Adaptive Embedded Boundary Discretizations for Multimaterial Simulation

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MultiMat 2013, SF
September 5th, 2013

Talk outline

- Finite volume cut cell background, idealism
- Embedded boundary examples
- Higher-order approaches?
- A little algebra – pros/cons of least squares
- Futures and conclusions

ANAG and Chombo

Applied Numerical Algorithms Group (ANAG) at LBNL,

Phil Colella, group lead, http://crd.lbl.gov/anag

- **Applications-driven fundamental research** in PDE discretization and solvers
- **Development and deployment of high-performance software** for numerical methods using locally-structured grids, particles.
- **Collaboration with DOE science and technology areas** on algorithms and software.

→ *Cross-linkage*: emerging science collaborations motivate algorithm and software research, software supports algorithms research, algorithms feed back into software.

Chombo: A Software Toolkit for Structured-Grid Applications, http://chombo.lbl.gov

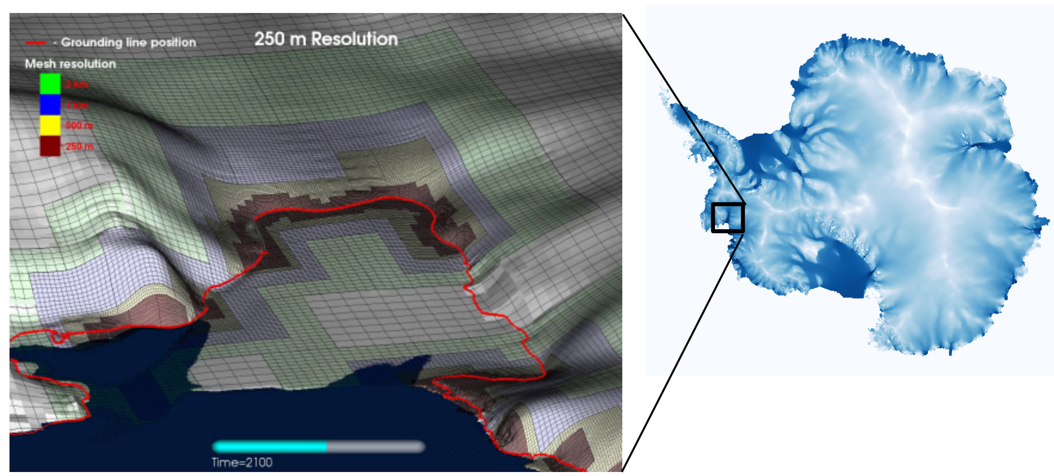
- **Supports a wide variety of applications** in a common software framework.
- Provides applications scientists with **open-source high-performance components** for developing complex applications with high-performance scalable implementations.
- **Parallel performance** (200k+ processors) with low-level details hidden from the applications developer using a layered software architecture.

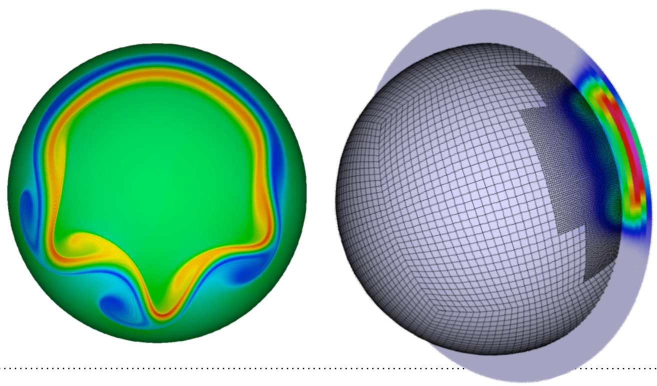
"Makes the easy things harder, but impossible things possible."

