$S_1 = (\mathbf{B}_{\mathrm{D}} - \mathbf{B}_{\mathrm{B}})/\left(\left(|\mathcal{F}_{\mathrm{D}}| + |\mathcal{F}_{\mathrm{B}}|\right)/2\right)$; $S_4 = (\mathbf{B}_{\mathrm{D}} - \mathbf{B}_{\mathrm{B}})/\left(|\mathcal{F}_{\mathrm{D}}|/2\right)$

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Extension to unstructured meshes

A. Robinson, P. Bochev, P. Rambo. `http://infoserve.sandia.gov/sand_doc/2001/012146p.pdf.`

CT Remap and Taylor expansion

$$\mathbf{B}_1(\mathbf{r}+\Delta\mathbf{r}) = \mathbf{B}_1(\mathbf{r}) + \frac{\partial \mathbf{B}_1(\mathbf{r})}{\partial x}\Delta x + \frac{\partial \mathbf{B}_1(\mathbf{r})}{\partial y}\Delta y + O\left(|\Delta\mathbf{r}|^2\right)$$

$$\mathbf{B}_2(\mathbf{r}+\Delta\mathbf{r}) = \mathbf{B}_2(\mathbf{r}) + \frac{\partial \mathbf{B}_2(\mathbf{r})}{\partial x}\Delta x + \frac{\partial \mathbf{B}_2(\mathbf{r})}{\partial y}\Delta y + O\left(|\Delta\mathbf{r}|^2\right)$$

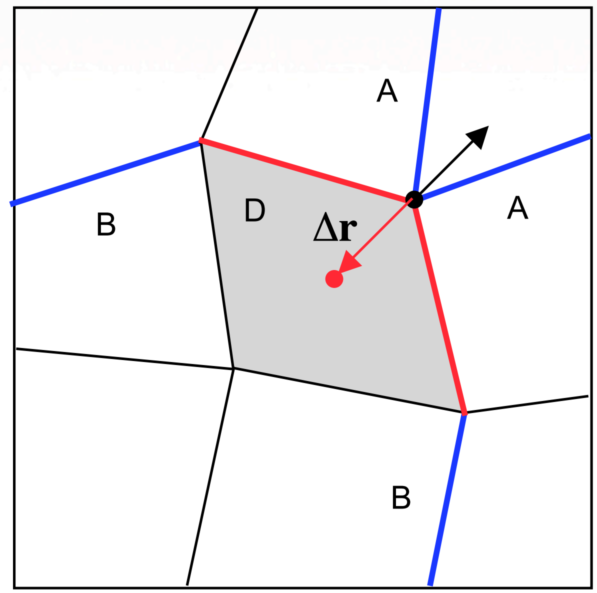
$$\nabla\cdot\mathbf{B} = \frac{\partial \mathbf{B}_1}{\partial x} + \frac{\partial \mathbf{B}_2}{\partial y} = 0$$

$$\mathbf{B}_1(\mathbf{r}+\Delta\mathbf{r}) = \mathbf{B}_1(\mathbf{r}) + \left(\frac{\partial \mathbf{B}_1(\mathbf{r})}{\partial x}\Delta x + \frac{\partial \mathbf{B}_2(\mathbf{r})}{\partial y}\Delta x\right) + \left(\frac{\partial \mathbf{B}_1(\mathbf{r})}{\partial y}\Delta y - \frac{\partial \mathbf{B}_2(\mathbf{r})}{\partial y}\Delta x\right) + O\left(|\Delta\mathbf{r}|^2\right)$$

$$\mathbf{B}_2(\mathbf{r}+\Delta\mathbf{r}) = \mathbf{B}_2(\mathbf{r}) + \left(\frac{\partial \mathbf{B}_2(\mathbf{r})}{\partial x}\Delta x - \frac{\partial \mathbf{B}_1(\mathbf{r})}{\partial x}\Delta y\right) + \left(\frac{\partial \mathbf{B}_2(\mathbf{r})}{\partial y}\Delta y + \frac{\partial \mathbf{B}_1(\mathbf{r})}{\partial x}\Delta y\right) + O\left(|\Delta\mathbf{r}|^2\right)$$

