Numerical Implementation of Anisotropic Diffusion

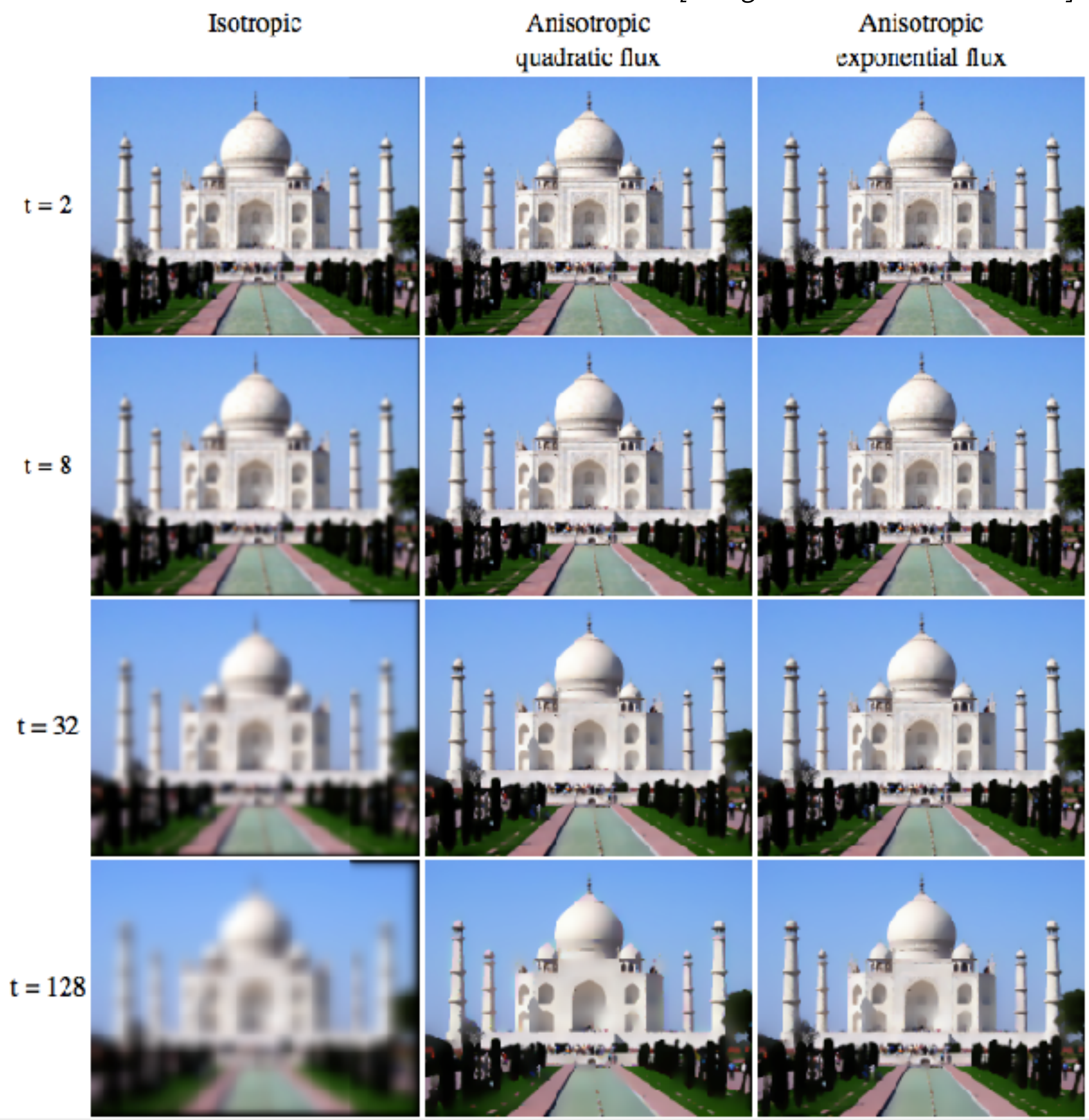
Prateek Sharma, IISc

Outline

- anisotropic diffusion eq. quite common: image processing, transport in magnetized plasmas, etc.
- finite difference scheme
- monotonicity & extremum principle
- limiters (minmod, van Leer)
- stability timestep & semi-implicit approach
- super-time-stepping

Diffusion in image processing

[Image Credit: Manasi Datar]



aims:

-maintain sharp edges

-no spurious edges at low resolution

-maximum detail with minimum storage

Diffusion in image processing

$$\frac{\partial}{\partial t} I(x,y,t) = c\nabla^2 I(x,y,t)$$

isotropic constant diffusion for intensity

$$I_{\vec{k}}(t) = I_{\vec{k}}(0)\exp(-ck^2 t)$$

Fourier space: larger k modes damped more
a low pass filter

$$G_\sigma \star I^0(\vec{x}) = \int G_\sigma(\vec{x}-\vec{x}')I^0(\vec{x}')d\vec{x}'$$

image convolved with a kernel

$$\widehat{G_\sigma \star I}^0(\vec{k}) = \widehat{G_\sigma}(\vec{k})\hat{I}^0(\vec{k})$$

convolution theorem

$$G_\sigma(\vec{x}) = \frac{1}{(2ct)^{d/2}}\exp\left(-\frac{\vec{x}\cdot\vec{x}}{4ct}\right)$$

isotropic diffusion equivalent to
isotropic Gaussian smoothing Kernel
in real space

AD in image processing

$$\frac{\partial}{\partial t} I(x,y,t) = \vec{\nabla} \cdot (c(x,y,t)\vec{\nabla} I)$$

more general diffusion equation
Perona-Malik 1990

$$c\left(\|\nabla I\|\right) = e^{-(\|\nabla I\|/K)^2}$$

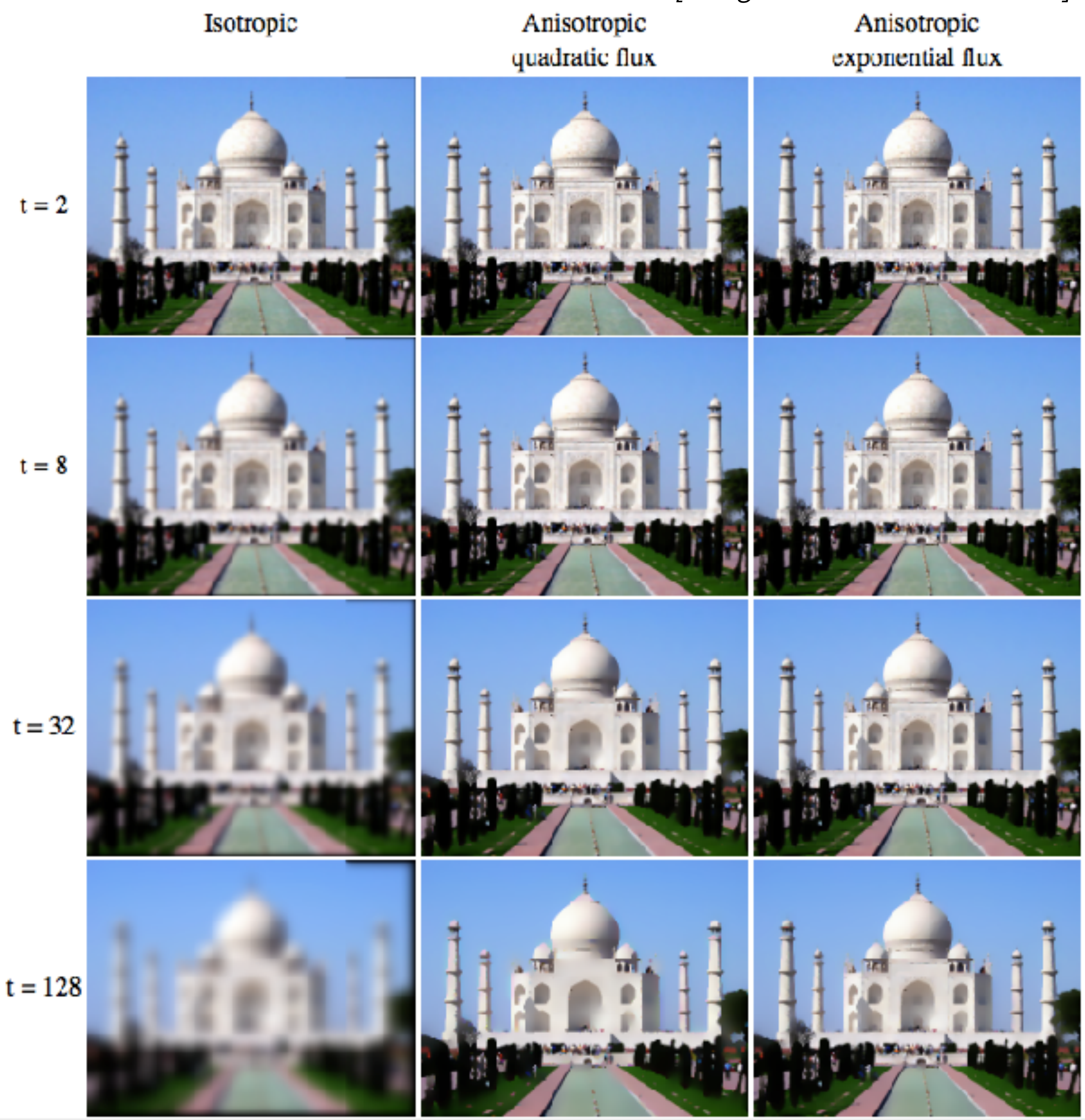
$$c\left(\|\nabla I\|\right) = \frac{1}{1 + \left(\frac{\|\nabla I\|}{K}\right)^2}$$

nonlinear diffusion equation
larger diffusion where I(x,y) is smooth
smaller where sharp changes in I (edges)

works quite well in practice
mathematical issues: ill-posed, regularization
noisy images can have spurious large gradients! these must be smoothened

Diffusion in image processing

[Image Credit: Manasi Datar]



AD indeed produces better results

Plasma Thermal Conductivity

diffusivity (cm^2s^{-1}) $\varkappa$: v_t x mfp; mfp~1/(nσ); σ~b^2 lnΛ; b~e^2/kT

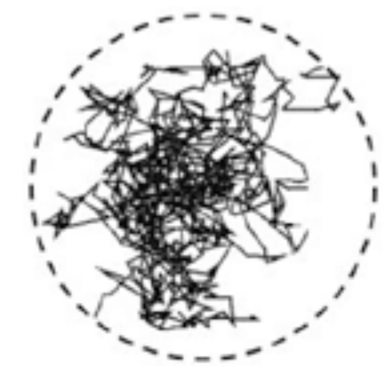
diffusivity∝$T^{5/2}$/n; e^-s conduct heat as they are 40 times faster than protons

$$nT\frac{ds}{dt} = -\nabla \cdot \mathbf{Q} \qquad s = \frac{k_B}{\gamma - 1}\ln\left(\frac{p}{\rho^\gamma}\right)$$ entropy

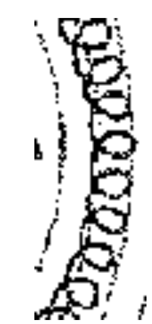
Plasma Thermal Conductivity

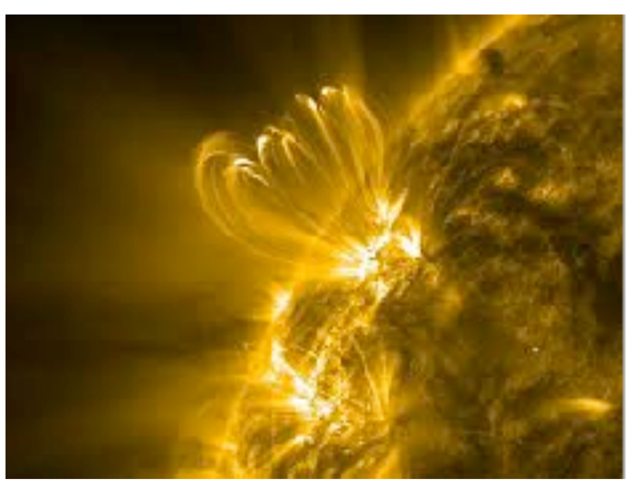
a tricky issue!

$$\mathbf{Q} = -\kappa \nabla T = -\chi n k_B \nabla T$$ for unmagnetized plasma



$$\mathbf{Q} = -\kappa \hat{b} \nabla_{||} T = -\kappa \hat{b} (\hat{b} \cdot \nabla) T$$ for magnetized plasma





particles move along B w. small Larmor radii but diffuse along B with a path length of mfp; mfp>>ρ_L

