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Algebraic Flux Correction FEM for Convection Dominated Transport

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Motivation

$$\frac{\partial u}{\partial t} + \vec{w} \cdot \nabla u - \nabla \cdot \nu \nabla u = 0$$

- Solve when convection dominated

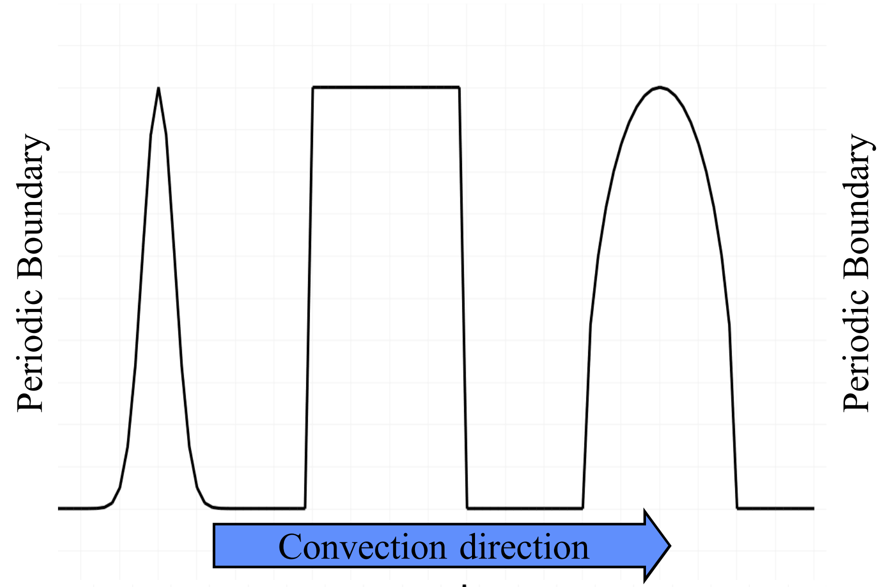
$$\nu < |\vec{w}| h$$

- Many physically relevant problems
  - Fluids, Drift-diffusion, Species transport
- Stability of solution is challenging
- Galerkin does poorly for shocks and steep gradients
- Considering stabilized FEM (SUPG) and Algebraic FCT

Shu-Osher Problem

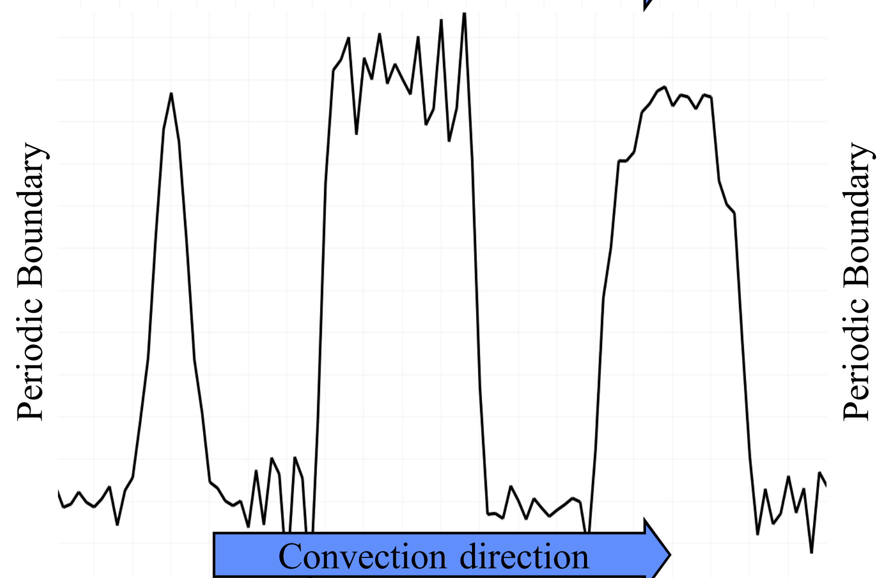
1D Transient Problem:

- smooth regions
- shock-like gradients
- sharp peak
- periodic solution



Galerkin solution (1 period):

- Crank-Nicolson
- clearly unstable
- dispersion disrupts hump



SUPG and DCO Stabilization

SUPG Stabilized Galerkin weak form

$$\int_\Omega \phi R(u)\,dx + \sum_e \int_e \tau(\vec{w}\cdot\nabla\phi)R(u)\,dx = 0 \quad \forall\phi$$

where R(u) is the PDE residual, and Φ is test function

- Diffusion is added in streamwise direction

Isotropic discontinuity capturing operator (DCO)

$$\int_\Omega \phi R(u)\,dx + \sum_e \int_e \tau(\vec{w}\cdot\nabla\phi)R(u)\,dx + \sum_e \int_e \nu\left(R(u)^2\right)\nabla\phi\cdot C\nabla u\,dx = 0 \quad \forall\phi$$

