A New Preconditioning Strategy for a Spectral-element-based Magnetohydrodynamics Solver

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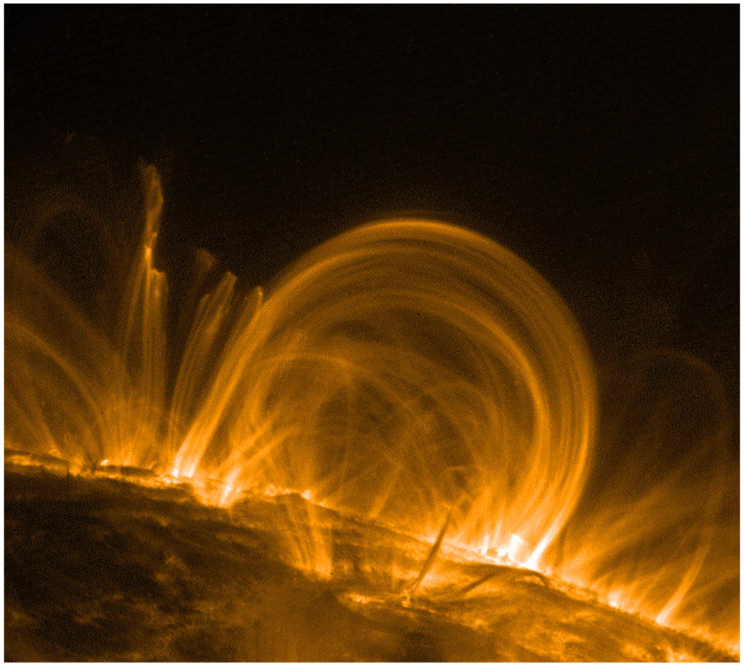
Outline

- Motivation
- Equations & discretization
- Maintaining continuity; adaptivity
- Explicit MHD
- Preconditioning strategy
- ORAS preconditioner
- Coarse correction
- Conclusions & future work

MHD & Hydro Turbulence: Interaction of structures with ambient turbulent fluid & with boundaries

- Phenomenological & fundamental:



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Kelvin-Helmholtz rolls
In match smoke

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Geophysics-Astrophysics Spectral-element Adaptive Refinement (GASpAR)

- Object-oriented framework for solving PDEs on adaptive grids
- Uses tensor product form for multi-dimensional operators (hence, matrix-matrix--BLAS-3--products)

- Equations are derived from standard interface: advection-diffusion, Navier-Stokes, MHD
- Adaptive grid mechanics independent of equations

Available at: /

http://www.image.ucar.edu/TNT/Software/GASpAR

MHD Equations: Implemented in GASpAR

Magnetohydrodynamics:

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mathbf{j} \times \mathbf{b} + \nu \nabla^2 \mathbf{u}$$

$$\partial_t \mathbf{b} = \nabla \times (\mathbf{u} \times \mathbf{b}) + \eta \nabla^2 \mathbf{b}$$

$$\nabla \cdot \mathbf{u} = 0, \quad \nabla \cdot \mathbf{b} = 0$$

Elsasser (1950) form:

$$\partial_t \mathbf{Z}^{\pm} + \mathbf{Z}^{\mp} \cdot \nabla \mathbf{Z}^{\pm} + \nabla \mathbf{p} - \nu^{\pm} \nabla^2 \mathbf{Z}^{\pm} - \nu^{\mp} \nabla^2 \mathbf{Z}^{\mp} = \mathbf{0}$$

$$\nabla \cdot \mathbf{Z}^{\pm} = \mathbf{0}$$

Via definitions: $\mathbf{Z}^{\pm} = \mathbf{u} \pm \mathbf{b}$ $\quad \nu^{\pm} = \frac{1}{2}(\nu \pm \eta)$

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Discretization via SEM method (Patera 1984)

- Problem well posed using spaces:

$$\mathbf{U}_\gamma := \left\{ \mathbf{w} = \sum_{\mu=1}^{d} w^\mu \vec{e}^\mu \;\middle|\; w^\mu \in \mathbf{H}^1(D)\ \forall \mu \ \&\ \mathbf{w} = \gamma \text{ on } \partial D \right\}$$

- Discrete spaces:

$$\left.\begin{aligned} \mathbf{Z}^\pm \in \mathbf{U}^N &= \mathbf{U}_{\mathbf{Z}_0} \bigcap \mathbf{P}_N \\ \zeta^\pm \in \mathbf{U}_0^N &= \mathbf{U}_0 \bigcap \mathbf{P}_N \\ p, q \in \mathbf{Y}^{N-2} &= \mathbf{L}_2(D) \bigcap \mathbf{P}_{N-2} \end{aligned}\right\} \quad \mathbf{P}_N - \mathbf{P}_{N-2}$$

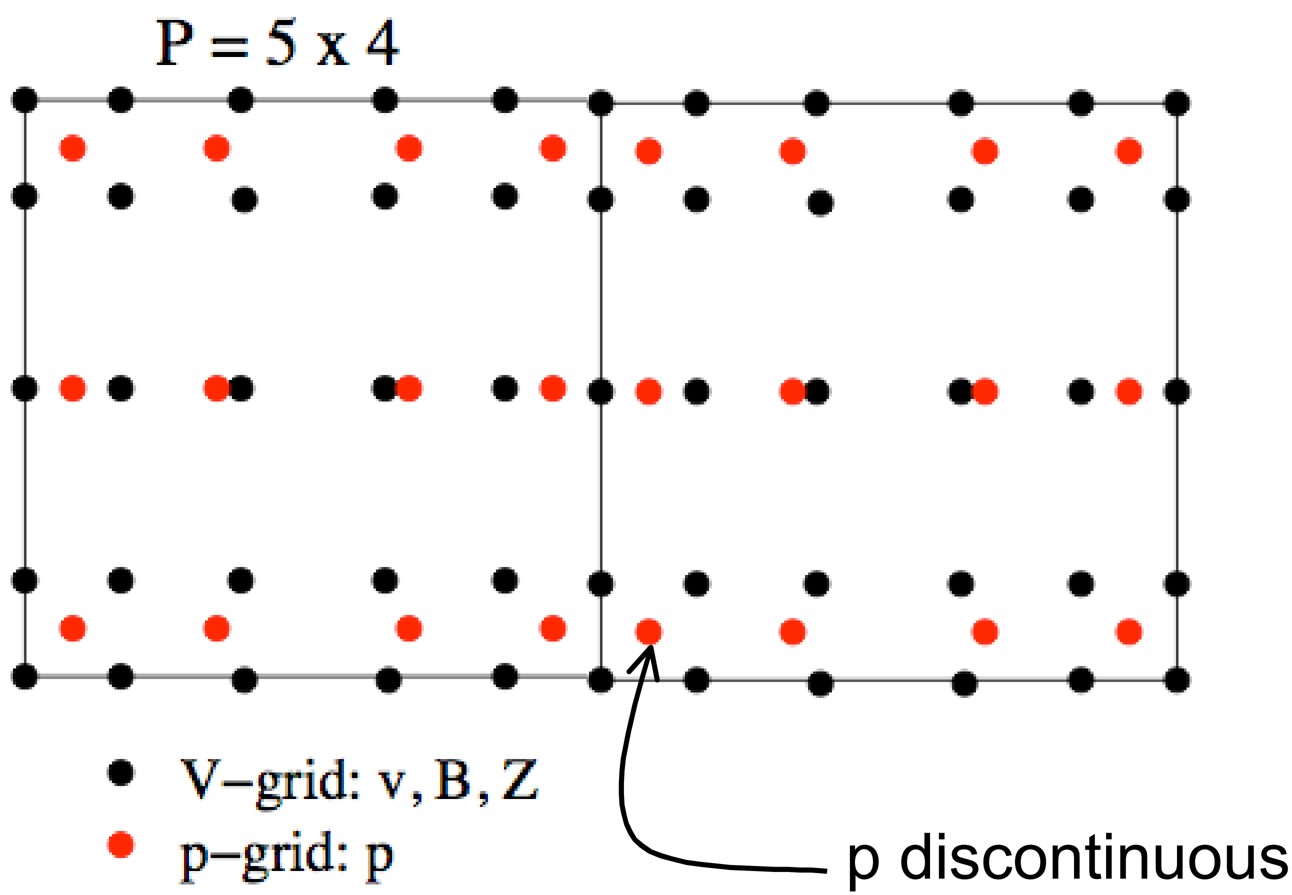
- Discrete problem:

$$\begin{aligned} \langle \zeta^\pm, \partial_t \mathbf{Z}^\pm \rangle_{\underline{GL}} + \langle \zeta^\pm, \mathcal{C}^\mp \mathbf{Z}^\pm \rangle_{\underline{GL}} - \frac{1}{\rho_0} \langle p, \nabla \cdot \zeta^\pm \rangle_{\underline{G}} &\\ = -\nu^\pm \sum_{\mu=1}^{d} \langle \partial_\mu \vec{\zeta}^\pm, \partial_\mu \vec{Z}^\pm \rangle_{\underline{GL}} &\\ \langle q, \nabla \cdot \mathbf{Z}^\pm \rangle_{\underline{G}} = 0, & \end{aligned}$$

$$\mathcal{C}^\pm := \mathbf{Z}^\pm \cdot \vec{\nabla}$$

Expand using GL or G polynomials…

Discrete staggered grid



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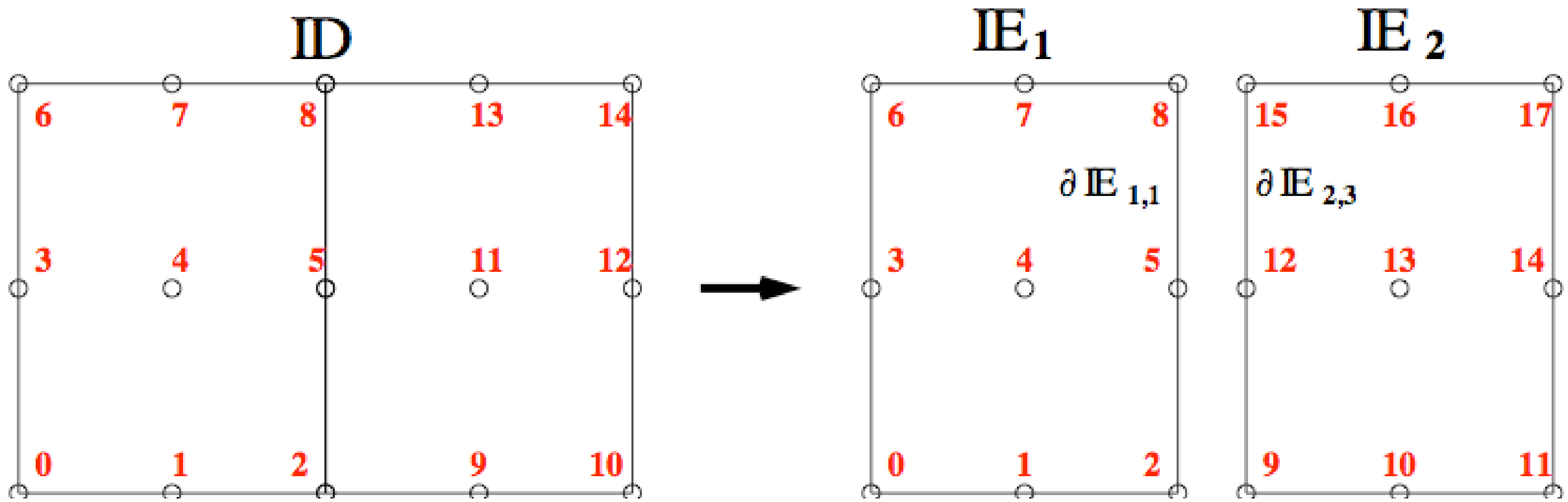
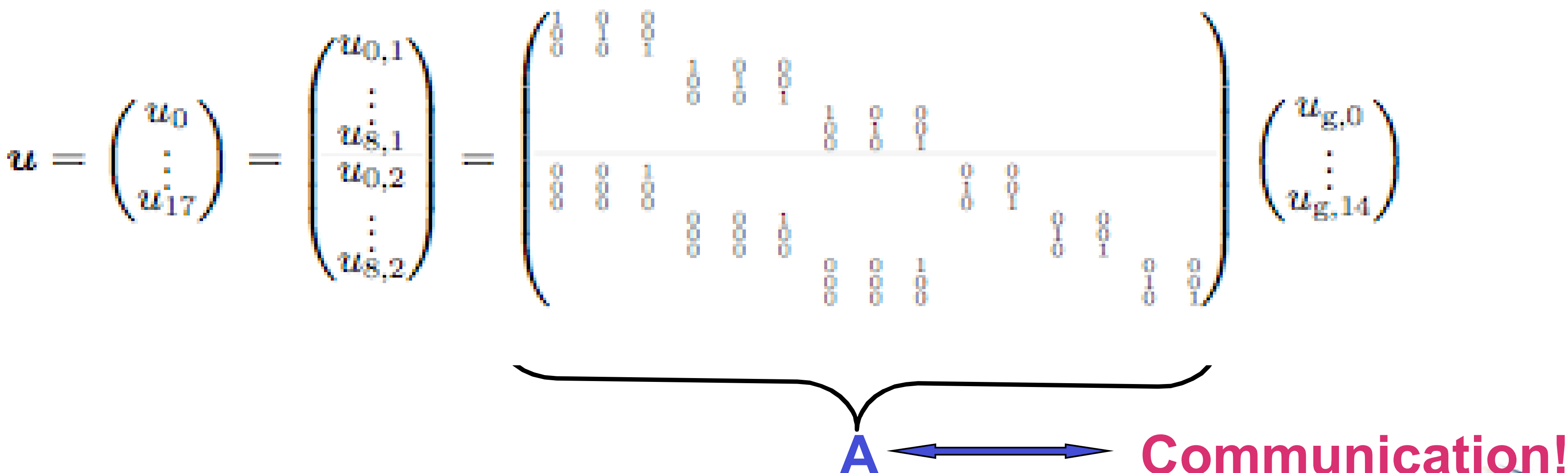
Conforming continuity: Associate local and global dofs





