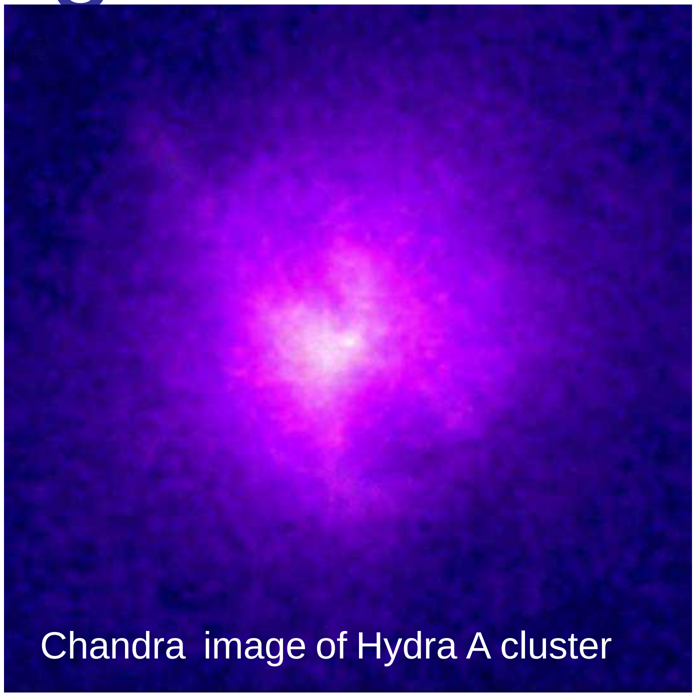
Anisotropic conduction with large temperature gradients



Prateek Sharma (Princeton)

(thanks to G. Hammett)

Motivation and Outline

- Anisotropic transport for hot, dilute plasmas ($\Omega_c \gg \nu \propto nT^{-3/2}$).
- Thermal conduction along B
- Finite differencing anisotropic conduction
- Symmetric, Asymmetric methods
- Negative temperature: simple tests
- Basic review of slope limiters in CFD.
- Limiting temperature gradient: slope, entropy limiters
- Tests
- Applications

Anisotropic thermal conduction

$$\frac{\partial e}{\partial t} = -\vec{\nabla} \cdot \vec{q}$$
$$\vec{q} = -\vec{b}n(\chi_{||} - \chi_{\perp})\nabla_{||}T - n\chi_{\perp}\vec{\nabla}T$$
$$\nabla_{||} = \vec{b} \cdot \vec{\nabla}$$

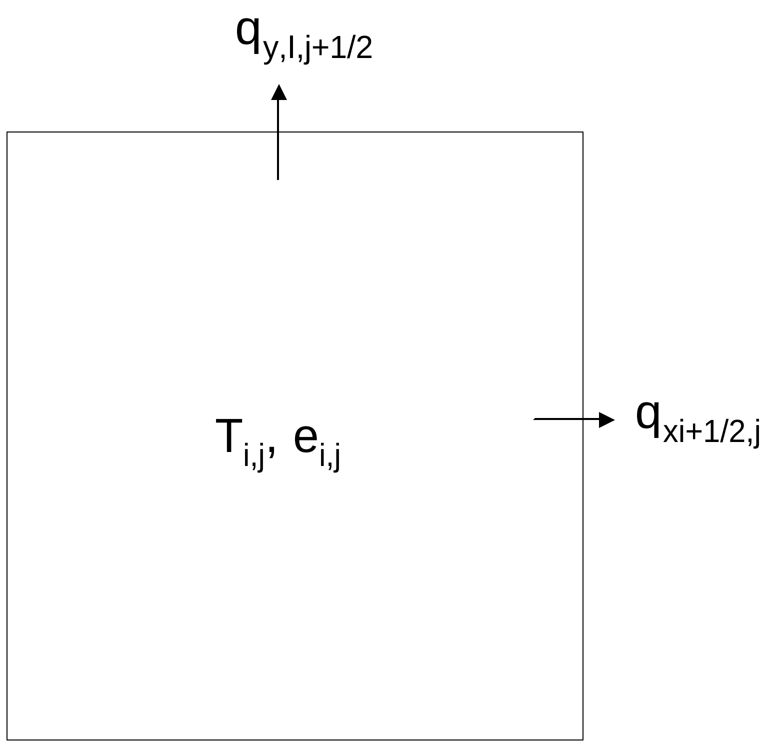
T = e/n($\gamma-1$), $\gamma=5/3$ for ideal gas in 3-D

e : internal energy density
q : anisotropic heat flux
T : temperature
t : time
$\chi_\perp$, $\chi_|$: conduction coefficients

Finite difference equation in conservative form in 2-D:

$$e_{i,j}^{n+1} = e_{i,j}^{n} - \Delta t \left[\frac{q_{x,i+1/2,j}^{n} - q_{x,i-1/2,j}^{n}}{\Delta x} + \frac{q_{y,i,j+1/2}^{n} - q_{y,i,j-1/2}^{n}}{\Delta y} \right]$$

Grid



Staggered grid with scalars at zone centers, vectors at zone faces.

Natural location for conservative form

Asymmetric differencing

- Most natural differencing

$$q_{x,i+1/2,j} = -\overline{n\chi} b_x \left[b_x \frac{\partial T}{\partial x} + \overline{b_y \frac{\partial T}{\partial y}} \right]$$

$$\overline{n} = \min \left[n_{i,j}, n_{i+1,j} \right]$$

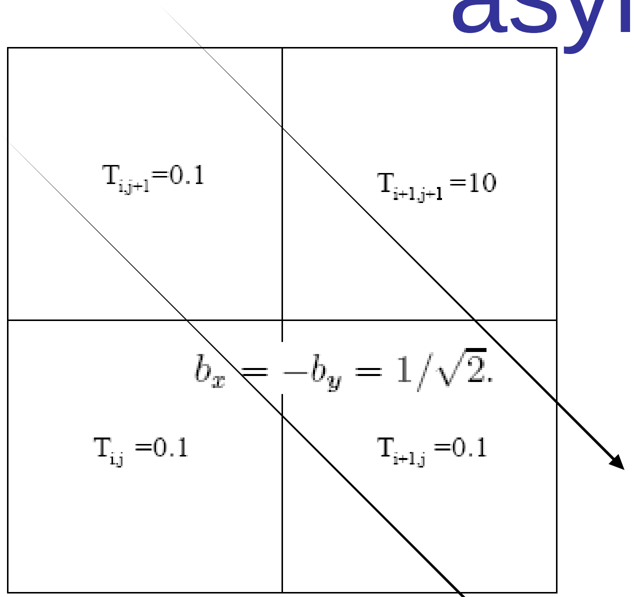
$$\overline{\chi} = \frac{\chi_{i,j} + \chi_{i+1,j}}{2}$$