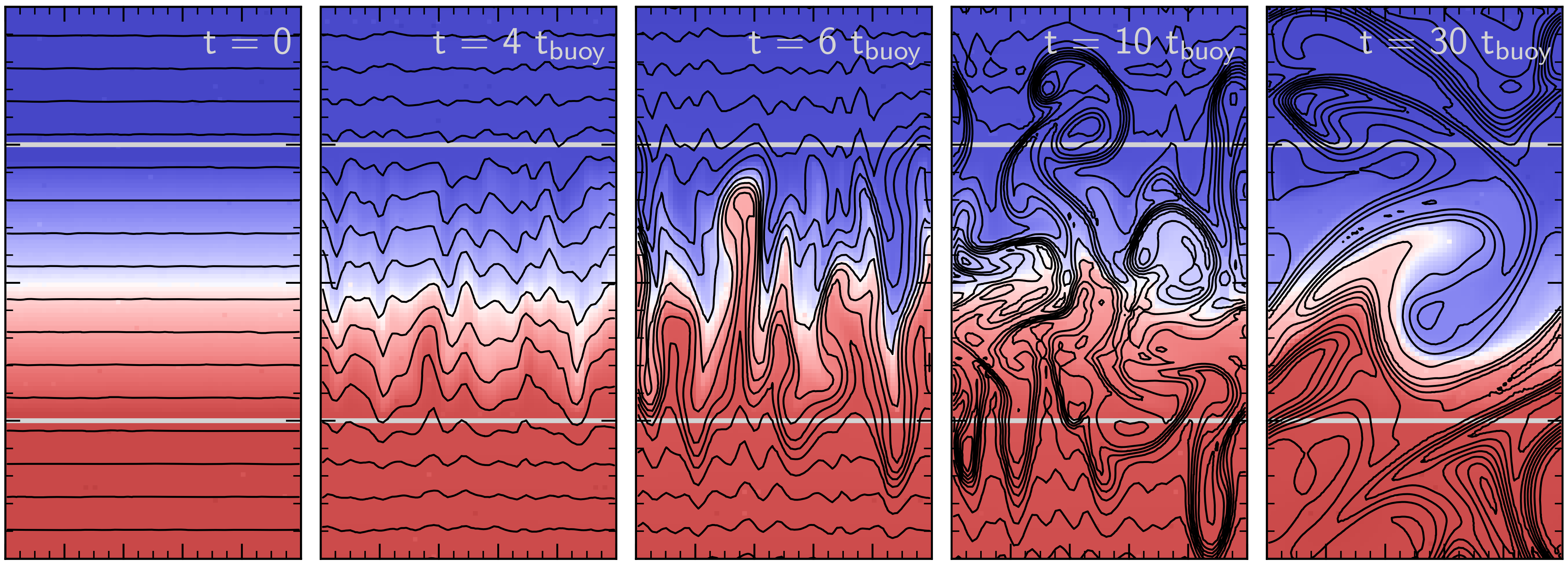
$$D_{||} \sim v_t^2 / \nu \gg D_{\perp} \sim \rho_L^2 \nu$$ true for all transport coeffts.

All this is fine for a given B, but B changes because of plasma currents, small scale instabilities! Observed perp. transport is enhanced. This is the key problem of tokamaks.

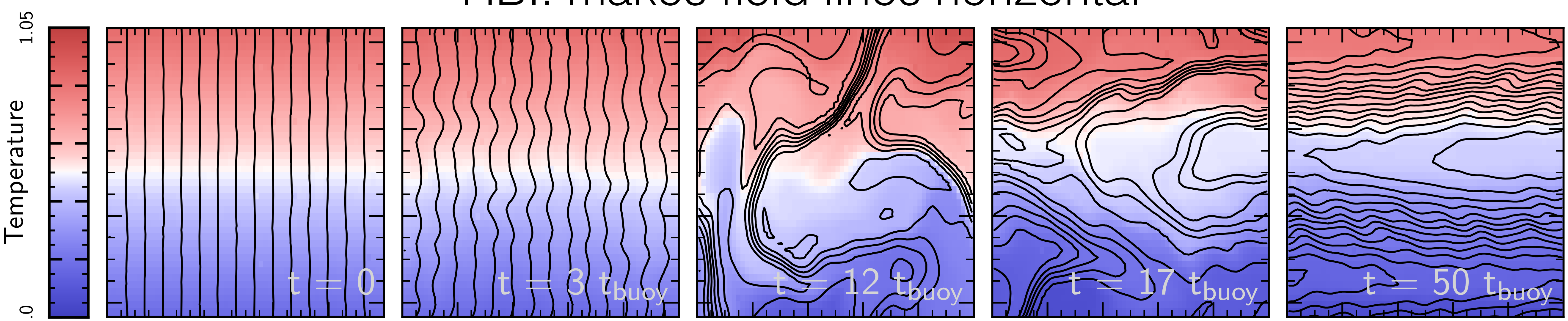
Buoyancy instabilities

buoyant response of gravitationally stratified fluids with anisotropic conduction fundamentally different from adiabatic fluids

MTI: makes field line vertical *[McCourt et al. 2011]*



HBI: makes field lines horizontal



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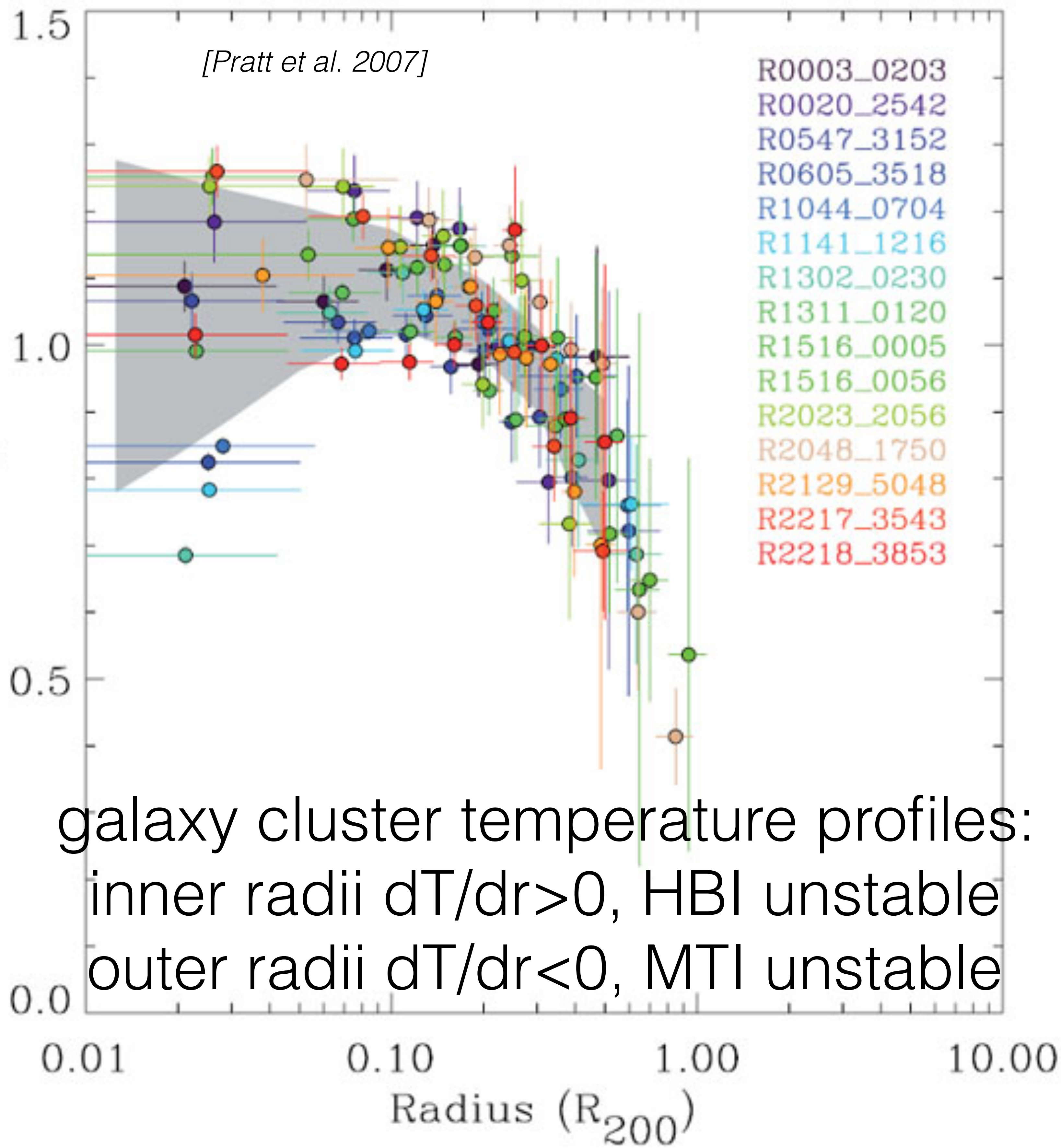
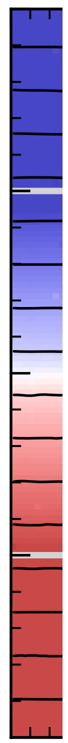
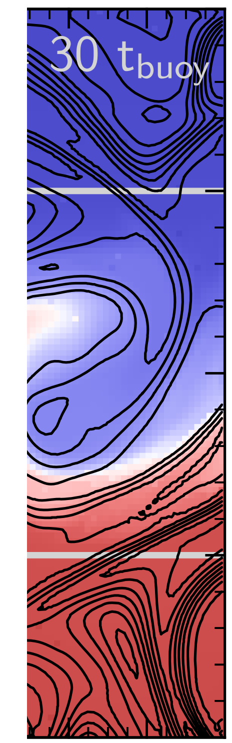
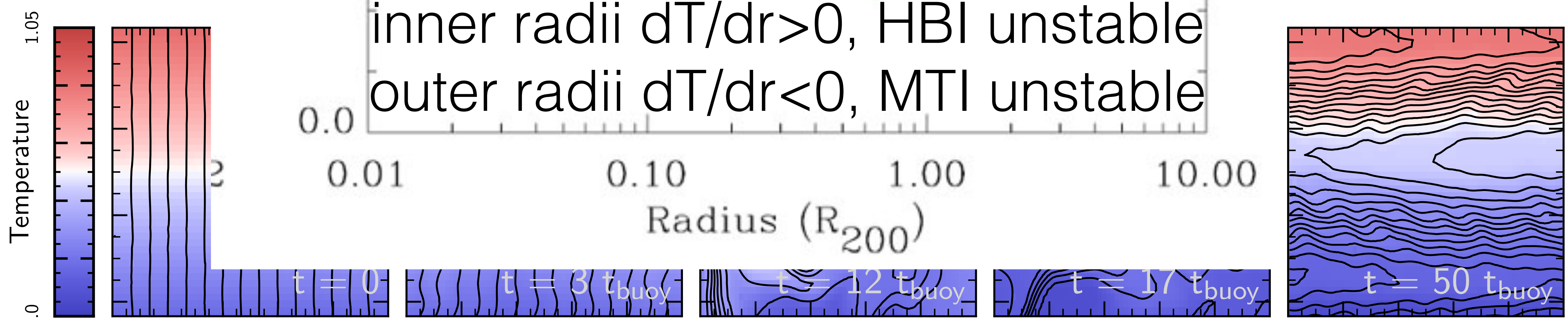


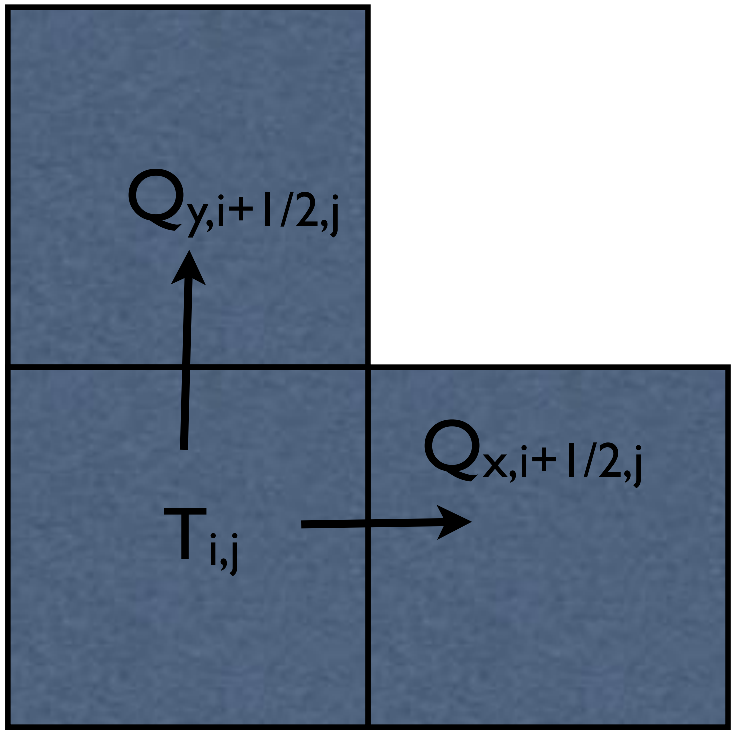






galaxy cluster temperature profiles:
inner radii dT/dr>0, HBI unstable
outer radii dT/dr<0, MTI unstable