Algebraic Flux Corrected Transport (AFCT)

Goals:

- Work with discrete algebraic system
- Parameter-less stabilization

High level algorithm:

1. Build diffusive problem from Galerkin system
2. Solve diffusive problem for “safe” solution
3. From “safe” solution determine how much Galerkin anti-diffusion can be added back (construct limiters)
4. Solve diffusive problem modified with limited Galerkin anti-diffusion

AFCT: Building Diffusive Problem

Discrete convection-diffusion (Galerkin FE)

$$M_C \frac{du}{dt} - Ku = 0$$

Diffusive convection-diffusion (algebraically constructed)

$$M_L \frac{du}{dt} - \tilde{K}u = 0$$

Anti-diffusive flux (difference of equations above)

$$(M_L - M_C)\frac{du}{dt} - Du$$

AFCT: Building Diffusive Problem

Use lumped mass approximation for transient operator

$$[M_L]_{ij} = \delta_{ij} \sum_k m_{ik}$$

Build and add in discrete diffusion operator

$$\tilde{K} = K + D$$

where

$$D_{ij} = \max(-K_{ij}, 0, -K_{ji}) \text{ and } D_{ii} = -\sum_{i \neq j} D_{ij}$$

Now anti-diffusive flux can be written nodally (from node j into i)

$$f_{ij} = m_{ij} \left(\frac{du_i}{dt} - \frac{du_j}{dt} \right) + D_{ij} \left(u_i - u_j \right)$$

AFCT: Building Diffusive Problem

Jacobian of diffusive system is M-matrix

$$A = \frac{1}{\Delta t} M_L + \theta \tilde{K}$$

implying

$$A^{-1} \geq 0$$

- important for *positivity preservation*

$$Au^{n+1} = Bu^n$$

if $B>0$ and $u^n>0$ then $u^{n+1}>0$

- M-matrix good for multigrid smoothers

AFCT: Limiter Construction

FCT residual

$$R_{fct}(u) = M_C \frac{du}{dt} - \tilde{K}u + \sum_j \alpha_{ij} f_{ij}$$

where $0 \leq \alpha_{ij} \leq 1$ are flux limiters

- Flux is difference between high-order and low-order solution

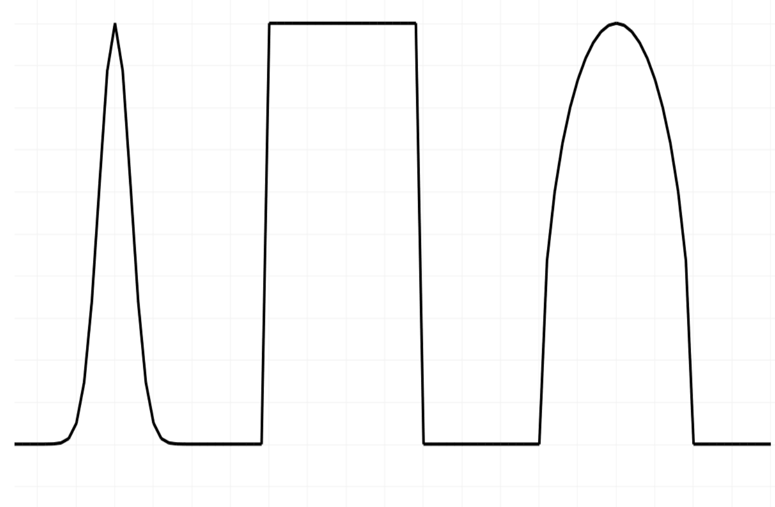
$$f_{ij} = m_{ij} \left(\frac{du_i}{dt} - \frac{du_j}{dt} \right) + D_{ij} \left(u_i - u_j \right)$$

Shu-Osher Problem

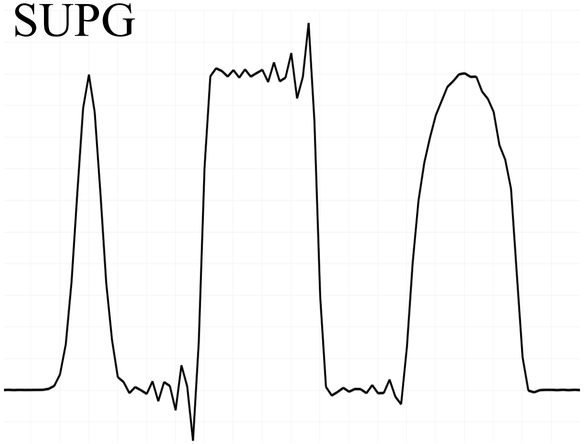
Shu-Oscher Test problem

- 200x2 elements (pseudo 1D)
- Δt=1e-4 implies CFL=0.02
- from "C.W. Shu, S. Osher, Efficient implementation of essentially non-oscillatory shock-capturing schemes, II, J. Comput. Phys (1989) 32-78."