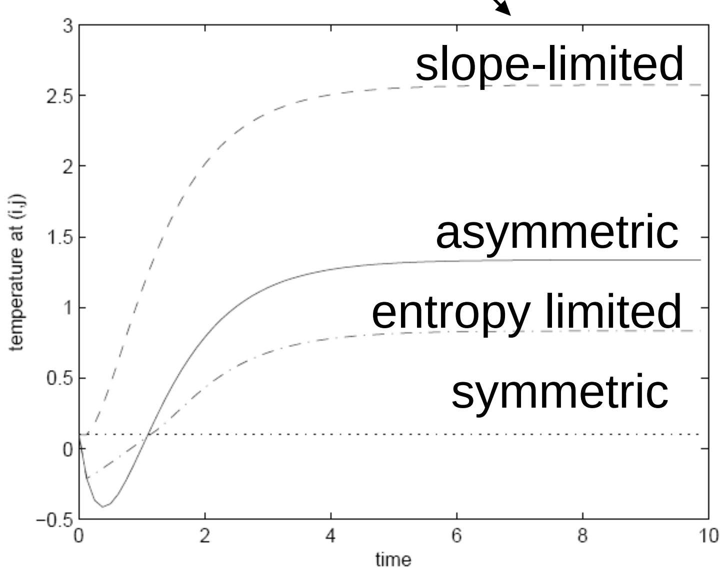
$$\overline{\frac{\partial T}{\partial y}} = \frac{T_{i,j+1} + T_{i+1,j+1} - T_{i,j-1} - T_{i+1,j-1}}{4\Delta y}$$

$$\overline{b_y} = \frac{b_{y,i,j-1/2} + b_{y,i+1,j-1/2} + b_{y,i,j+1/2} + b_{y,i+1,j+1/2}}{4}$$

Min used so that Courant stability condition is not severe.

Negative temperature with asymmetric method





Reflecting BC for temperature

$$q_{x,i-1/2,j} = 0$$
$$q_{y,i,j-1/2} = 0$$
$$q_{x,i+1/2,j} = -n\chi b_x \left[b_x \frac{\partial T}{\partial x} + b_y \overline{\frac{\partial T}{\partial y}} \right]$$
$$\overline{\frac{\partial T}{\partial y}} = \frac{10 + 0.1 - 0.1 - 0.1}{4\Delta y} = \frac{9.9}{4\Delta y}$$
$$q_{x,i+1/2,j} = q_{y,i,j+1/2} = -n\chi b_x b_y \frac{9.9}{4\Delta y} > 0$$

Symmetric method

$$q_{x,i+1/2,j+1/2} = -\overline{n}\overline{\chi}\overline{b_x}\left[\overline{b_x}\overline{\frac{\partial T}{\partial x}} + \overline{b_y}\overline{\frac{\partial T}{\partial y}}\right]$$

$$\overline{n} = \min\left[n_{i,j}, n_{i+1,j}, n_{i,j+1}, n_{i+1,j+1}\right]$$

$$\overline{\chi} = \frac{\chi_{i,j} + \chi_{i+1,j} + \chi_{i,j+1} + \chi_{i+1,j+1}}{4}$$

$$\overline{b_x} = \frac{b_{x,i+1/2,j} + b_{x,i+1/2,j+1}}{2}$$

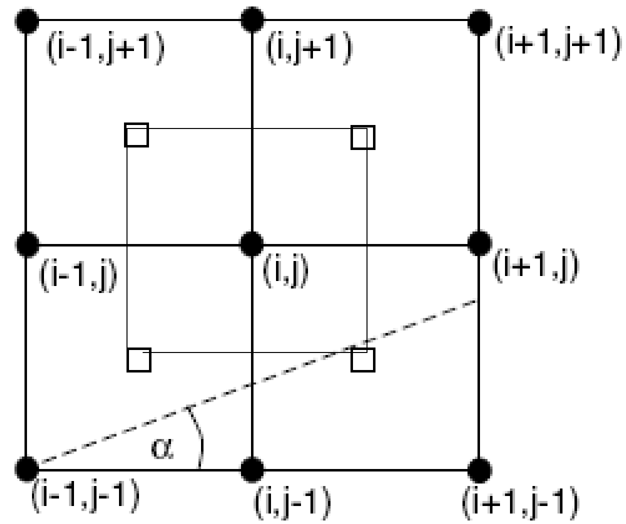
$$\overline{b_y} = \frac{b_{y,i,j+1/2} + b_{x,i+1,j+1/2}}{2}$$

$$\overline{\frac{\partial T}{\partial x}} = \frac{T_{i+1,j} + T_{i+1,j+1} - T_{i,j} - T_{i,j+1}}{2}$$

$$\overline{\frac{\partial T}{\partial y}} = \frac{T_{i,j+1} + T_{i+1,j+1} - T_{i,j} - T_{i+1,j}}{2}$$

$$q_{x,i+1/2,j} = \frac{q_{x,i+1/2,j+1/2} + q_{x,i+1/2,j-1/2}}{2}$$

$$q_{y,i,j+1/2} = \frac{q_{x,i+1/2,j+1/2} + q_{y,i-1/2,j+1/2}}{2}$$



Primary heat fluxes at cell corners
[Gunter et al., JCP, 2005]

Why Symmetric method?

- Numerical cross-field diffusion does not scale with $\chi_{|}$ /$\chi_{\perp}$,Sovinec’s test
- Self-adjointness of $\vec{\nabla} \cdot \chi_{||}(\vec{b} \cdot \vec{\nabla} T)\vec{b}$, matrix is symmetric, good for Krylov methods
- Entropy condition satisfied at the cell corners, -q.Ñ T³ 0
- good when temperature gradients are not enormous
- Less sensitive to angle between b and coordinate axes

Problems with symmetric method

- Small scale overshoots are not damped.
- Unable to diffuse away a chess-board pattern.

