Gyrokinetic Turbulence simulations of an NSTX SOL with model geometry, and Exponential Reconstructions and Positivity for Discontinuous Galerkin Algorithms

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Gkeyll Tokamak References

Gkeyll is apparently the first successful *continuum* gyrokinetic code doing turbulence on open field lines, sheath boundary conditions & toroidal bad curvature (XGC, and recently ELMFIRE, are only other codes, using a PIC approach. XGC can also do X-points). COGENT making progress, has more advanced collision operator, 2D general geometry. Essential to have independent codes to cross-check on difficult turbulence problems.

* LAPD-like case with straight field lines: E.L. Shi, G.W. Hammett, T. Stoltzfus-Dueck, A. Hakim, J. Plasma Physics (2017) http://dx.doi.org/10.1017/S002237781700037X

* First extension to a helical model of a tokamak SOL including bad-curvature drive, for NSTX-type parameters:
  - "Gyrokinetic Continuum Simulation of Turbulence in Open-Field-Line Plasmas", Eric L. Shi, Ph.D. Dissertation, Princeton U., (Arxiv, 2017). https://arxiv.org/abs/1708.07283
  - “Full-f gyrokinetic simulation of turbulence in a helical open-field-line plasma” E.L. Shi et al., Phys. Plasmas 26, 012307 (2019) https://doi.org/10.1063/1.5074179

* Key papers (so far) on DG algorithms in Gkeyll:
  - J. Juno, A. Hakim, et al., J. Comp. Phys. (2018) https://doi.org/10.1016/j.jcp.2017.10.009
  - A. Hakim, M. Francisquez et al., 2019, “Conservative Discontinuous Galerkin Schemes for Nonlinear Fokker-Planck Collision Operators” https://arxiv.org/abs/1903.08062

Collaborated with Q. Pan, et al., extended GENE to full-F for SOL and LAPD-like straight fields : Q. Pan, D. Told, E. Shi, G. Hammett, F. Jenko (PoP 2018)

(* gwh: updated 4019.04.26.)

Gkeyll using novel algorithms, has multiple spinoffs

Novel version of Discontinuous Galerkin algorithm, conserves energy for Hamiltonian system even with upwinding. High-order algorithms that reduce communication costs helpful for Exascale computers.

4 Main Versions / spinoffs (consolidating kinetic versions some):

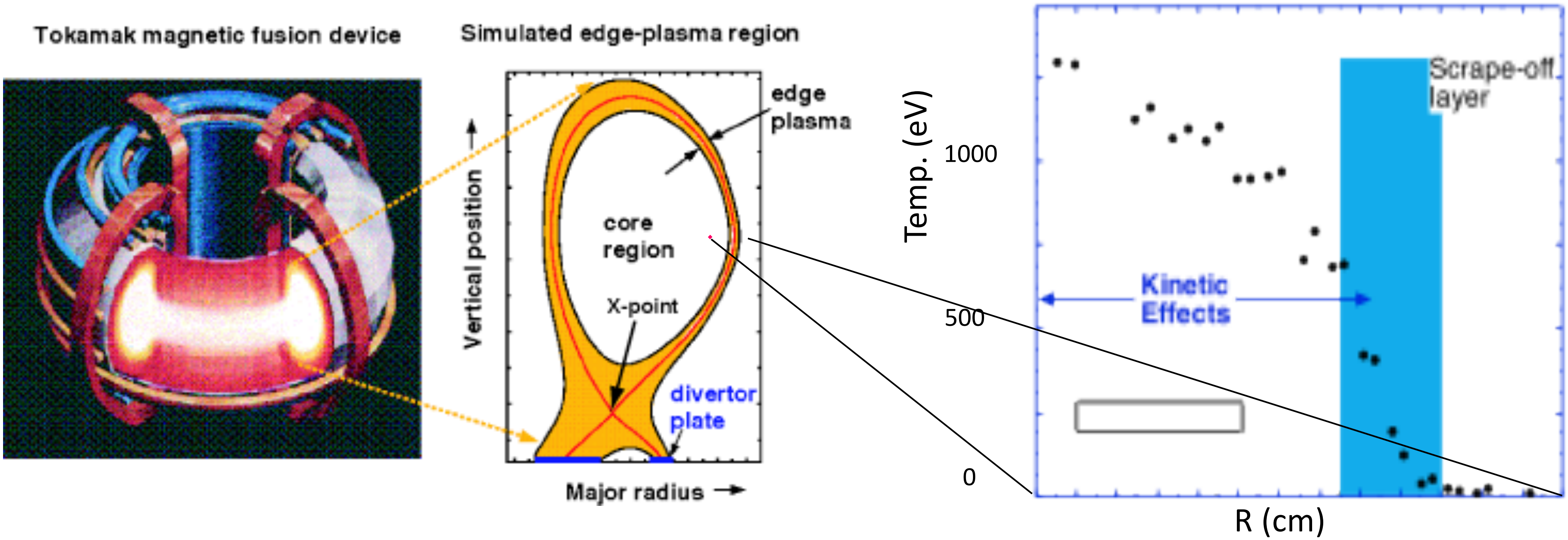
- Gyrokinetic DG version for edge turbulence in fusion
  NSTX: E. Shi et al. Phys. Plasmas (2019), Helimak: T.N. Bernard et al. Phys. Plasmas (2019), LAPD results: E. Shi,et al. J. Plasma Physics (2017), Shi Ph.D. 2017 (arxiv)

- Vlasov/Poisson DG version for plasma thrusters (AFOSR/Virginia Tech)
  Cagas et al. Phys. Plasmas (2017)

- Vlasov/Maxwell DG version for solar wind turbulence (U. Maryland, NSF)
  J. TenBarge, Sherwood Inv. Talk (2017), J. Juno et al., JCP 2018,
  Shocks in Laser-Plasma Interaction: Pusztai et al., (2018), Sundström (JPP 2019)

- Multi-moment multi-fluid (~extended MHD) finite-volume version, studying magnetospheres and reconnection (Princeton Center for Heliophysics).
  C. Dong et al. 2019 https://arxiv.org/abs/1904.02695 , J. Ng PoP 2015, L. Wang PoP 2015

Edge region very difficult



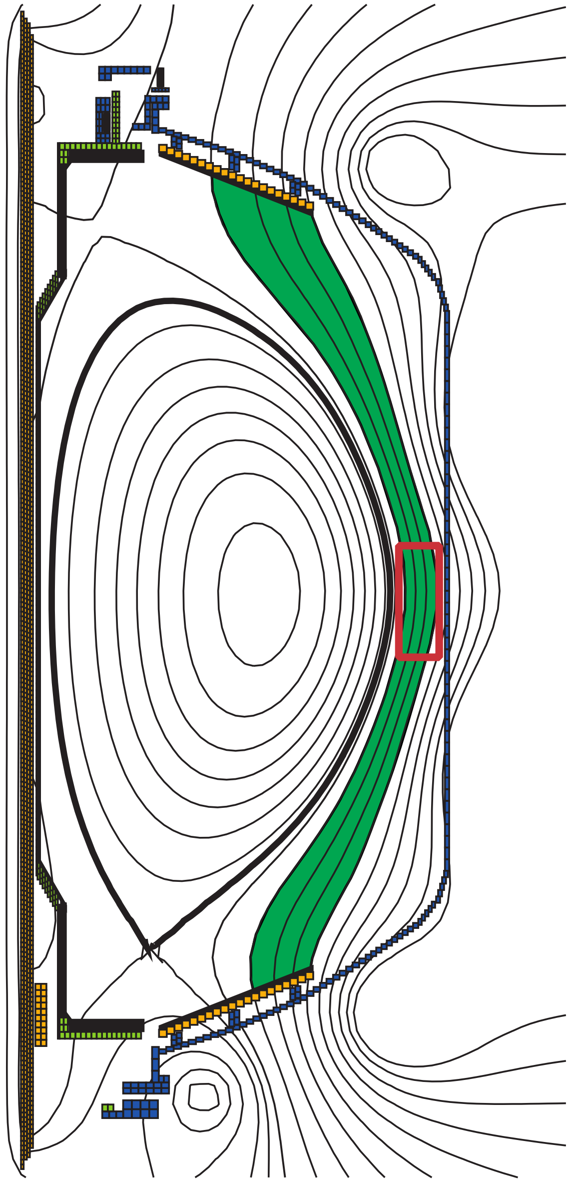
Edge pedestal temperature profile near the edge of an H-mode discharge in the DIII-D tokamak. [Porter*2000*]. Pedestal is shaded region.