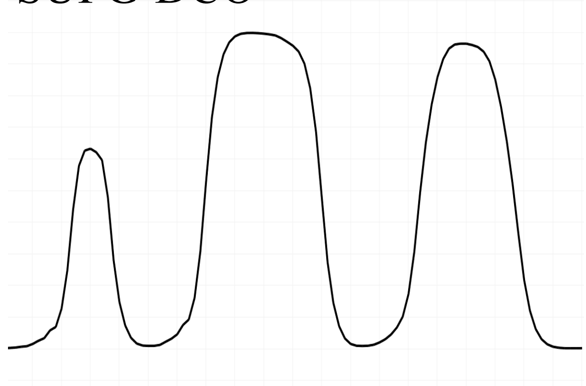
Initial Condition



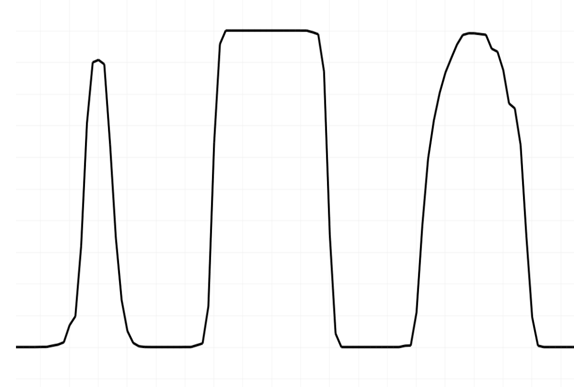
SUPG



SUPG-DCO



FCT



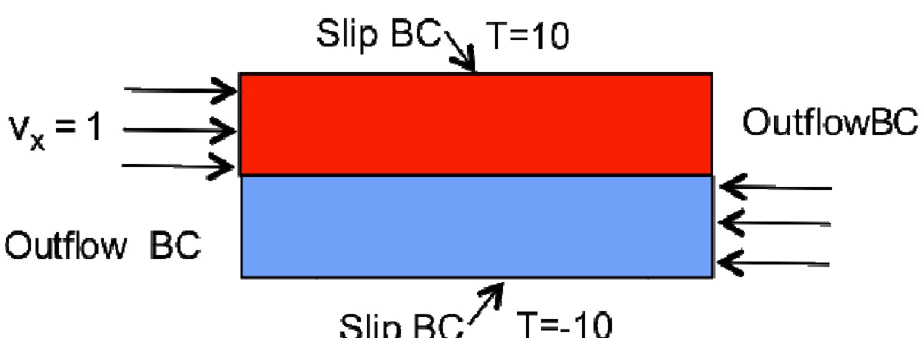
Semi-Implicit Shear Layer Simulation

Semi-Implicit Navier-Stokes

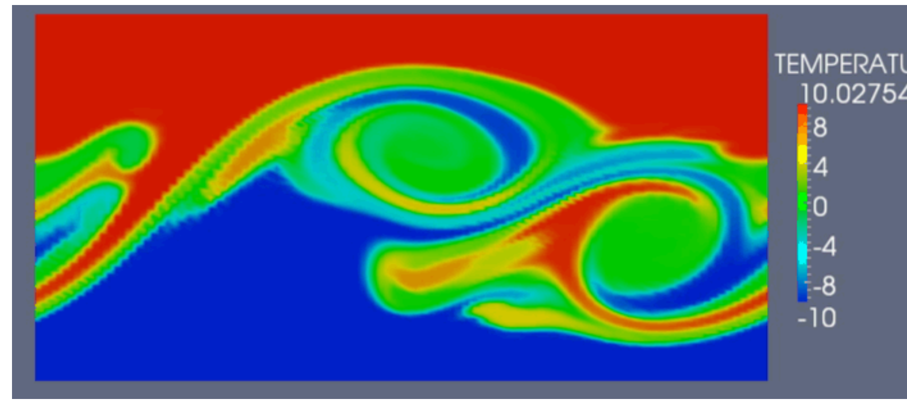
- Pure advection of temperature field
- FCT applied only to temperature
- CFLs around 0.6 and 3
- Run for ~10 simulation seconds