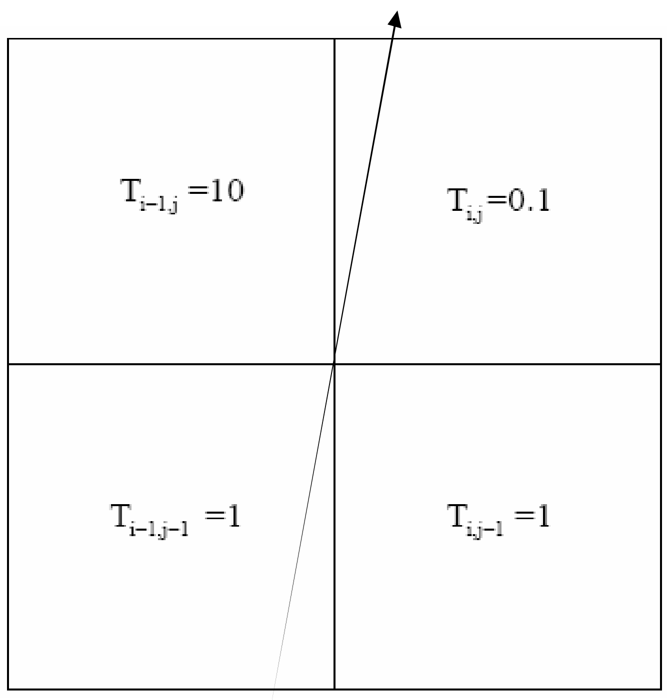
+	-	+	-
-	+	-	+
+	-	+	-
-	+	-	+

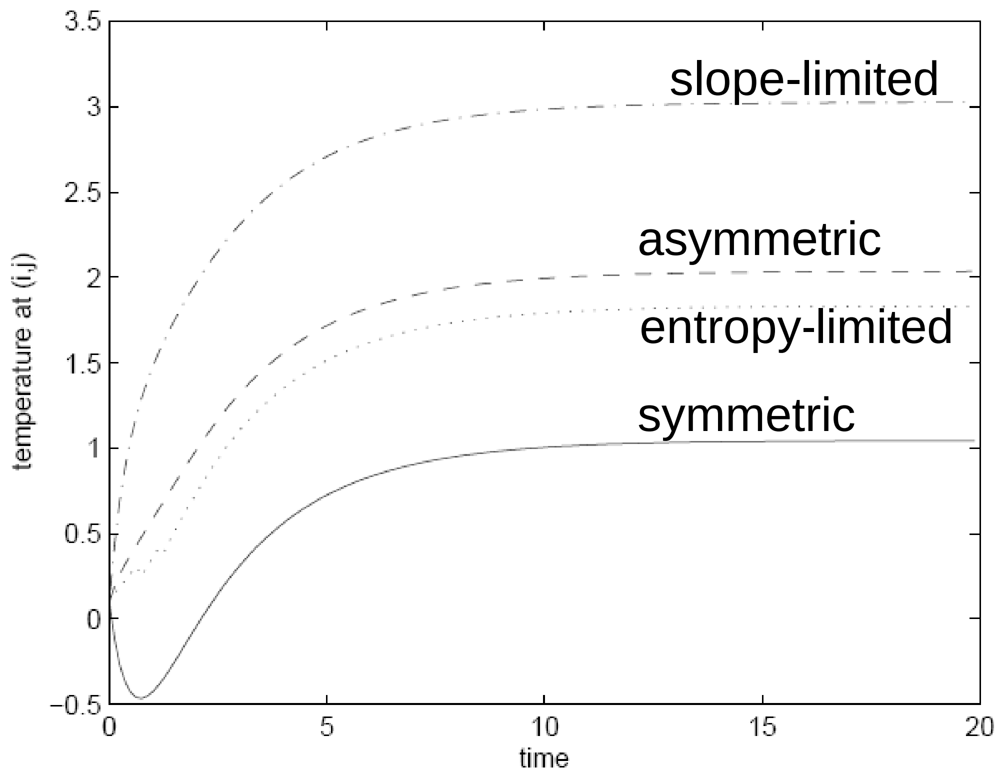
$$\overline{\frac{\partial T}{\partial x}} = 0$$

$$\overline{\frac{\partial T}{\partial y}} = 0$$

, $q=0$

Negative temperature with symmetric method





$$b_x = 1/\sqrt{5}, b_y = 2/\sqrt{5}$$

Heat flows out of (i,j) despite it being a minimum.
Reflective BC.
q_x, q_y at (i-1/2,j-1/2) <0

Why negative temperature?

$$q_x = q_{xx} + q_{xy}$$

$$q_{xx} = -\overline{n}\chi b_x^2 \frac{\partial T}{\partial x}$$

$$q_{xy} = -\overline{n}\chi b_x \overline{b_y}\,\overline{\frac{\partial T}{\partial y}}$$

q_{xx} satisfies the entropy condition, with heat flowing from higher to lower temp., but q_{xy} can have any sign.

Need to limit transverse term q_{xy}
Responsible for heat flowing in wrong direction

What is the best interpolation?

Arithmetic average for dT/dy?

Limiters for averaging?

Basic Eulerian/Continuum Advection Algorithms

$$\frac{\partial f}{\partial t} + \frac{\partial (\mathrm{v} f)}{\partial z} = 0$$

thanks to Greg Hammett for introductory slides on limiters.

Discrete grid, $f(z_j) = f_j$ Conservative differencing:

$$\frac{\partial f_j}{\partial t} = -\frac{\mathrm{v}_{j+1/2} f_{j+1/2} - \mathrm{v}_{j-1/2} f_{j-1/2}}{\Delta z}$$

Std 2nd order centered differencing (okay for smooth regions, phase errors too large for sharp-gradient regions, gives unphysical oscillations):

$$f_{j+1/2} = \frac{1}{2}\left(f_j + f_{j+1}\right)$$

1st order upwind (eliminates unphysical oscillations, but too dissipative):

$$f_{j+1/2} = f_j$$

Higher-order upwind Methods with clever monotonicity-preserving slope limiters

Reconstruct f(z) in each cell, extrapolate to bdys: $f(z) = f_j + s_j (z - z_j)$

Piecewise constant = 1st order upwind : $s_j = 0$

Simplest, minmod limiter: minmod(a,b) = sign(a,b). min(|a|,|b|)