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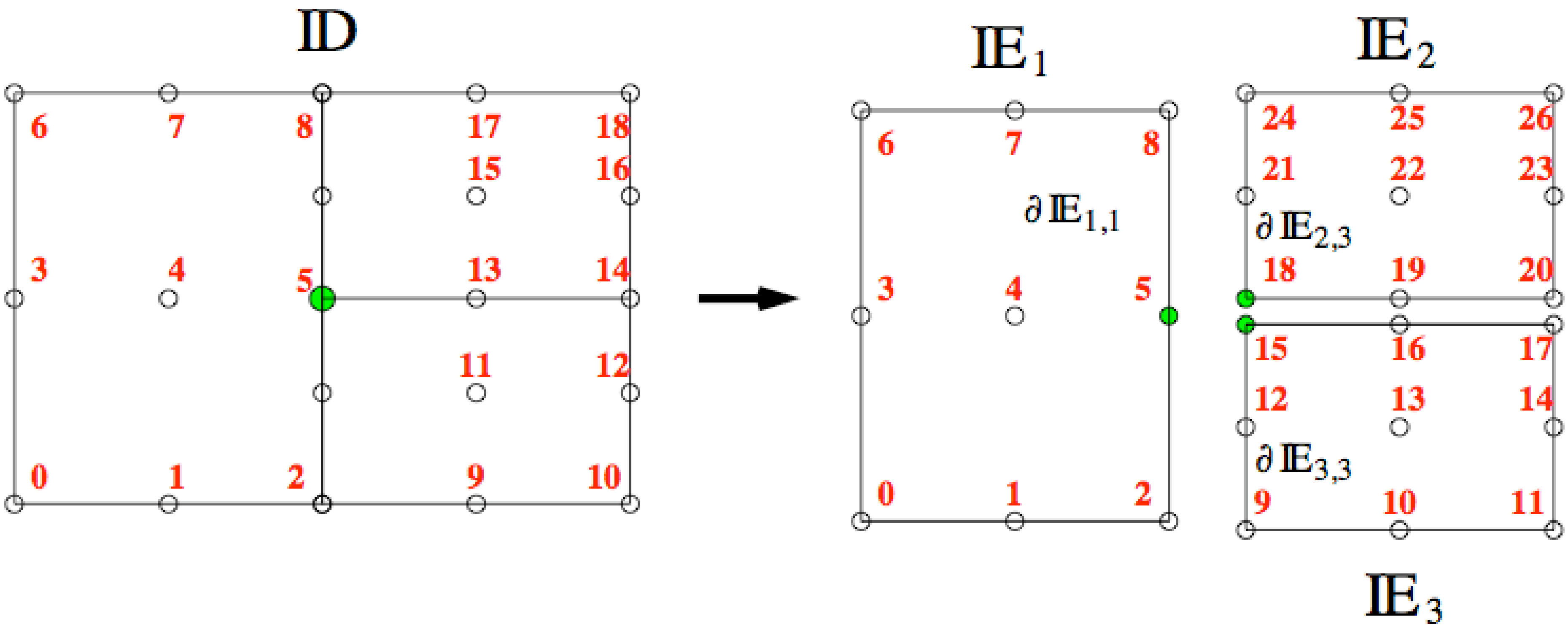
Nonconforming continuity (1)



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Nonconforming continuity (2): Interpolation implied

$$
u = \begin{pmatrix} u_0 \\ \vdots \\ u_{26} \end{pmatrix} = \begin{pmatrix} u_{0,1} \\ \vdots \\ u_{8,1} \\ u_{0,2} \\ \vdots \\ u_{8,2} \\ u_{0,3} \\ \vdots \\ u_{8,3} \end{pmatrix} = \left(\begin{array}{ccccccccccccccccccc}
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0&0&0&&&&&&&0&1 \\
0&0&3/8&0&0&3/4&0&0&-1/8&&&0&0 \\
0&0&0&0&0&0&0&0&0&&&1&0 \\
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\end{array}\right) \begin{pmatrix} u_{g,0} \\ \vdots \\ u_{g,18} \end{pmatrix}
$$

$$
= \underbrace{\begin{pmatrix}
1 &&&&&&&&& \\
& \ddots &&&&&&&& \\
&&& 1 &&&&&& \\
0\;0\;3/8 & 0\;0\;3/4 & 0\;0\;-1/8 &&&&&&& \\
0\;0\;0 & 0\;0\;0 & 0\;0\;0 && 1 &&&&& \\
&&&&& \ddots &&&& \\
0\;0\;0 & 0\;0\;0 & 0\;0\;0 &&&& 1 &&& \\
0\;0\;-1/8 & 0\;0\;3/4 & 0\;0\;3/8 &&&&&&& \\
0\;0\;0 & 0\;0\;0 & 0\;0\;0 &&&&& 1 && \\
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0\;0\;0 & 0\;0\;0 & 0\;0\;0 &&&&&&& 1
\end{pmatrix}}_{\Phi}
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1 &&&&&&&&& \\
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& \begin{smallmatrix}0&0&1\\0&0&0\\0&0&0\end{smallmatrix} &&&&& \begin{smallmatrix}0&0\\1&0\\0&1\end{smallmatrix} &&& \\ \hline
& \begin{smallmatrix}0&0&1\\0&0&0\\0&0&0\end{smallmatrix} &&&&& \begin{smallmatrix}0&0\\1&0\\0&1\end{smallmatrix} &&& \\
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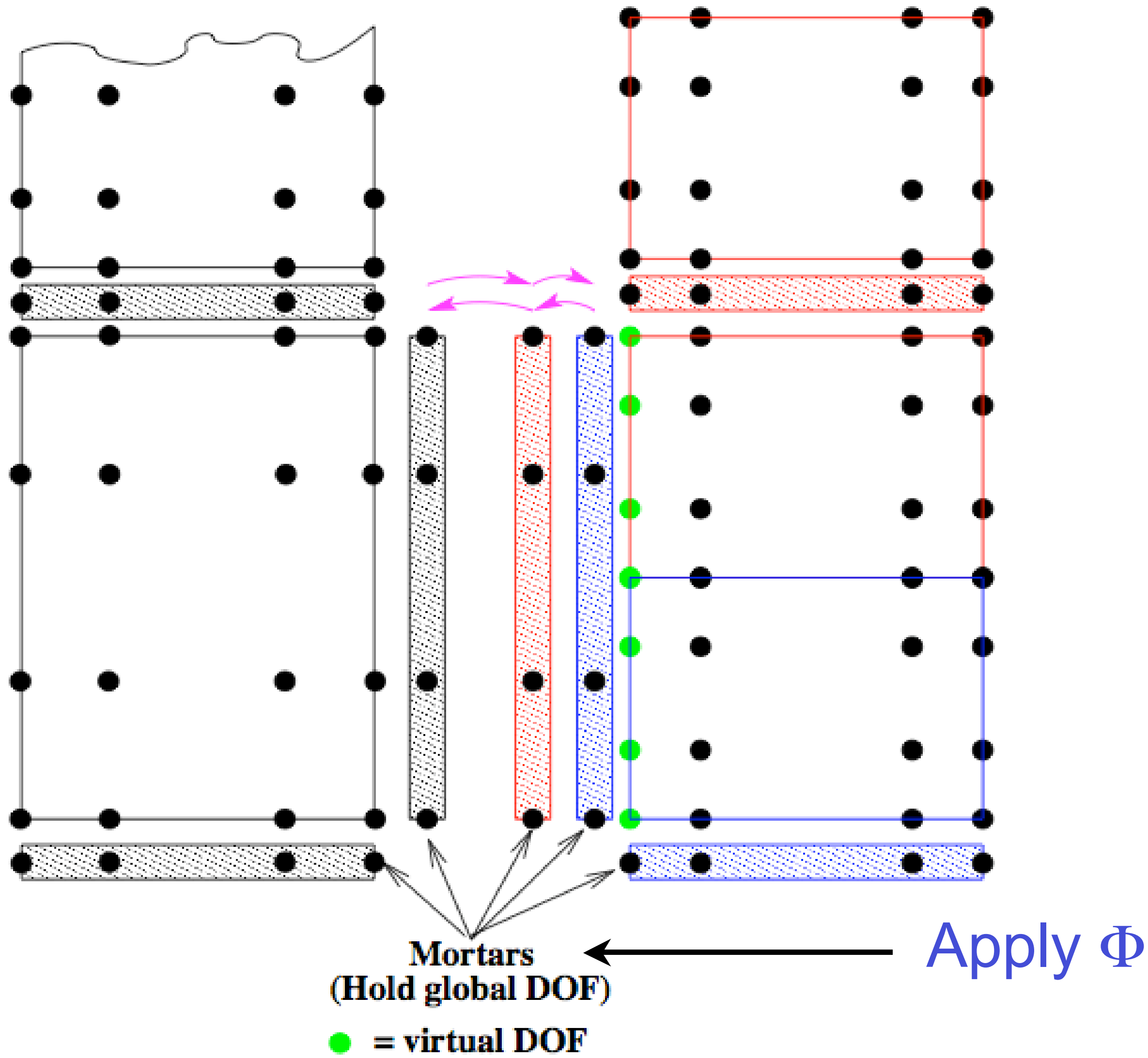
&& \begin{smallmatrix}0&0&1\\0&0&0\\0&0&0\end{smallmatrix} &&&&&&& \begin{smallmatrix}0&0\\1&0\\0&1\end{smallmatrix}
\end{array}\right)}_{A}
\begin{pmatrix} u_{g,0} \\ \vdots \\ u_{g,18} \end{pmatrix}
$$

Interpolation operator → Φ

Mortar Data Structures: Perform interpolations



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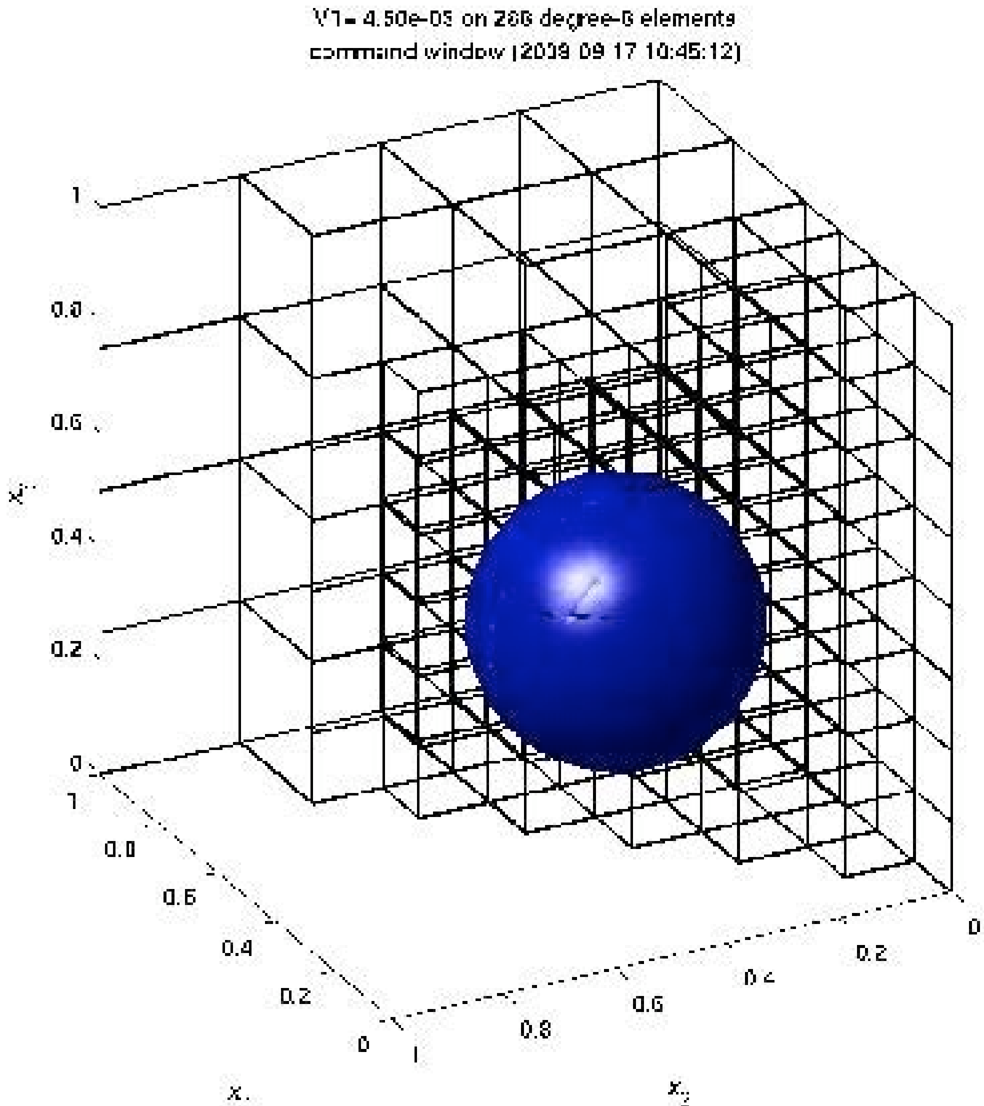
Adaptivity: IConnAMR

Rosenberg, Fournier, Fischer, Pouquet, *J.Comp.Phys.*, **215**:59 (2006)

- Applies 'forest of oct-trees', weak data structures
- Uses a 2^d:1 isotropic refinement decomposition
- Employs voxel database (VDB) to locate element neighbors and to set mortar properties
- Variety of a-posteriori refinement criteria; also user-defined
- 2-d and 3-d

Advection-diffusion: Adaptive 3-d linear advection



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MHD Discretization

Rosenberg, Pouquet, Mininni, *New J. Phys.*, **9**:304 (2007);

Ng, et al. Ap. J. Suppl., **177**(2):613 (2008)

- Semi-discrete equations

$$\mathbf{M}\frac{d\hat{\mathbf{Z}}_j^{\pm}}{dt} = -\mathbf{M}\mathbf{C}^{\mp}\hat{\mathbf{Z}}_j^{\pm} + \mathbf{D}_j^{T}\hat{p}^{\pm} - \nu_{\pm}\mathbf{L}\hat{\mathbf{Z}}_j^{\pm} - \nu_{\mp}\mathbf{L}\hat{\mathbf{Z}}_j^{\mp}$$

$$\mathbf{D}^{j}\hat{\mathbf{Z}}_j^{\pm} = 0\,,$$

- DNS==>one-step explicit time discretization:

$$\hat{\mathbf{Z}}_j^{\pm} = \hat{\mathbf{Z}}_j^{\pm,n} - \frac{1}{k}\Delta t\,\mathbf{M}^{-1}\left(\mathbf{M}\mathbf{C}^{\mp}\hat{\mathbf{Z}}_j^{\pm} - \mathbf{D}_j^{T}\hat{p}^{\pm} + \nu_{\pm}\mathbf{L}\hat{\mathbf{Z}}_j^{\pm} + \nu_{\mp}\mathbf{L}\hat{\mathbf{Z}}_j^{\mp}\right).$$

- **Apply divergence constraint to discretized system**:

Pseudo-Poisson operator

Fischer JCP 133:84 (1997);

Kruse et al, J Sci Comp. 17(1):81 (2002)

$$\mathbf{D}^j \mathbf{M}^{-1} \mathbf{D}_j^T \hat{p}^{\pm} = \mathbf{D}^j g_j^{\pm}.$$