Present core gyrokinetic codes are highly optimized for core, need new codes to handle additional complications of edge region of tokamaks (& stellarators):

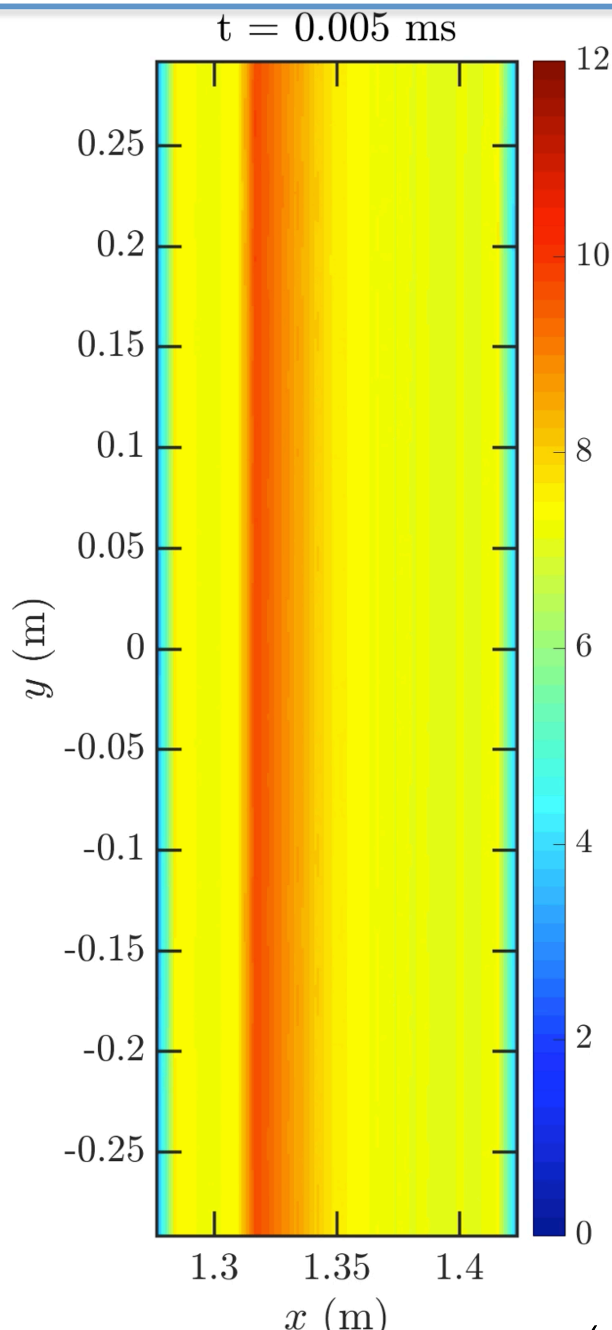
open & closed field lines, plasma-wall-interactions, large amplitude fluctuations, (positivity constraints, non-Maxwellian full-F), atomic physics, non-axisymmetric RMP / stellarator coils, magnetic fluctuations near beta limit, stable sheath model…

Hard problem: but success of core gyrokinetic codes and progress of XGC PIC code makes me believe this is tractable, with a major initiative

Gkeyll: First Continuum 5D Gyrokinetic Simulations of Turbulence in SOL with sheath model boundary conditions



Edge region has been computationally very difficult.



Various simplifications at present, such as helical model of SOL (toroidal + vertical B field).
XGC is only gyrokinetic turbulence code that can handle separatrix at present.

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(movie)

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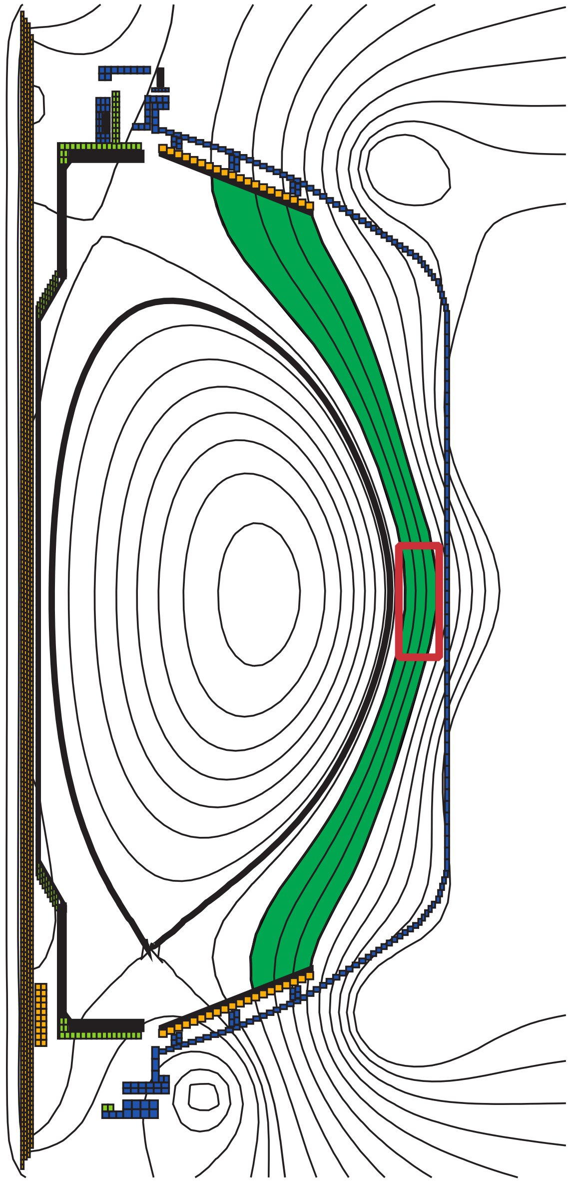

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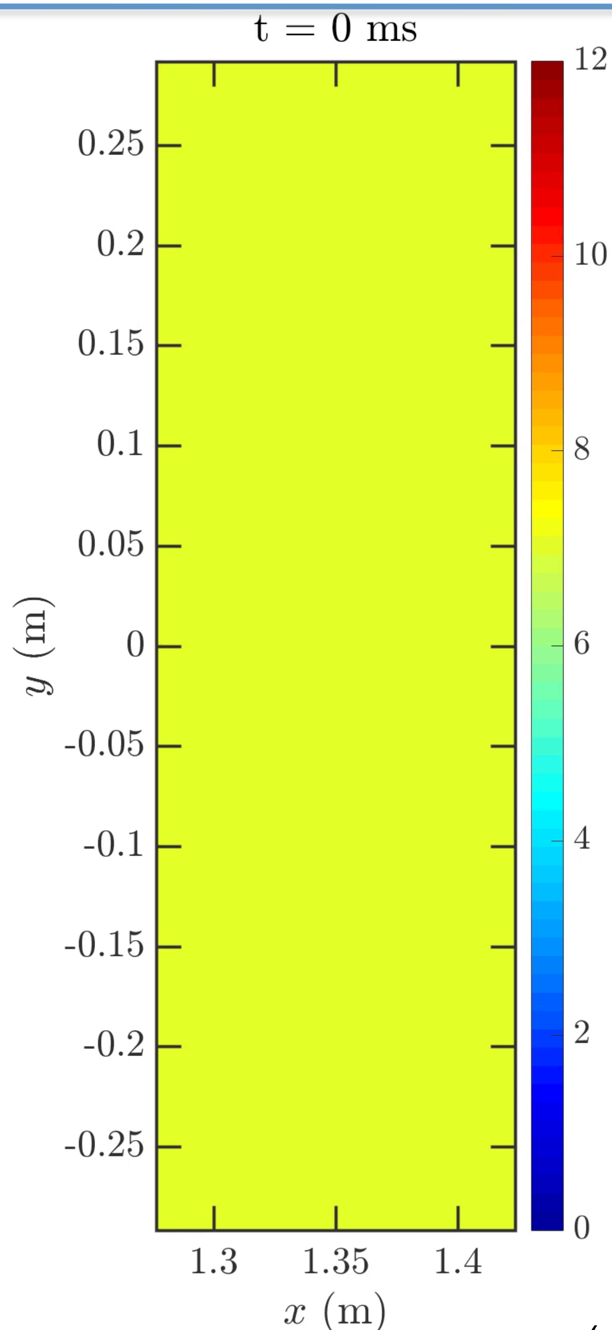