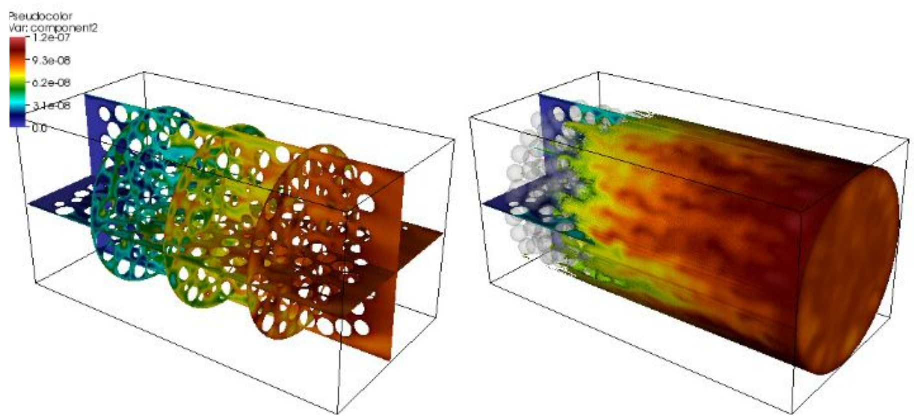
ANAG Algorithms Research

- High-order, finite-volume methods, space-time AMR algorithms
- Multiscale models for complex fluids, phase space, multi-physics
- Embedded boundary for complex geometries, mapped multiblock for high-order methods.
- Fast solvers that minimize communication, memory access.

"Mathematical engineering" for science and software on HPC platforms.





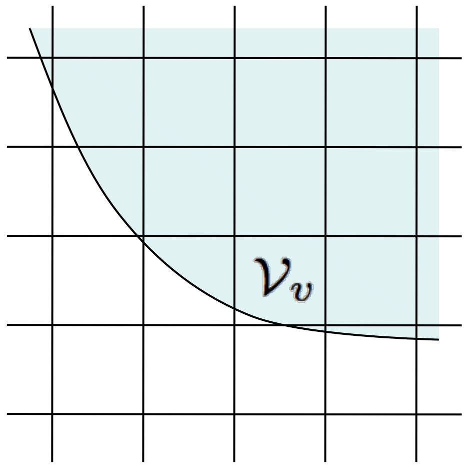


Adaptive Embedded Boundary Discretizations for Multimaterial Simulation
(*Hans Johansen, LBNL)*

COMPUTATIONAL RESEARCH DIVISION

BERKELEY LAB

"EB" Chombo: Finite Volume for Cut Cells



Operator: defined from divergence theorem on a "cut cell"

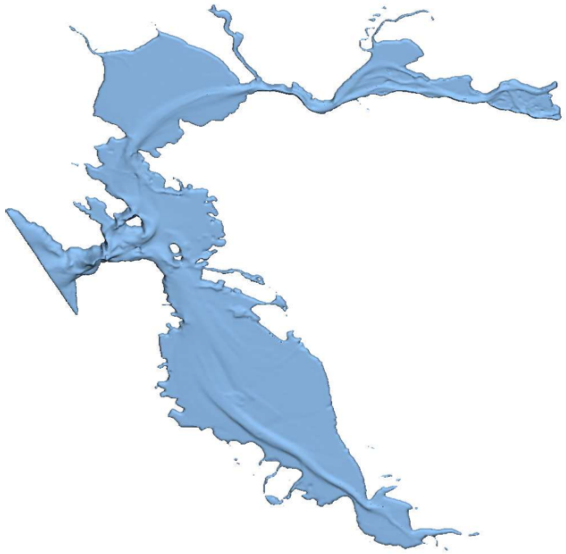
$$\int_{\mathcal{V}_v} \nabla \cdot \boldsymbol{F} dV = \sum_{f \in f(v)} \int_{\mathcal{F}_f} \boldsymbol{F} \cdot \boldsymbol{n}_f \, dA$$

$$\nabla \cdot \beta(\nabla u) = \rho, \quad \boldsymbol{F}(u) = \beta(\nabla u)$$

$$\frac{\partial u}{\partial t} = \nabla \cdot \rho(\nabla u), \quad \boldsymbol{F}(u) = \rho(\nabla u)$$

$$\frac{\partial u}{\partial t} + \nabla \cdot \boldsymbol{F}(u) = S(u), \quad \boldsymbol{F}(u) \text{ is given.}$$

SF Bay digital elevation map
[Ligocki et al, 2008]



Why cut cells?

- Conservative discretizations important for physics
- AMR effective for smaller number of boundary cells
- Move/refine boundary without "global regridding"
- Regular grid calculations very scalable, optimized
- Compatible with mapped grids, too (for accuracy)

“EB” Chombo: AMR Finite Volume for Cut Cells

Hyperbolic: FV discretizations important for coupling

- Conservative convection-diffusion-reaction
- Accurate jump conditions (shock speeds, fluid-solid coupling, moving boundaries, etc.)
- Non-linear fluxes use limiters, min/max preservation