Notice temperature range

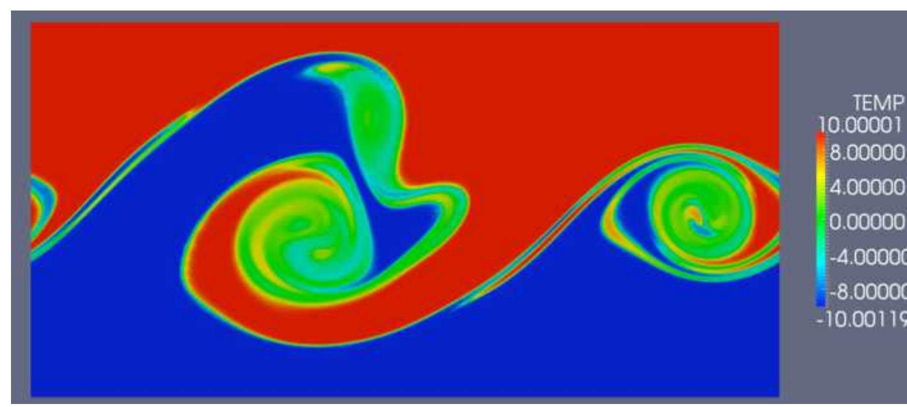
- FCT not LED for CFL>0.5



Coarse Mesh: 100x100



Fine Mesh: 512x512

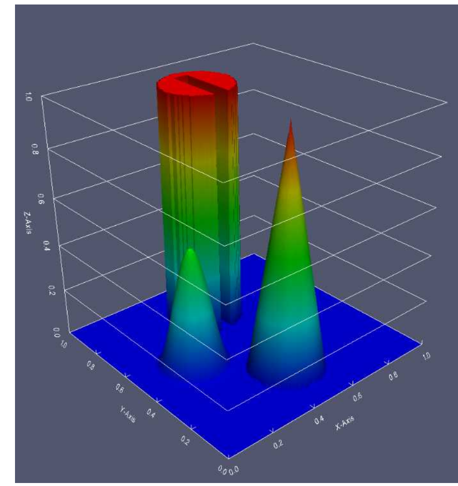


Solid Body Rotation

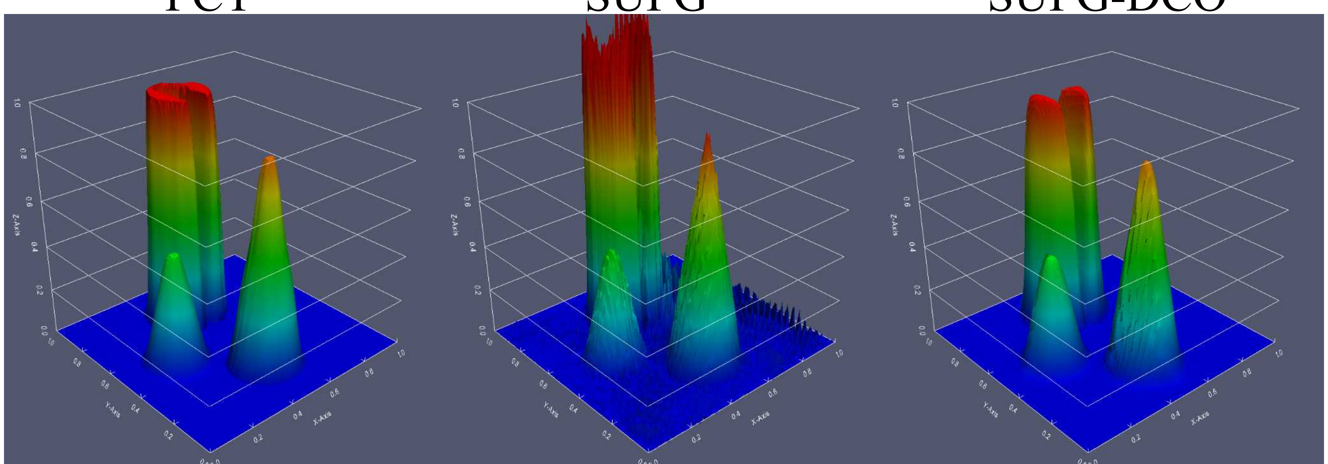
- Solid body rotation benchmark
  - 628 steps theta method $\Delta t=0.001$, $\theta=0.5$
- Weak scaling study

Mesh	Cores
128x128	8
256x256	32
512x512	128
1024x1024	512

Initial Cond.