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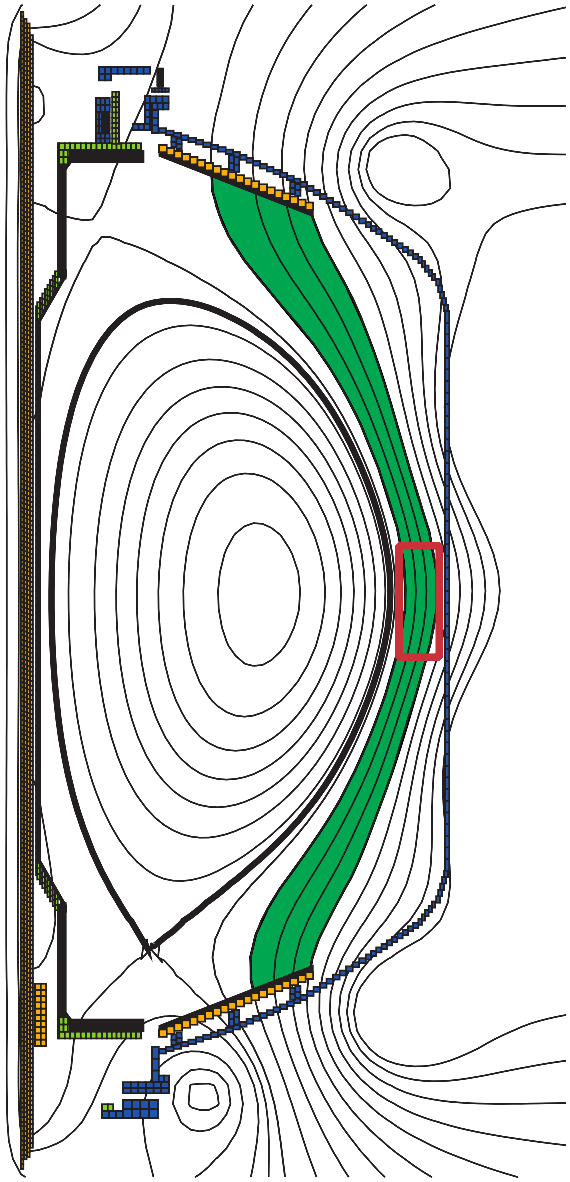

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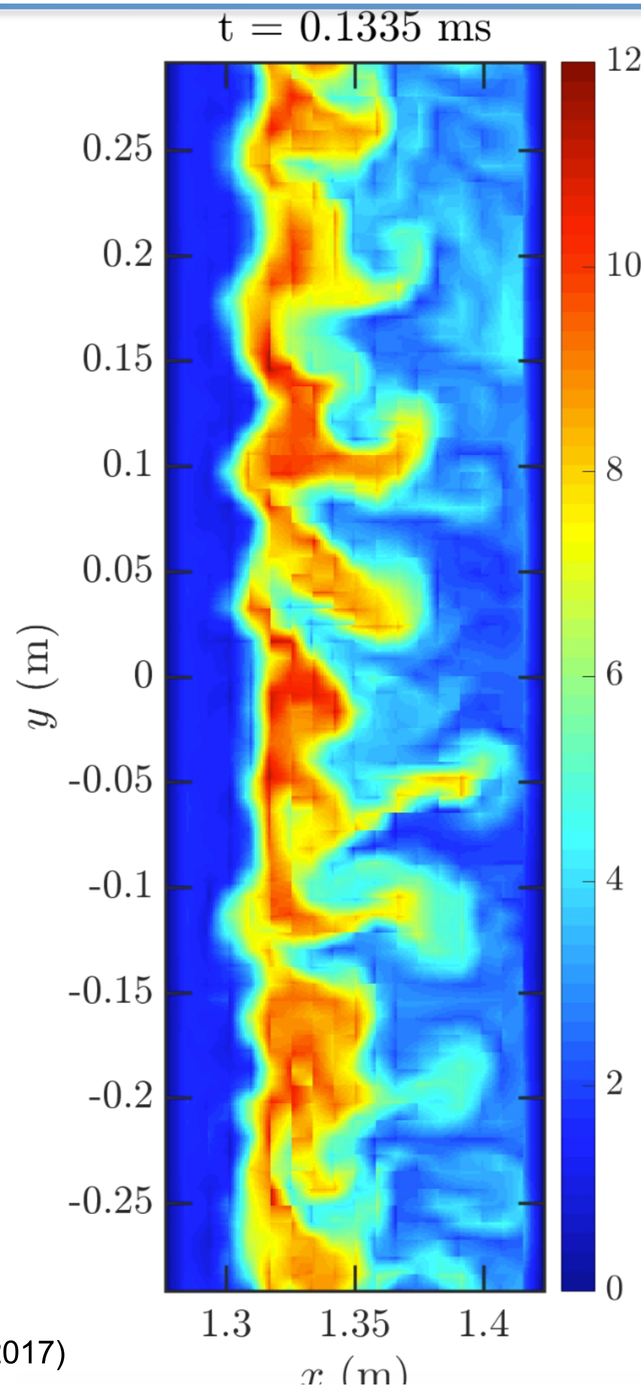