Inhomogeneity:

$$g_j^{\pm} = \frac{1}{k}\Delta t\, \mathbf{M}^{-1}(\mathbf{M}\mathbf{C}^{\mp}\hat{\mathbf{Z}}_j^{\pm} + \nu_{\pm}\mathbf{L}\hat{\mathbf{Z}}_j^{\pm} + \nu_{\mp}\mathbf{L}\hat{\mathbf{Z}}_j^{\mp}) - \hat{\mathbf{Z}}_j^{\pm,n}$$

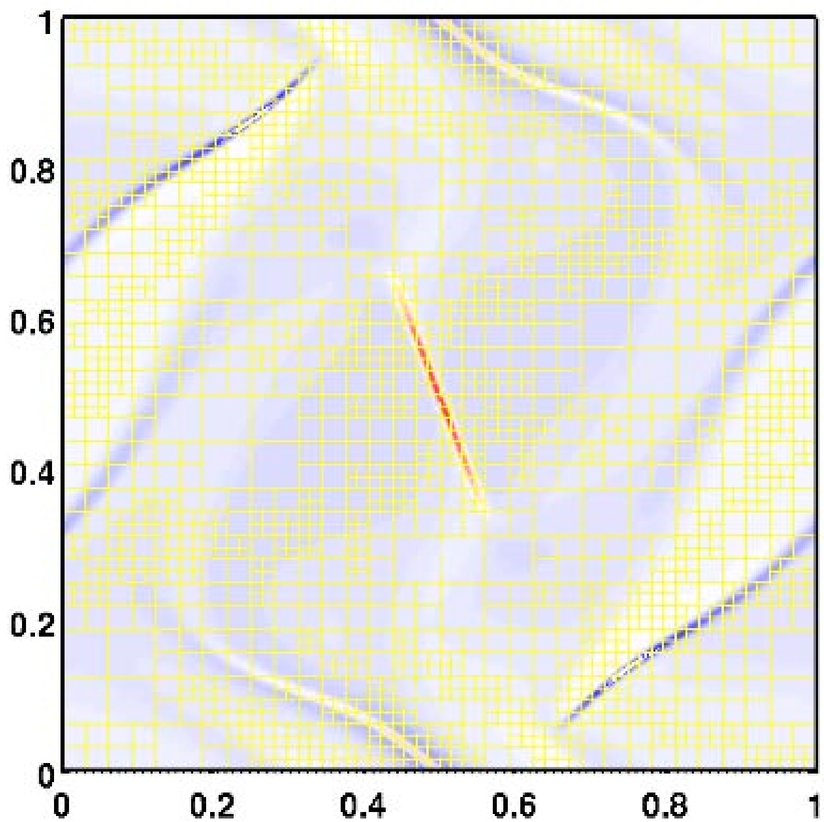
Communication is hidden in Stokes operators:

$$\mathbf{D}_j \rightarrow \mathbf{D}_j \mathbf{\Phi} \mathbf{A}$$

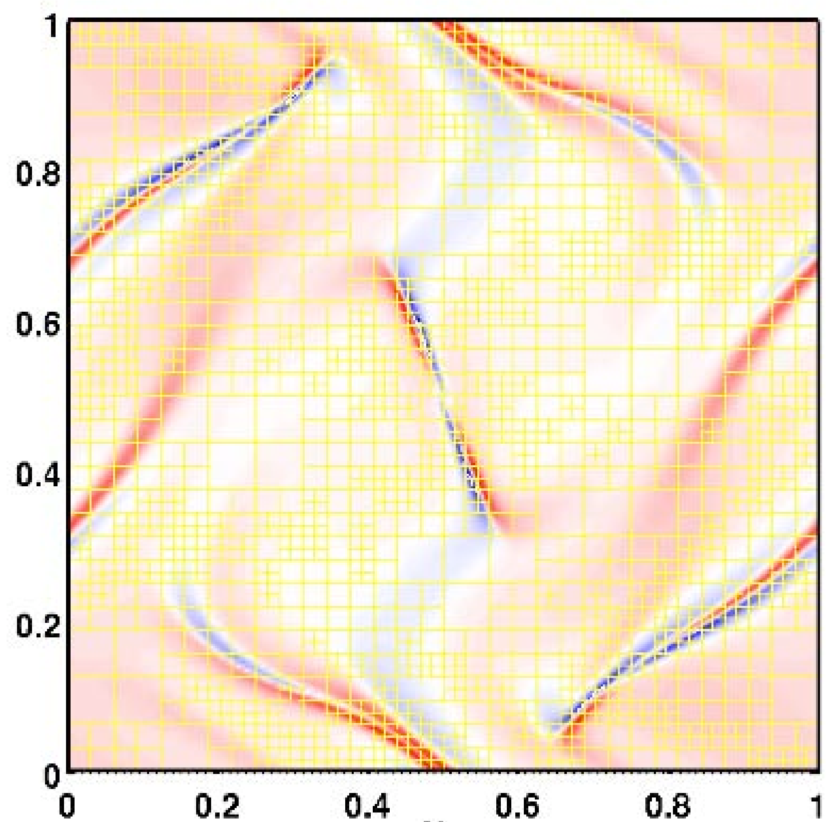
This operator also appears in Navier-Stokes from a Schur decompostion of discretized equations accurate to second order in Δt.

Orszag-Tang (OT) Problem: SEM AMR has excellent accuracy on challenging problem

•Current Density



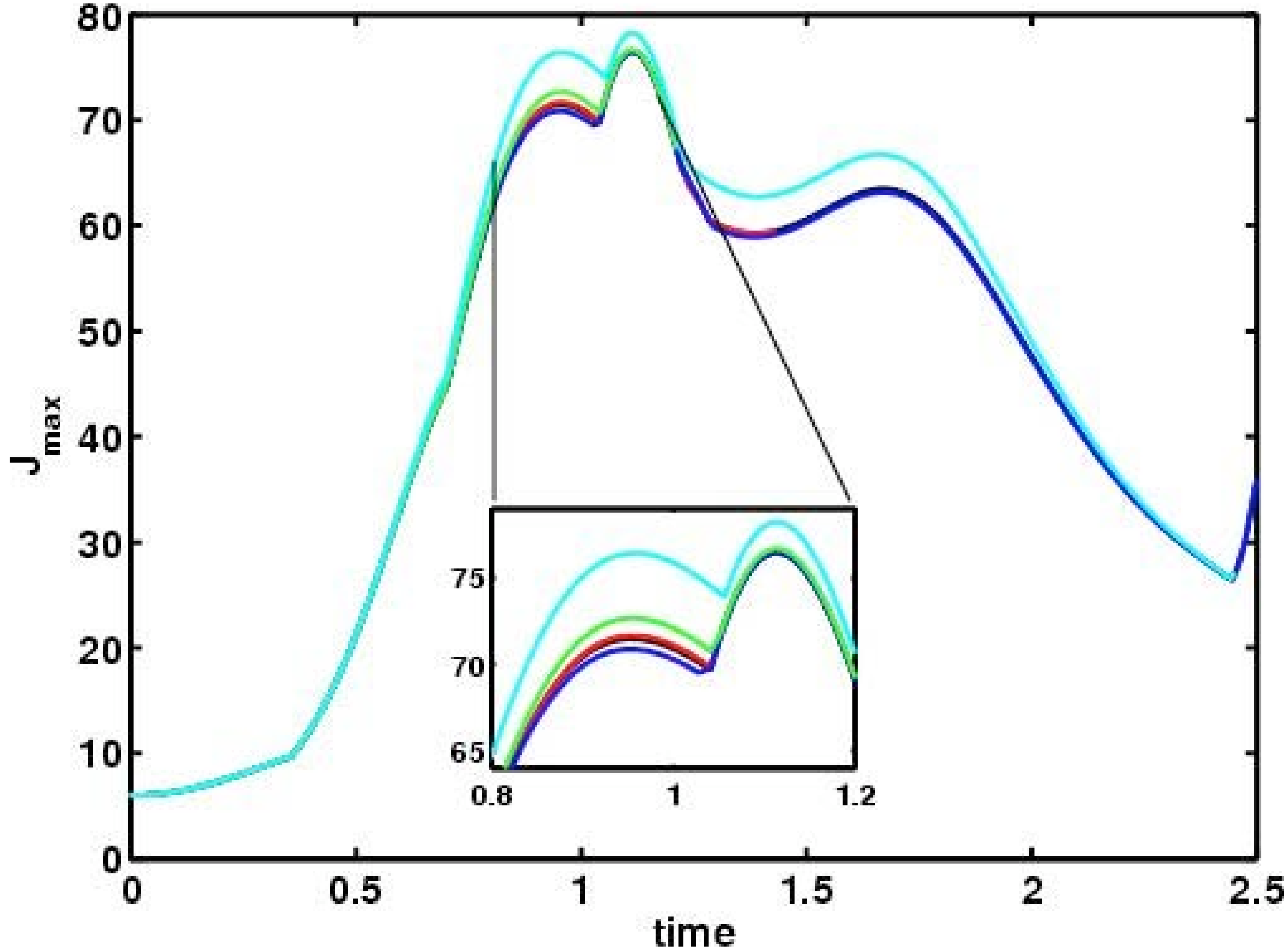
•Vorticity



Rosenberg, Pouquet, & Mininni. New J. Phys, 9, 304 (2007).

For OT, see: JFM 90, 129, 1979

OT SEM convergence: Truncation order matters!



Black: pseudo-spectral
Red: p=8
Blue: p=6
Green: p=4
Cyan: p=3

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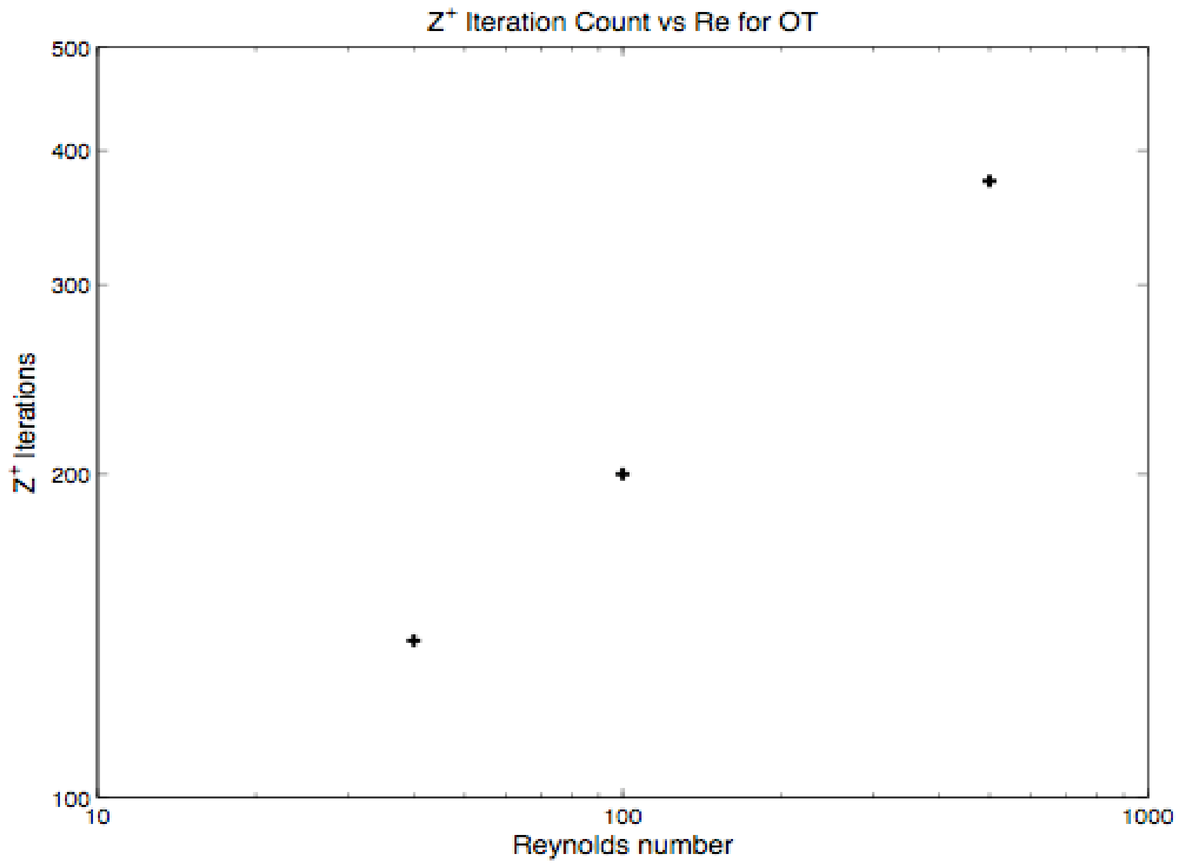
Iteration count scaling with Re in OT: Block Jacobi



Preconditioning clearly required!

Preconditioning strategy

St-Cyr, Rosenberg, Kim, in press; arXiv:0805.0025v1 (2008)

Precondition the following pseudo-Laplacian operator:

$$A \equiv \mathbf{D}_j \mathbf{M}^{-1} \mathbf{D}_j^T$$

•Restricted Additive Schwarz (RAS); begin with conforming grids

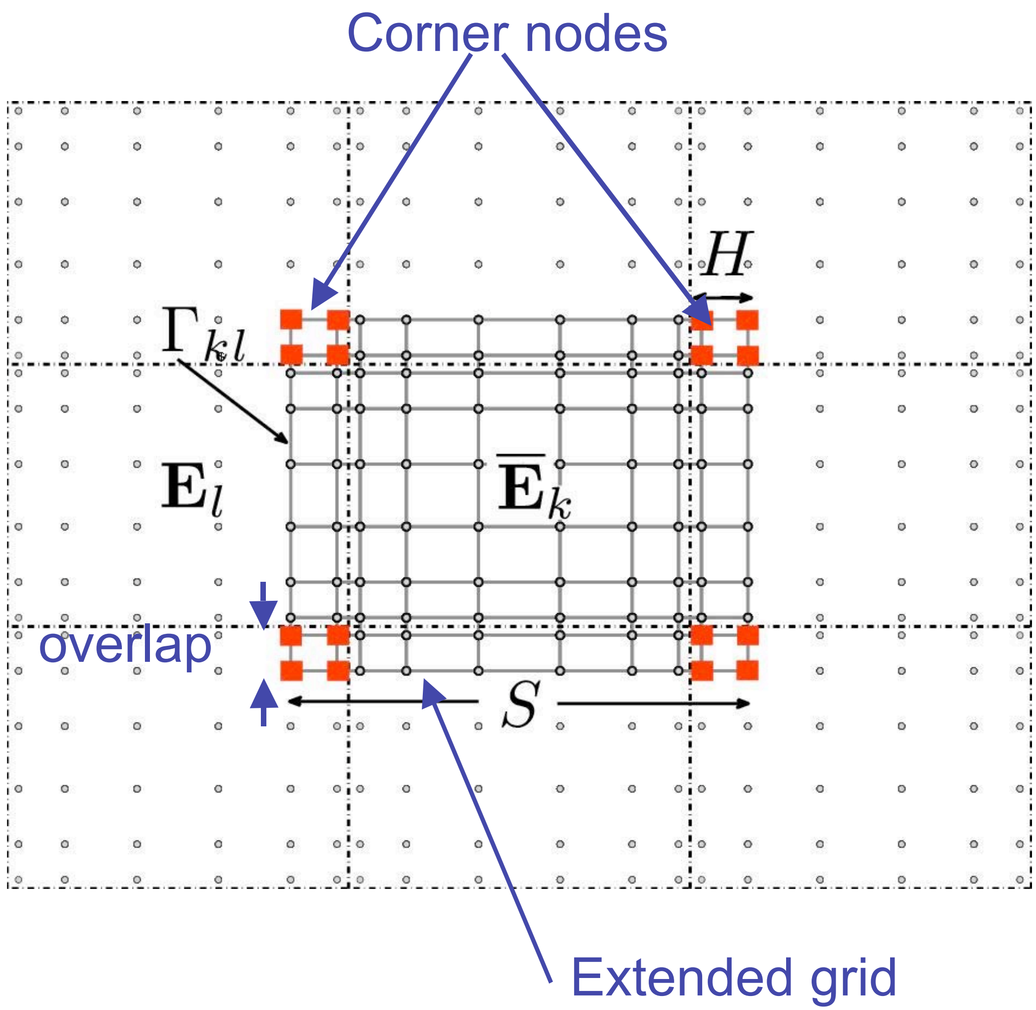
•Apply results of St-Cyr, et al. (2007) to optimize Q1 blocks