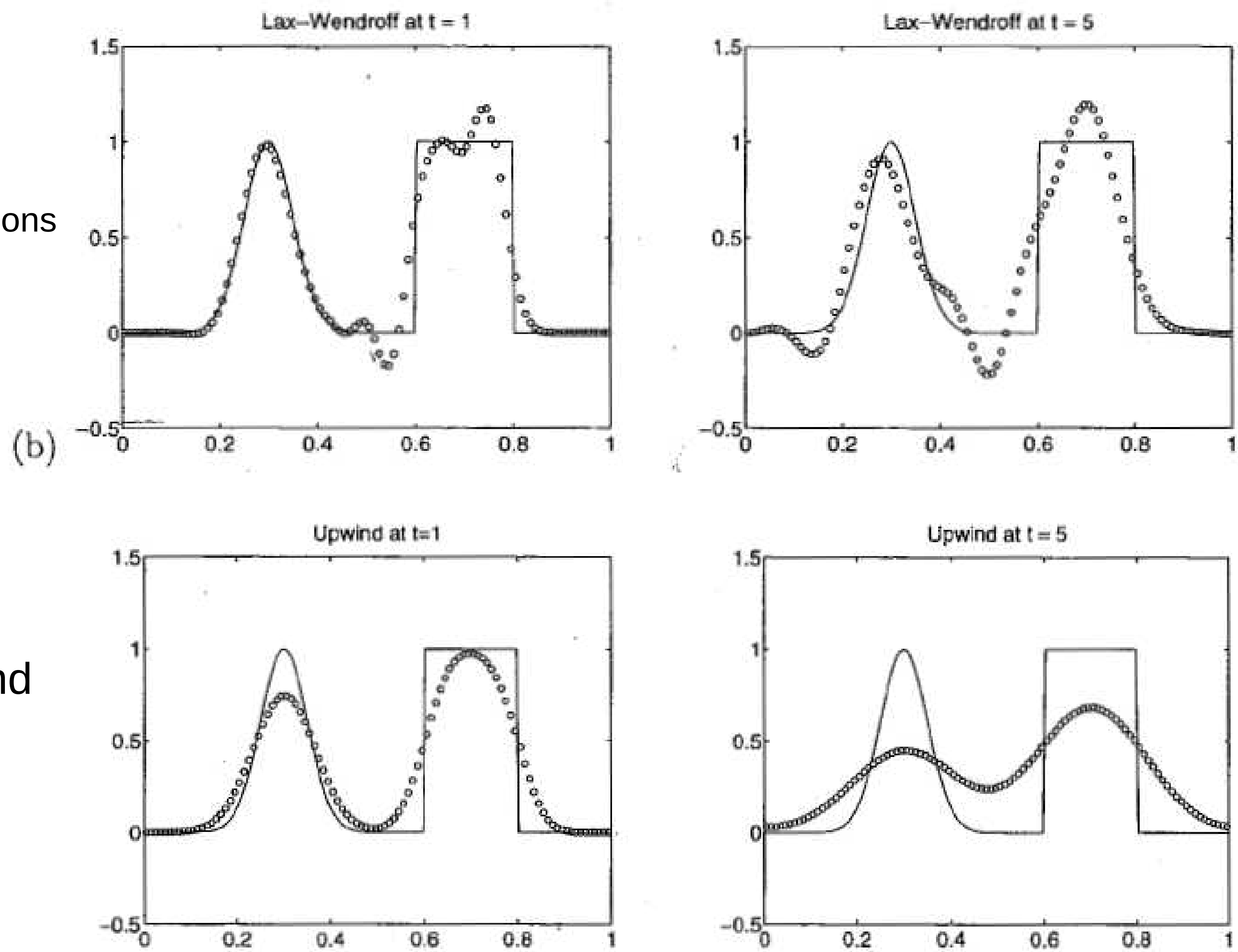
van Leer's (MC) limiter:
"Monotonized Central"

$$s_j = \mathrm{minmod}\left(\frac{f_{j+1} - f_{j-1}}{2\Delta z}, 2\frac{f_{j+1} - f_j}{2\Delta z}, 2\frac{f_j - f_{j-1}}{2\Delta z} \right)$$

Higher order extensions, e.g., 2nd order PPM of Colella & Woodward

Advection tests

2cd order Centered
Algorithm
okay in smooth regions
Phase errors large
for sharp gradients



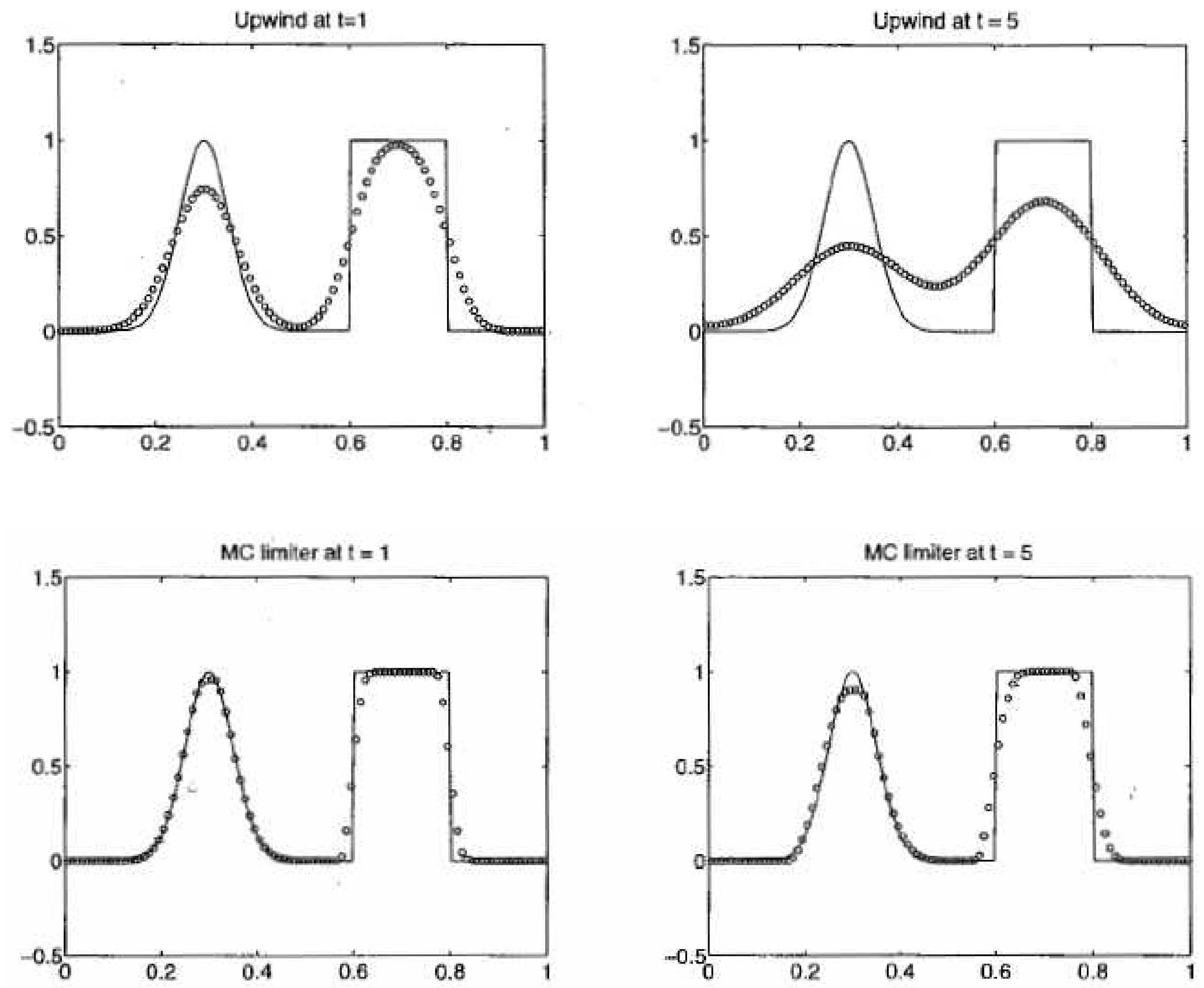
1st Order upwind
Too dissipative

From R.J. Leveque, Finite Volume Methods for Hyperbolic Problems, Cambridge Univ. Press (2002).