Numerical implementation



$$\frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{Q} = \nabla \cdot (\chi \hat{b}\hat{b} \cdot \nabla T)$$

$$\mathbf{Q} = -\chi \hat{b} \nabla_{\|} T$$

with constant ϰ

$$Q_x = -\chi b_x \left(b_x \frac{\partial T}{\partial x} + b_y \frac{\partial T}{\partial y} \right) \quad Q_y = -\chi b_y \left(b_x \frac{\partial T}{\partial x} + b_y \frac{\partial T}{\partial y} \right)$$

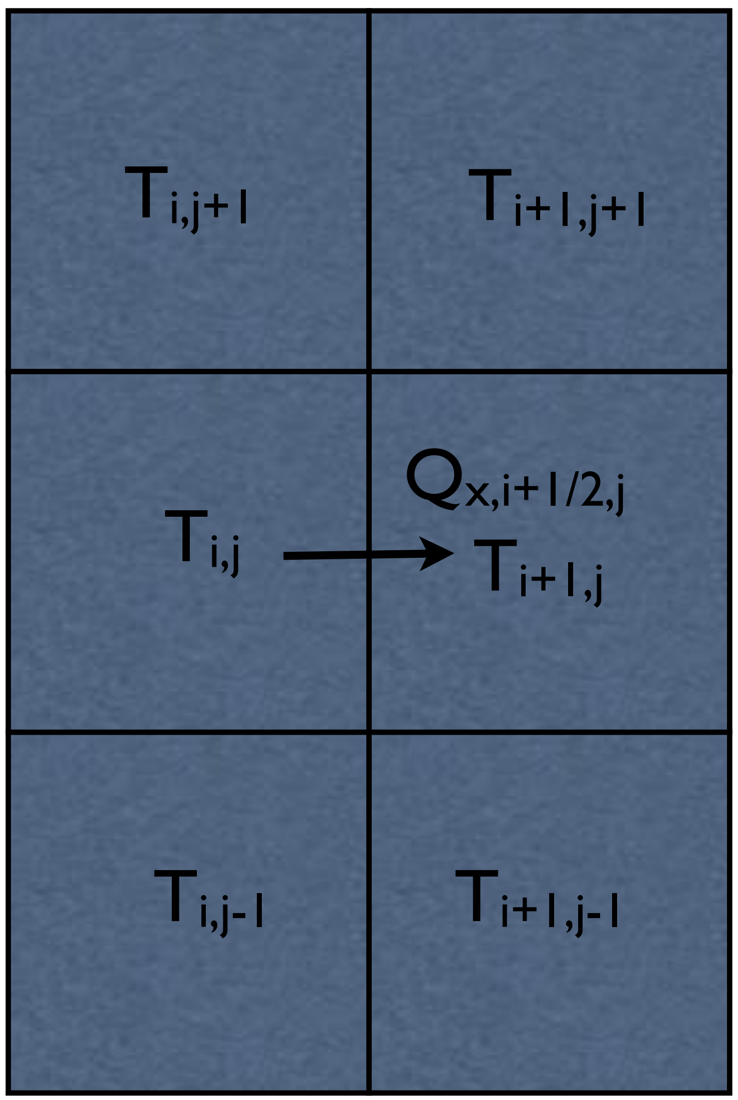
$$\frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t} = -\frac{Q_{x,i+1/2,j} - Q_{x,i-1/2,j}}{\Delta x} - \frac{Q_{y,i,j+1/2} - Q_{y,i,j-1/2}}{\Delta y}$$

$$Q_{x,i+1/2,j} = -\chi b_x \left(b_x \frac{T_{i+1,j} - T_{i,j}}{\Delta x} + b_y \overline{\frac{\partial T}{\partial y}} \right)$$

conservative differencing s.t., internal fluxes cancel

needs to be interpolated at (i+1/2,j)

Centered Differencing



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

similarly,

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

in general,

$$\overline{\frac{\partial T}{\partial y}} = \mathcal{L}\left(\left.\frac{\partial T}{\partial y}\right|_{i+1,j+1/2}, \left.\frac{\partial T}{\partial y}\right|_{i,j+1/2}, \left.\frac{\partial T}{\partial y}\right|_{i+1,j-1/2}, \left.\frac{\partial T}{\partial y}\right|_{i,j-1/2} \right)$$

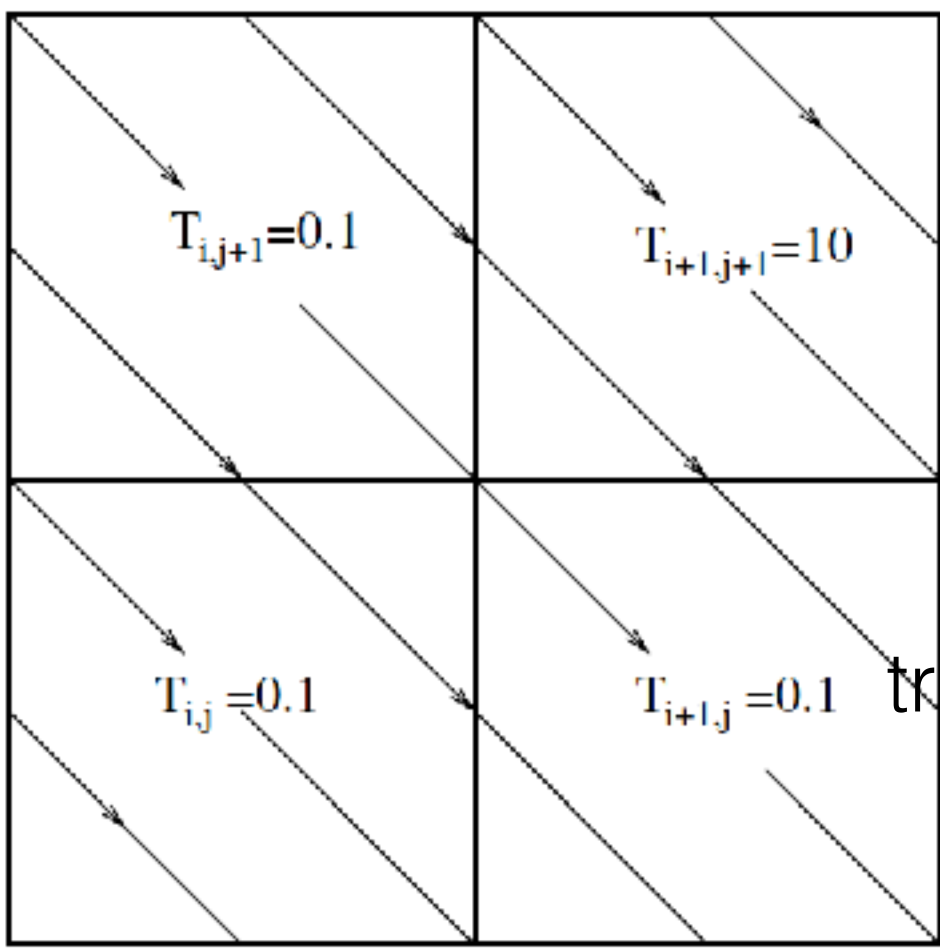
Problem w. CD

its not monotonicity preserving! can give -ve temperatures!

$$Q_{x,i+1/2,j} = -b_x \left(b_x \cancel{\frac{\partial T}{\partial x}} + b_y \overline{\frac{\partial T}{\partial y}} \right)$$

$$= \frac{1}{2} \frac{(10 - 0.1)}{4\Delta y} = \frac{9.9}{8\Delta y} > 0!$$

similarly, $Q_{y,i,j+1/2} = \dfrac{9.9}{8\Delta y} > 0!$



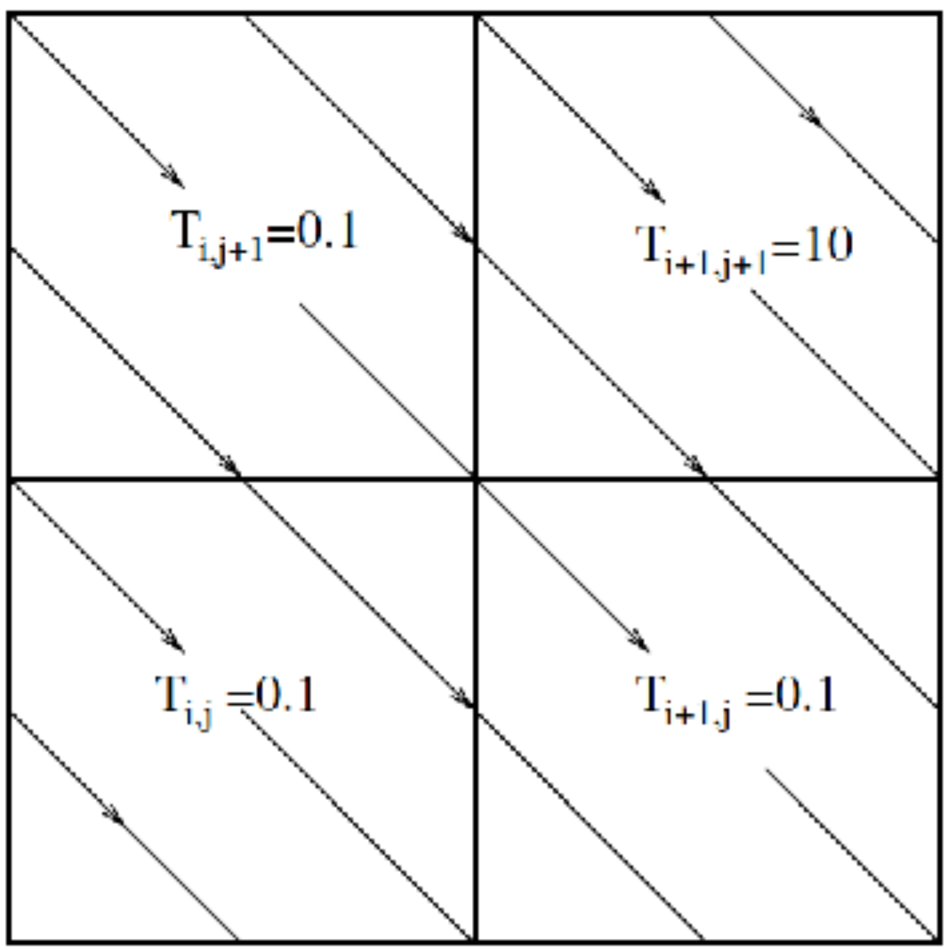
reflective BC

transverse term can be made arbitrarily large and of any sign!

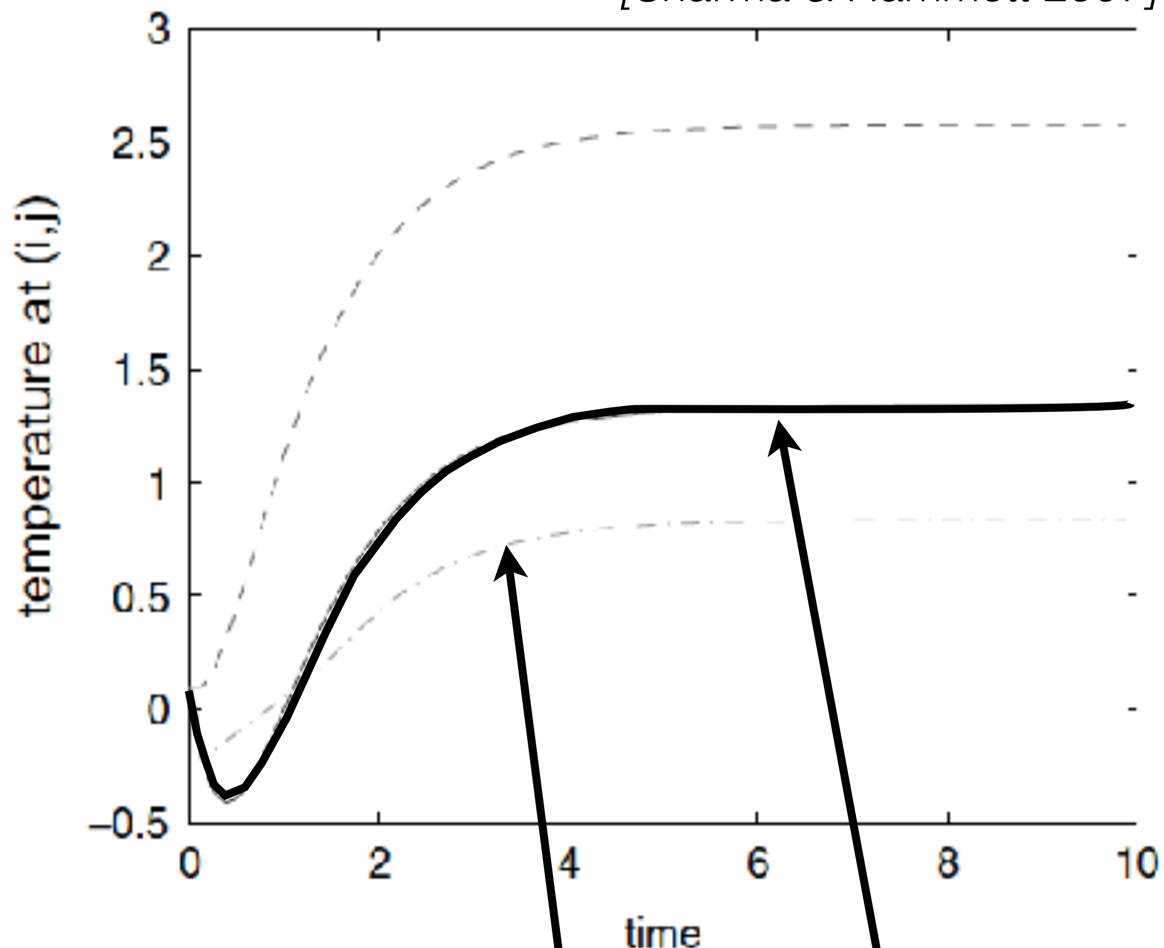
heat flux is out of temperature minimum!
=> not extrema preserving

Problem w. CD

its not extrema preserving! can give -ve temperatures!