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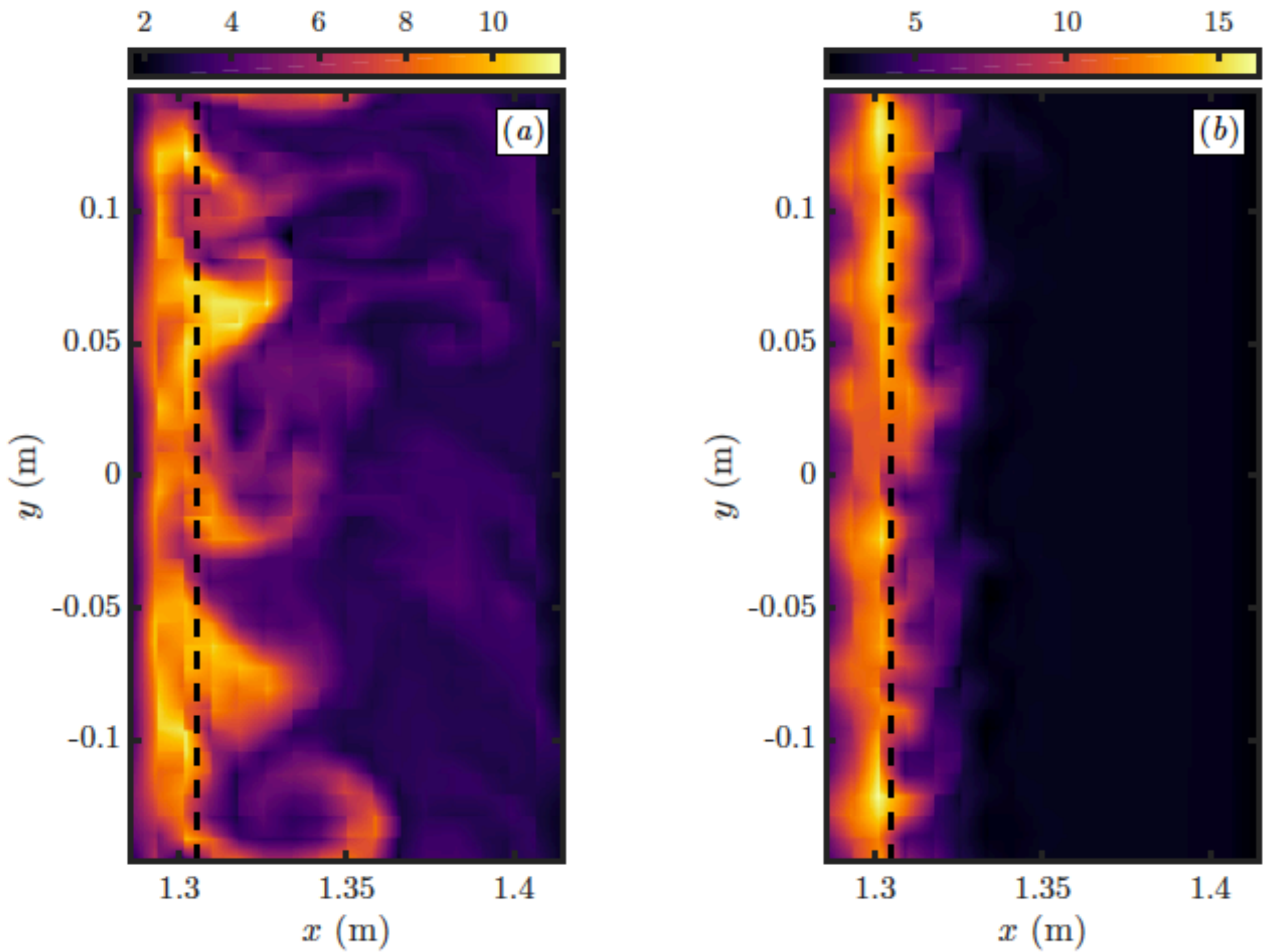
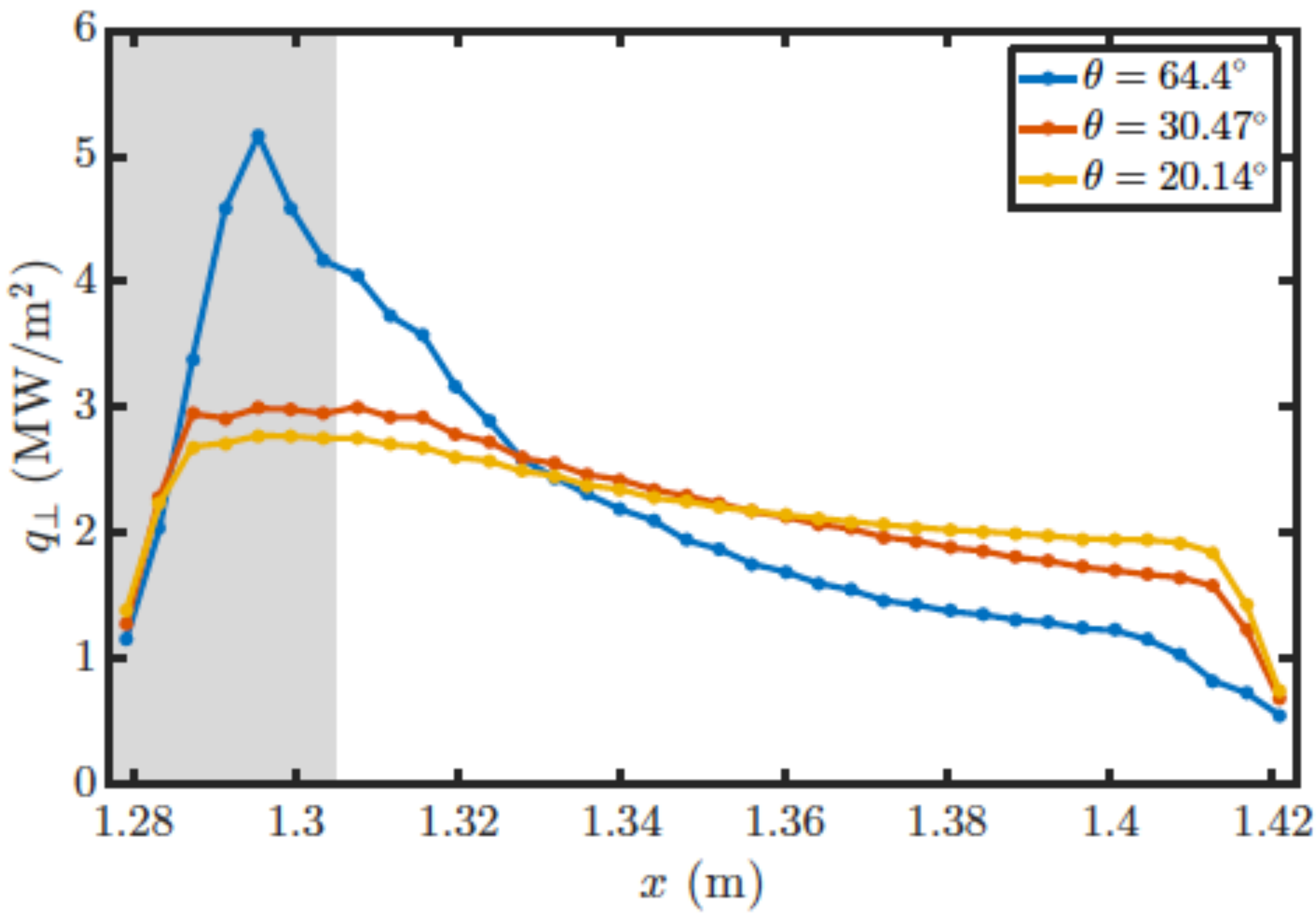
Toroidal case (left) vs. Slab case (right)



Clearly shows bad curvature enhances instability drive

Divertor heat flux broadens ~ theta ~ 1/B_pol



E. Shi (Ph.D. 2017)

(Present simulation neglects magnetic shear and related stabilization near x-point, shortened parallel length to divertor plates to approximately compensate.)