•Use multilevel idea of Fischer (1997)

Use equivalence between Q1 and SEM

RAS: Tiling extended grid

Fischer, JCP, **133:84 (1997)**



- Variable overlap
- Assemble 1d FE mass & stiffness matrices between nodes (Q1)_
- Allow for communication of corner data

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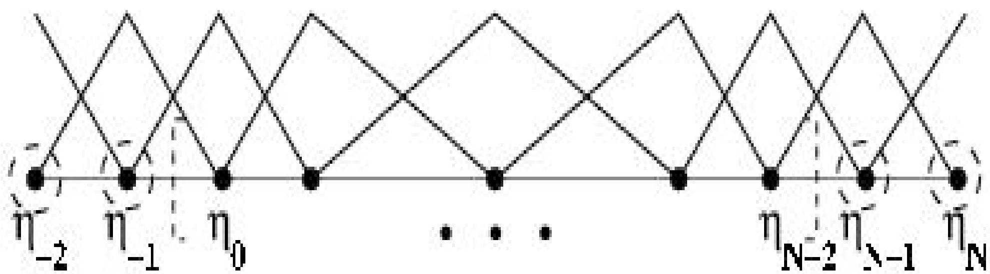
RAS FEM Operator Assembly



- Gauss grid node ⋮ Gauss–Lobatto node end–point (•) Extended Gauss grid node

-Use linear shape functions to build 1-d mass and stiffness operators;

-Do DSS.

-Construct 2- and 3-d Laplacian operators using tensor products..

$$P^{-1} = \sum_{k=1}^{K} R^{T}_{\mathbb{E}_k} \tilde{A}_k^{-1} R_{\bar{\mathbb{E}}_k}$$

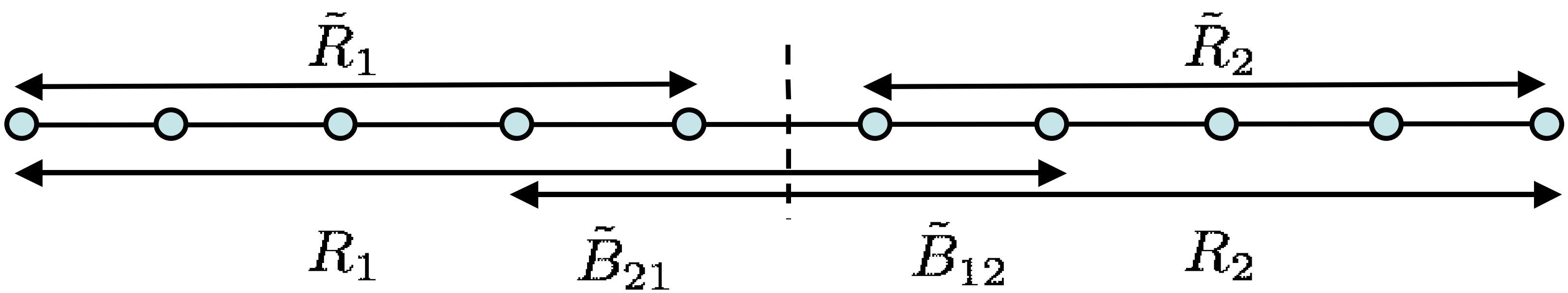
RAS optimization

St-Cyr, Gander & Thomas, SIAM JSC, **29**:2402 (2007);
Dubois, et al (2009);
Gander, SIAM J. Num. Anal. **44**:699 (2006)

- Given a Schwarz method transform to optimized versions (RAS case)

$$P_{RAS}^{-1} = \sum_{i=1}^{K} \tilde{R}_i^T A_i^{-1} R_i \xrightarrow{?} P_{ORAS}^{-1} = \sum_{i=1}^{K} \tilde{R}_i^T \tilde{A}_i^{-1} R_i$$

- St-Cyr et al. (2007) find under which conditions this is possible
- Conditions in the RAS case: $\tilde{B}_{jk} R_k \tilde{R}_m^T = 0, \quad m \neq k.$



In this case, transmission operator must have 2 points

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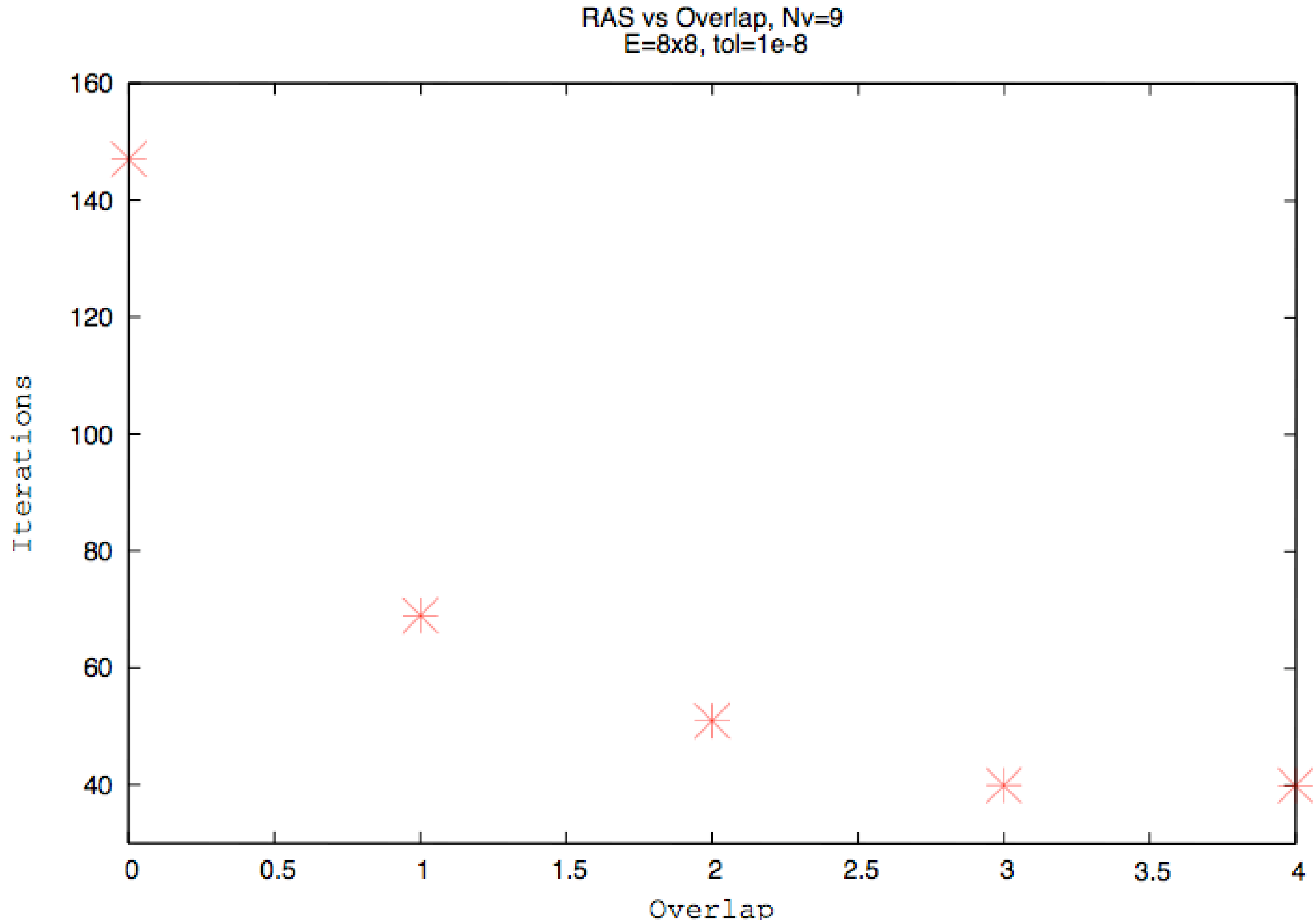
Numerical Experiments

- Native stand-alone pseudo-Poisson solver
- Periodic boundary conditions
- Use BiCGStab
- Krylov vector initialized with random noise
- Corner communication
- Embedding: replace FE operator with SEM
- Extrapolation: allowed when not using corner communication

RAS vs overlap: Saturation at overlap of 2



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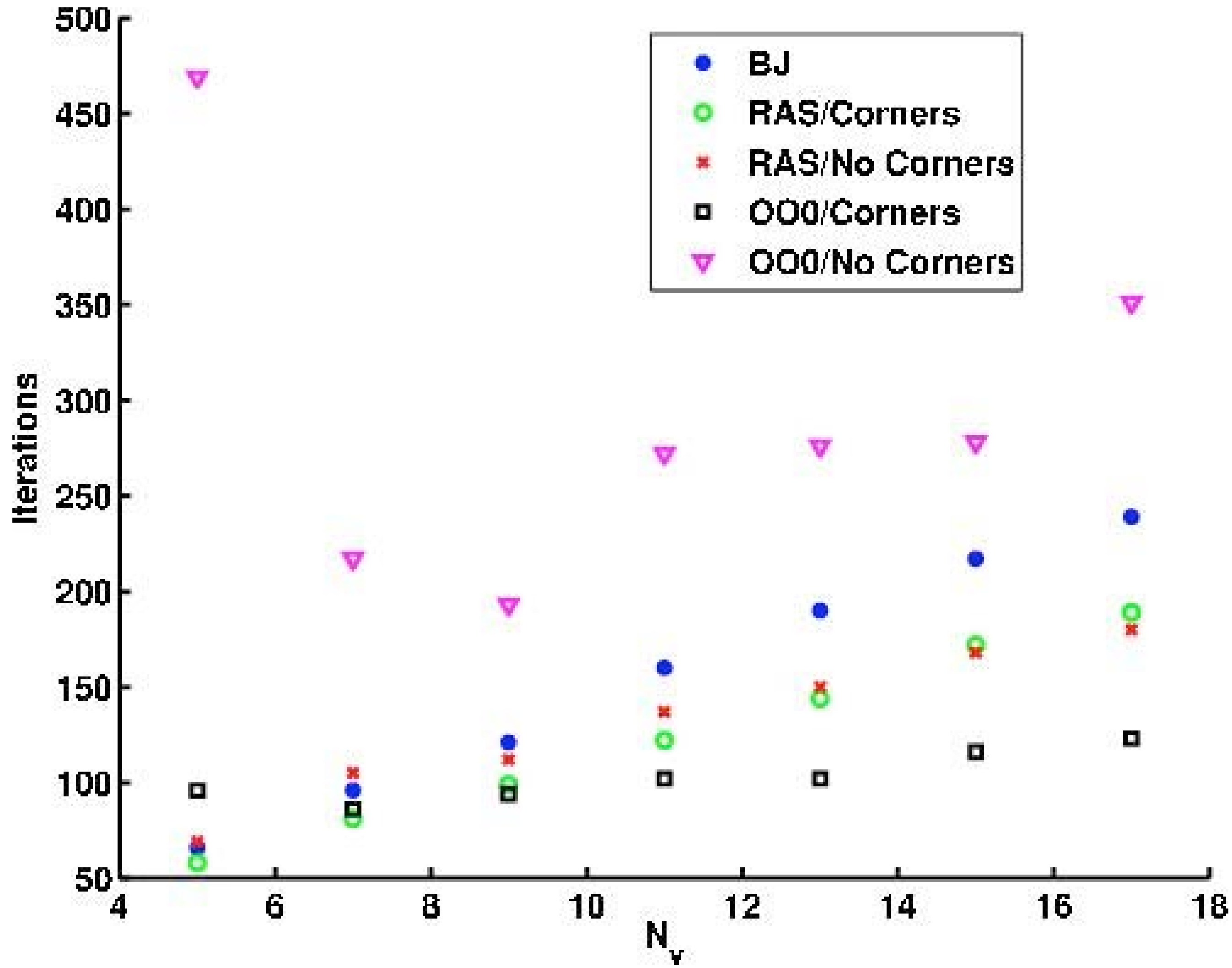
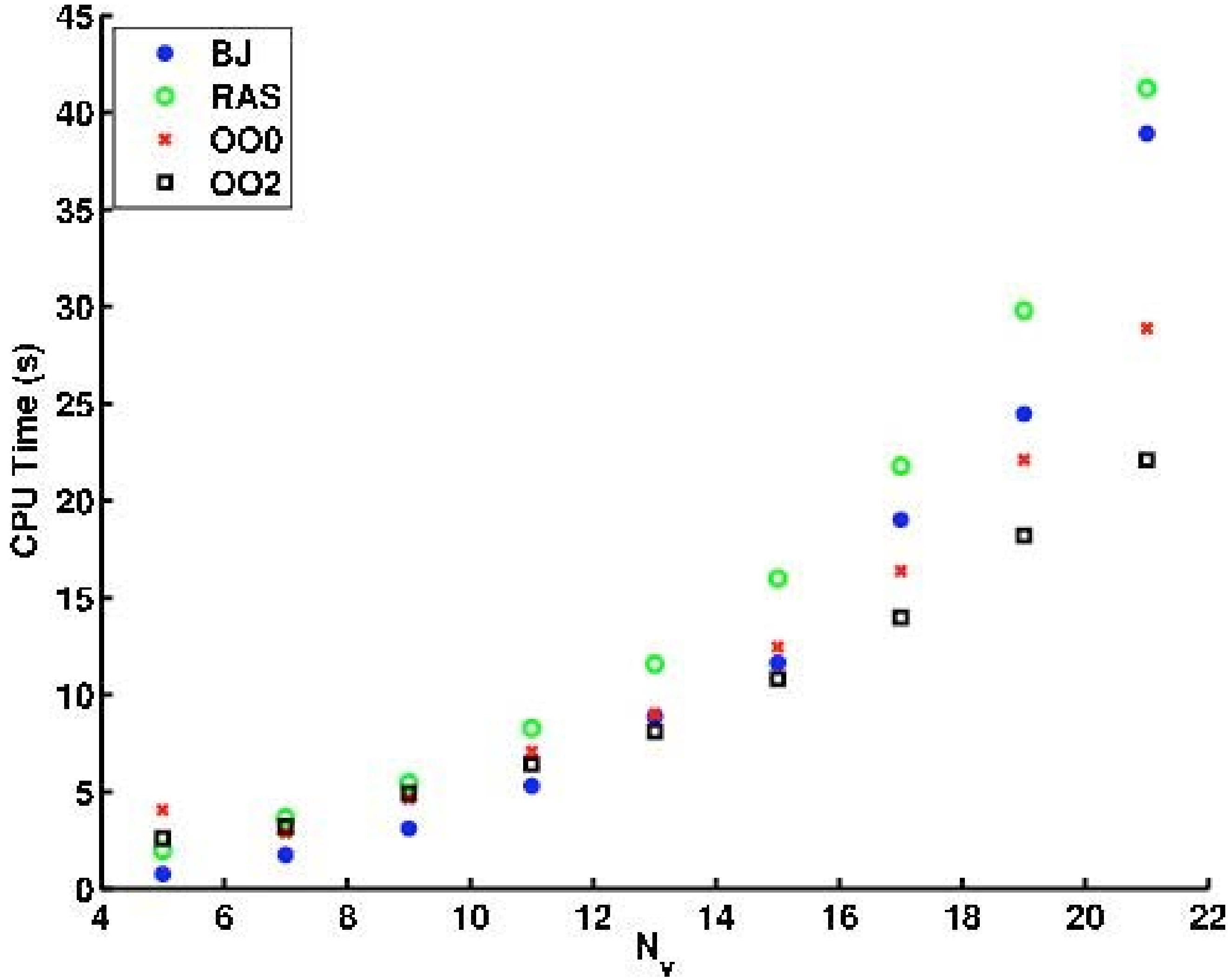
ORAS corner communication: Corners necessary!