[Sharma & Hammett 2007]



simple averaging of transverse T gradients gives non-monotonicity!

Solution?

normal terms: $Q_{x,N} = -b_x^2 \frac{\partial T}{\partial x}, Q_{y,N} = -b_y^2 \frac{\partial T}{\partial y}$ flux always down the gradient

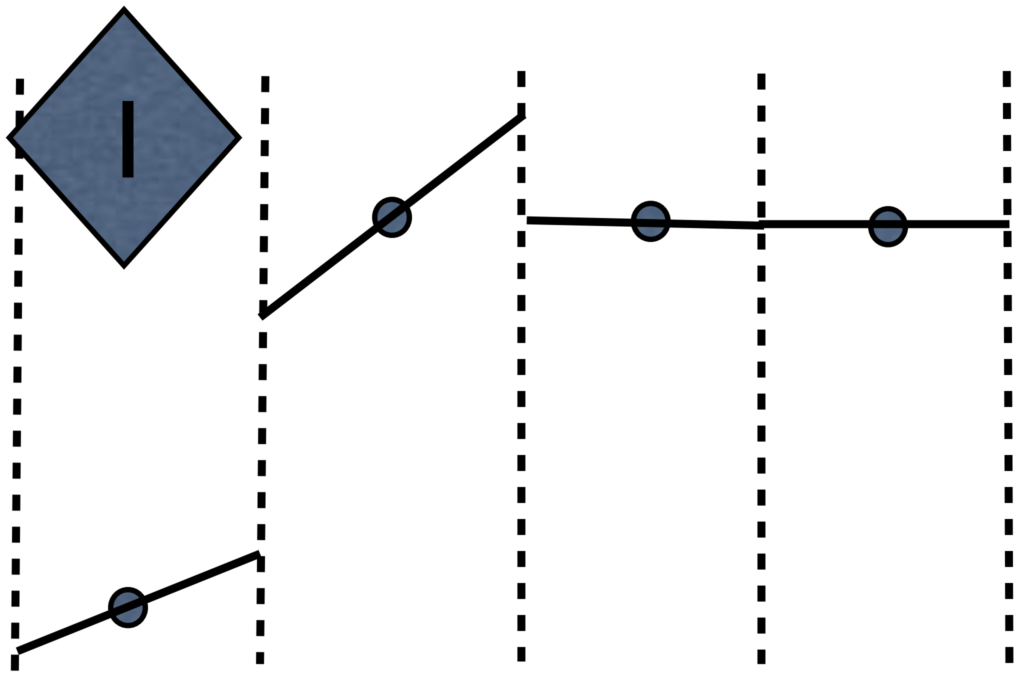
transverse terms: $Q_{x,T} = -b_x b_y \overline{\frac{\partial T}{\partial y}}, Q_{y,T} = -b_x b_y \overline{\frac{\partial T}{\partial x}}$ can have any sign!

$$\overline{\frac{\partial T}{\partial y}} = \mathcal{L}\left(\left.\frac{\partial T}{\partial y}\right|_{i+1,j+1/2}, \left.\frac{\partial T}{\partial y}\right|_{i,j+1/2}, \left.\frac{\partial T}{\partial y}\right|_{i+1,j-1/2}, \left.\frac{\partial T}{\partial y}\right|_{i,j-1/2} \right)$$

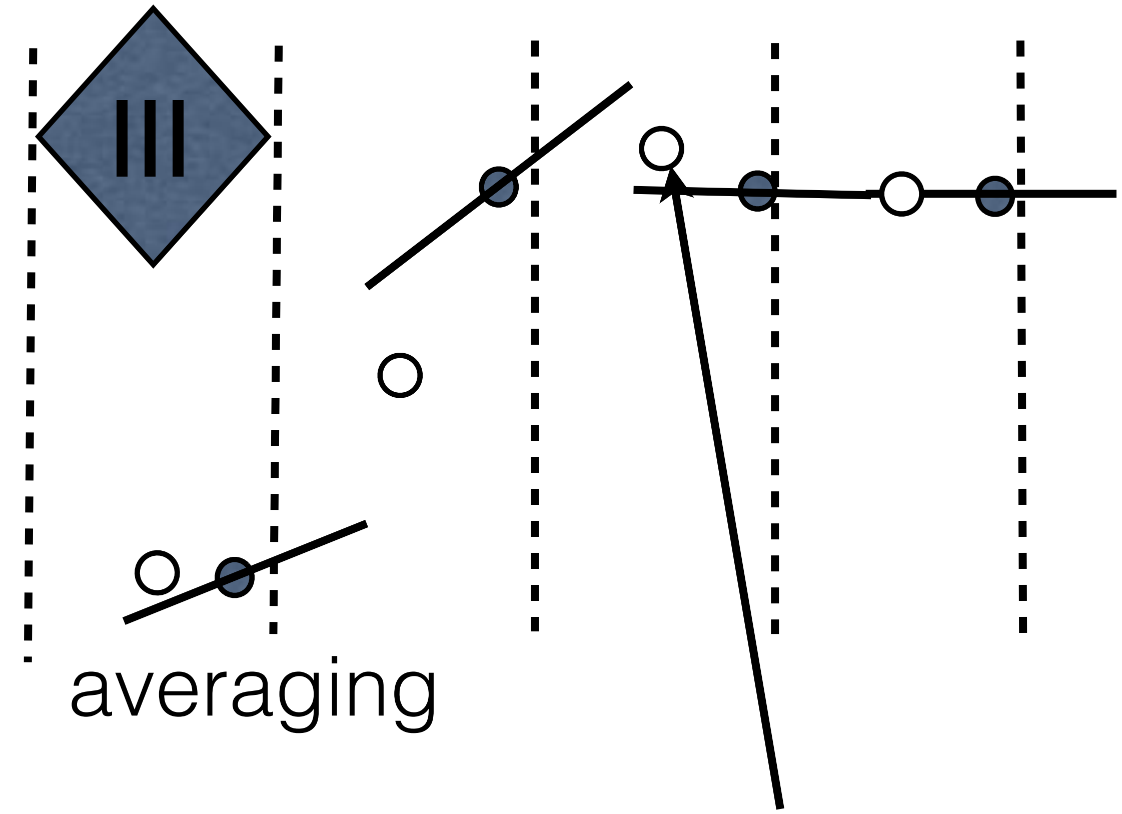
choosing arithmetic averaging does not work!
can be arbitrarily large and of any sign

need to have a better interpolation which is not affected by a large +/- value of the argument

Limiters in advection

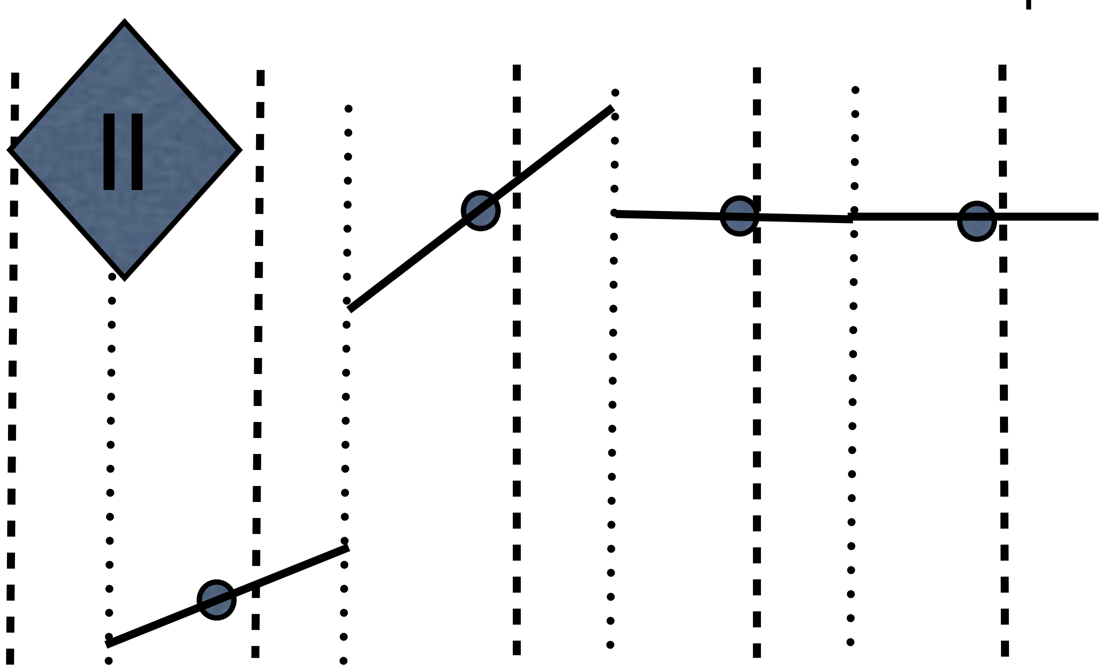


linear reconstruction: AM of slopes



averaging

non-monotonic
causes oscillations
at discontinuities

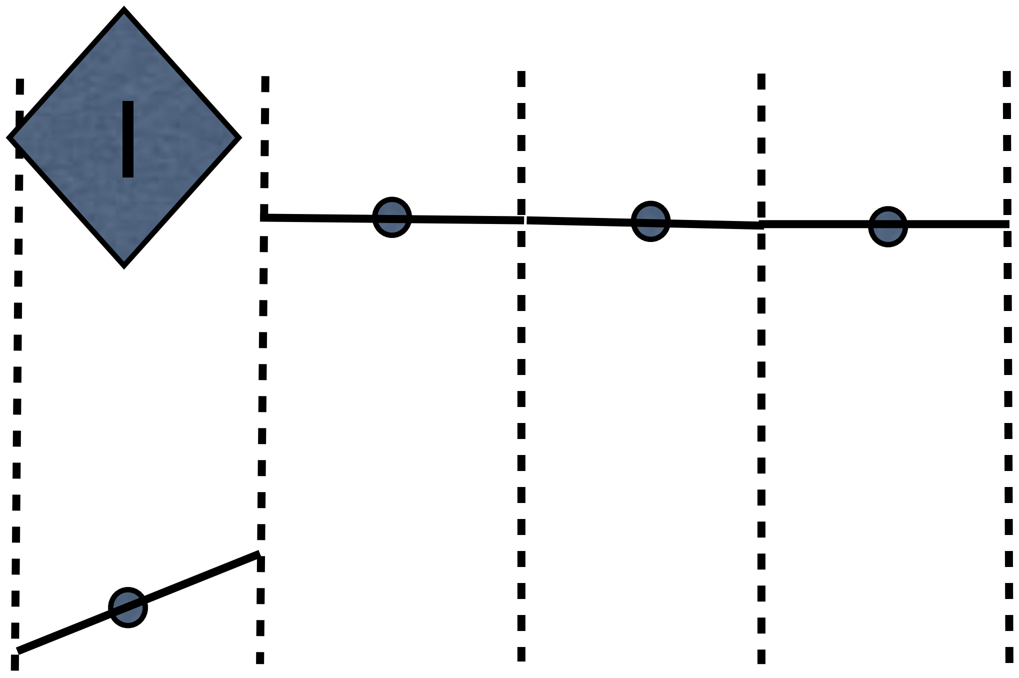


advection with v>0

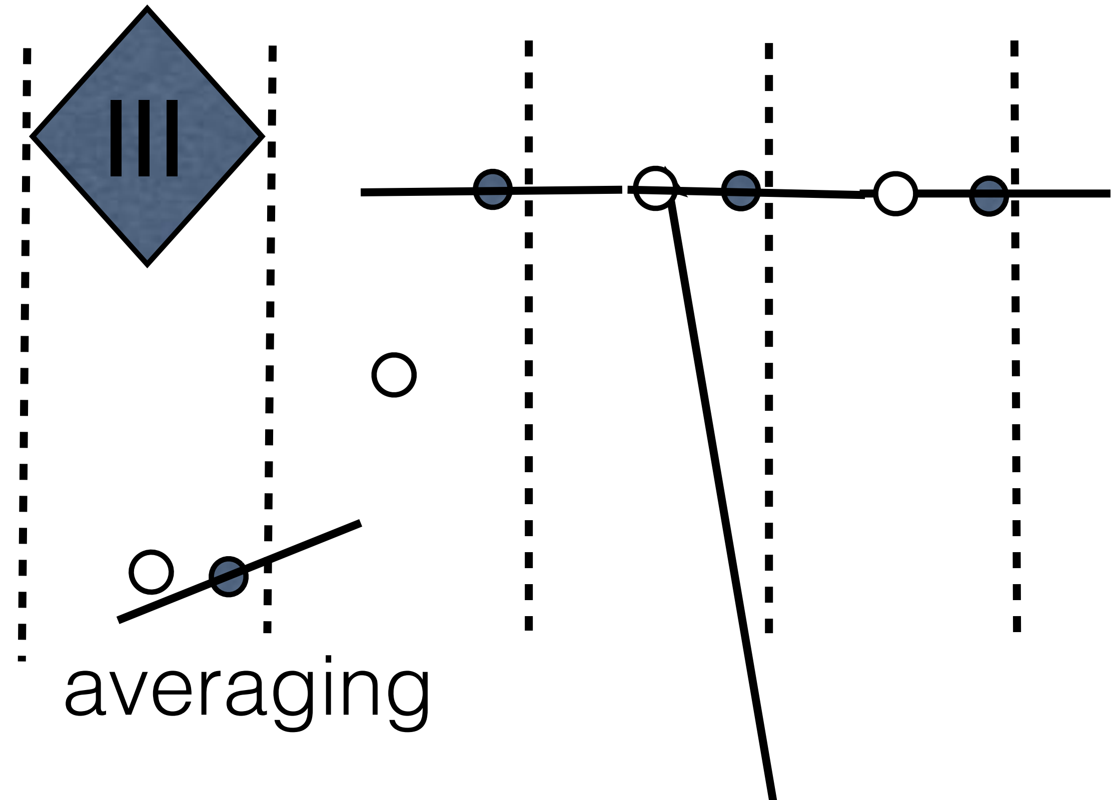
$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0$$