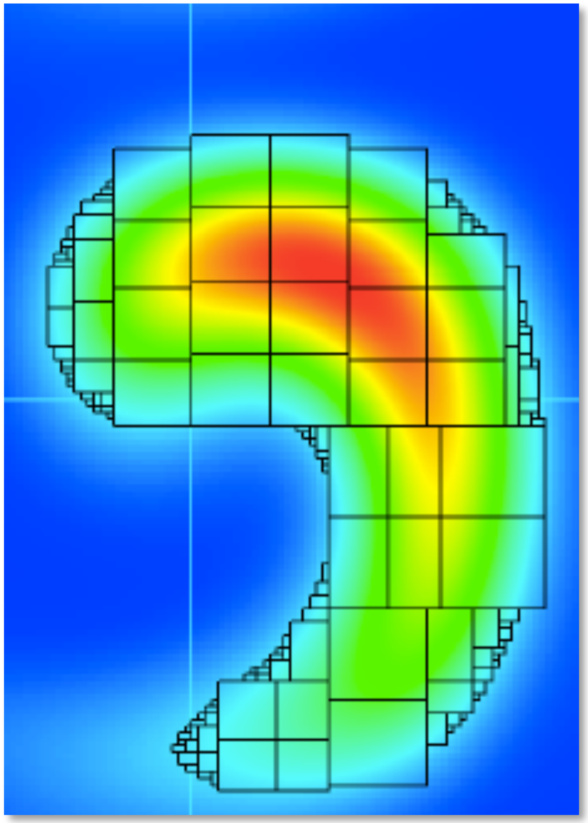
→ Primary issue is explicit time-stepping for “small cells”

Parabolic: discretization in time, space (“method of lines”)

- Conservative convection-diffusion-reaction
- Fast solvers available (such as multi-grid, FMM)
- “Small cell” problem expressed in matrix conditioning

→ Primary issue is stability for operator (eg. PD matrix)

Adaptivity: to contain error (both spatial and temporal)

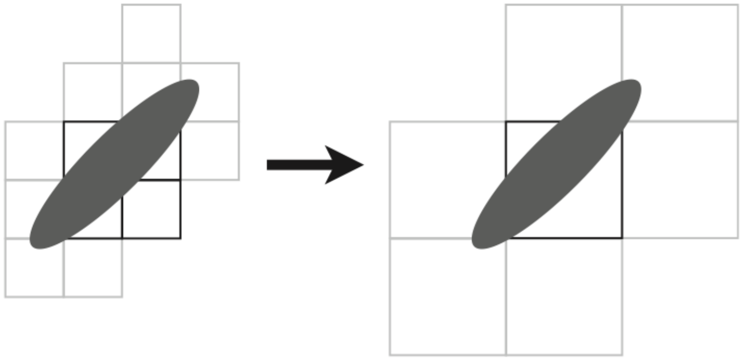


Stiff CDR AMR example [Zhang, HJ 2012]

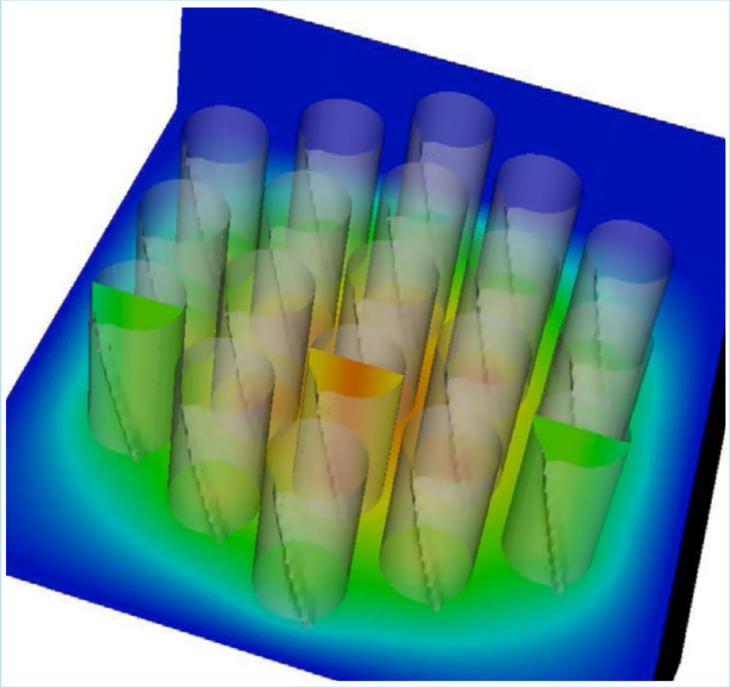
"MF" Chombo for Multimaterial

Material interfaces with flux-balance conditions:

- "Jump" conditions important for multi-fluid physics
- Boundary refinement requires additional, but local data structures (like octree)
- Regular grid calculations still very scalable, optimized for threading / vector processors