Advection tests: Higher order upwind w/ limiters

1st Order upwind
Too dissipative

2cd order upwind
With MC limiter
Much better



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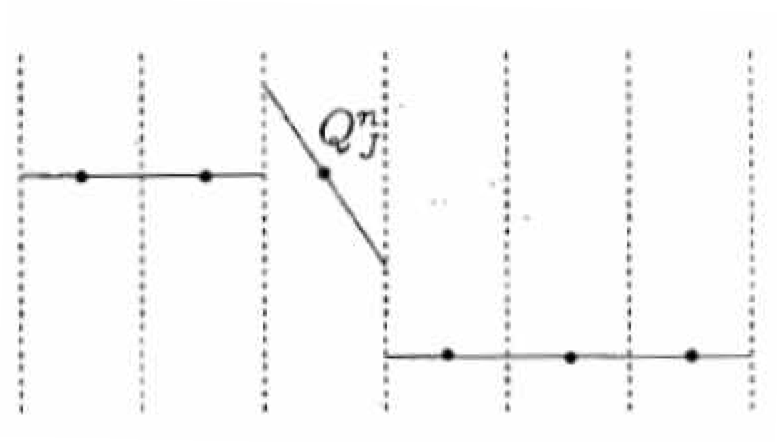


Lax-Wendroff equivalent to downwind Slope. Can lead to overshoots in reconstruction

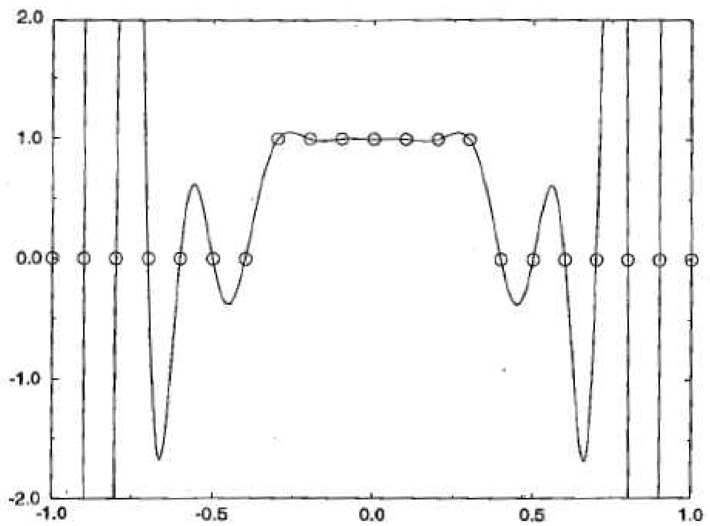
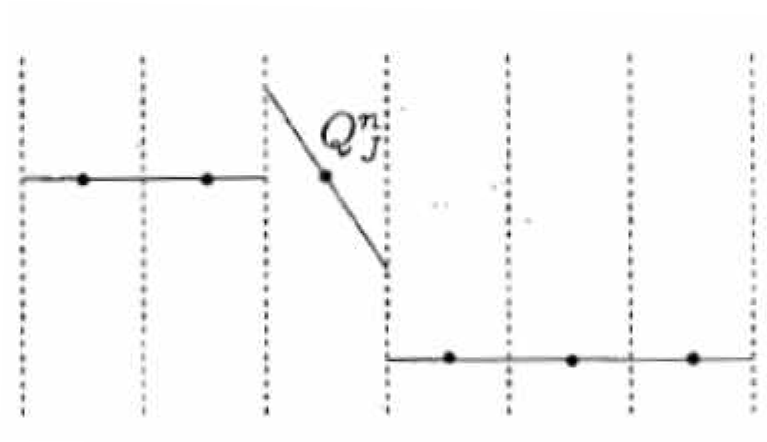


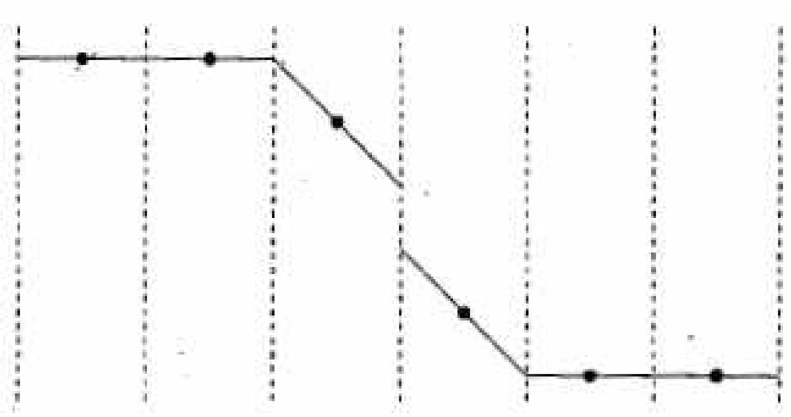
Figure 8.5 Twentieth-order polynomial interpolation for a square wave.

Just going to higher order doesn't help near sharp gradient regions (Gibb's phenomena)

Top Fig. From R.J. Leveque, Finite Volume Methods for Hyperbolic Problems, Cambridge Univ. Press (2002).
2cd Fig. From C.B. Laney, Computational Gasdynamics, Cambridge Univ. Press (1998).



Central differencing to determine slopes can lead to overshoots in reconstruction, Slope limiter uses s=0 at extrema to avoid oscillations



MC limiter gives much more robust and accurate result.

From R.J. Leveque, Finite Volume Methods for Hyperbolic Problems, Cambridge Univ. Press (2002).