advection equation: REA approach

Limiters in advection

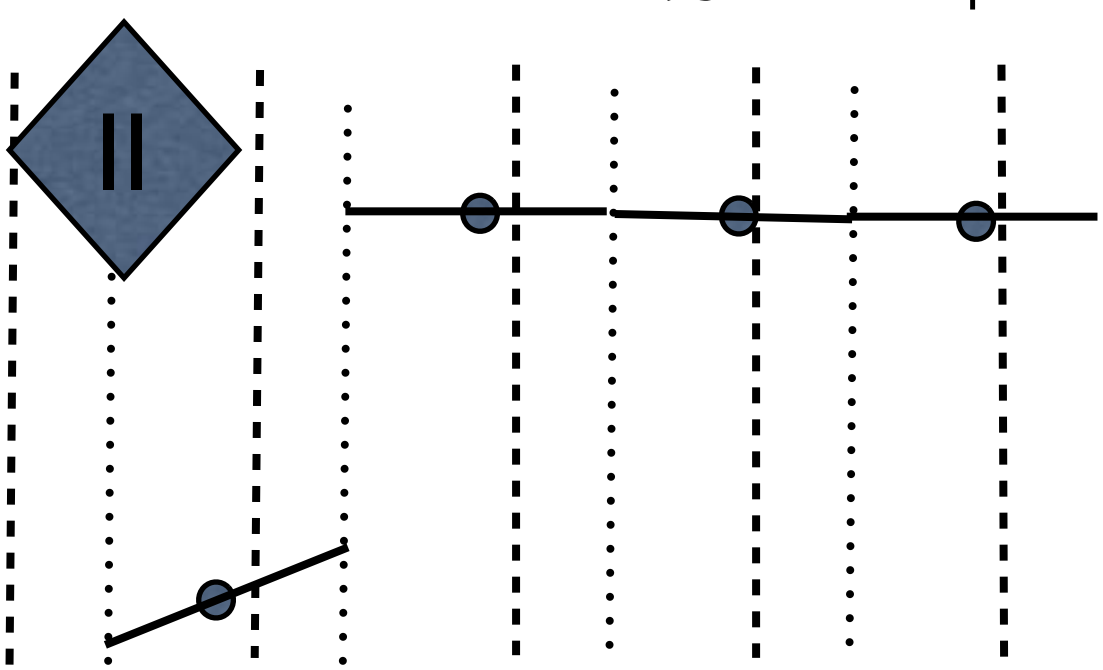


linear reconstruction: $\mathcal{L}$ of slopes



averaging

monotonic
prevents oscillations
at discontinuities if
limited reconstruction



advection with v>0

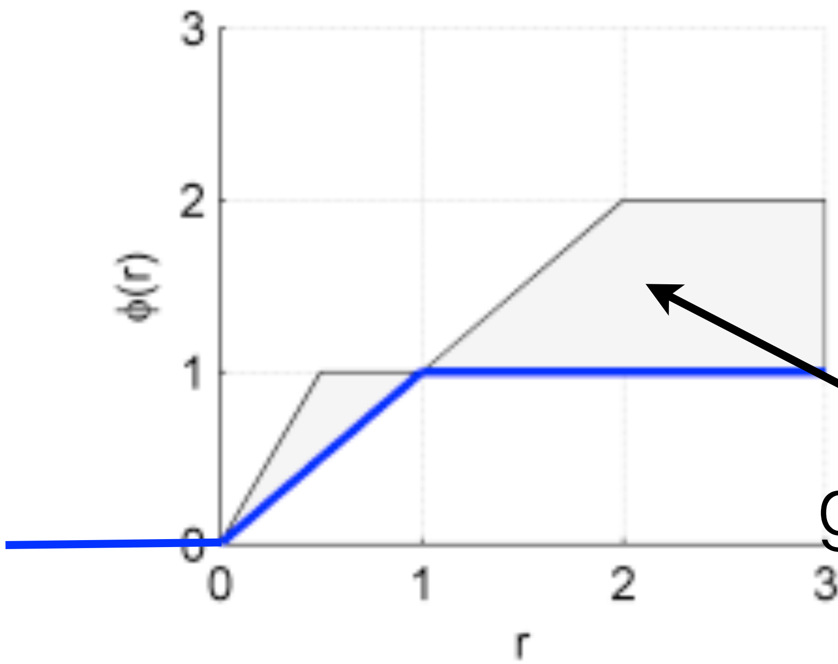
$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0$$

advection equation: REA approach

Minmod limiter

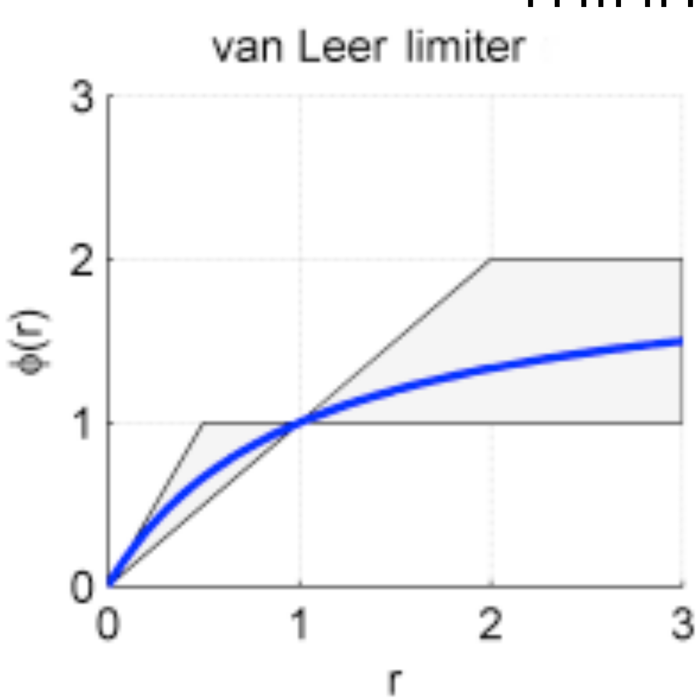
$$\mathcal{L}(a,b) = a\phi(1, r = b/a) = b\phi(1, r = a/b)$$

$\mathcal{L}$=0 if arguments have opposite sign



grey: monotonicity zone

minmod(a,b)=0 if ab<=0, min(a,b) if ab>0



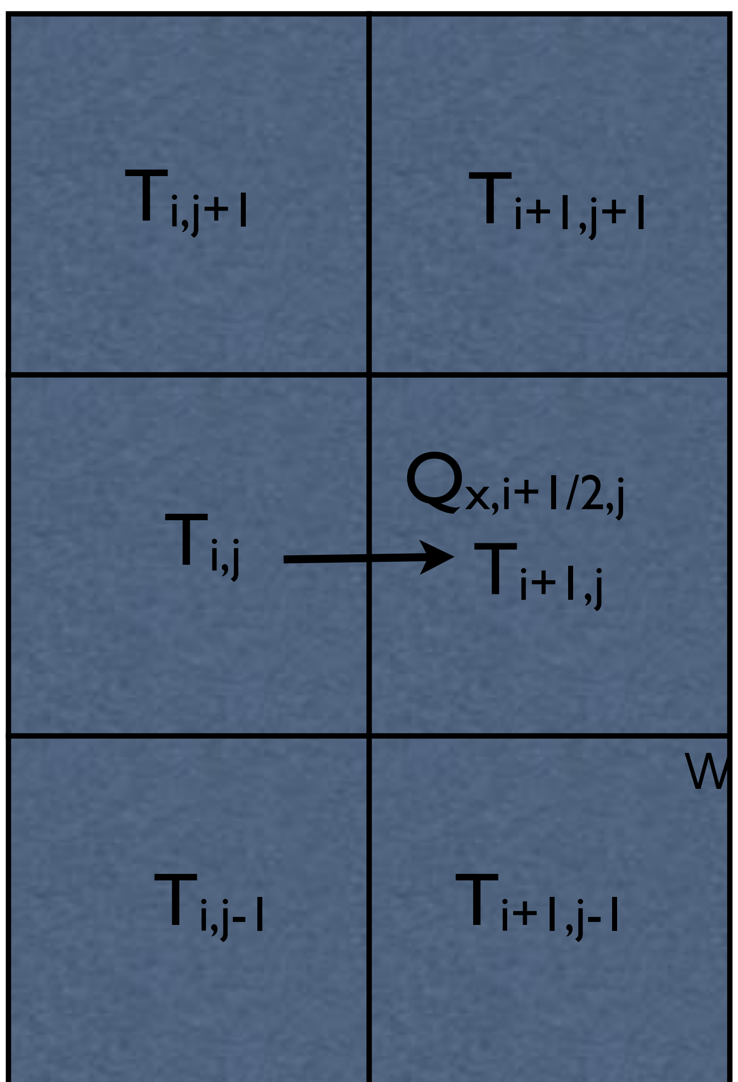
smoother, higher order accuracy, still nonlinear

van Leer(a,b)=0 if ab<=0, 2ab/(a+b) if ab>0

Limited averaging

$$\overline{\frac{\partial T}{\partial y}} = \mathcal{L}\left(\left.\frac{\partial T}{\partial y}\right|_{i+1,j+1/2}, \left.\frac{\partial T}{\partial y}\right|_{i,j+1/2}, \left.\frac{\partial T}{\partial y}\right|_{i+1,j-1/2}, \left.\frac{\partial T}{\partial y}\right|_{i,j-1/2} \right)$$ symmetric in arguments

limited averaging which vanishes if all 4 arguments don't have the same sign



if $T_{i,j}$ is a local extremum

$$\left.\frac{\partial T}{\partial y}\right|_{i,j+1/2} \times \left.\frac{\partial T}{\partial y}\right|_{i,j-1/2} \leq 0$$

and

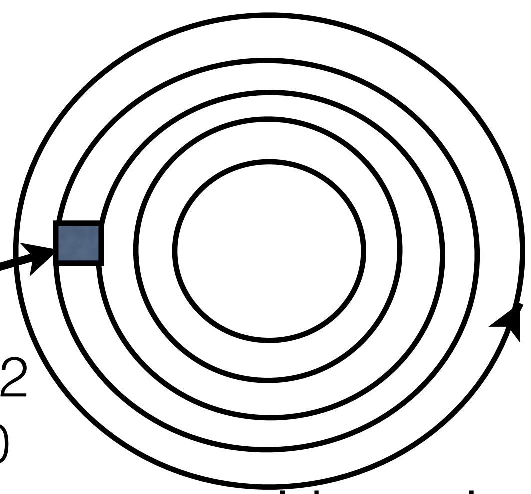
$$\left.\frac{\partial T}{\partial x}\right|_{i+1/2,j} \times \left.\frac{\partial T}{\partial x}\right|_{i-1/2,j} \leq 0$$

with limiter averaging transverse temperature gradients vanish and heat flux is down the temperature gradient

extrema won't be accentuated!