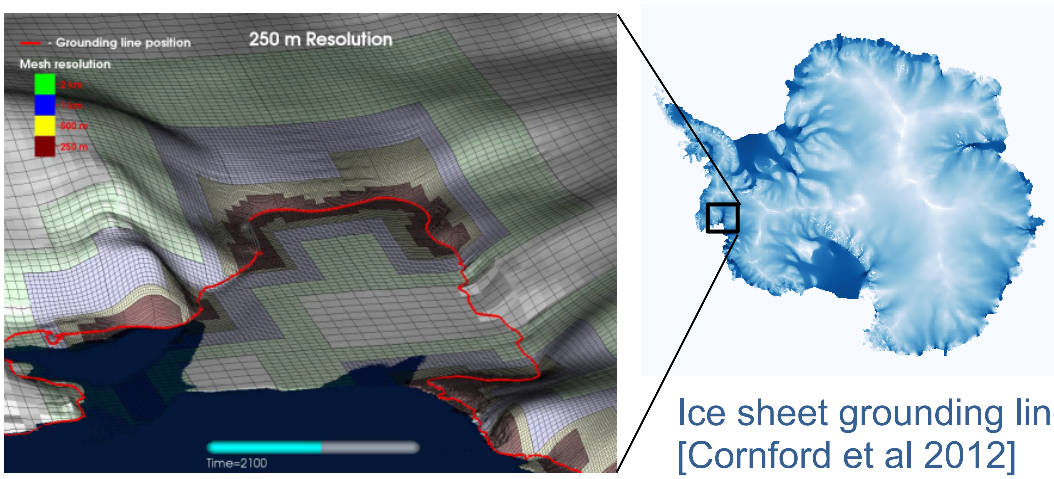


Support for sub-grid scale grid connectivity, data structures [Crockett et al 2011]



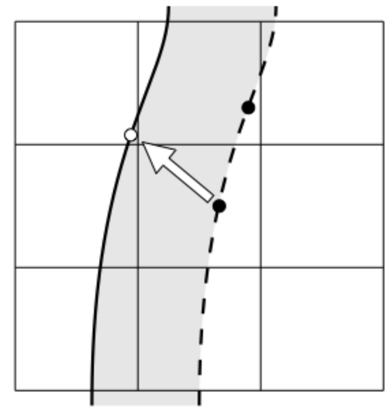
Multi-material heat transfer problem using AMR embedded boundary approach [Crockett et al 2011]

In progress: Multimaterial Moving Interfaces



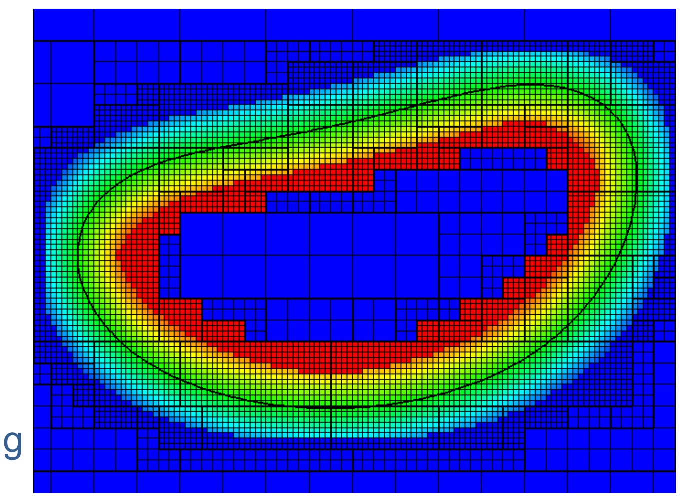
Ice sheet grounding line
[Cornford et al 2012]

Moving boundary INS [Miller et al 2012]



Track interfaces with conservation in mind

- Front motion connected to fluxes / physics
- Dynamic AMR required to control error
- Move/refine boundary without "global regridding"
- Volume conservation vs. reactions, phase change



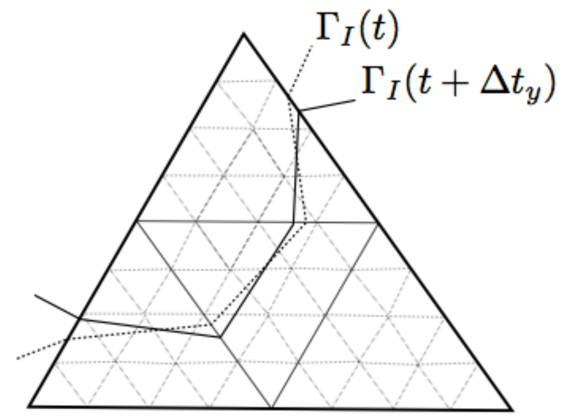
Higher-order AMR front tracking
[Lee, HJ, work in progress]