ORAS asymptotic scaling



Coarse grid correction

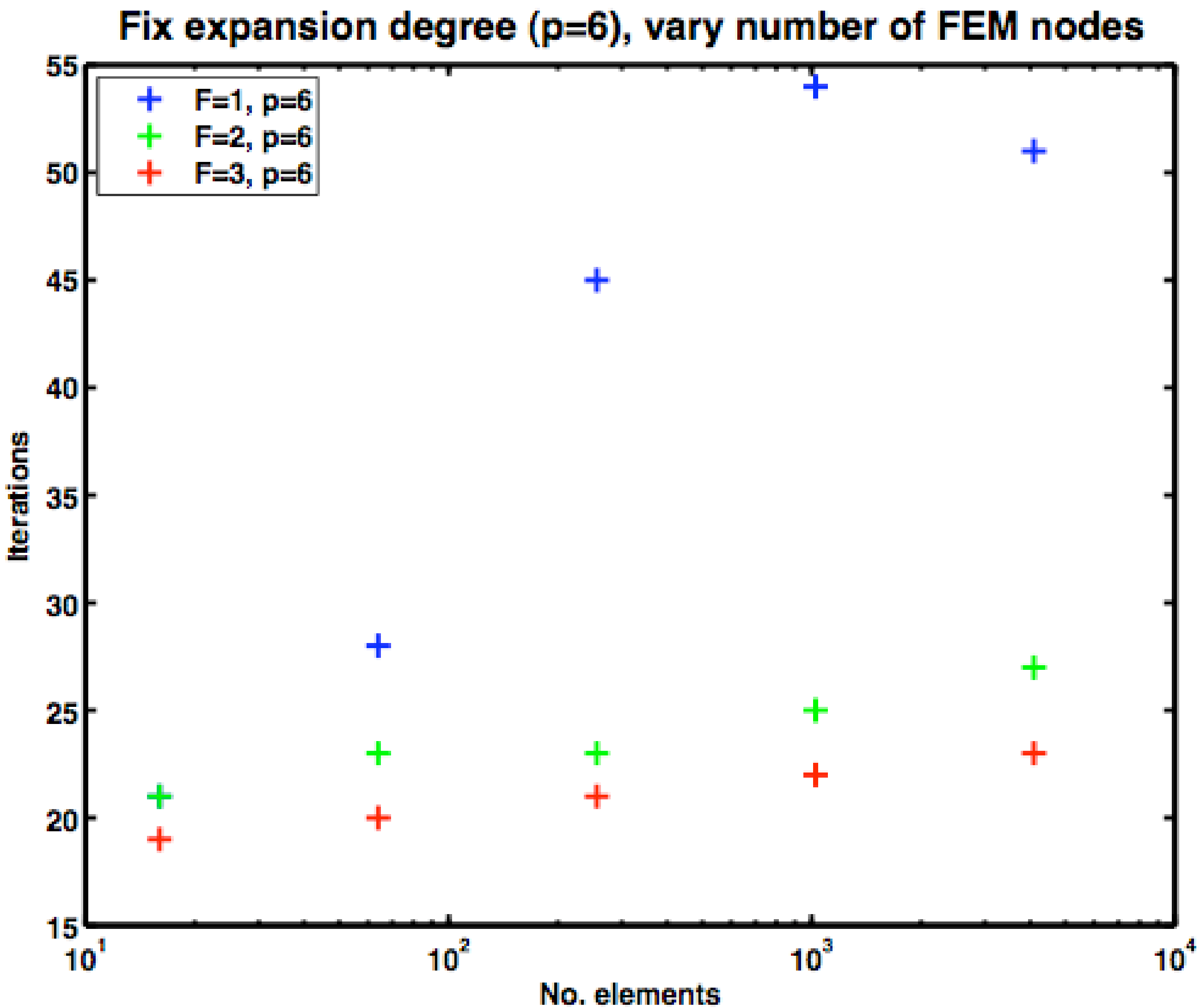
Coarse

$$P^{-1} = \underbrace{R_c^T \tilde{A}^{-1} R_c}_{\text{Coarse}} + \underbrace{\sum_{k=1}^{K} R_{\bar{\mathbb{E}}_k}^T \tilde{A}_k^{-1} R_{\bar{\mathbb{E}}_k}}_{\text{Fine: ORAS}}$$

Fine: ORAS

- Coarse grid is fine grid <u>skeleton</u> but at low no. Fes (F=1, 2 or 3)
- R_c is simple interpolation from fine to coarse grid
- A-operator is <u>FEM Laplacian</u>; tiling same as in RAS w/o overlap

Coarse grid scaling: Conforming grids: Vary no. FEs: asympotics look good!



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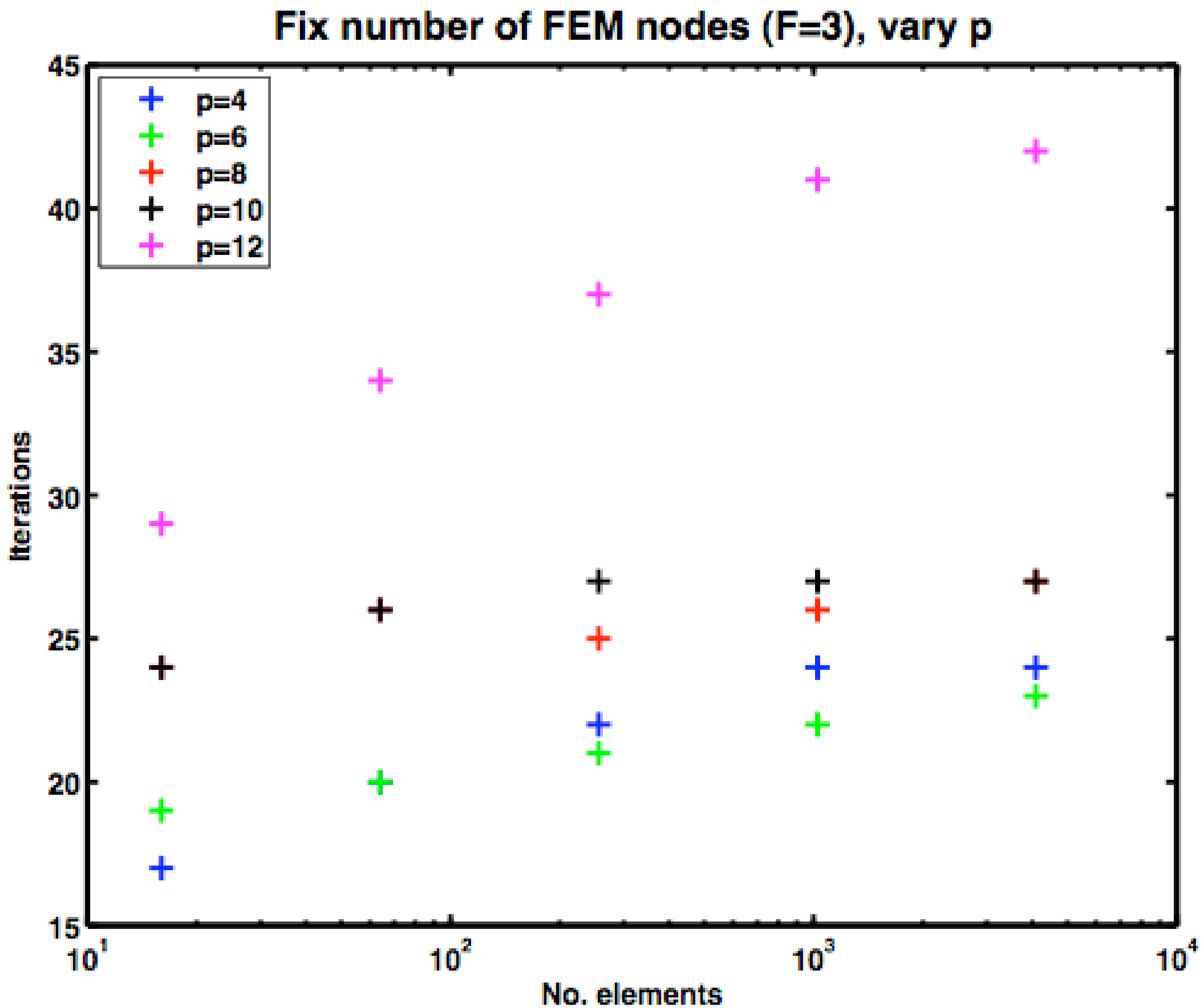
Coarse grid scaling: Conforming grids: Vary degree: asymptotics again look good!



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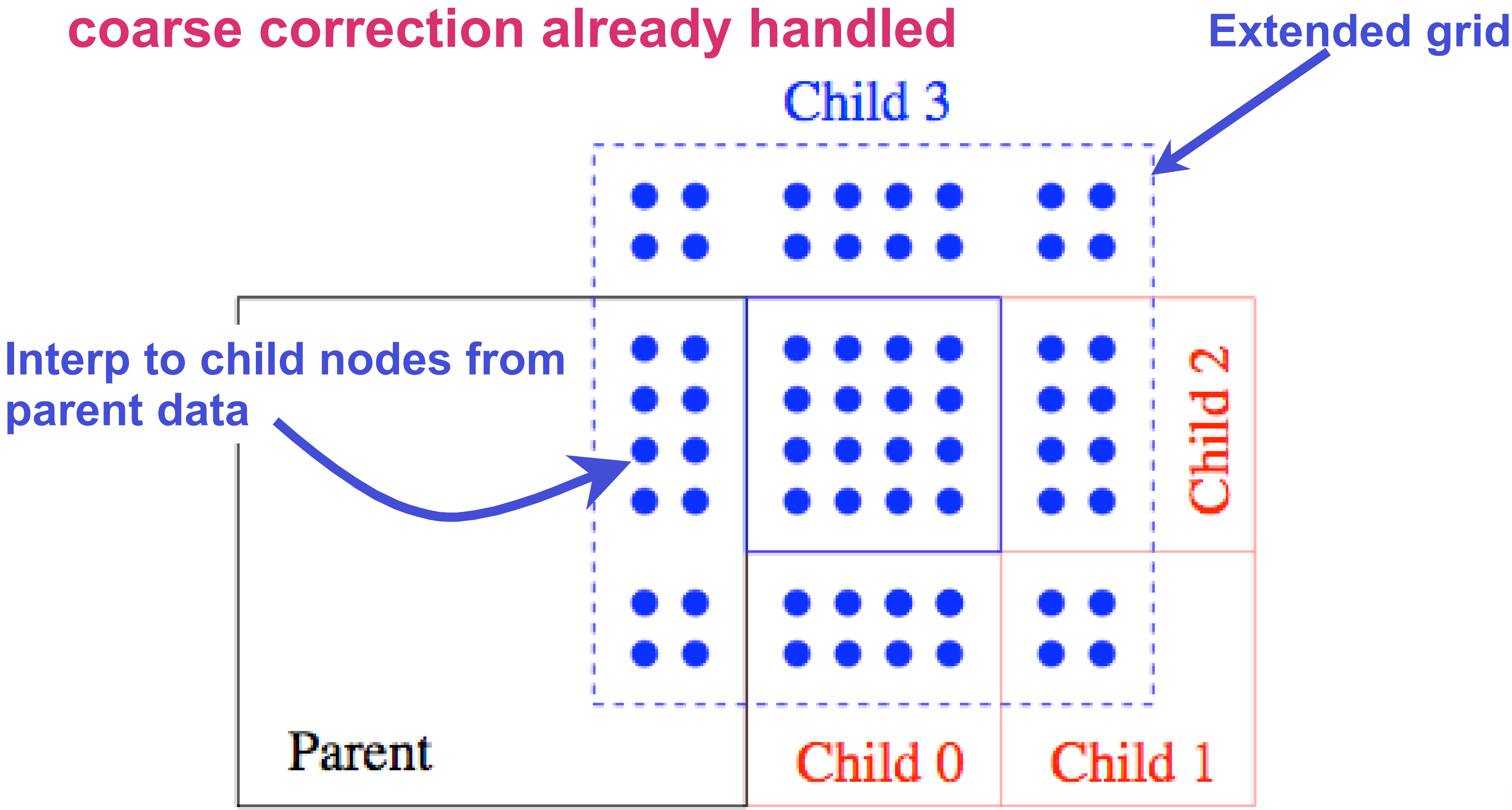
Considerations for nonconforming overlap