Ring test problem

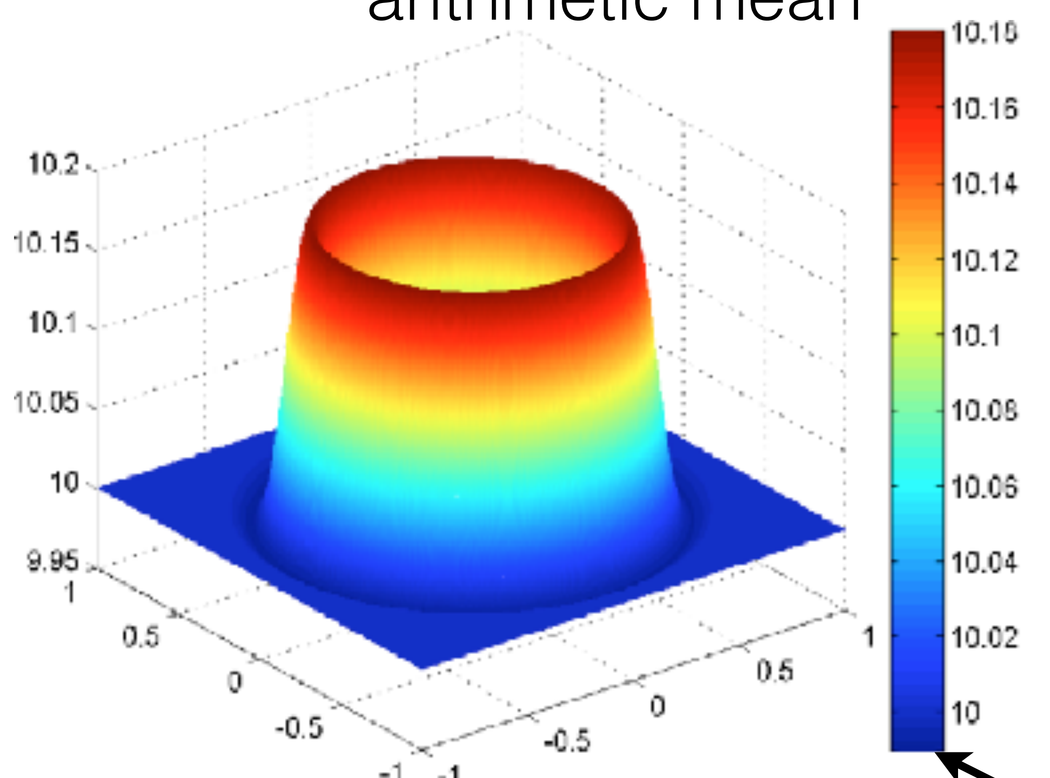
[Parrish & Stone 2005]



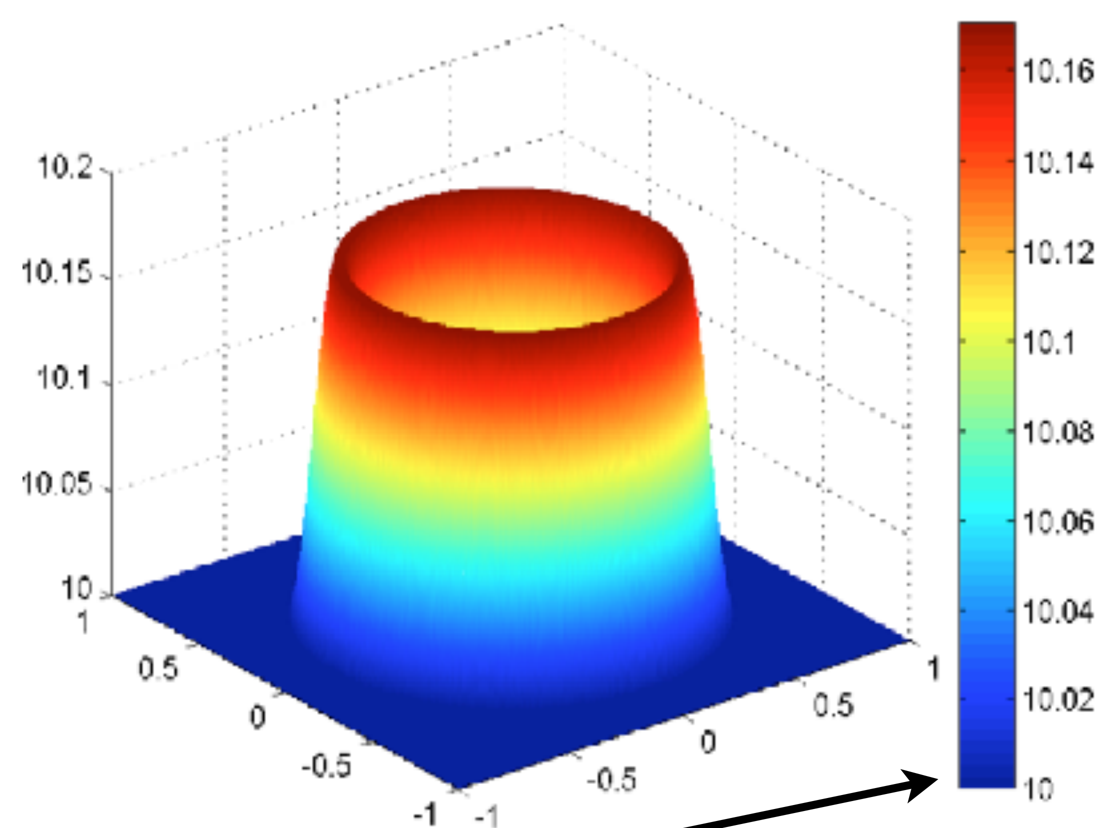
hot patch=12
ambient=10

$$b_x = -y/(x^2 + y^2)^{1/2}, b_y = x/(x^2 + y^2)^{1/2}$$

arithmetic mean



limited averaging: van Leer

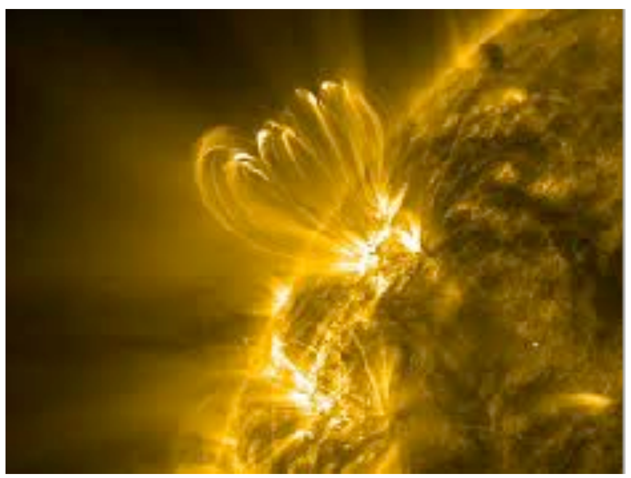


notice minimum temperature
non-monotonic even at late times

Negative temperature!

with large temperature gradients

negative temperature => sound wave becomes unstable =>code blows up



large temperature gradients are natural in plasmas; e.g., solar prominences in corona, 3 phases of the ISM

our method is essential for simulating such plasmas robustly from first principles

Another problem

the scheme is explicit and governed by a stability CFL constraint

$$\Delta t \leq \frac{\Delta x^2}{2\chi}$$

for high conductivity plasma such as ICM, this can be 1000s time smaller than $\dfrac{\Delta x}{c_s}$

one can subcycle: for every hydro timestep apply many conduction cycles but this is slow; better to go implicit where there is no stability constraint

$$\frac{T^{\star}_{i,j} - T^{n}_{i,j}}{\chi_{\parallel}\Delta t} = b^2_{x,i+1/2,j}\frac{T^{\star}_{i+1,j} - T^{\star}_{i,j}}{\Delta x^2} - b^2_{x,i-1/2,j}\frac{T^{\star}_{i,j} - T^{\star}_{i-1,j}}{\Delta x^2} + \frac{b_{x,i+1/2,j}b_{y,i+1/2,j}}{\Delta x \Delta y}\overline{\Delta T}^{n}_{i+1/2,j} - \frac{b_{x,i-1/2,j}b_{y,i-1/2,j}}{\Delta x \Delta y}\overline{\Delta T}^{n}_{i-1/2,j},$$

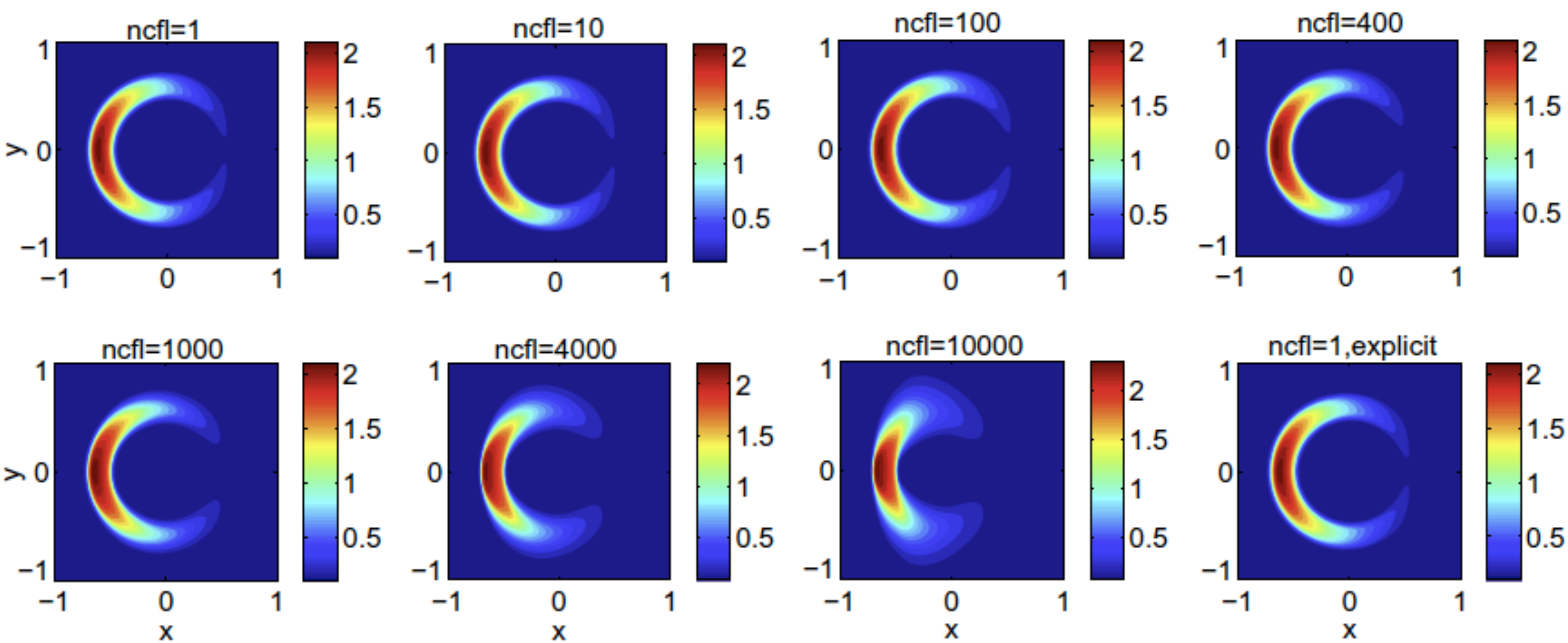
$$\frac{T^{n+1}_{i,j} - T^{\star}_{i,j}}{\chi_{\parallel}\Delta t} = b^2_{y,i,j+1/2}\frac{T^{n+1}_{i,j+1} - T^{n+1}_{i,j}}{\Delta y^2} - b^2_{y,i,j-1/2}\frac{T^{n+1}_{i,j} - T^{n+1}_{i,j-1}}{\Delta y^2} + \frac{b_{y,i,j+1/2}b_{x,i,j+1/2}}{\Delta x \Delta y}\overline{\Delta T}^{\star}_{i,j+1/2} - \frac{b_{y,i,j-1/2}b_{x,i,j-1/2}}{\Delta x \Delta y}\overline{\Delta T}^{\star}_{i,j-1/2},$$

this requires solving a tridiagonal matrix (O[N]): simply use LAPACK

Does implicit work?

ring diffusion test

[Sharma & Hammett 2011]