Larger amplitude & more intermittent blobs in far SOL

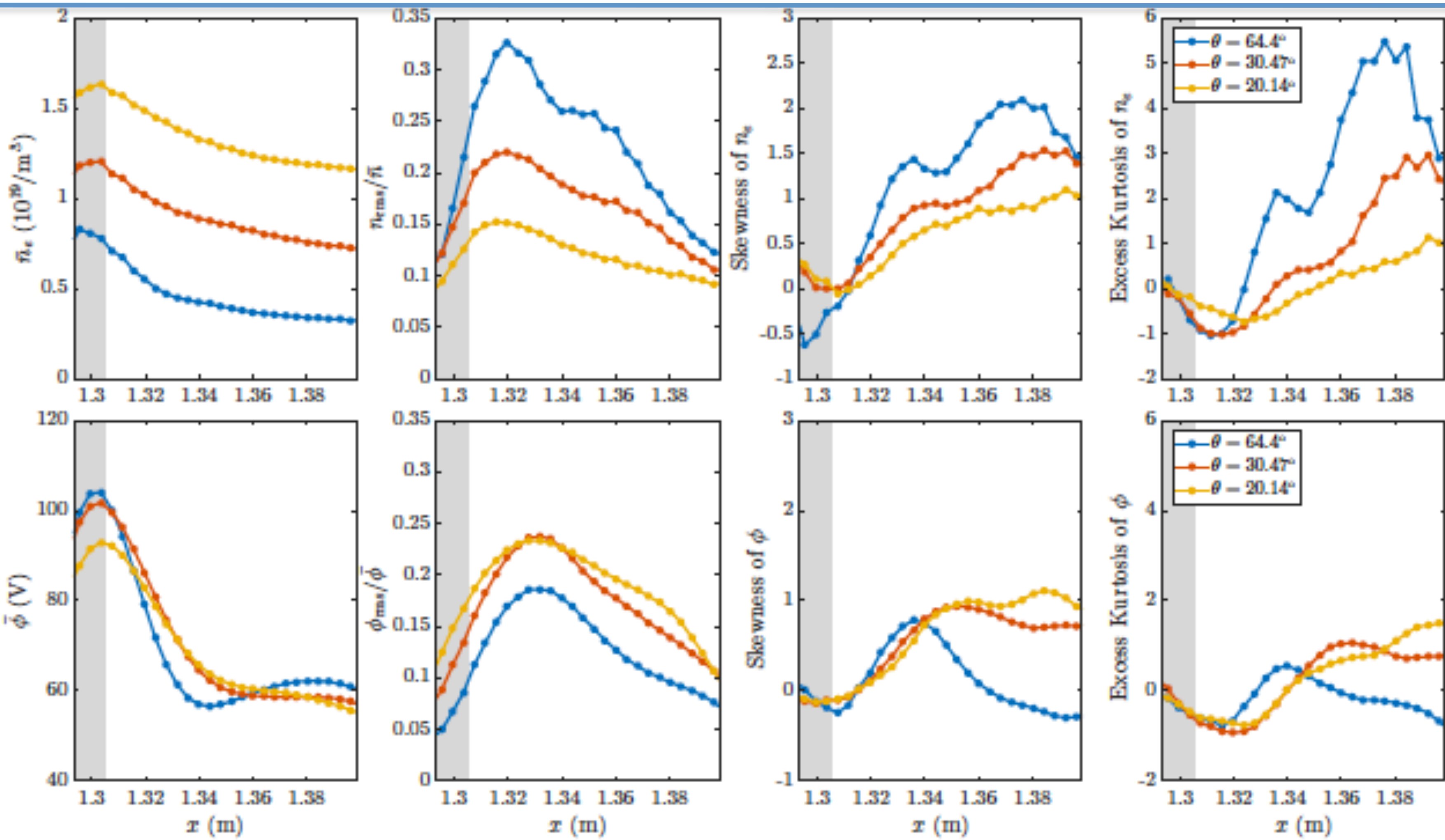


Figure 5.13: Electron density fluctuation statistics (top row) and potential fluctuation statistics (bottom row) computed near the $z = 0$ m plane for three cases with different magnetic field line incidence angle θ. The potential fluctuations are notably less intermittent than the density fluctuations. The shaded area indicates the region in which the source is concentrated.

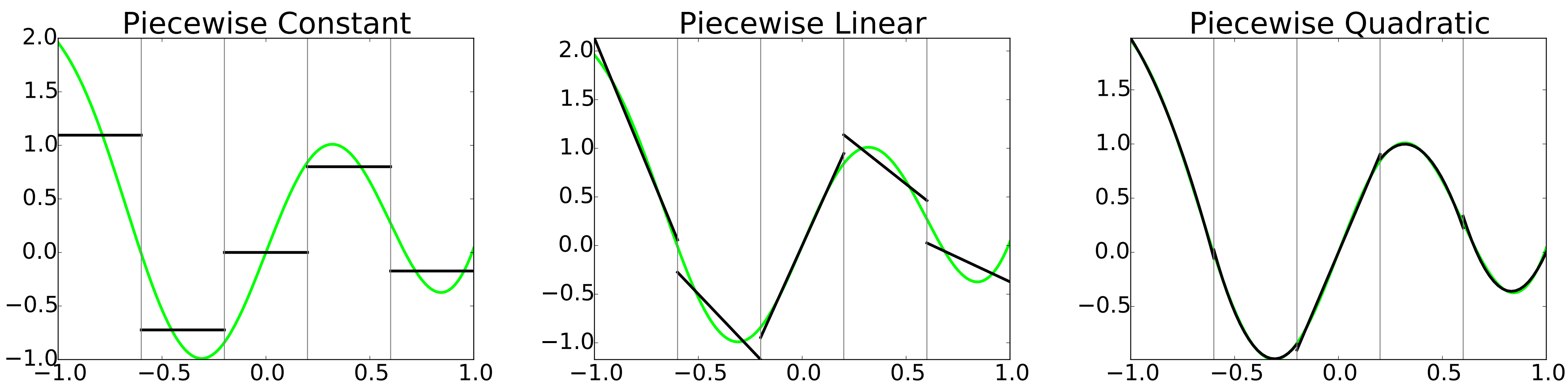
E. Shi (Ph.D. 2017)

Discontinuous Galerkin Algorithms

and modifications to ensure positivity of solution

(density of particles, energy, etc. should be non-negative,
otherwise may cause numerical problems with sheaths, collision operator, …)

Discontinuous Galerkin (DG) Combines Attractive Features of Finite-Volume & Finite Element Methods



Don't get hung up on the word "discontinuous". Simplest DG is piecewise constant: equivalent to standard finite volume methods that evolve just cell averaged quantities. Can reconstruct smooth interpolations between adjacent cells when needed.

Need at least piecewise linear DG for energy conservation (conserves energy even with upwinding). Standard Finite Volume methods do not conserve energy exactly for Vlasov-type problems (except Arakawa method, which can have artificial oscillations). Unlike Navier-Stokes fluid eqs., energy conservation in kinetic/Vlasov-Boltzmann equations is indirect, involving integration-by-parts and particle-field energy exchange.

Simple Example of the DG algorithm

The standard form of the Discontinuous Galerkin (DG) algorithm, illustrated on the simple passive advection problem:

$$\frac{\partial f(x,t)}{\partial t} = -v\frac{\partial f}{\partial x}$$

Within each cell (normalized to $x \in [-1,1]$), expand with piecewise-linear functions:

$$f(x,t) = \sum_j f_j(t) b_j(x) = f_0(t) + f_1(t)x$$

Require that the error projected onto the space of basis functions in each cell vanish, and integrate by parts to remove derivative on f:

$$\int dx\, b_j \frac{\partial f}{\partial t} = -\int dx\, b_j\, v \frac{\partial f}{\partial x} = -v\; b_j(x)\hat{f}(x)\Big|_{x_{j-1/2}}^{x_{j+1/2}} + v\int dx\, \frac{\partial b_j}{\partial x} f$$

