

Higher-Order Finite-Volume Methods

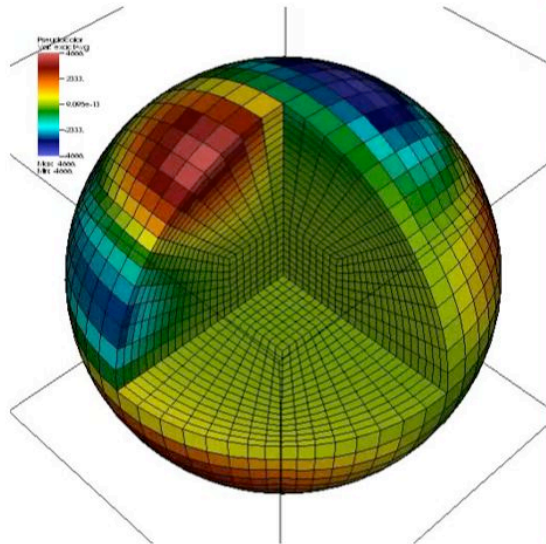
Phillip Colella

Applied Numerical Algorithms Group, LBNL

Joint work with Milo Dorr, Jeff Hittinger (LLNL); Dan Martin,
Peter McCorquodale (LBNL).

Mapped Multiblock Algorithms

Want to compute solutions to fluid dynamics problems in near-spherical symmetry without pole singularities.



Want to use finite-volume discretizations on multiblock grid obtained from cubed-sphere mapping. High-order accuracy (fourth-order or better) essential due to the discontinuities in the grid mapping at block boundaries.

Applications: Large-scale dynamics for supernovae; gyrokinetic edge plasmas in tokamaks; atmospheric fluid dynamics.

High-Order Finite-Volume Methods on Structured Grids

Local conservation form:

$$\nabla \cdot \vec{F} \rightarrow \frac{1}{h} \sum_{d=1}^D F_{i+\frac{1}{2}e^d}^d - F_{i-\frac{1}{2}e^d}^d \quad F_{i+\frac{1}{2}e^d}^d \approx \frac{1}{h^{D-1}} \int_{A_{i+\frac{1}{2}e^d}} F^d dA$$

Greater than second-order accuracy requires one to distinguish between point values and averages over control volumes, faces (Barad and Colella, 2006).

$$\frac{1}{h^{D-1}} \int_{A_{i+\frac{1}{2}e^d}} F^d dA = F^d(\mathbf{x}_{i+\frac{1}{2}e^d}) + \frac{h^2}{24} \sum_{d' \neq d} \frac{\partial^2 F^d}{\partial x_{d'}^2} + O(h^4)$$

Drivers:

- Applications requiring long-time integration.
- Lessens impact of loss of accuracy at boundaries where mesh is not smooth (e.g. AMR, multiblock): 2nd order \rightarrow 1st order \Rightarrow 4th order \rightarrow 3rd order.
- Phase space problems (4-6 space dimensions).

High-Order Finite-Volume Methods on Structured Grids

Extension to mapped grids:

$$\mathbf{x} = \mathbf{X}(\xi) , \mathbf{X} : [0, 1]^D \rightarrow \mathbf{R}^D$$

$$\nabla_{\mathbf{x}} \cdot \vec{F} \equiv \frac{1}{J} \nabla_{\xi} \cdot (\mathbf{N}^T \vec{F})$$

$$J \equiv \det(\nabla_{\xi} \mathbf{X}) , \mathbf{N}_{p,q} = \det((\nabla_{\xi} \mathbf{X})(p|\mathbf{e}^q))$$

Finite-volume discretization: if V_i is a rectangular cell in the mapping space,

$$\int_{X(V_i)} \nabla_x \cdot \mathbf{F} d\mathbf{x} = \int_{V_i} \nabla_{\xi} \cdot (\mathbf{N}^T \mathbf{F}) d\xi = \sum_{\pm=+,-} \sum_{d=1}^D \pm \int_{A_d^{\pm}} (\mathbf{N}^T \mathbf{F})_d dA_{\xi}$$

Fourth-order accurate approximation to face integrals:

$$\int_{A_d} (\mathbf{N}^T \vec{F})_d dA_{\xi} = \left(\left(\int_{A_d} \mathbf{N}^T dA_{\xi} \right) \cdot \left(\int_{A_d} \vec{F} dA_{\xi} \right) \right)_d + \frac{h^2}{12} \int_{A_d} \sum_{d' \neq d} \left(\frac{\partial}{\partial \xi_{d'}} (\mathbf{N}^T) \cdot \frac{\partial}{\partial \xi_{d'}} (\vec{F}) \right)_d dA_{\xi} + O(h^4)$$

Constant fluxes require cancellation of face integrals of metric terms.