Limiting transverse gradient

$$\overline{\frac{\partial T}{\partial y}}\bigg|_{i+1/2,j} = L\left\{ L\left[\frac{\partial T}{\partial y}\bigg|_{i,j-1/2}, \frac{\partial T}{\partial y}\bigg|_{i,j+1/2} \right], \; L\left[\frac{\partial T}{\partial y}\bigg|_{i+1,j-1/2}, \frac{\partial T}{\partial y}\bigg|_{i+1,j+1/2} \right] \right\}$$

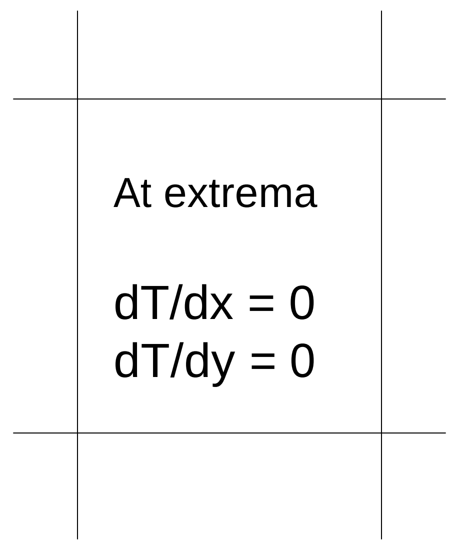
We limit transverse temperature gradient to calculate q_x

L is a limiter like: minmod, van Leer, monotonized central (MC)

Limiters return a zero if arguments are of opposite sign

Temperature extrema are not amplified

Only normal term remain nonzero at extrema



Limiting symmetric method

$$q_{xx,i+1/2,j+1/2} = -\overline{n\chi}\overline{b_x^2} L2\left[\left.\frac{\partial T}{\partial x}\right|_{i+1/2,j}, \left.\frac{\partial T}{\partial x}\right|_{i+1/2,j+1}\right]$$

$$q_{xx,i+1/2,j-1/2} = -\overline{n\chi}\overline{b_x^2} L2\left[\left.\frac{\partial T}{\partial x}\right|_{i+1/2,j}, \left.\frac{\partial T}{\partial x}\right|_{i+1/2,j-1}\right]$$

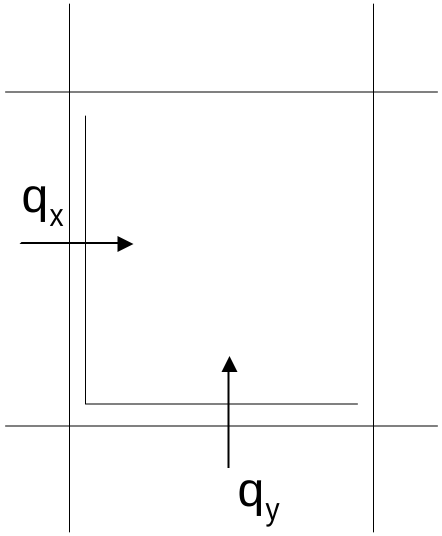
$$q_{xx,i+1/2,j} = (q_{xx,i+1/2,j+1/2} + q_{xx,i+1/2,j-1/2})/2$$

$$\begin{aligned} L2(a,b) = &(a+b)/2,\ \text{if } \alpha a \lessgtr (a+b)/2 \gtrless a/\alpha,\ \text{otherwise},\\ &\alpha a,\ \text{if } \mathrm{sgn(a)} \neq \mathrm{sgn(b)},\\ &a/\alpha,\ \text{if } \mathrm{sgn(a)} = \mathrm{sgn(b)}. \end{aligned}$$

$\alpha=0.75$, L2 not symmetric in its arguments
Need to limit both normal and transverse gradients.
Normal derivative limited so that q_{xx} is always from higher to lower temp.
Chess-board pattern will not diffuse if normal derivative not limited!

Entropy limiting

- Using face pairs to satisfy entropy condition $\dot{s} = -\vec{q} \cdot \nabla T \geq 0$



$$\dot{s} = -q_x \frac{\partial T}{\partial x} - q_y \frac{\partial T}{\partial y} \geq 0$$

If dT/dx=0, then an arbit. q_x can give neg. temp.

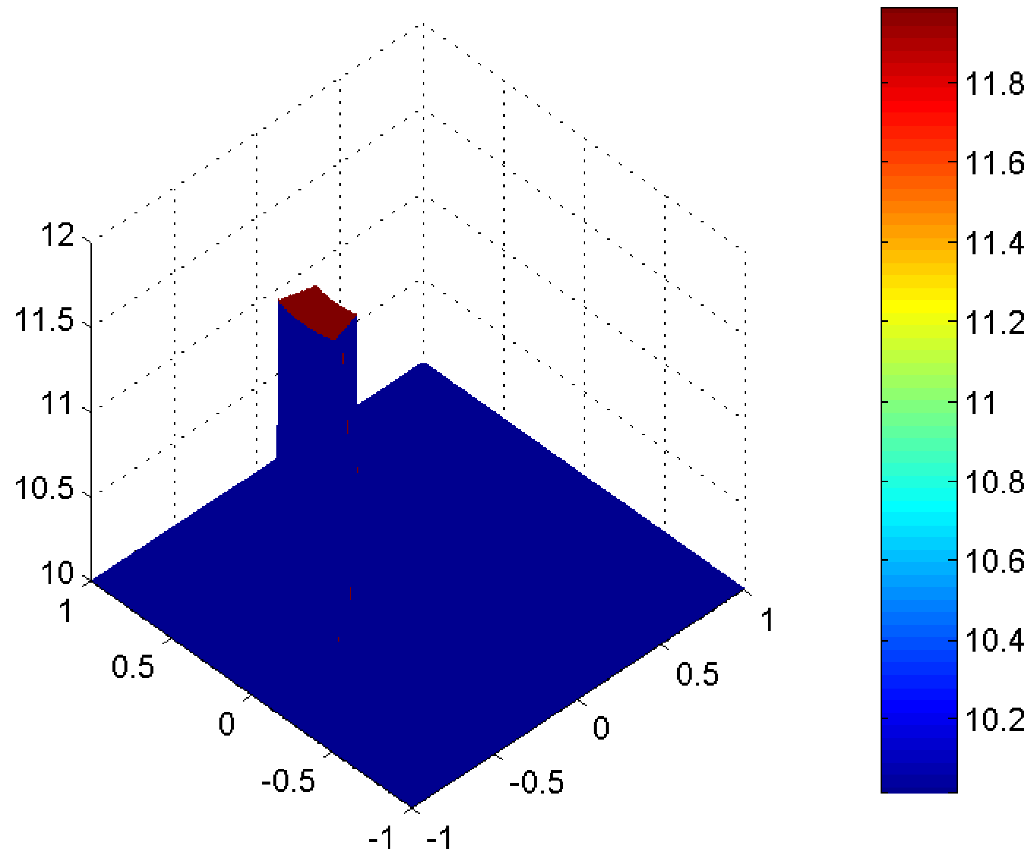
Not strictly monotonic, but overshoots highly damped

Entropy condition satisfied at some point is not a sufficient condition for heat flowing in the right dirn.