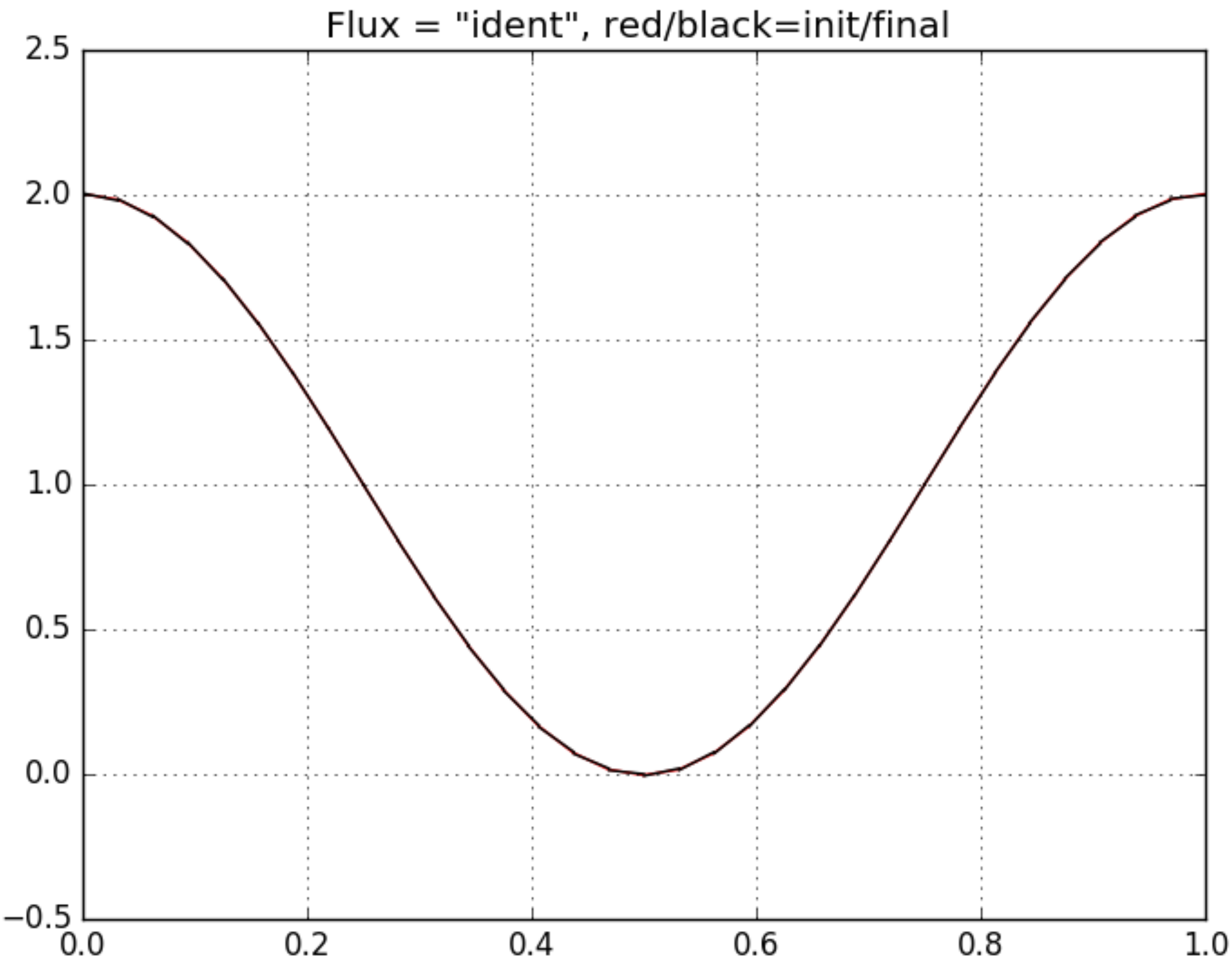
Define a unique (upwind) value at the boundary, $\hat{f}(x_{j+1/2})$. Using linear basis set:

$$df_0/dt = -v(f(x_{j+1/2}) - f(x_{j-1/2}))/\Delta x$$

$$df_1/t = -3v(x_{j+1/2}\hat{f}(x_{j+1/2}) - x_{j-/2}\hat{f}(x_{j-1/2}))/\Delta x + 6vf_0/\Delta x$$

and use an upwind flux, $\hat{f}(x_{j+1/2}) = f_0 + f_1$ for the j'th cell.

Standard DG on a simple advection problem works well for smooth initial conditions.



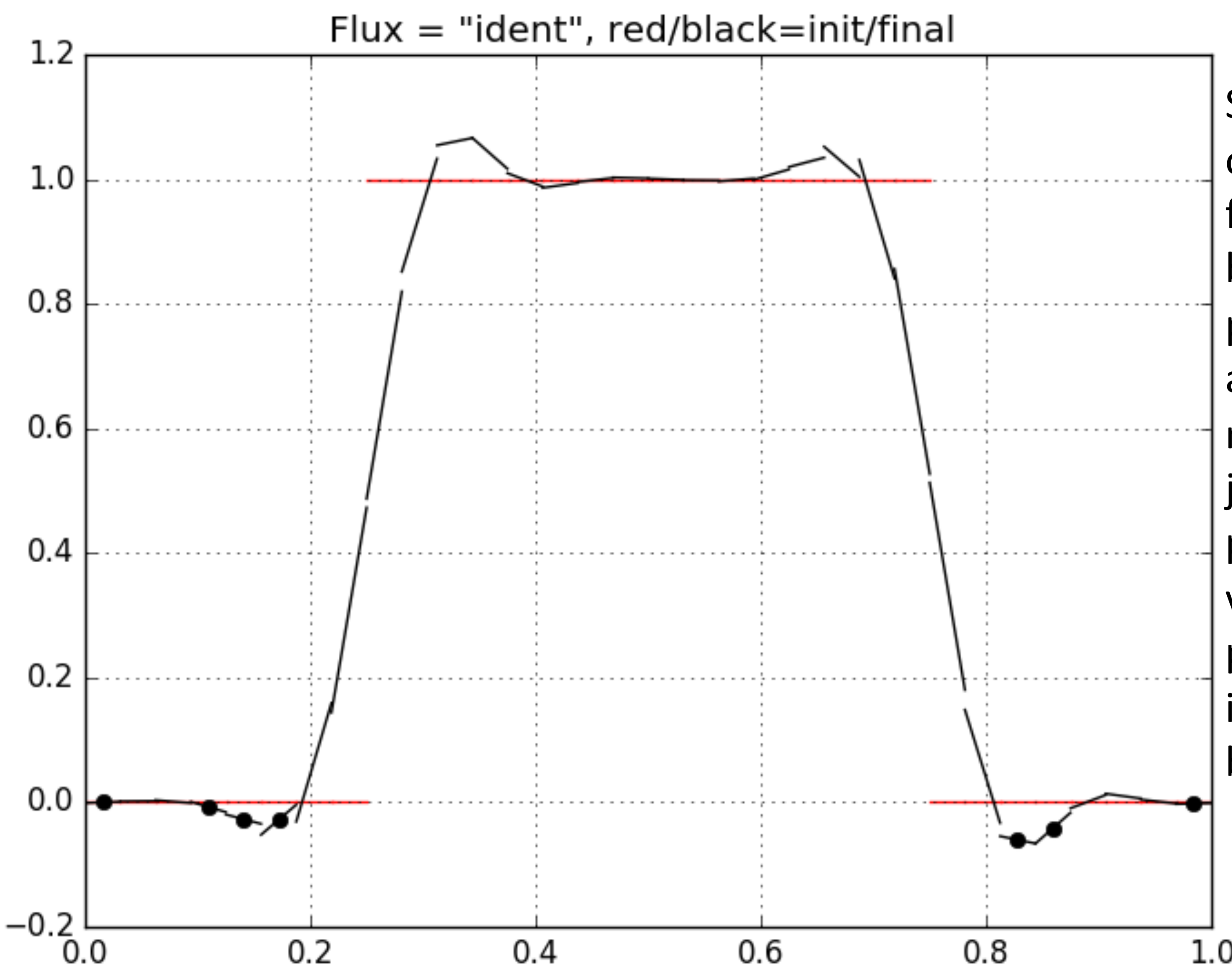
Solution of

$$\frac{\partial f}{\partial t} = -v\frac{\partial f}{\partial x}$$

with periodic boundary conditions. After 1 period, the solution (black) overlays the initial condition (red) very well.