High-Order Finite-Volume Methods on Structured Grids

Freestream-preservation \leftrightarrow equality of mixed partials:

$$\nabla_{\xi} \cdot \mathbf{N}^T = \sum_{\pm=+,-} \sum_{d=1}^D \pm \int_{A_{d,\pm}} \mathbf{N}_d^T dA_{\xi} = 0$$

Poincare lemma:

$$\exists \mathcal{N}_{d,d'}^s, d \neq d' \quad \text{such that} \quad N_d^s = \sum_{d' \neq d} \frac{\partial \mathcal{N}_{d,d'}^s}{\partial \xi_{d'}} , \mathcal{N}_{d,d'}^s = -\mathcal{N}_{d',d}^s$$

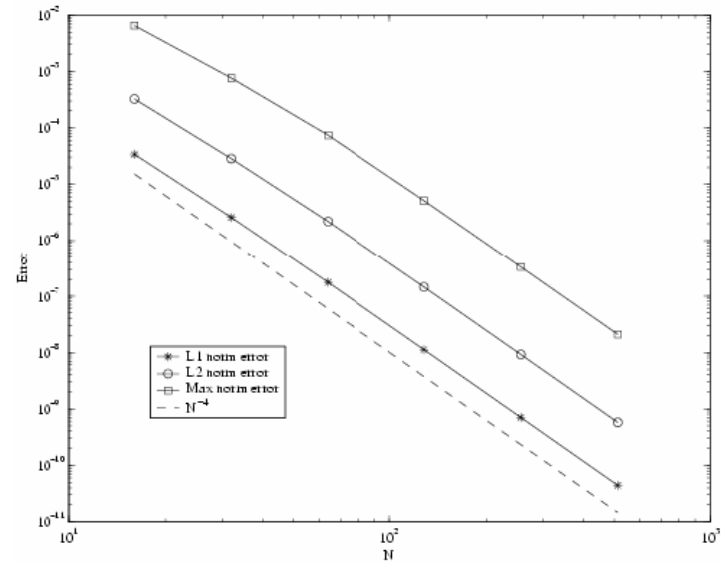
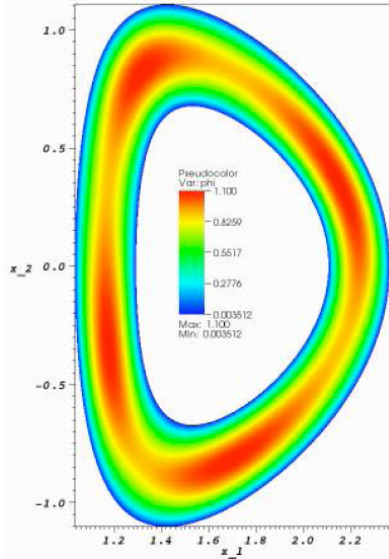
Use Stokes' theorem to compute face averages of \mathbf{N} :

$$\int_{A_d} N_d^s dA_{\xi} = \sum_{\pm=+,-} \sum_{d' \neq d} \pm \int_{E_{d,d'}^{\pm}} \mathcal{N}_{d,d'}^s dE_{\xi}$$

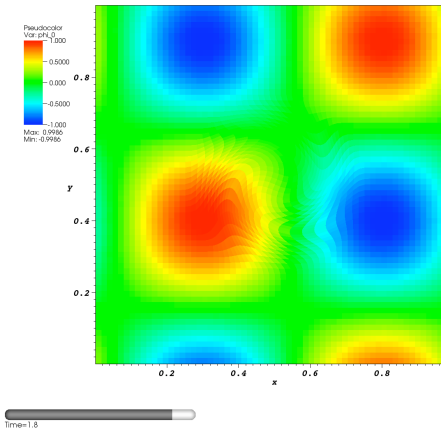
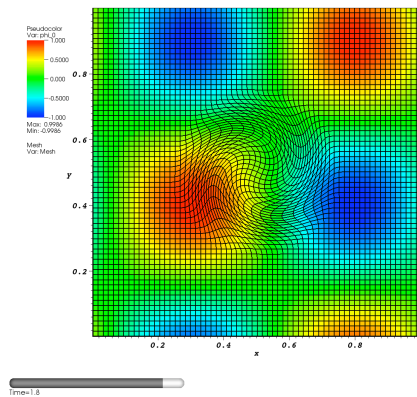
Any quadrature for the integrals on the RHS that preserves antisymmetry implies that we get the required cancellation. $\mathcal{N}_{d,d'}^s$ is known as an explicit local function of the mapping and its gradient, for any number of dimensions.