$$\mathbf{B}(\mathbf{r}+\Delta\mathbf{r}) = \mathbf{B}(\mathbf{r}) + \begin{pmatrix} \frac{\partial}{\partial y}(\mathbf{B}_1(\mathbf{r})\Delta y - \mathbf{B}_2(\mathbf{r})\Delta x) \\ -\frac{\partial}{\partial x}(\mathbf{B}_1(\mathbf{r})\Delta y - \mathbf{B}_2(\mathbf{r})\Delta x) \end{pmatrix} + O\left(|\Delta\mathbf{r}|^2\right) = \mathbf{B}(\mathbf{r}) - \nabla\times(\Delta\mathbf{r}\times\mathbf{B})$$

$$\mathbf{B}(\mathbf{r}+\Delta\mathbf{r}) = \mathbf{B}(\mathbf{r}) - \nabla\times\left(\Delta\mathbf{r}\times\mathbf{B}\right) + O\left(|\Delta\mathbf{r}|^2\right)$$



Reconstruction must be exact for the 1st derivatives to get 2nd order accuracy. Not easy on unstructured meshes!

return

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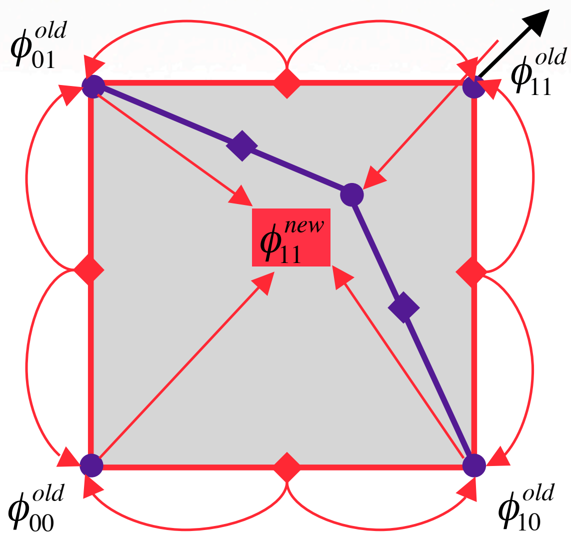
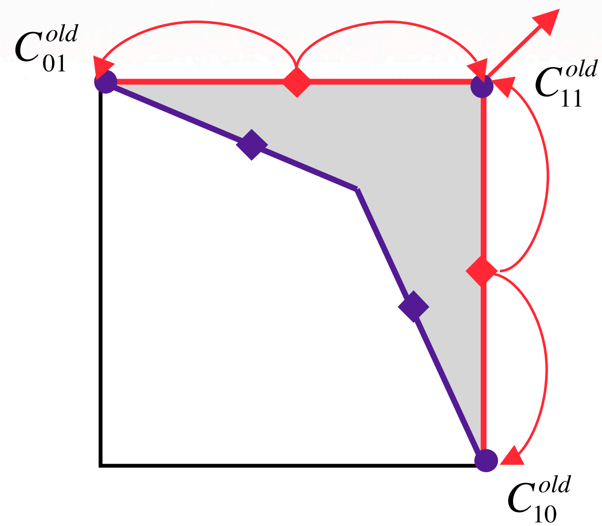
Base CI Uses Information Better Than Donor Cell CT





$$\Phi_U^{new} = \left(\phi_{01}^{new} - \phi_{11}^{new}\right)$$
$$\Phi_R^{new} = \left(\phi_{11}^{new} - \phi_{10}^{new}\right)$$

$$\Phi_U^{new} = \Phi_U^{old} + \Delta t\left(C_{01}^{old} - C_{11}^{old}\right)$$
$$\Phi_R^{new} = \Phi_R^{old} + \Delta t\left(C_{11}^{old} - C_{10}^{old}\right)$$

ϕ_{ij}^{new} depend on **all 4 old** flux values

C_{ij}^{old} depend **only on 2 old** flux values