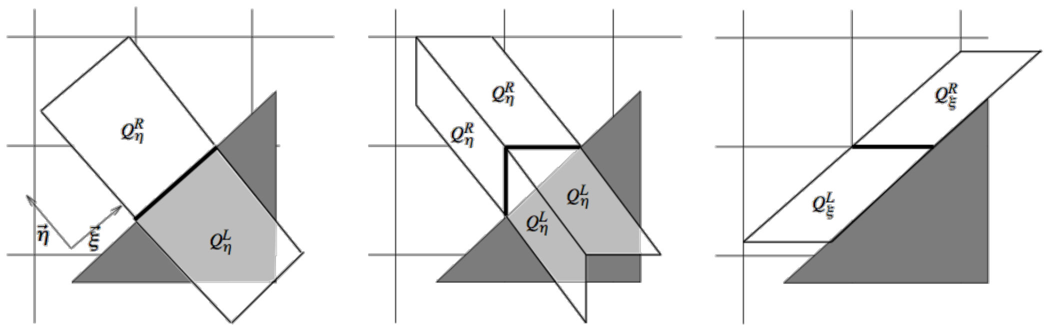
Difficulties with finite volume cut cells

Design criteria: (+AMR)

- **Conservative**: flux-based discretization
- **Accuracy**: $O(h^P)$ but ok with order P-1 near EB
- **Stability**: no "small cell problem," has stability characteristics of the differential operator
- **Consistency**: free stream preservation, polynomials
- **Simplification**: in the limit of full cells, low-memory regular discretization away from boundary
- **Usability**: for linear, non-linear, etc. problems in a framework that works for small or large problems

X-FEM DG for Stefan problem [Bernauer et al 2011]





H-box configuration [Helzel, Berger 2012]

Conservative fluxes using geometric moments

Fluxes: approximated by Taylor expansion on faces

$$\int_{\mathcal{F}_f} \nabla\phi \cdot \boldsymbol{n}_f \, dA = \sum_{d=1}^{D} \int_{\mathcal{F}_f} \phi^{(\boldsymbol{e}^d)} \, n_d \, dA$$

$$\boxed{m_{d,f}^{\boldsymbol{p}}}$$

$$= \sum_{d=1}^{D} \sum_{\boldsymbol{p}:|\boldsymbol{p}|<P} \frac{1}{\boldsymbol{p}!} \left[\phi^{(\boldsymbol{e}^d+\boldsymbol{p})}\right]_{\boldsymbol{x}=\bar{\boldsymbol{x}}_f} \boxed{\int_{\mathcal{F}_f} n_d (\boldsymbol{x}-\bar{\boldsymbol{x}}_f)^{\boldsymbol{p}} \, dA} + O(h^{P+D-1})$$

Parabolic fluxes: quadrature in time and on faces

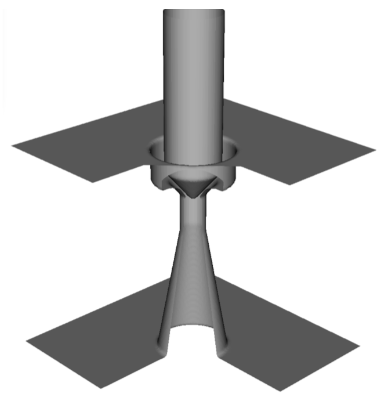
$$\int_{t^n}^{t^{n+1}} \left(\int_{\mathcal{F}_f} \nabla\phi \cdot \boldsymbol{n}_f \, dA \right) dt = \sum_{s=1}^{S} \omega_s \sum_{d=1}^{D} \sum_{\boldsymbol{p}:|\boldsymbol{p}|<P} \frac{1}{\boldsymbol{p}!} \left[\phi^{(\boldsymbol{e}^d+\boldsymbol{p})}(t_s)\right]_{\boldsymbol{x}=\bar{\boldsymbol{x}}_f}$$

$$\boxed{m_{d,f}^{\boldsymbol{p},t^n \to t^{n+1}}} \quad \boxed{\int_{t^n}^{t^{n+1}} \int_{\mathcal{F}_f} n_d (\boldsymbol{x}-\bar{\boldsymbol{x}}_f)^{\boldsymbol{p}} \, dA \, dt} + O(h^{\min(P,S)+D-1})$$