High-Order Finite-Volume Methods on Structured Grids

Gyrokinetic Poisson equation (variable-coefficient elliptic problem):



Advection on a twisted grid using centered differences, RK4 time discretization.

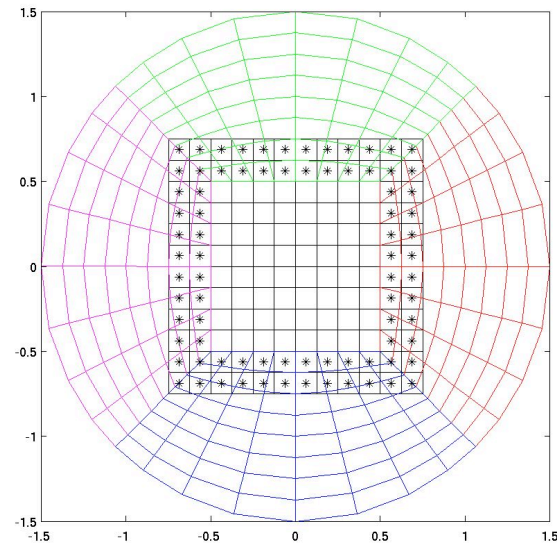


Mapped Multiblock Interpolation

Can extend higher-order mapped grid algorithms if one can compute sufficiently accurate ghost cell values on smooth extensions of each block.

Use polynomial interpolation:

$$\varphi(\mathbf{x}) \approx \sum_{\mathbf{p}} a_{\mathbf{p}} \mathbf{x}^{\mathbf{p}}, \quad \mathbf{x}^{\mathbf{p}} = \prod_{d=1}^D x_d^{p_d}$$
$$\int_{V_v} \varphi(\mathbf{x}) d\mathbf{x} = \sum_{\mathbf{p}} a_{\mathbf{p}} \int_{V_v} \mathbf{x}^{\mathbf{p}} d\mathbf{x}, \quad v \in \mathcal{V}$$



We use a set of control volumes such that the above system of equations for the expansion coefficients is of maximal rank, and can be solved using least-squares. Then we evaluate the polynomial or its moments to obtain the ghost values.

High-Order Limiters (Colella and Sekora, JCP 2008)

Example: PPM (first step)

Linear deconvolution:

$$a_{j+\frac{1}{2}} = \frac{7}{12}(a_j + a_{j+1}) - \frac{1}{12}(a_{j-1} + a_{j+2})$$

Constrain face values so that

$$\min(a_j, a_{j+1}) \leq a_{j+\frac{1}{2}} \leq \max(a_j, a_{j+1})$$

At smooth extrema, this leads to a first-order accurate method. ENO / WENO / CENO, other methods provide remedies, but they are complicated - want a simpler solution.

High-Order Limiters (Colella and Sekora, JCP 2008)

At extrema (and only at extrema) replace the constraint

$$\min(a_j, a_{j+1}) \leq a_{j+\frac{1}{2}} \leq \max(a_j, a_{j+1})$$

with the following:

$$D^2a = \frac{3}{h^2}(a_j + a_{j+1} - 2a_{j+\frac{1}{2}})$$

$$D^2a_L = \frac{1}{h^2}(a_{j-1} + a_{j+1} - 2a_j)$$

$$D^2a_R = \frac{1}{h^2}(a_j + a_{j+2} - 2a_{j+1})$$

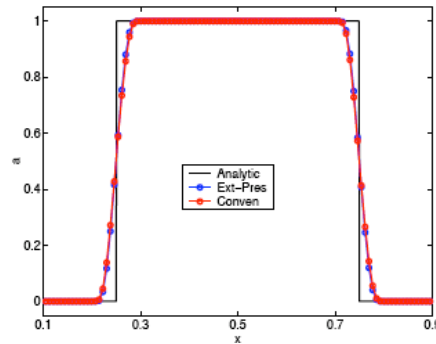
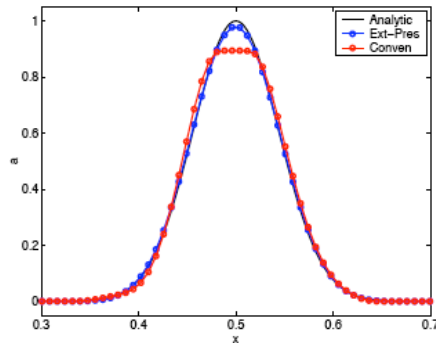
$$D^2a_{lim} = s \cdot \min(C|D^2a_L|, C|D^2a_R|, |D^2a|) \text{ if signs match} \\ = 0 \text{ otherwise}$$

$$a_{j+\frac{1}{2}} = \frac{1}{2}(a_j + a_{j+1} - \frac{h^2}{3}D^2a_{lim})$$

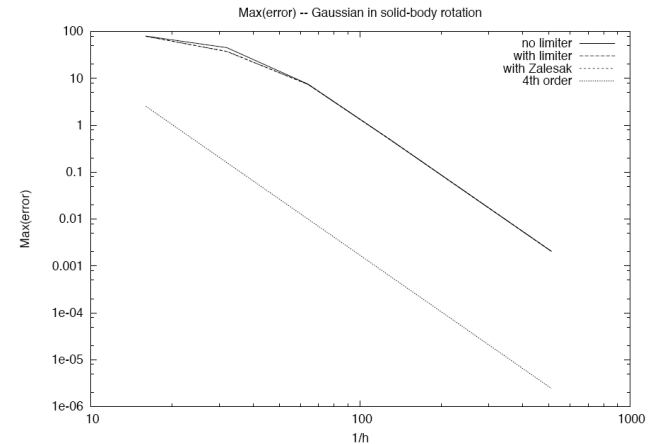
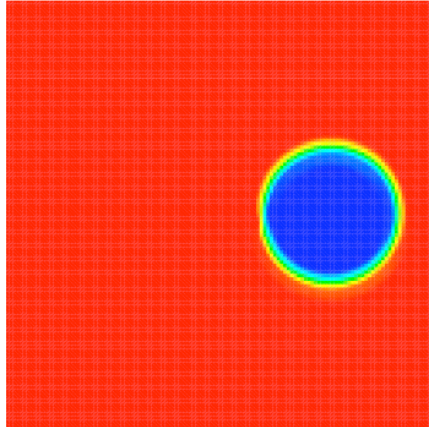
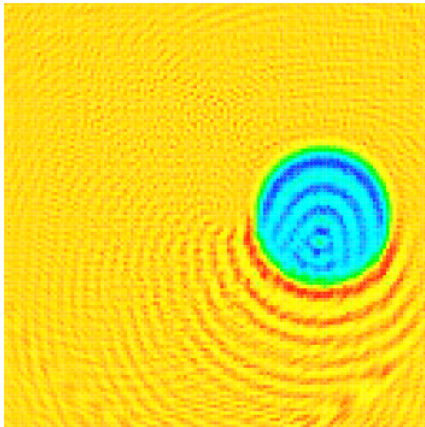
$C > 1$, independent of the mesh spacing. If the solution is smooth, edge value is unchanged. At a discontinuity, one of the estimates of D^2a is much smaller than the others. Can apply the same idea to limiting the parabolic profiles. Combine with Zalesak FCT limiter for positivity preservation.

High-Order Limiters (Colella and Sekora, JCP 2008)

1D PPM advection results:



2D RK4 advection results (Colella, Dorr, Hittinger, Martin, 2008):



Other Issues

Model issues. Splitting of three time scales (advective, gravity-wave, acoustic). Well-posed BVP for local refinement. Hydrostatic vs. non-hydrostatic behavior as a function of horizontal scale, within a non-hydrostatic model.

Other discretization Issues.

- High-order semi-implicit temporal discretization methods. Multiply-implicit spectral-deferred corrections in time, based on integral equation formulation ?
- Representation of orography: body-fitted grids vs. cut-cell.

Software Issues: retooling parallel AMR infrastructure for multiblock.

Planned Work

- Finish initial implementation of the mapped-multiblock infrastructure (less than six months).
- Advection, SWE on a sphere test cases (six months).
- Simplified dynamical core based on Helmholtz splitting of full compressible equations. No orography, column physics. Apply to test suite.
- Add column physics, for specialized two-scale simulation of the tropics ?