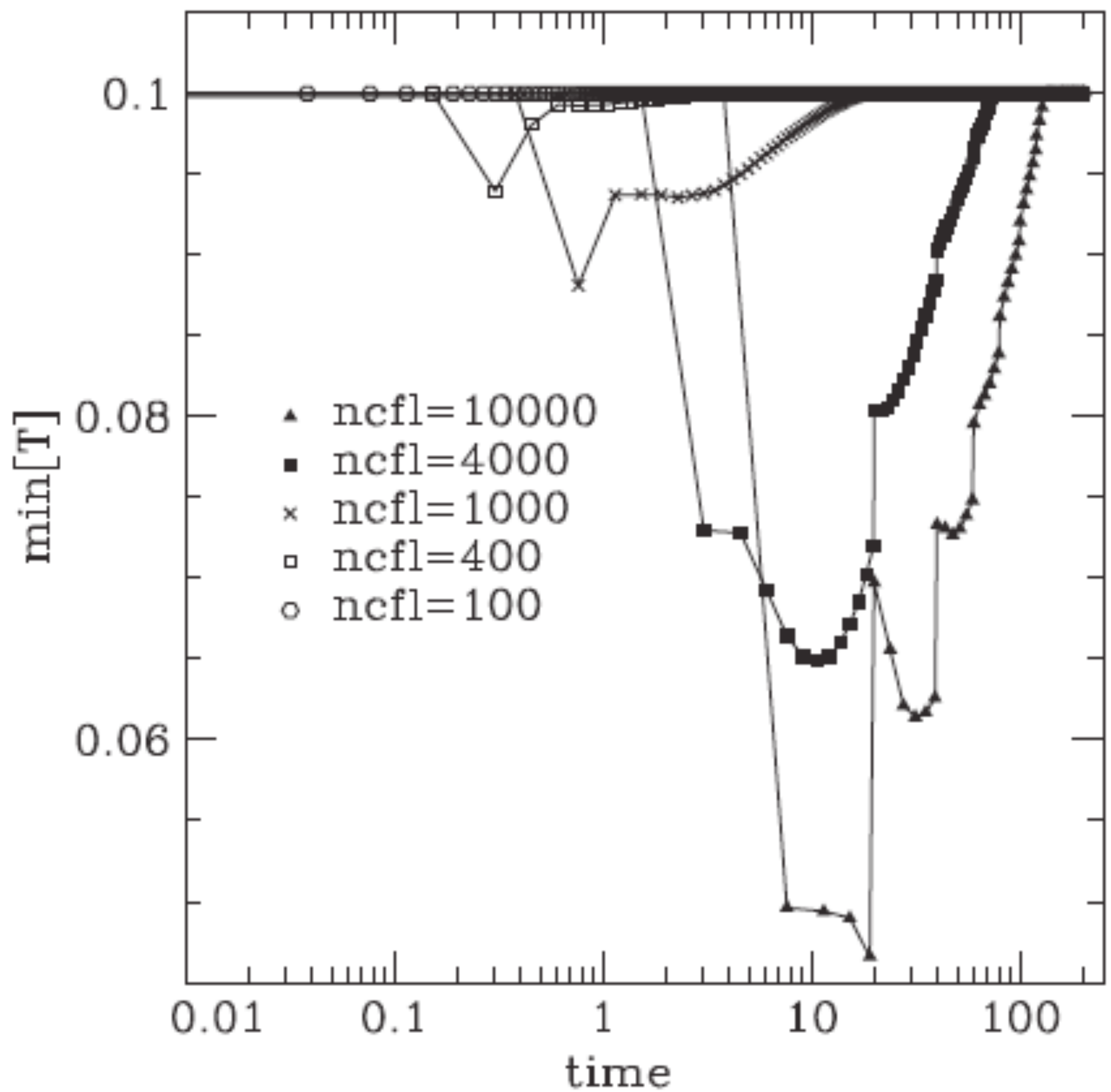


indeed it does; here, T_{hot}=10, T_{cold}=0.1

Does implicit work?

ring diffusion test

[Sharma & Hammett 2011]

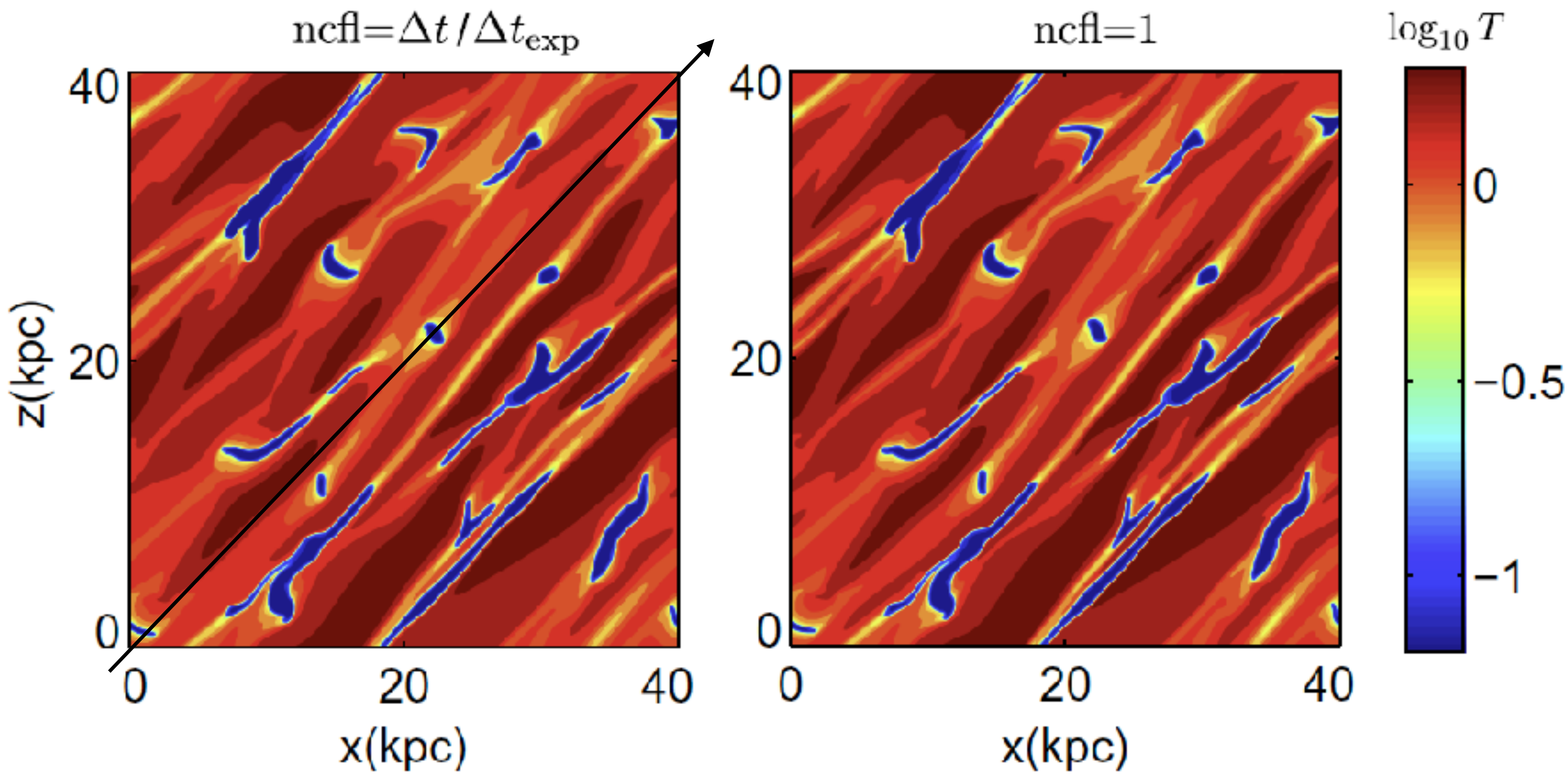


non-monotonicity not guaranteed but much better than without limiters!

non-monotonicity much less & only for early times

A real application: TI

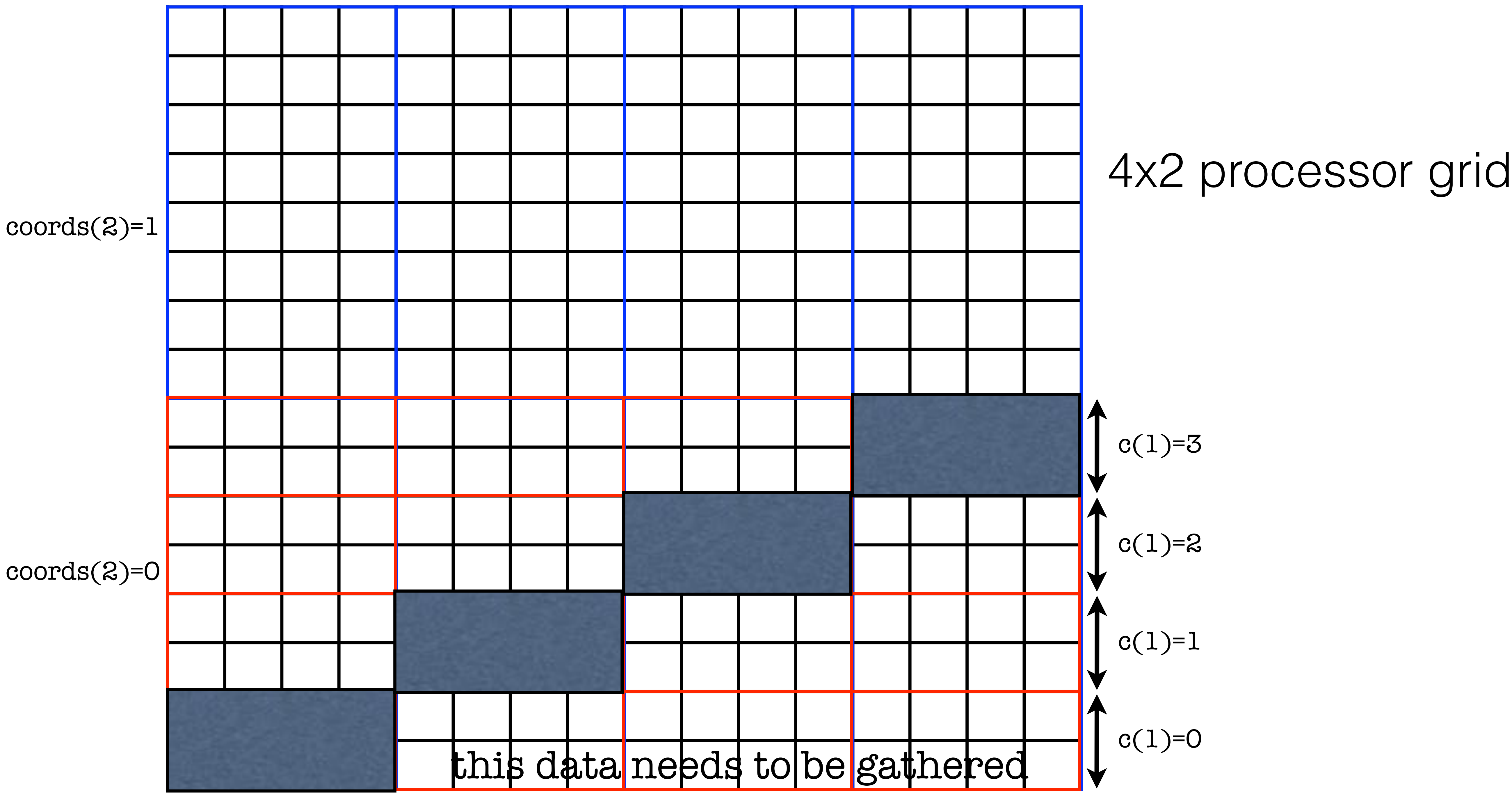
initially small density perturbations with global thermal balance
overdense regions cool and underdense are heated



this is 100 times faster!

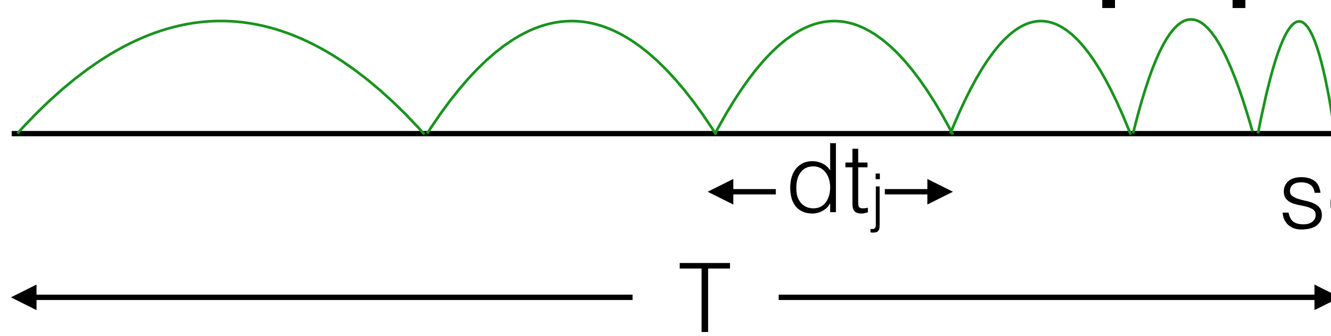
Parallel implementation

the implicit method is not yet parallel
parallelization strategy is clear but work needs to be done
another approach is to use parallel iterative packages like PETSc



a faster explicit method

Super time stepping



several variants

$$T = \sum_{j=1}^{j=N} dt_j$$

super timestep — substep j

diffusion eq. non-positive eigenvalues = $-Dk^2$

$$\frac{df}{dt} = -|\lambda| f$$

stability polynomial $p_N(\lambda)$

$|p_N(\lambda)|$ must be < 1 for numerical stability for all λ

$$f^N = \left(\prod_{j=1}^{j=N} (1 - |\lambda| dt_j) \right) f^1$$

for a given N, choose largest T such that $| p_N(\lambda) | < 1$

$$T \xrightarrow[\nu \to 0]{\lambda_{\max}} N^2 \Delta t_{\exp}$$

factor of N speed-up!