Applies to fine grid only;
coarse correction already handled



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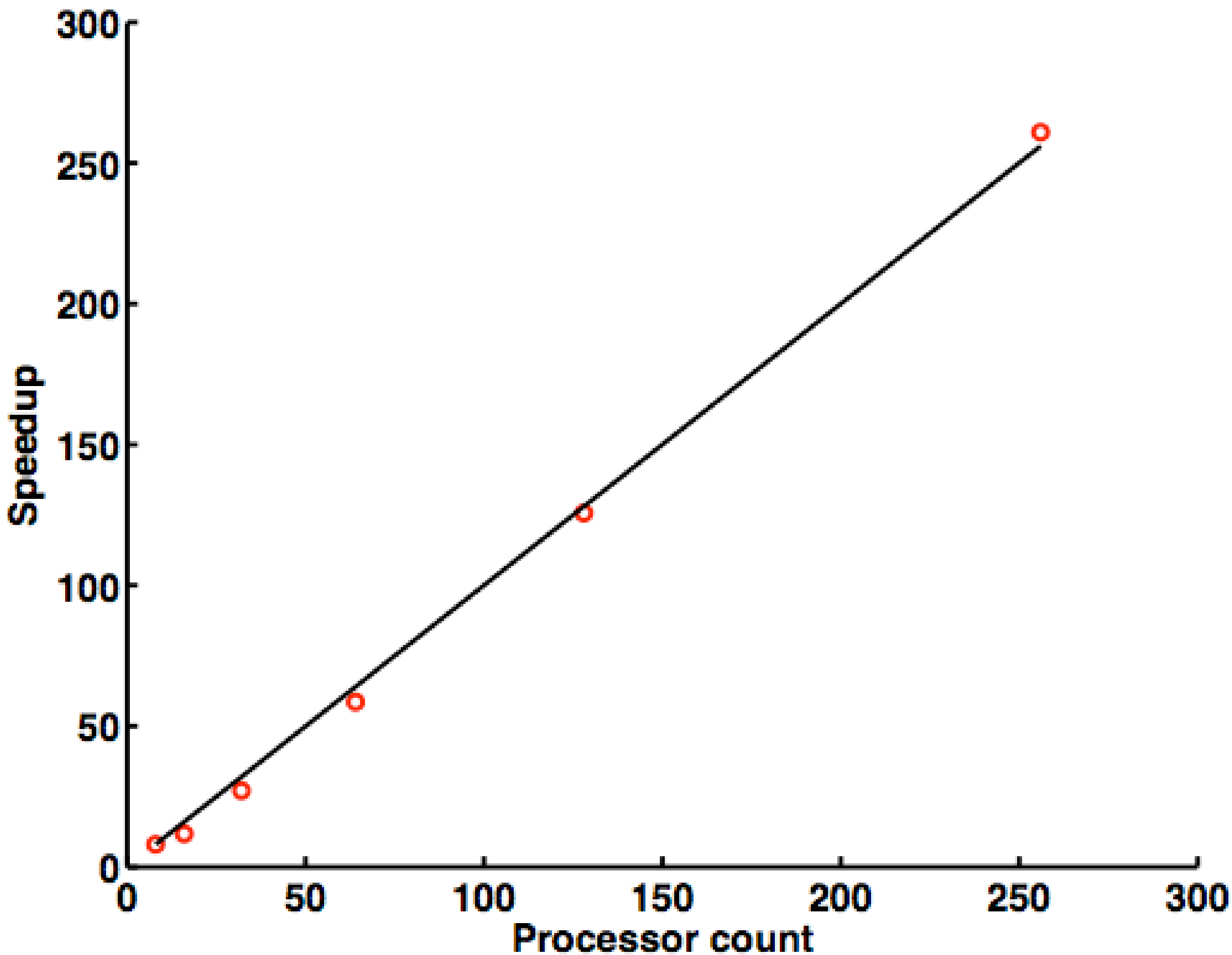
Conclusions & (near-)future work

- Demonstrated asymptotics of ORAS for pseudo-Laplacian operator on staggered grid,
- Demonstrated iteration plateauing/optimization with coarse grid correction
- Coarse solve using ‘factor once, use many’: e.g. AMG, SuperLU, XXT, MUMPS
- Complete 3D ORAS

Thank you!

Speedup



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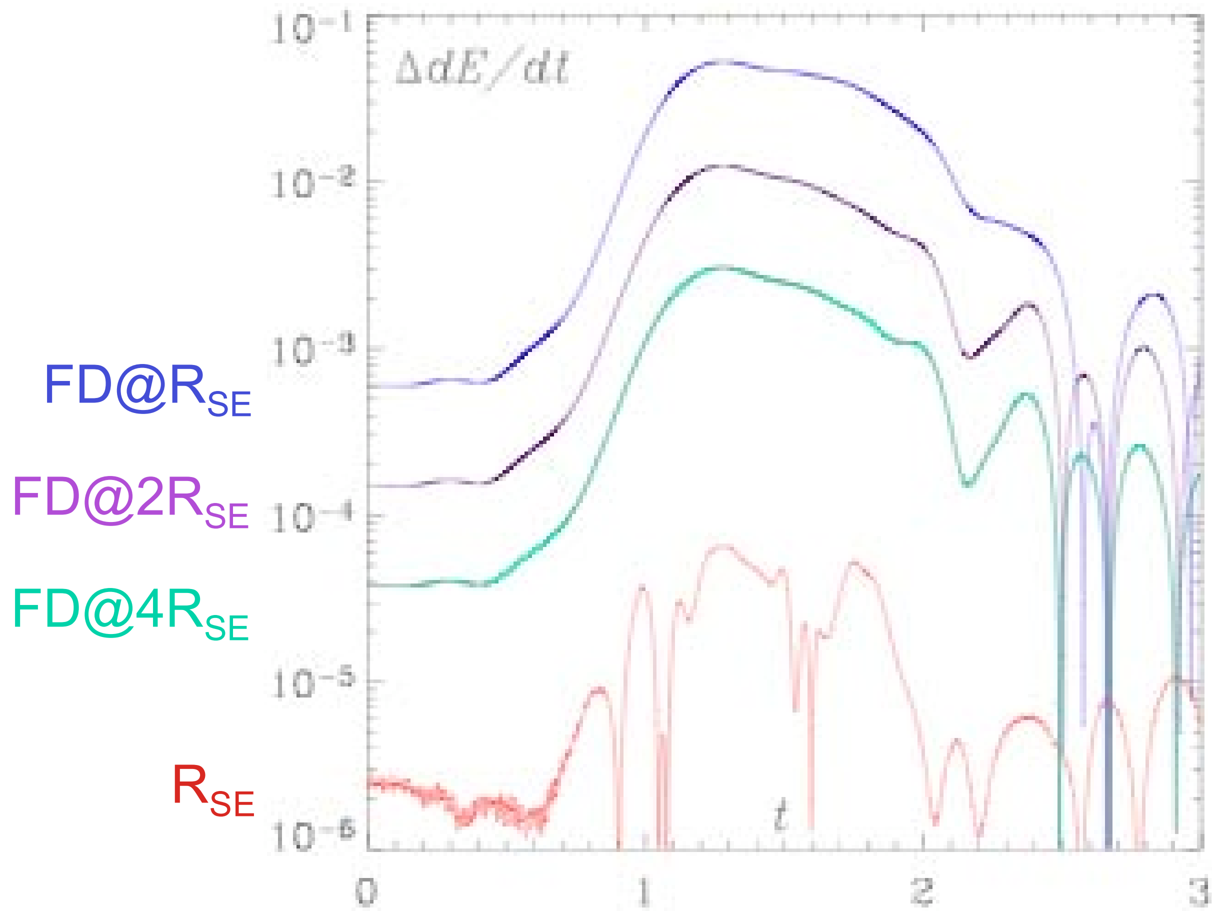
Adaptive SEM vs uniform FD on MICI problem



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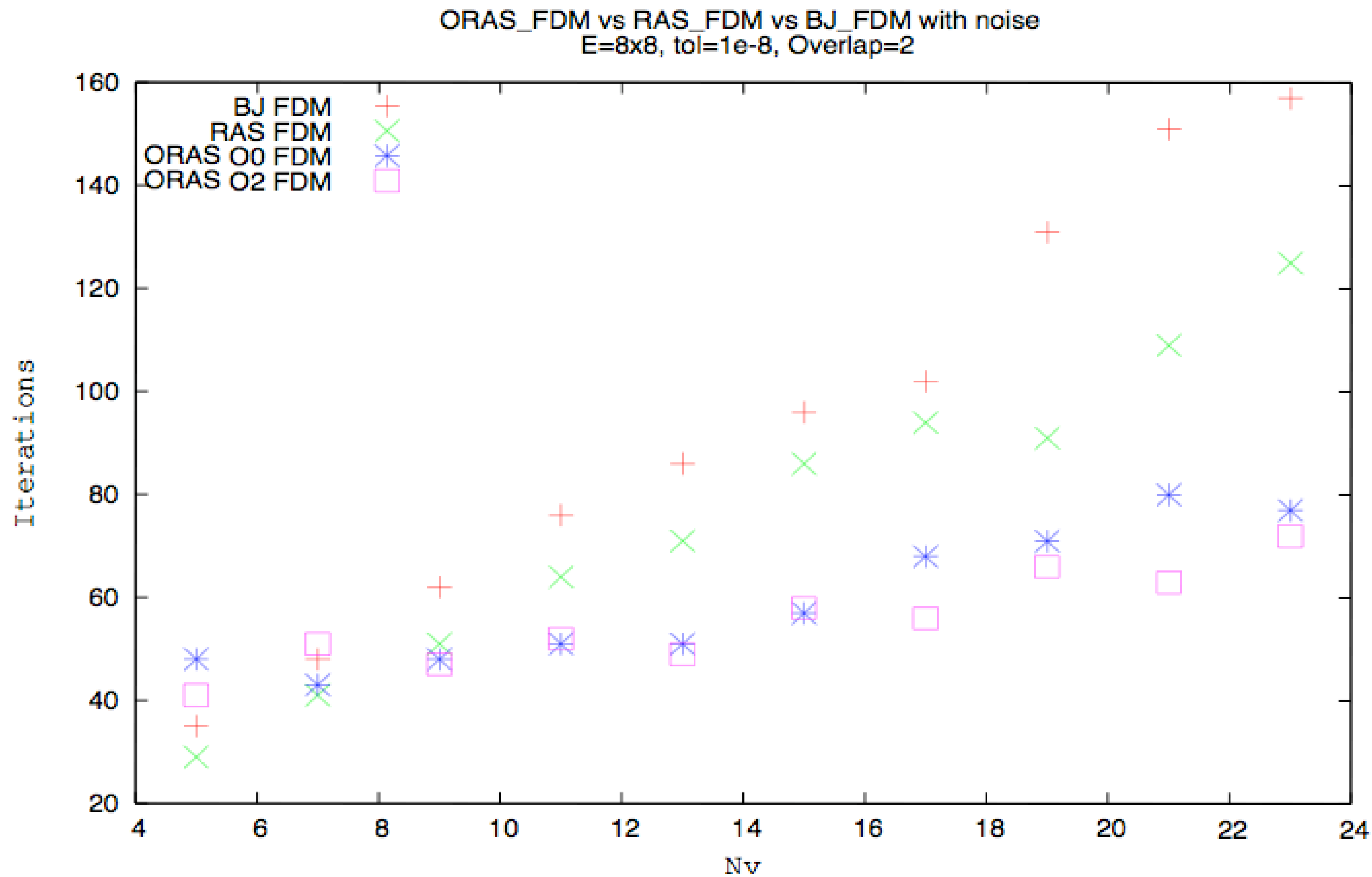
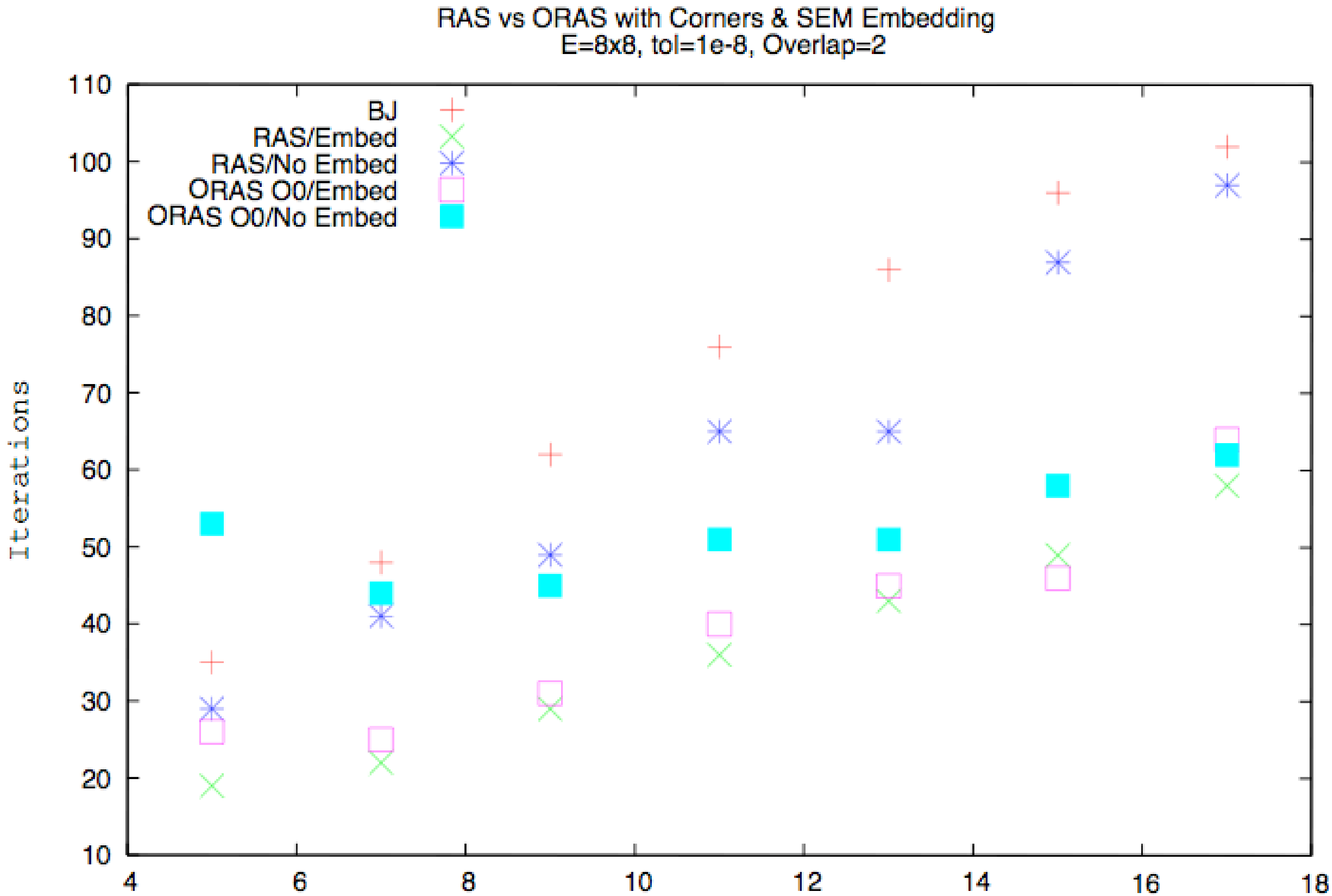
ORAS vs RAS and Block Jacobi