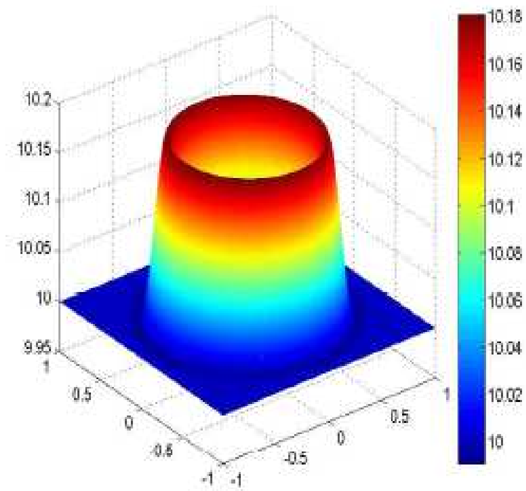
Ring diffusion test

- Initial hot patch $0.5<r<0.7$, $11\pi/12<\theta<13\pi/12$
- Coefft. $\chi_{|}=0.01$,
- $\chi_{\perp}=0$, $t_{end}=200$

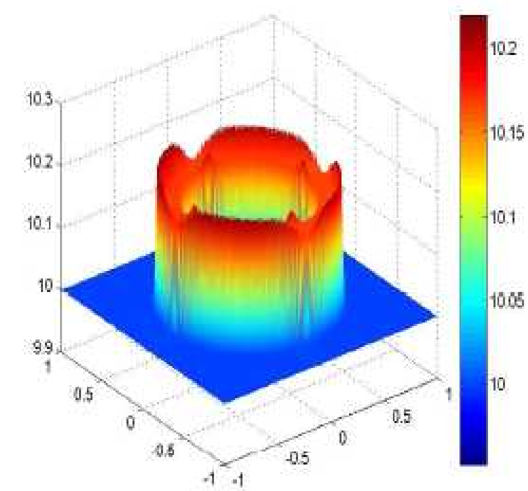
- Reflective BC
- Circular magnetic field lines



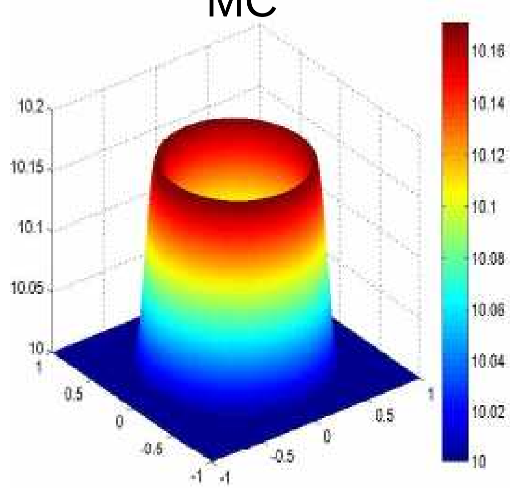
Small temperature gradient

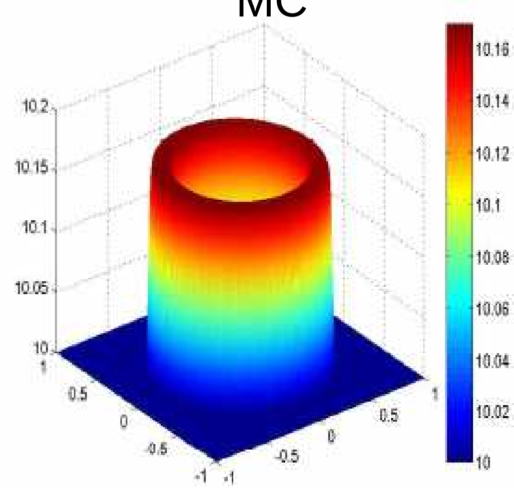


Asymmetric MC



Symmetric MC





400 X 400 box

Asymmetric and symmetric methods non-monotonic even late times

Slope limited methods monotonic

Sharp boundaries even with limiting

For lower resln. slope lim. methods are more diffusive.

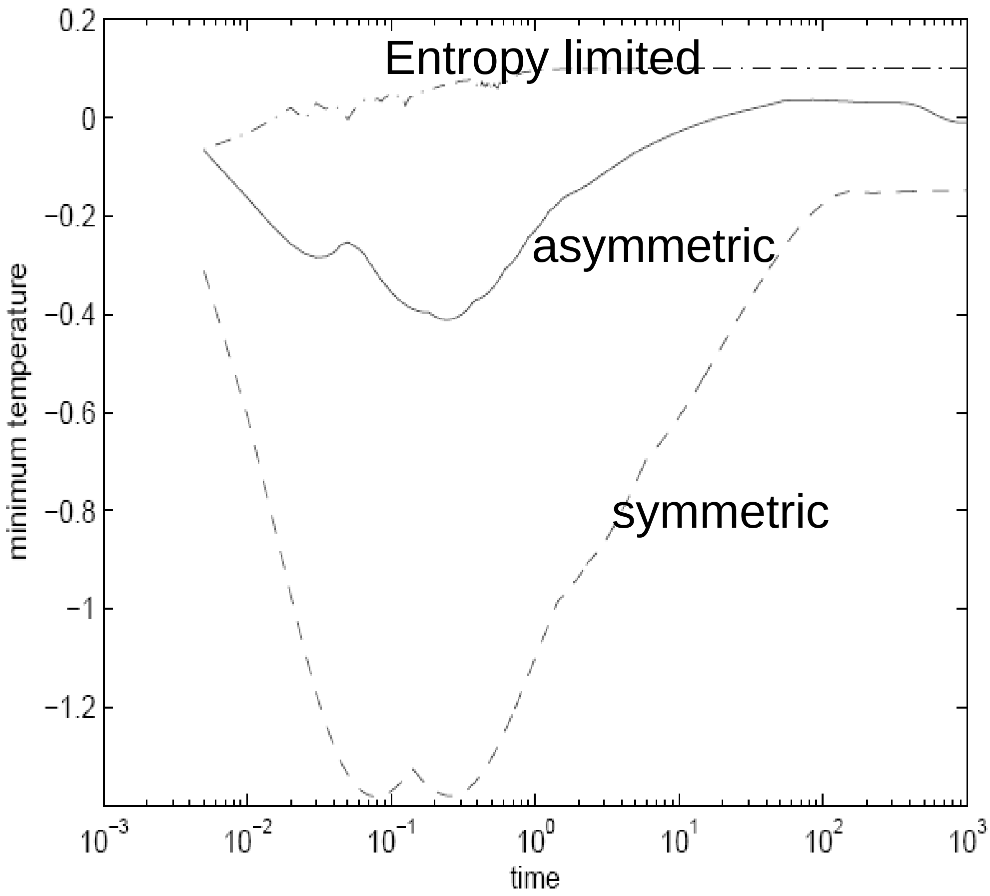
Ring diffusion with large temp. gradient

Initially T_{max}=10, T_{min}=0.1

Both symmetric and asymmetric methods give negative temp. at late times

Slope limited methods are strictly monotonic with T_{min}=0.1 at all times

Entropy limiting damps the undershoots.