COMMUNICATIONS IN NUMERICAL METHODS IN ENGINEERING, Vol. 12, 31–42 (1996)

SUPER-TIME-STEPPING ACCELERATION OF EXPLICIT SCHEMES FOR PARABOLIC PROBLEMS

VASILIOS ALEXIADES

Mathematics Department, University of Tennessee, Knoxville, TN 37996-1300, U.S.A. and Mathematical Sciences Section, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6367, U.S.A.

GENEVIÈVE AMIEZ

Laboratoire de Calcul Scientifique, Université de Franche-Comté, 25030 Besançon, France

AND

PIERRE-ALAIN GREMAUD

Department of Mathematics and Center for Research in Scientific Computation, North Carolina State University, Raleigh, NC 27695, U.S.A.

$$\tau_j = \Delta t_{\text{expl}} \left((-1+\nu)\cos\left(\frac{2j-1}{N} \frac{\pi}{2} \right) + 1 + \nu \right)^{-1} \qquad j = 1, \ldots N$$

$$\Delta t_{\text{expl}} = 2/\lambda_{\max}$$

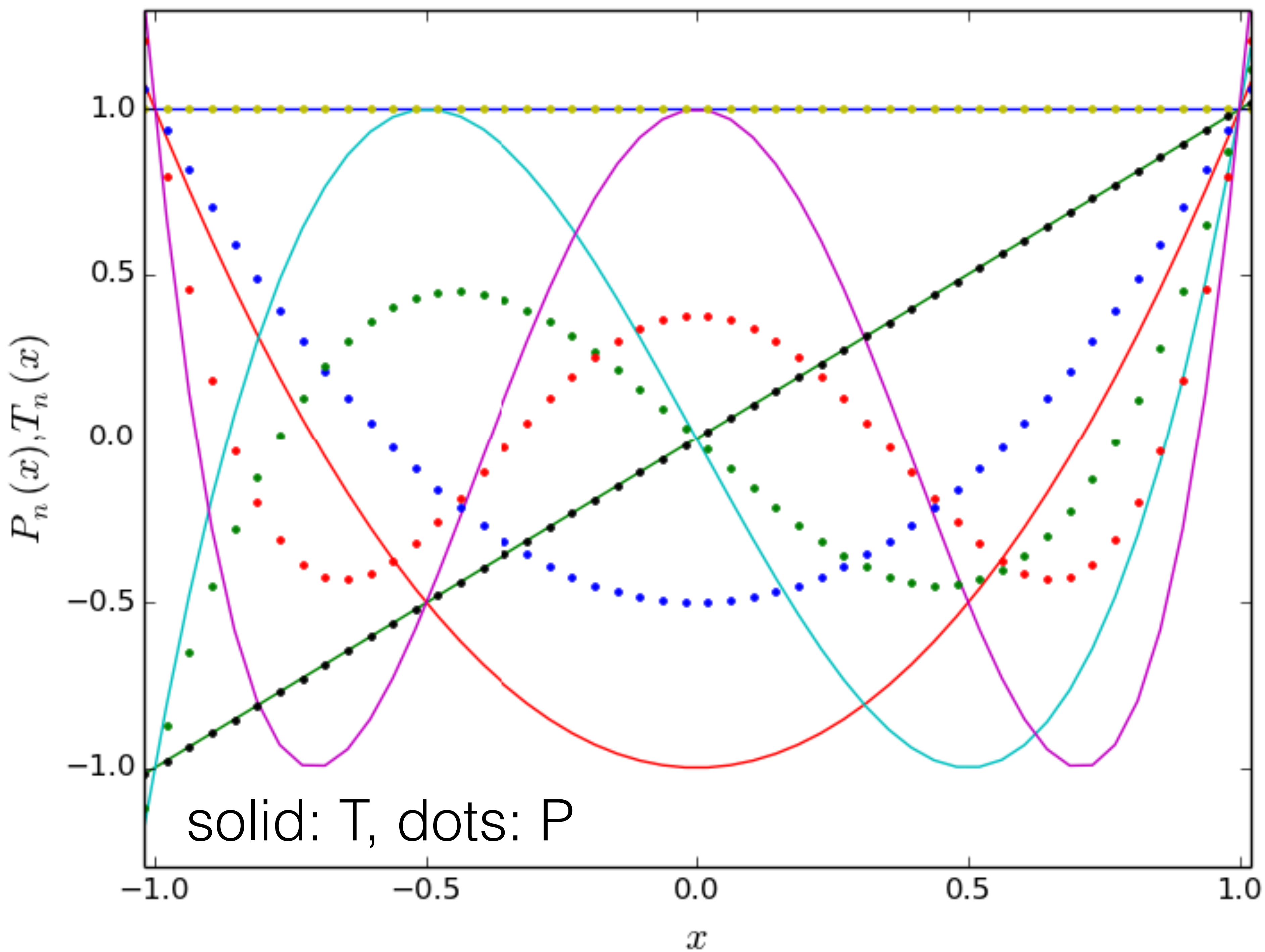
stability parameter <<1

$$T = \sum_{j=1}^{N} \tau_j = \Delta t_{\text{expl}} \frac{N}{2\sqrt{\nu}} \left(\frac{(1+\sqrt{\nu})^{2N} - (1-\sqrt{\nu})^{2N}}{(1+\sqrt{\nu})^{2N} + (1-\sqrt{\nu})^{2N}} \right)$$

super timestep

prescription based on enforcing $p_N(\lambda)$ to be Chebyshev polynomial with |argument| < 1

Chebyshev vs Legendre



Comparison of $T_n(x)$ & $P_n(x)$: since $|P|<1$ in (-1,1) => better stability

Stabilized Runge-Kutta (RK)

A stabilized Runge–Kutta–Legendre method for explicit super-time-stepping of parabolic and mixed equations *[JCP, 2014]*

Chad D. Meyer [a,*], Dinshaw S. Balsara [a], Tariq D. Aslam [b]

typically multiple stages in RK introduced for higher accuracy
here it is for stability with as long a timestep as possible

$$\frac{du}{dt} = \mathbf{M}u(t) \qquad u(t) = e^{t\mathbf{M}}u(0) \approx \left(1 + t\mathbf{M} + \frac{1}{2}(t\mathbf{M})^2 + \cdots\right)u(0)$$

analytic solution   Taylor series expansion

$R_s(z) = a_s + b_s P_s(w_0 + w_1 z)$ stability polynomial for s-stage RKL, $z=\lambda T$

for first order accuracy: $R_s(0)=1$, $R'_s(0)=1$,=> $u^{(j)} = P_j\left(1 + \frac{2}{s^2+s}z\right)u^n$

RKL1

first order Runge-Kutta Legendre scheme:

$$Y_0 = u(t_0)$$

$$Y_1 = Y_0 + \tilde{\mu}_1 \tau \mathbf{M} Y_0$$

$$Y_j = \mu_j Y_{j-1} + \nu_j Y_{j-2} + \tilde{\mu}_j \tau \mathbf{M} Y_{j-1}; \quad 2 \leqslant j \leqslant s$$

$$u(t+\tau) = Y_s$$

$$\mu_j = \frac{2j-1}{j}; \qquad \nu_j = \frac{1-j}{j}$$

$$\tilde{\mu}_j = \frac{2j-1}{j}\frac{2}{s^2+s}$$

stability polynomial at jth substep

$$u^{(j)} = P_j\left(1 + \frac{2}{s^2+s}z\right)u^n$$

$$\tau_{\max} = \Delta t_{expl}\frac{s^2+s}{2}$$

RKL1

compare with LP's recursion relations

growth polynomial at each time substep matched to P_j

$$(j)P_j(x) = (2j-1)xP_{j-1}(x) - (j-1)P_{j-2}(x)$$

$$Y_j = \mu_j Y_{j-1} + \nu_j Y_{j-2} + \tilde{\mu}_j \tau \mathbf{M} Y_{j-1}; \quad 2 \leqslant j \leqslant s$$

$$u(t+\tau) = Y_s$$

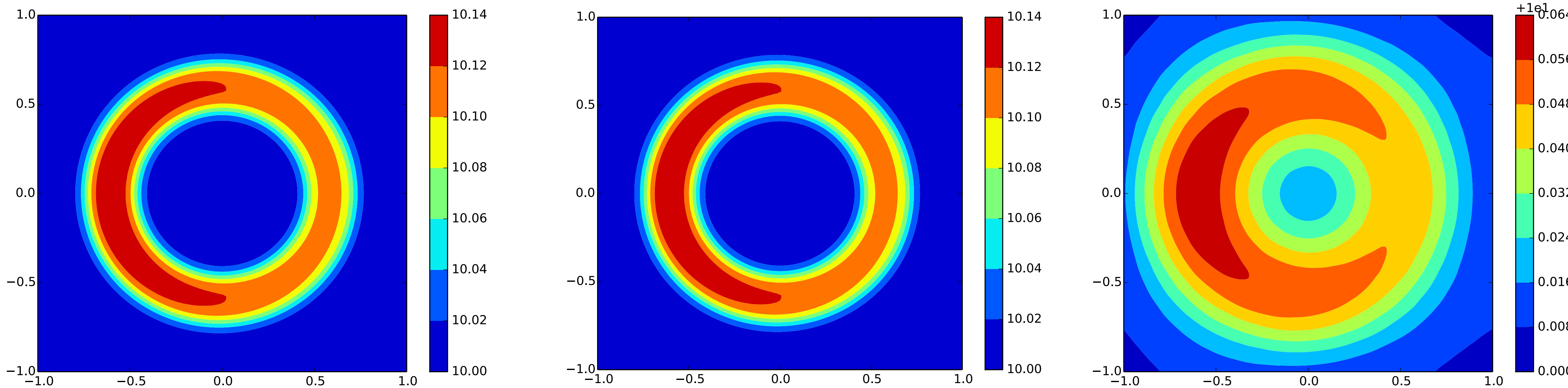
$$\mu_j = \frac{2j-1}{j}; \qquad \nu_j = \frac{1-j}{j}$$

$$\tilde{\mu}_j = \frac{2j-1}{j}\frac{2}{s^2+s}$$

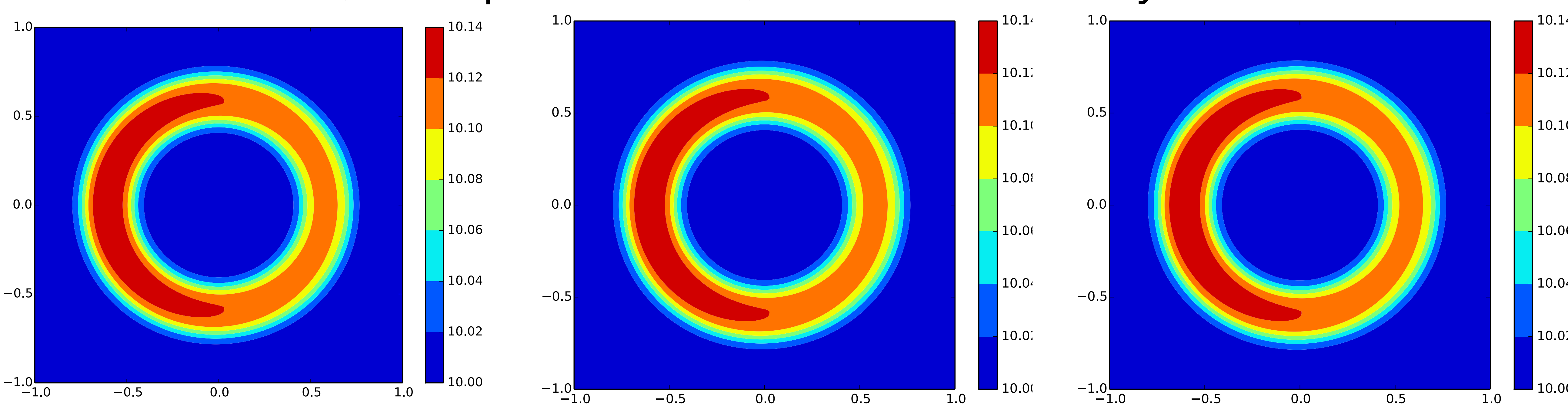
similar schemes for RKL2, RKC1, RKC2

Comparison on ring diffusion

AAG STS, v=0.01 for N=5, 10, 20; blows up for 50



RKL1; ok up to N=20; inaccurate beyond that



Conclusions

- anisotropic diffusion important in plasmas
- monotonicity, extrema-preservation
- Limiters can maintain extrema
- implicit scheme; parallelization is difficult
- super-time-stepping: AAG, RKC, RKL

Thank You!

References

- Sharma & Hammett 2007: extrema problem, limiters
- Sharma & Hammett 2011: semi-implicit scheme, tridiagonal, large speed-up
- Alexiades, Amiez & Gremaud 1996: super-time-stepping
- Verweer, Hundsdorfer & Sommeijer 1990: RKC
- Meyer, Balsara & Aslam 2014: RKL