Embedding Results



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Semi-discrete equations

Advection-Diffusion:

$$\mathbf{M}\frac{d\mathbf{u_j}}{dt} = -\mathbf{MCu_j} - \nu\mathbf{Lu_j}$$

Navier-Stokes:

$$\begin{cases} \mathbf{M}\frac{d\mathbf{u_j}}{dt} = -\mathbf{MCu_j} + \mathbf{D_j^T p} - \nu\mathbf{Lu_j} \\ \mathbf{D}^j\mathbf{u_j} = 0 \end{cases}$$

Continuity: Operators

Advection-Diffusion, semi-implicit form:

$$\mathbf{H} = \frac{\beta}{\Delta t}\mathbf{M} + \nu \mathbf{L}$$

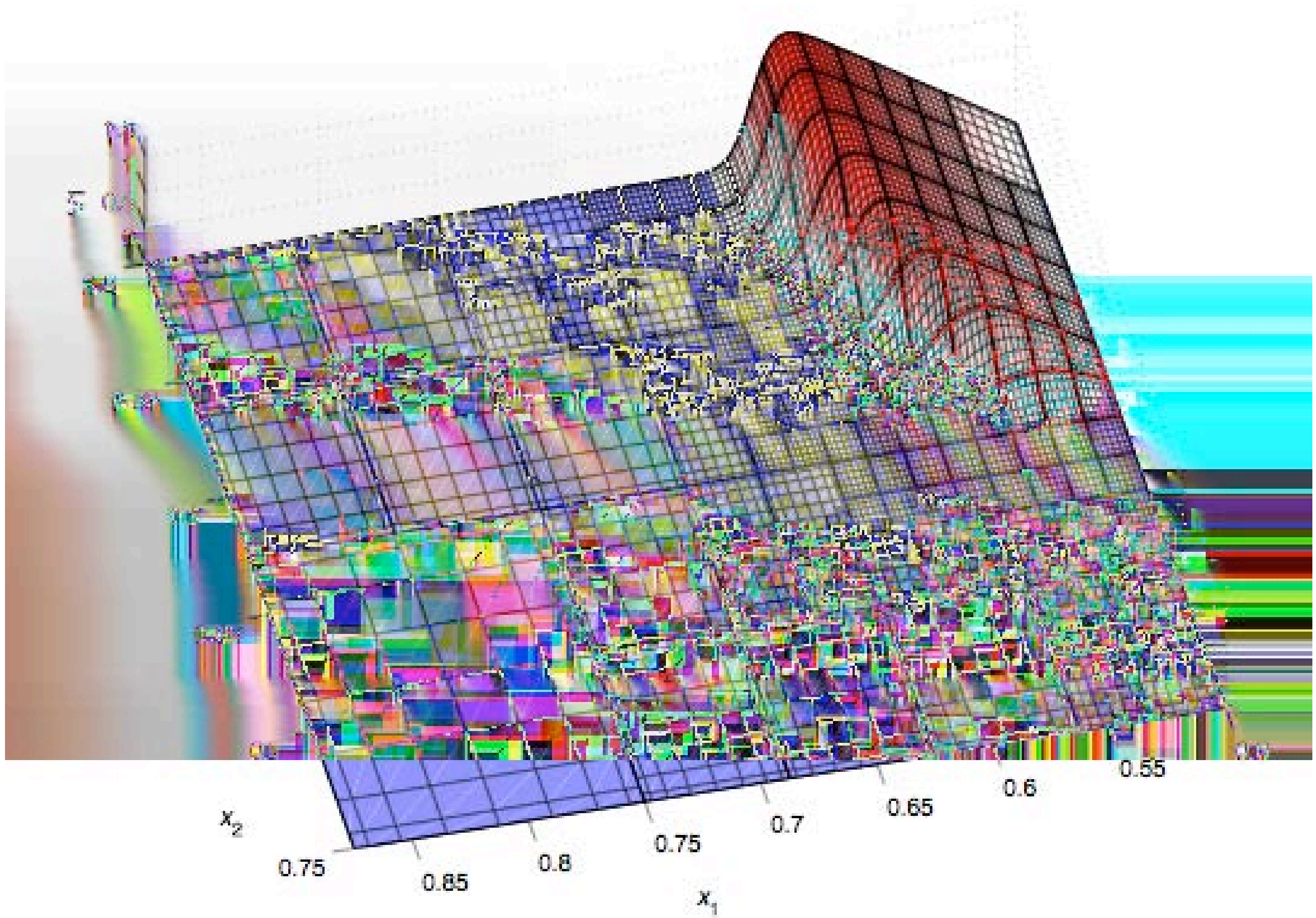
$$\underbrace{\mathbf{\Phi A A^T \Phi^T}}_{\text{DSS operator}}\mathbf{H \Phi A u} = \mathbf{\Phi A A^T \Phi^T f}$$

DSS operator

Navier-Stokes & MHD:

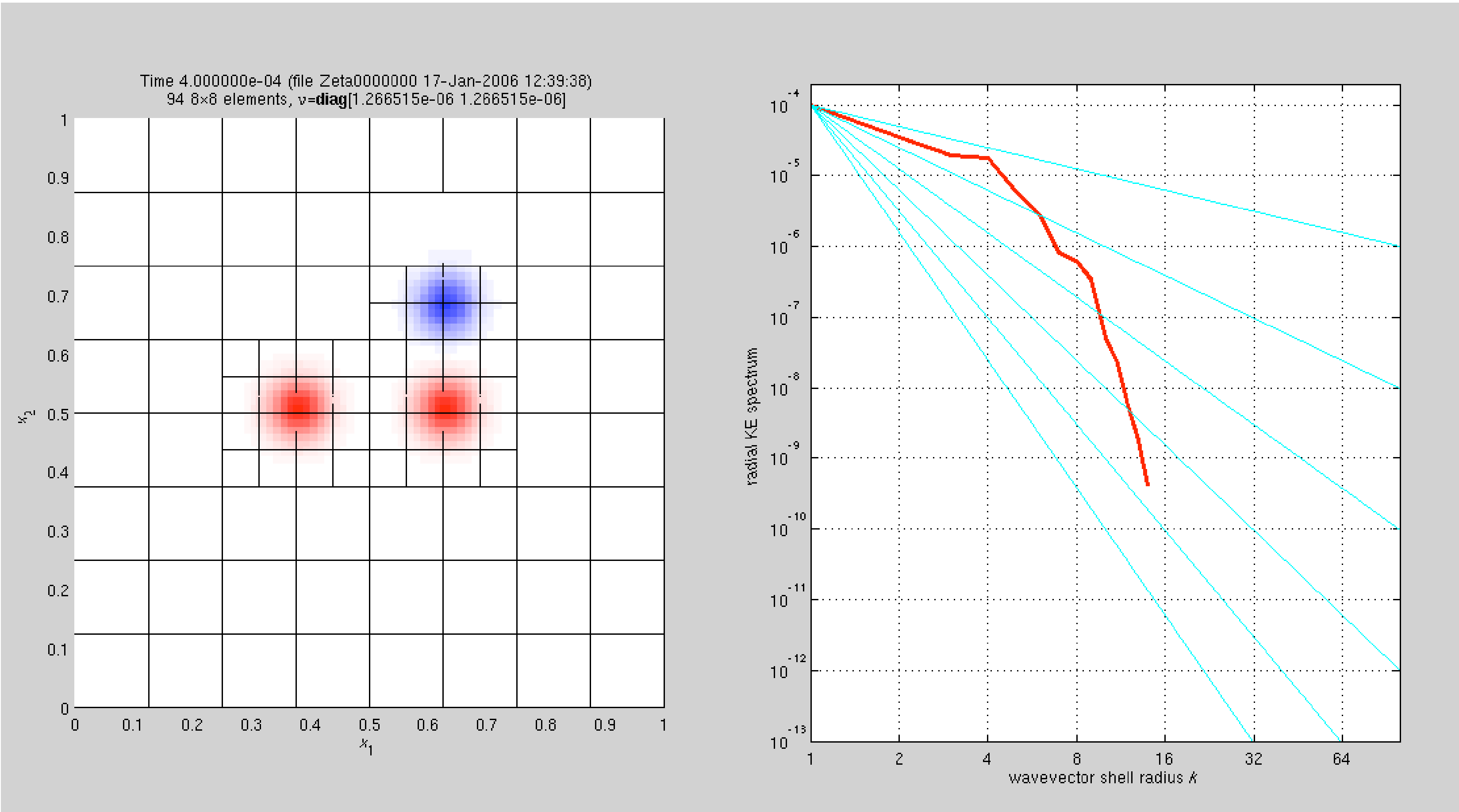
$$\mathbf{D}_j \rightarrow \mathbf{D}_j \mathbf{\Phi A}$$

Advection-diffusion: 2-d N-Wave



Navier Stokes: 3-vortex simulation

Fournier, Rosenberg, Pouquet, GAFD, 103(2), 245--268 (2009).



Vorticity (left) and energy spectra (right; Fournier, J. Comp. Phys., 215(1), (2006)) for Re=10^4. Note power law spectral behavior with filament formation

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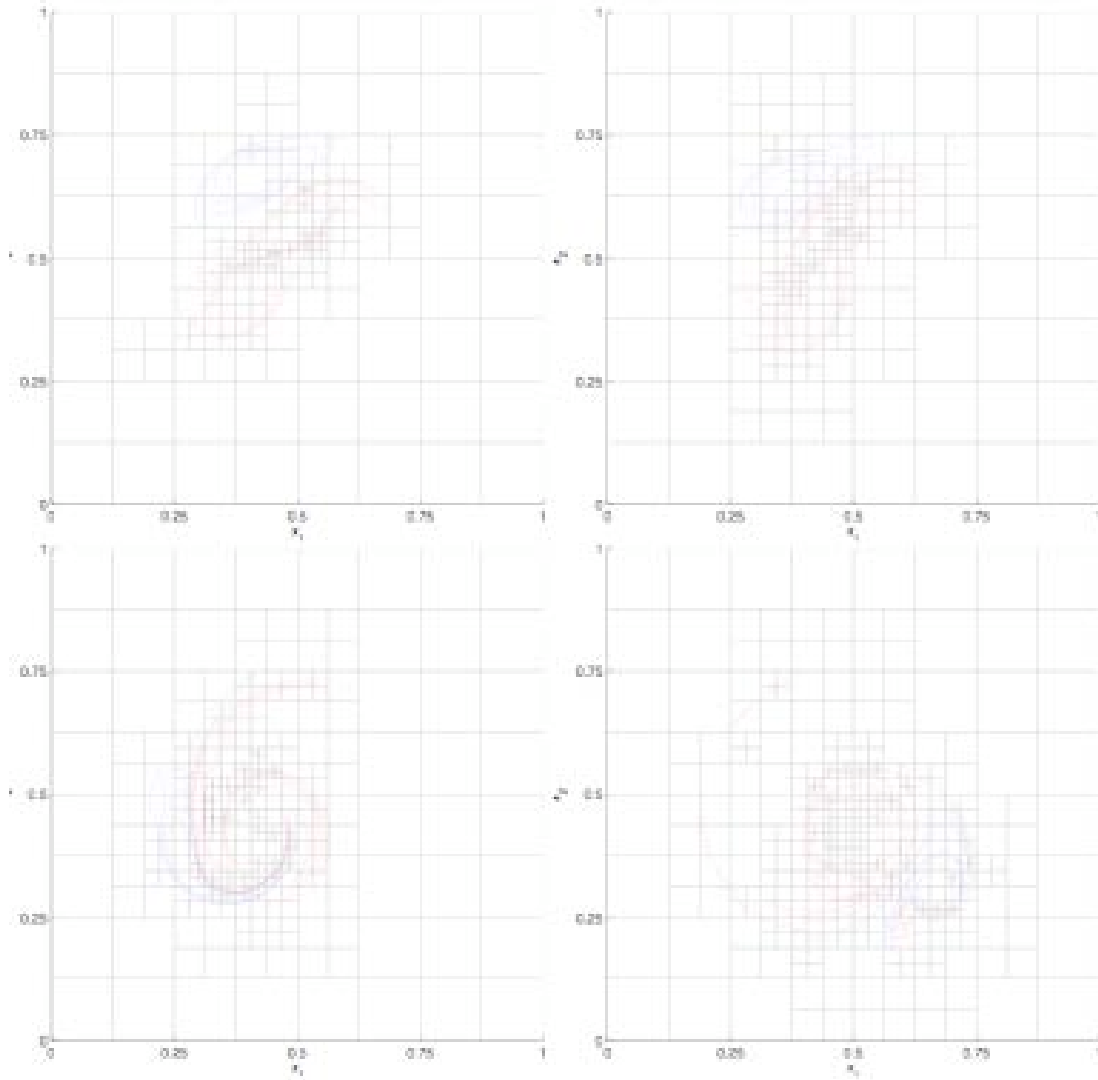
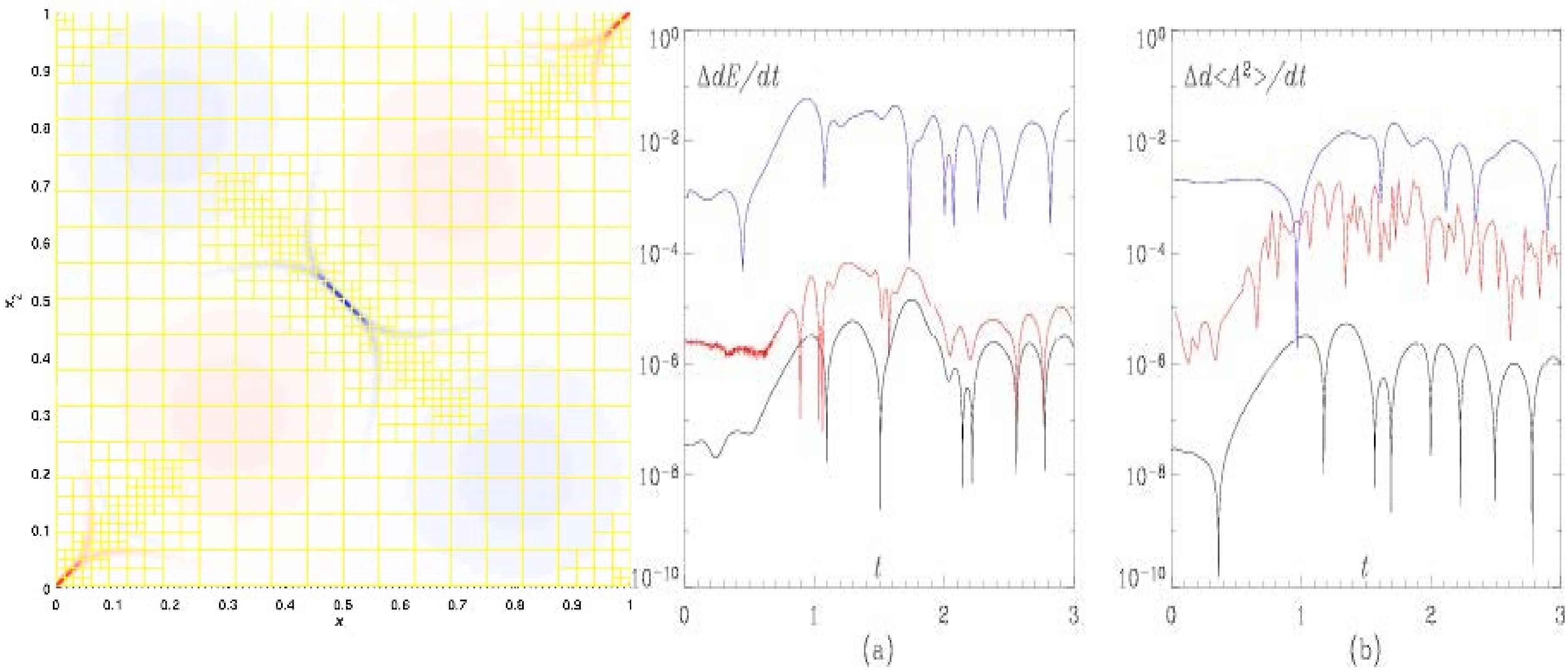
Fournier, Rosenberg, Pouquet, GAFD (2008)

Navier-Stokes: 3-vortex simulation



MHD: Island coalescence instability



Ng, Rosenberg, Germaschewski, Pouquet, Bhattacharjee, Ap. J. Suppl., 177(2), 613--625 (2008).