Calculating geometric moments on cut cells

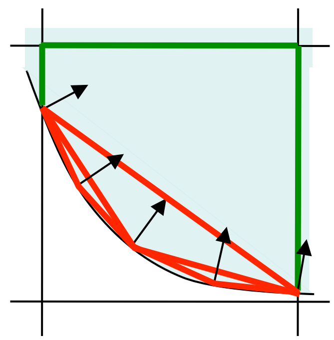
Moments: use divergence theorem to build a P^{th}-order least-squares system for volumes, moments, and normals based on implicit functions [Ligocki, et al, 2008]

- This is EB's "grid generation," but localized to cut cells
- With constraints, reproduces "water tight" combinations of moments
- Least-squares residual errors: *h*-scaled in higher-order moments that matter less
- Easily generated from level sets, surface triangulation, or CSG (implicit functions)
- Same approach works for mapped grids as well



Exact face moments from intersections

Exact normals, gradients from implicit function



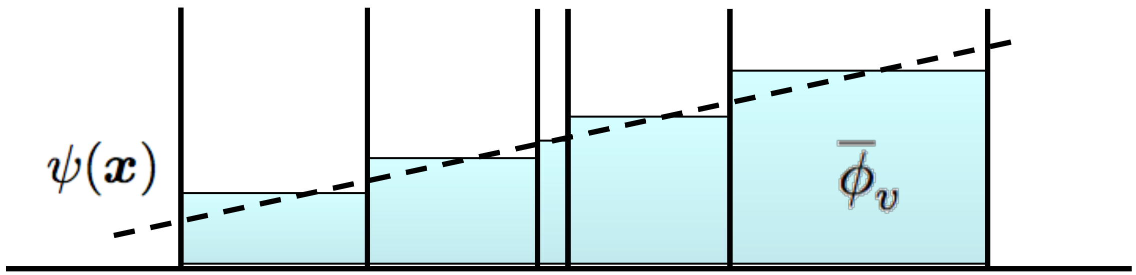
Subdivide for accuracy

Divergence theorem for volume / area moments

Least Squares Fit to Averages

Averages: approximated via a Taylor expansion for cell-average quantities and their derivatives (Note this is different than finite differences - point-wise).

$$\overline{\phi}_v = \frac{1}{|\mathcal{V}_v|}\left(\sum_{\boldsymbol{p}:\,|\boldsymbol{p}|<P} \frac{1}{\boldsymbol{p}!}\partial^{\boldsymbol{p}}\phi(\boldsymbol{x}_0)\, m_v^{\boldsymbol{p}}\right) + O(h^P) \qquad m_v^{\boldsymbol{p}} = \int_{\mathcal{V}_v} (\boldsymbol{x}-\boldsymbol{x}_0)^{\boldsymbol{p}}\, d\mathcal{V}$$



$$\psi(\boldsymbol{x}) = \sum_{\boldsymbol{k}:\,|\boldsymbol{k}|<P} c_{\boldsymbol{k}}(\boldsymbol{x}-\boldsymbol{x}_0)^{\boldsymbol{k}} \qquad \overline{\psi}_v = \frac{1}{|\mathcal{V}_v|}\sum_{\boldsymbol{p}:\,|\boldsymbol{p}|<P} c_{\boldsymbol{p}}\, m_v^{\boldsymbol{p}}(\boldsymbol{x}_0)$$

Least Squares Fit to Averages

Averages: least-square approximation using a polynomial fit:

$$\min_{c} ||\Phi - \Psi||_{2,W}\,, \text{ where}$$

$$||\Phi - \Psi||_{2,W} \equiv \sum_{v} w_v \left(\overline{\phi}_v - \overline{\psi}_v\right)^2 ,$$

$$\Psi = A\,c\,, \text{ where } A_{vp} = \frac{m_v^{\boldsymbol{p}}(\boldsymbol{x}_0)}{m_v^{\boldsymbol{0}}}$$