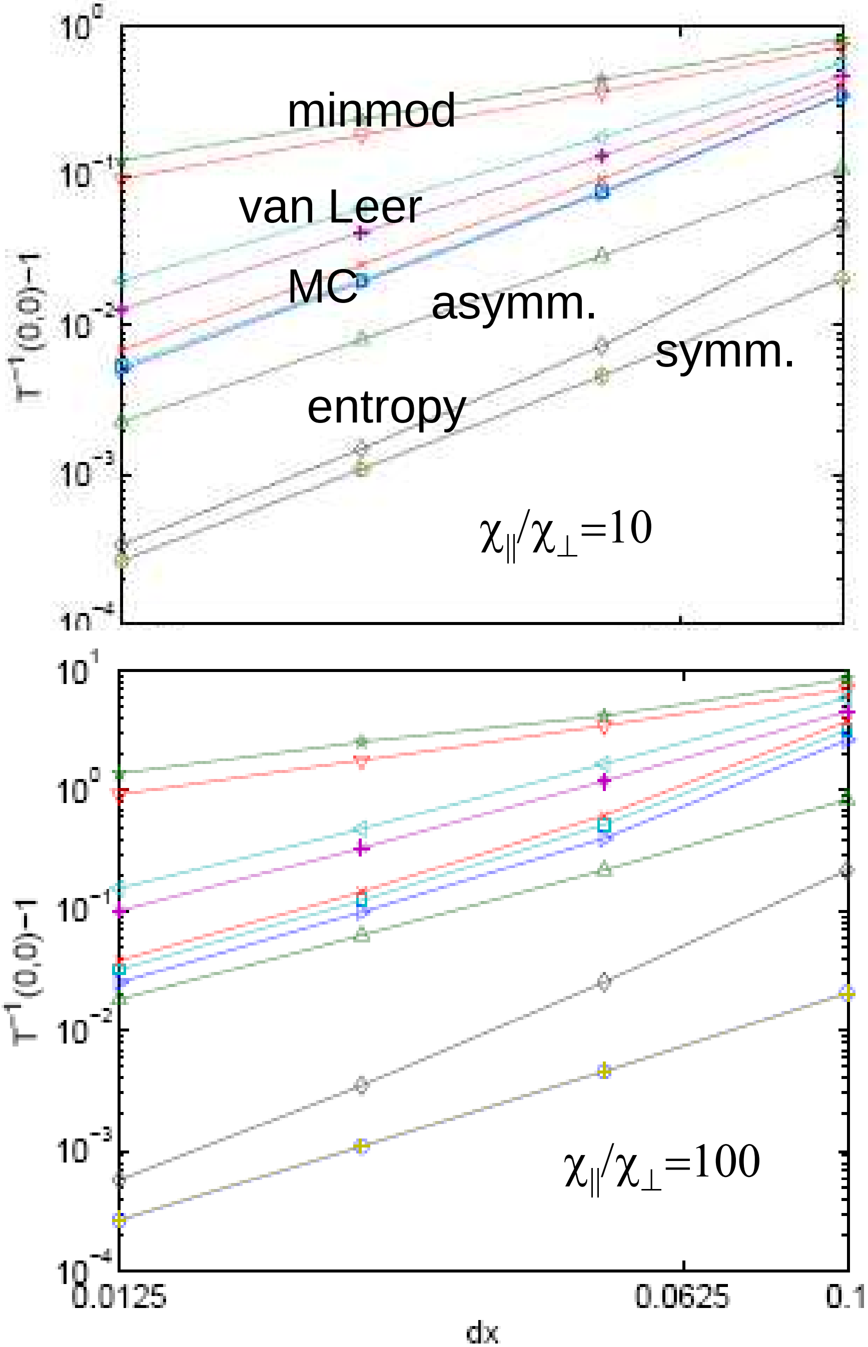


Perpendicular numerical diffusion

- Test problem by *Sovinec et al. 2005*
- Solve anisotropic diffusion with source term to get steady state, circular field lines
- L_x=L_y=1, in SS heat diffusion balances Q
- Q = $2\pi^2 \cos(\pi x) \sin(\pi x)$
- An explicit $\chi_\perp$, $T_{anal}(0,0)=1/\chi_\perp$

□ $\chi_{\perp num}$ = 1/T(0,0)-1, correct defn. is

□ $\chi_{\perp num}$ = 1/T(0,0)-1/T_{iso}(0,0)



Symmetric method is least diffusive (also entropy limited)
$\chi_{\perp num}$ independent of $\chi_{\parallel}/\chi_{\perp}$

Asymmetric method & MC limiter close, $\chi_{\perp num}$ scales with $\chi_{\parallel}/\chi_{\perp}$

Second order convergence for all except minmod

Correct defn. for $\chi_{\perp num}$ implies even tinier diffusion

$\chi_{\parallel}/\chi_{\perp num}$ = few 10^3 for N=100

Applications

- Problems with large temperature gradients where negative temperature cause numerical problems (spurious instabilities)
- Astrophysical systems e.g., Disk-corona interface, warm-hot phase interface in ISM
- Systems where a huge $\chi_{||}/\chi_{\perp}$ is not reqd., or where $\chi_{\perp}$ need not be resolved.

Future Directions

- Methods that are both monotonic and less diffusive, higher order reconstructions
- Faster implicit methods for anisotropic conduction
- Applications to problems with large temperature gradients and anisotropic thermal conduction, e.g., global models of RIAFs

Conclusions

- -Non-monotonic behavior of centered differencing in presence of large temp. gradients
- -simple test problems for negative temp.
- -slope limited methods are monotonic, second order convergence
- -test problem to measure $\chi_{\perp num}$
- - Astrophysical applications, ISM, disk-corona interface

Thank you for your attention!