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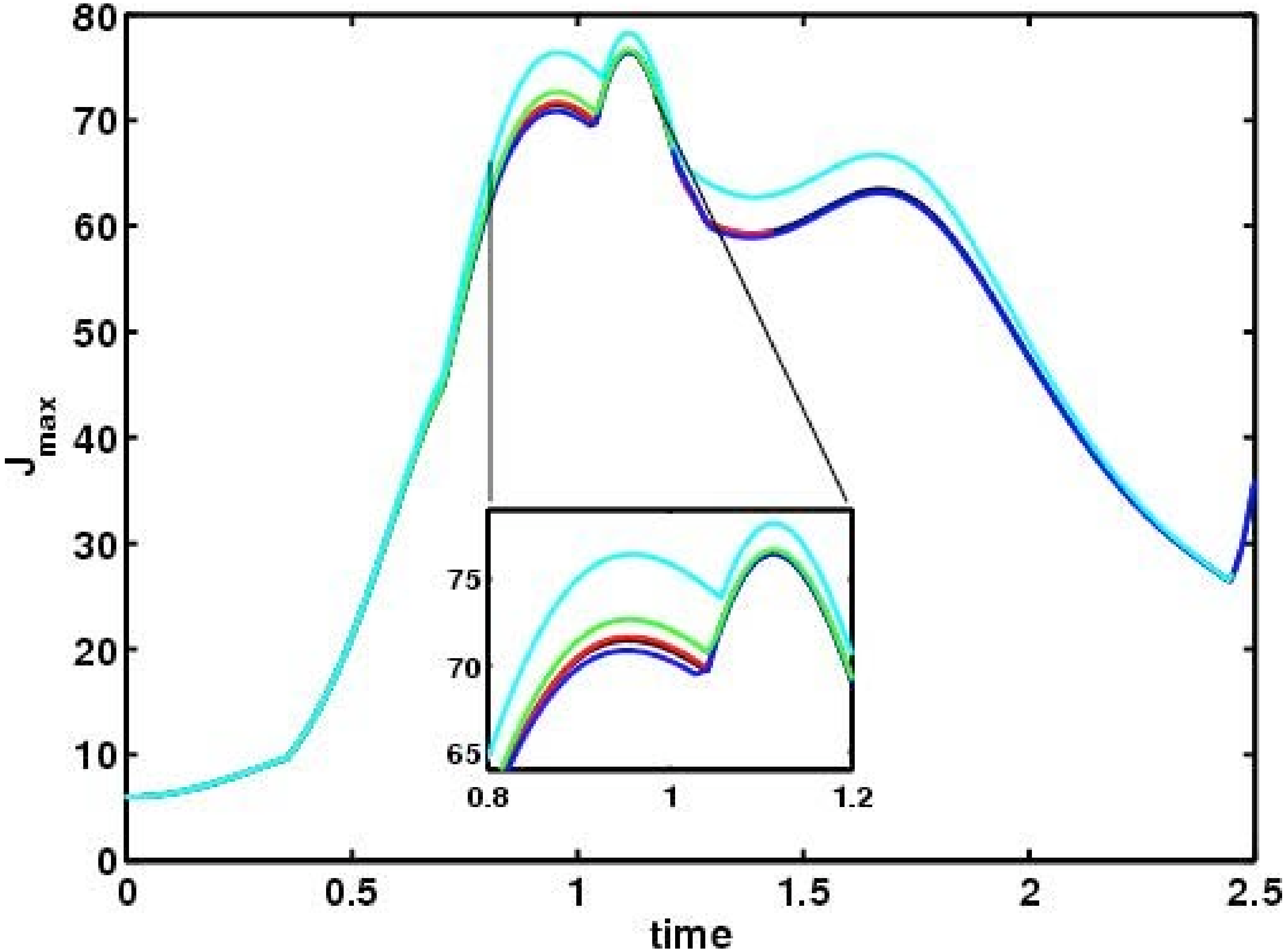
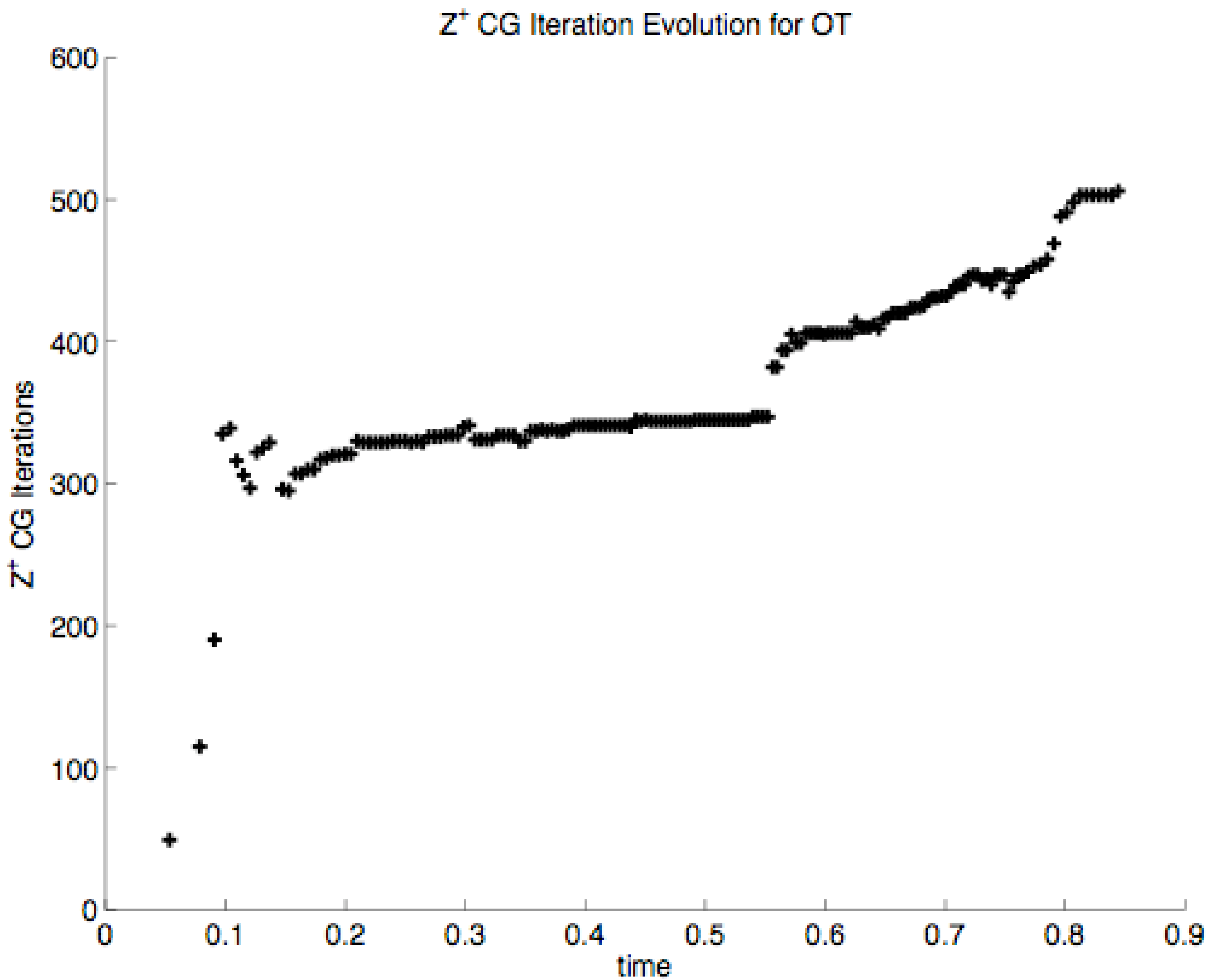
OT SEM convergence



Black: pseudo-spectral
Red: p=8
Blue: p=6
Green: p=4
Cyan: p=3

Evolution of iteration count for OT: Block Jacobi



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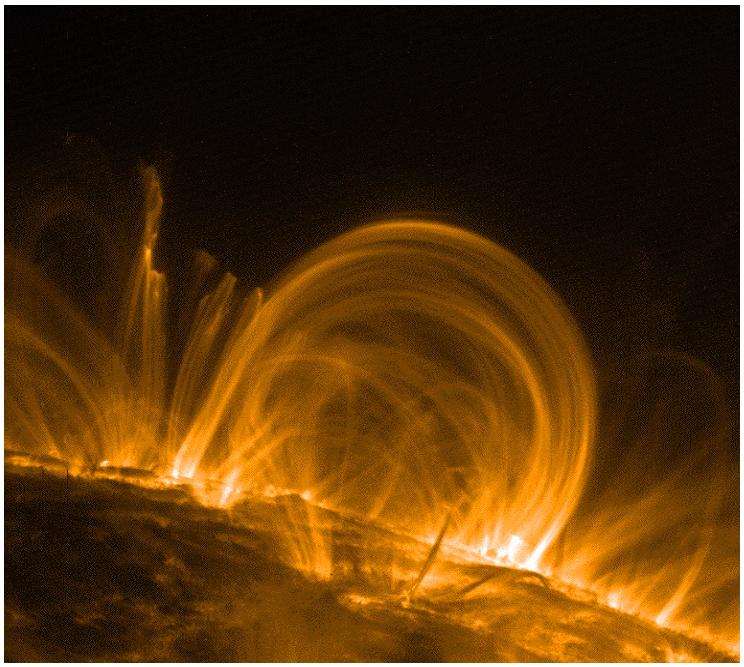
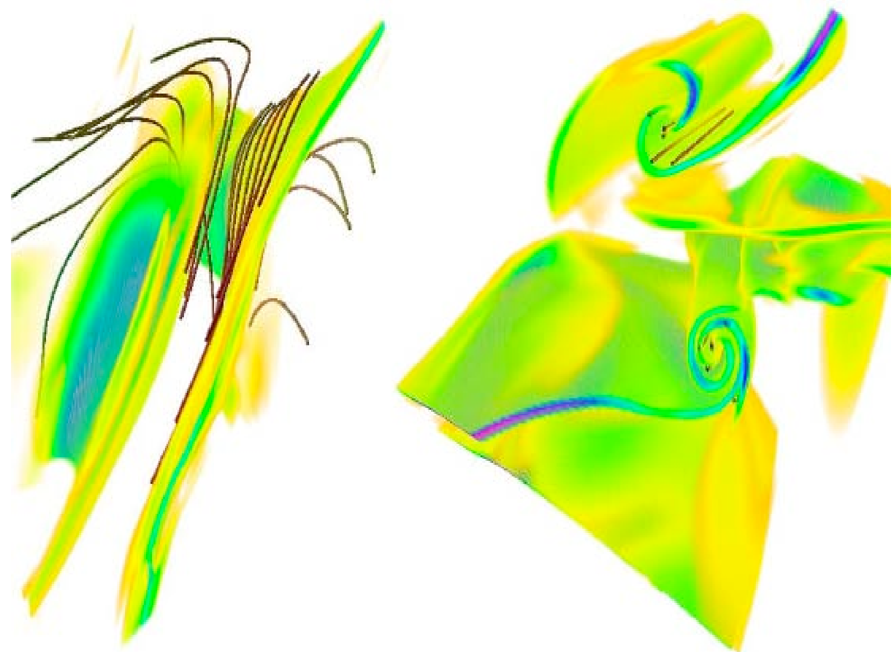
MHD Turbulence

- Phenomenological & fundamental:

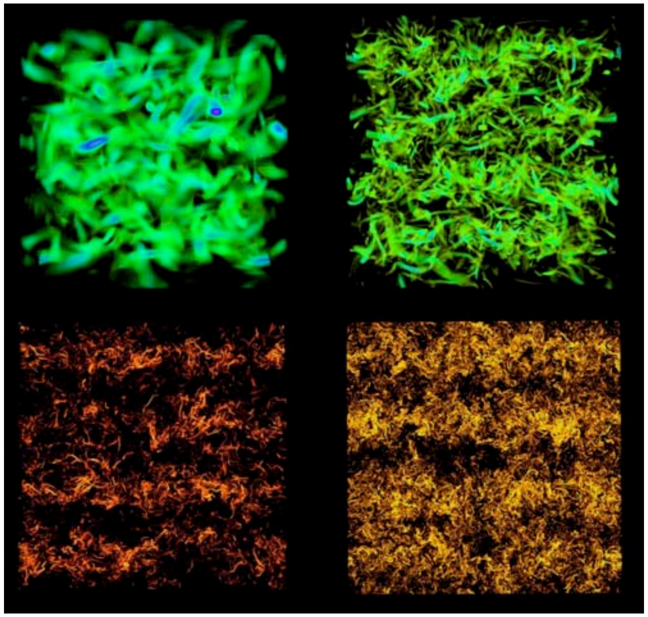


Trace



Mininni & Pouquet (2007)

Hydro Turbulence



Taylor-Green flow at 64^3, 256^3, 1024^3, 2048^3 (Mininni, Alexakis, Pouquet 2007)

Kelvin-Helmholtz rolls
In match smoke

NCAR