(N_x = 32 cells)

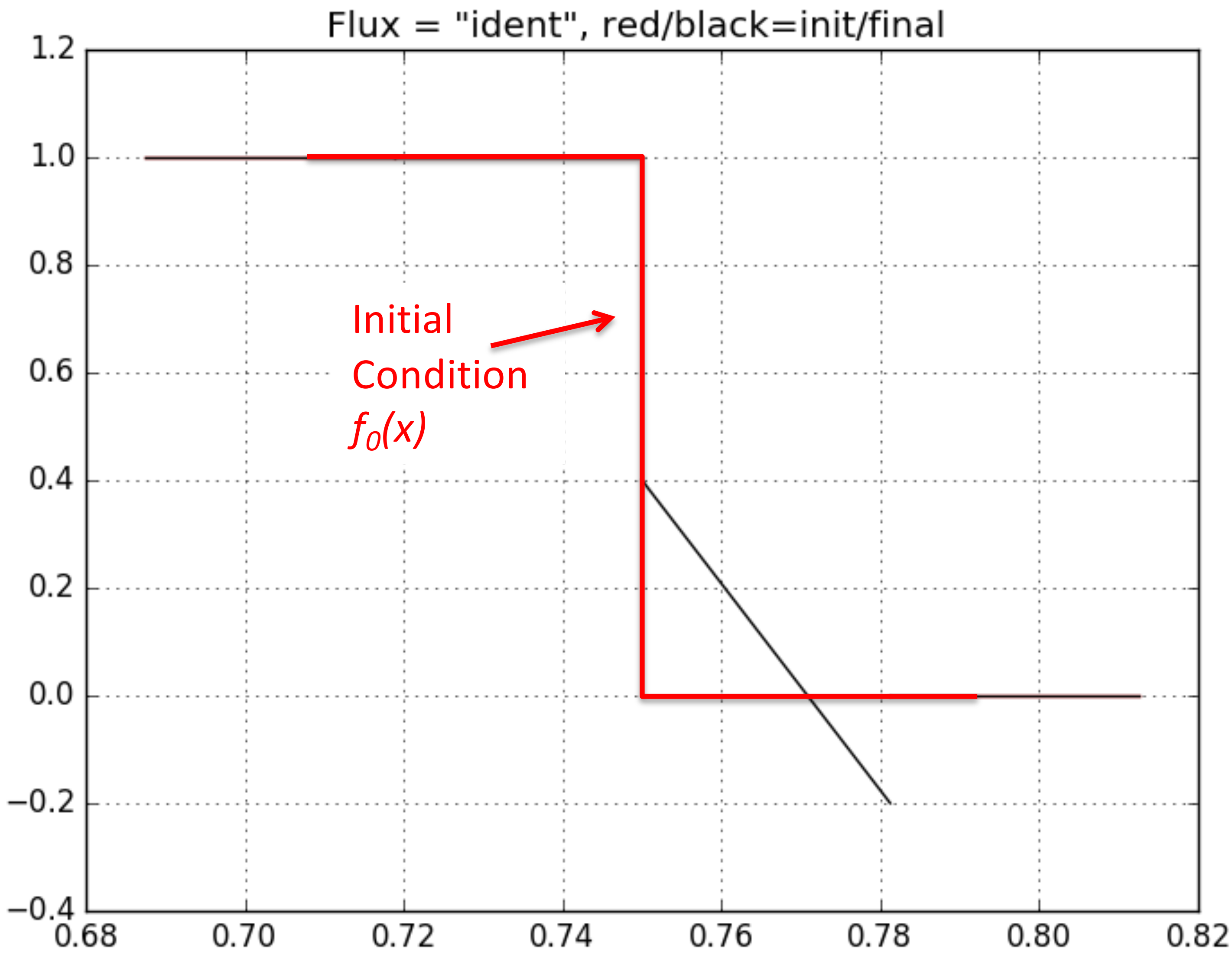
Standard DG approximately ok on discontinuous case, but negative overshoots bad for plasma



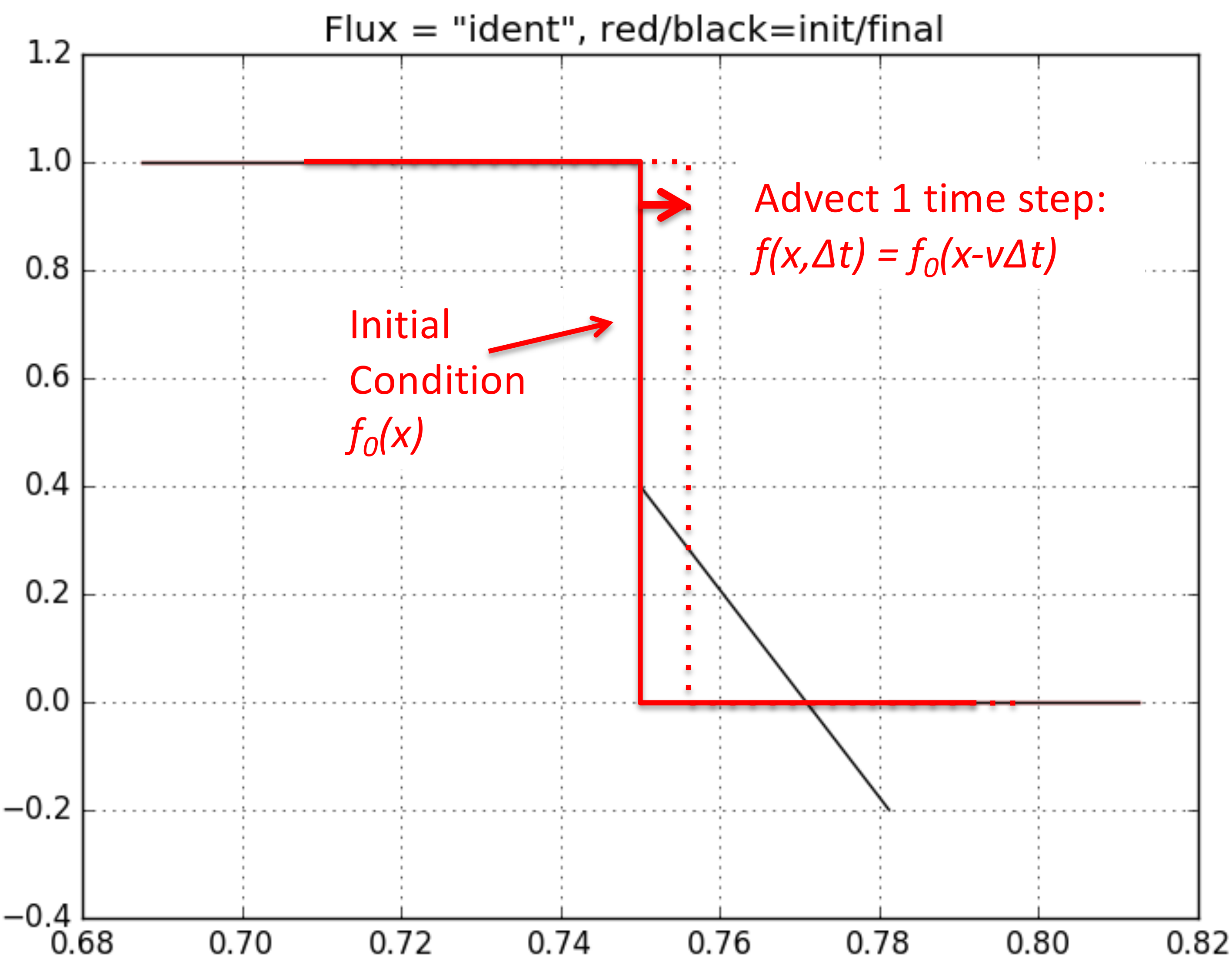
Small negative overshoots not a big deal for some applications, but might cause serious problems for other applications. Negative mass densities, or even just negative f in part of phase space, might cause various problems in plasmas, or in their interaction with sheath boundary conditions.

(Dots indicate f_0 in cells with mean f_0<0.)