Averages: least-square approximation to calculate flux leads to a flux stencil

$$\begin{aligned}\overline{\mathbf{F} \cdot \boldsymbol{n}_f} &= \frac{1}{|\mathcal{A}_f|} \sum_{d=1}^{D} \left(\sum_{\boldsymbol{p}:\, |\boldsymbol{p}|<P} \frac{1}{\boldsymbol{p}!} \partial^{\boldsymbol{p}} F_d(\boldsymbol{x}_0) m_f^{d,\boldsymbol{p}} \right) \\ &= \frac{1}{m_f^0} \sum_{d=1}^{D} \sum_{|\boldsymbol{p}|<P} c_{d,\boldsymbol{p}}\, m_{d,f}^{\boldsymbol{p}} \\ &\equiv f^T\, c\,.\end{aligned}$$

$$\begin{aligned} s^T &= f^T C \\ &= f^T (A^T W A)^{\dagger} A^T W \end{aligned}$$

Least Squares Fit for Fluxes

- **Fluxes:** stencils specified by system derived from fit:

$$\int_{\mathcal{F}_f} \nabla\phi \cdot \boldsymbol{n}_f \, dA \approx \boxed{\sum_{d=1}^{D} \sum_{\substack{\boldsymbol{k}:\boldsymbol{k}\geq \boldsymbol{e}^d \\ \boldsymbol{k}<P\boldsymbol{u}+\boldsymbol{e}^d}} k_d \, C_{\boldsymbol{k}} \, m_{d,f}^{\boldsymbol{k}-\boldsymbol{e}^d}} + O(h^{P+D-1})$$

$$\boxed{\equiv A_{v'}(\boldsymbol{k}, f) \, \langle\phi\rangle_{v'}}$$

- **Boundary conditions** can be specified generally
  - **Dirichlet,** add to system for C: $$\int_{\mathcal{F}_f} g \, dA = \sum_{\boldsymbol{p}:|\boldsymbol{p}|<P} C_{\boldsymbol{p}} m_f^{\boldsymbol{p}}$$
  - **Neumann,** flux is specified (and can be added to system): $$\int_{\mathcal{F}_f} \nabla\phi \cdot \boldsymbol{n}_f \, dA = \int_{\mathcal{F}_f} g \, dA$$

Example: free stream preservation

- Free stream preservation for $\mathbf{F} = \phi \mathbf{u}$:

$$\nabla \cdot (\phi \mathbf{u}) = \phi (\nabla \cdot \mathbf{u}) + \cancelto{0}{(\nabla \phi)} \mathbf{u}$$

$$\nabla \cdot (\phi \mathbf{u}) = \sum_{k} C_k (x - \bar{x})^k \Big|_{\nabla \hat{\phi} = \mathbf{0}} (\nabla \cdot \mathbf{u})$$

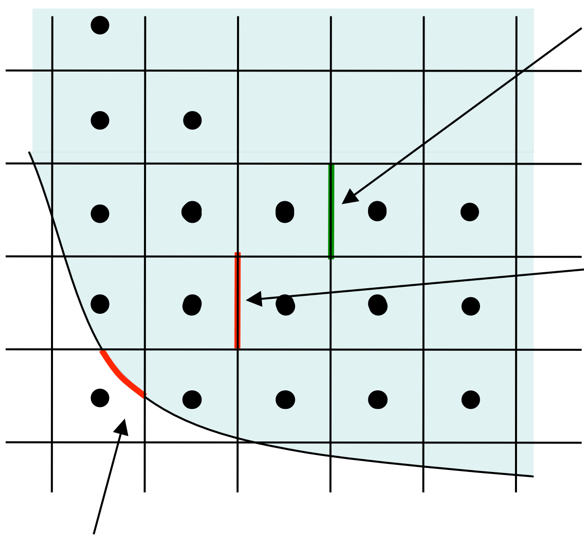
$$\nabla \cdot (\phi \mathbf{u}) = C_0 (\nabla \cdot \mathbf{u})$$

- For $\nabla \cdot \mathbf{u} = 0$:

$$\nabla \cdot \mathbf{u} = \frac{1}{V_v} \sum_{d=1}^{D} \sum_{f \in \partial v} n_d A_f \langle u_d \rangle_f = 0, \langle u_d \rangle_f \approx \frac{1}{A_f} \sum_{k} m_f^k \frac{1}{k!} u_d^{(k)}$$

Least Squares Fit *(cont.)*

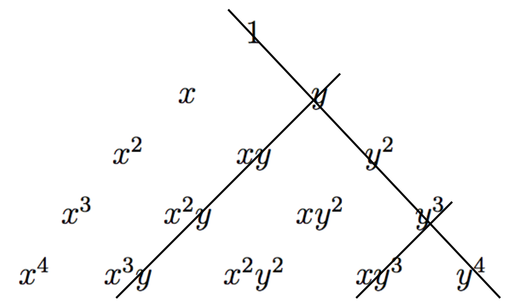
Stencil: sufficient points to make system full-rank



"Regular" 4th order stencil

$$\int \phi^{(\mathbf{e}^d)}\, dA \approx \frac{h^{D-2}}{16}\,[1 \quad -15 \quad 15 \quad -1]\,\langle \phi \rangle + O(h^{D+3})$$

"Irregular" 4th-order stencil, needs some additional cross-derivatives to complete the stencil:



"Boundary" flux requires all of these and must include boundary conditions (Dirichlet, etc.) as well.