FCT SUPG SUPG-DCO



Solid Body Rotation

AFCT (Gauss-Seidel Smoother)

Processors	Iters/GMRES	GMRES/Newton	Total Time
8	1.000	2.049	489.4
32	1.000	2.068	611.0
128	1.000	2.049	742.0
512	1.965	2.005	982.9

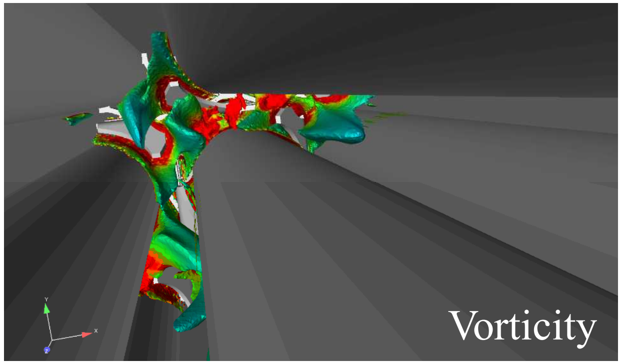
SUPG-DCO (ILU Smoother)

Processors	Iters/GMRES	GMRES/Newton	Total Time
8	6.470	3.089	302.6
32	12.188	3.293	436.2
128	23.974	4.414	909.1
512	54.090	6.830	4167.0

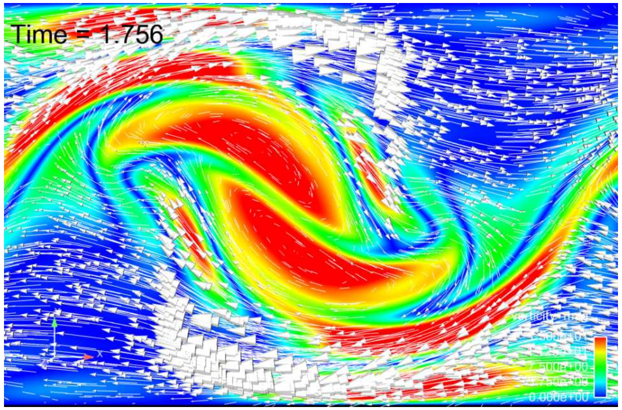
Conclusions

- Presented several stabilization methods for scalar advection
  - SUPG, SUPG-DCO, Algebraic FCT
- Algebraic FCT is Local Extremum Diminishing (implies positivity presevering)
- Presented results comparing performance of Algebraic FCT to residual based stabilization (eyeball-norm!)
- Compared algebraic multigrid performance on
  - Algebraic FCT: with Gauss-Seidel smoothers
  - SUPG-DCO: with ILU smoothers
- Preliminary demonstration of Algebraic FCT scalability using multigrid

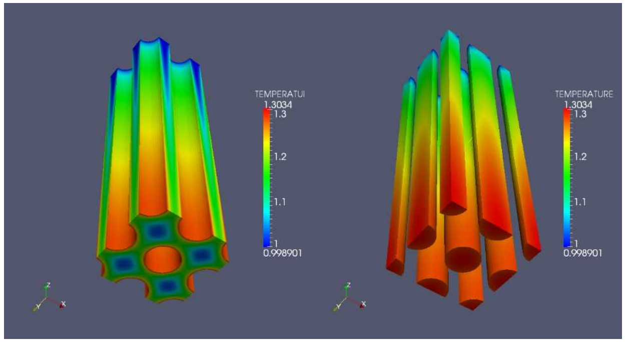
Drekar (JN Shadid, RP Pawlowski, EC Cyr, TM Smith, T Wildey)



LES: Flow over spacer grid



MHD: Hydromagnetic Kelvin-Hemlholtz



Conjugate Heat Transfer

Scalable parallel implicit FE code

- Includes: Navier-Stokes, MHD, LES, RANS
- Architecture admits new coupled physics
- Support of advanced discretizations
  - ➢ mixed, compatible and high-order basis functions
  - ➢ multi-physics capable (conjugate heat transfer)
- Advanced UQ techniques
  - ➢ Embedded stochastic Galerkin
  - ➢ Adjoint based sensitivities and error-estimates
- Advanced solution methods
  - ➢ Parallel solvers from SNL's Trilinos framework
  - ➢ Physics-based preconditioning
  - ➢ Fully-coupled multigrid for monolithic systems