- *All stencils automatically derived from least squares approach given set of neighbors that makes system full-rank*

Least Squares Fits – Dirty Secrets

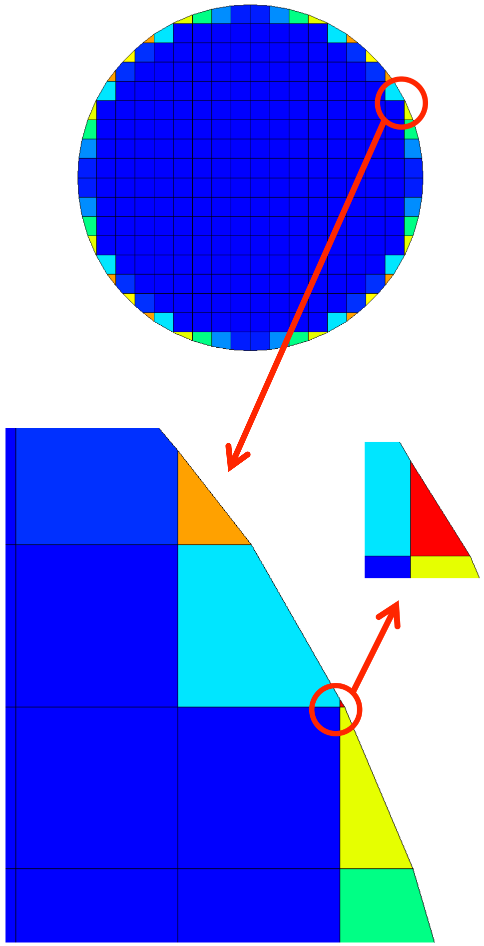
Stencils: *N* points, *P* polynomial coefficients:

- *N > P*
  - Coefficients are *over-determined*, 2-norm minimization
  - Stencils are *under-determined* - additional degrees of freedom that don't change consistency
  - Can lead to down-winding, Runge phenomenon, etc.
  - Need criteria for selecting the correct stencil: sparsity (L1 norm minimization), stability (but without studying entire matrix?), etc.
- *P > N*
  - Stencils are *over-determined*, may not be 4th-order
  - Coefficients are under-determined – need additional criteria to identify "best" choice
  - Leads to minimum Sobolev norm, WENO, other approximations

Results: 2D Laplacian, Dirichlet BC's

Truncation error for polynomials on a circle

$h =$	$1/16$	$1/32$	$1/64$	$1/128$	
$\min(\lambda)$	3.1e-2	4.2e-3	7.7e-4	4.5e-4	
Test	error in $\|\|\Lambda\Delta\phi\|\|_1$				Order
$\phi = xy$	3.78e-14	2.45e-13	8.13e-13	2.55e-12	N/A
$\phi = 1 - r^4$	1.26e-13	7.15e-13	6.43e-12	9.61e-12	N/A
$\phi = r^2(1 - r^4)$	9.15e-5	5.98e-6	3.83e-7	2.42e-8	3.96
Test	error in $\|\|F(\phi)\|\|_1$				Order
$\phi = xy$	5.74e-14	2.28e-13	6.13e-13	8.85e-13	N/A
$\phi = 1 - r^4$	7.56e-13	1.15e-12	2.04e-12	2.61e-11	N/A
$\phi = r^2(1 - r^4)$	2.86e-5	9.69e-7	2.99e-8	1.02e-9	4.93



Conclusions and Future Research

We have been researching a new, general cut-cell approach:

- Simple "grid generation" even with complex geometries
- 4^{th}-order, but may be generalized to 6^{th} or higher
- No "small cell problem," relatively insensitive to errors in geometry generation, boundary conditions

Active research areas:

- Good conditioning → multigrid, fast parabolic solvers, time integrators (RKC)
- Limiters for non-linear hyperbolic problems
- Conditions that guarantee positive definiteness?
- Combine with moving boundary → space-time moments
- Multi-physics flux matching conditions (multi-phase flow vs. porous media)

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Work supported by
Office of Science, ASCR

Thank you!

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