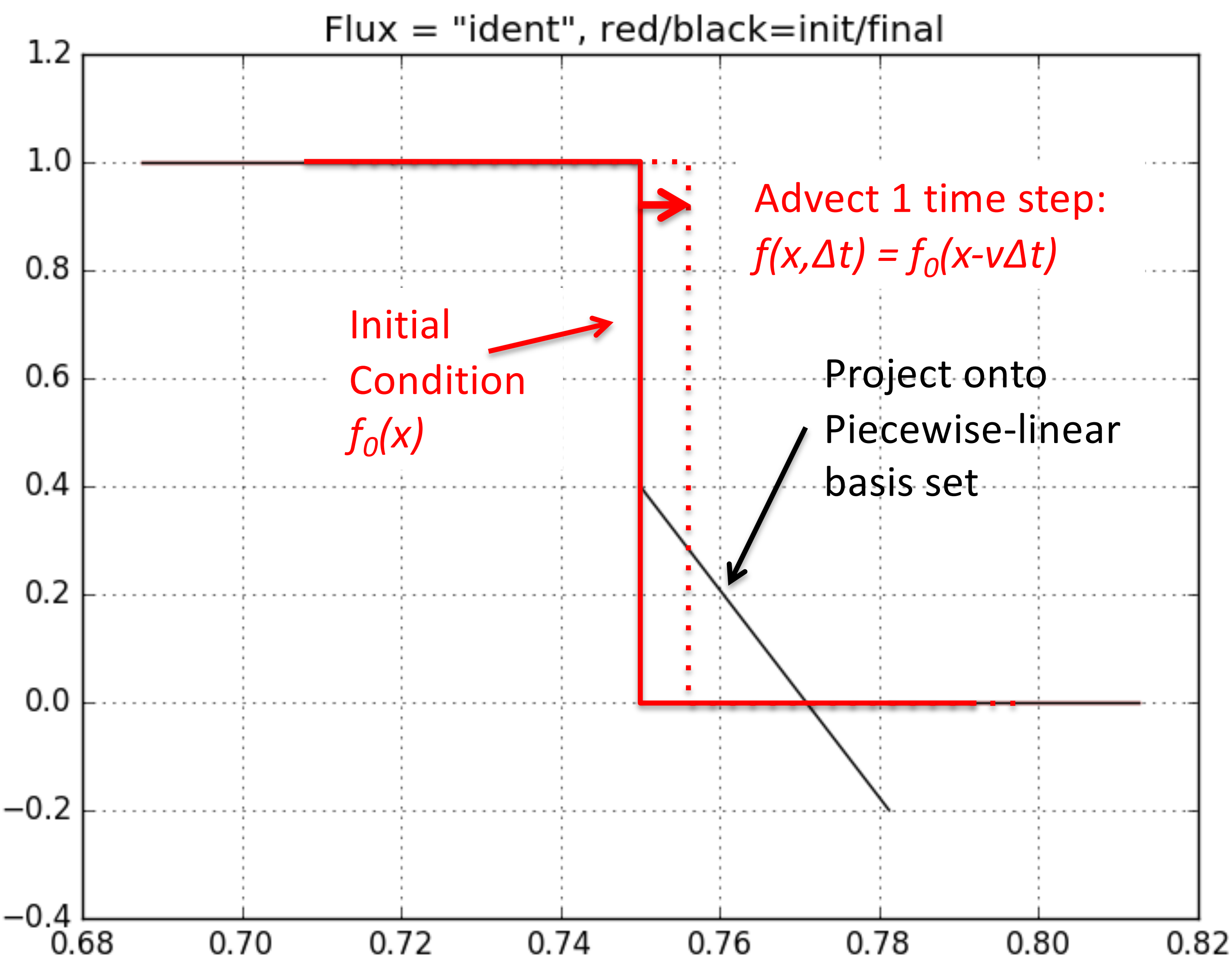
First place where f goes <0 is leading edge, Here is algorithm sequence for 1st step



First place where f goes <0 is leading edge, Here is solution after 1 time step



First place where f goes <0 is leading edge, Here is solution after 1 time step



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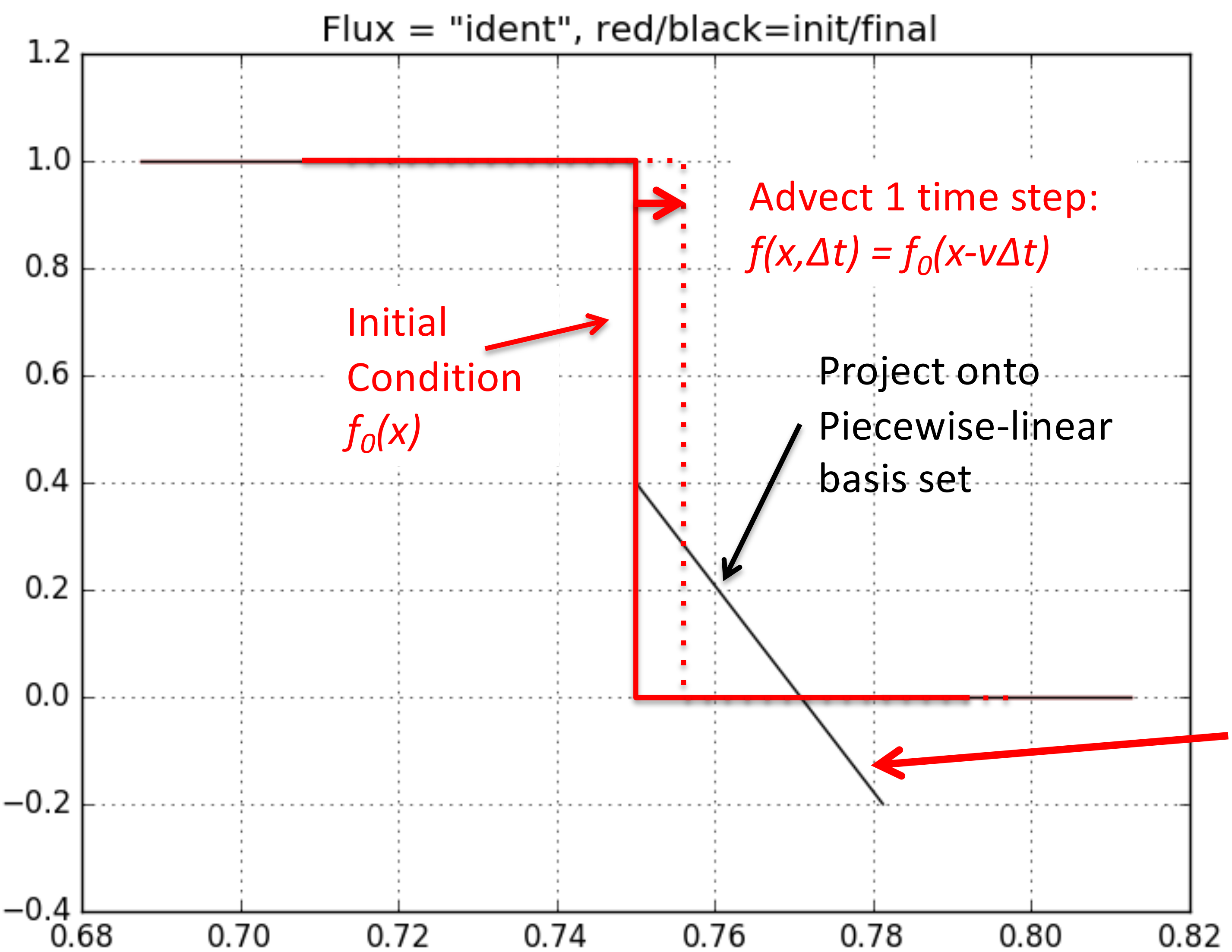
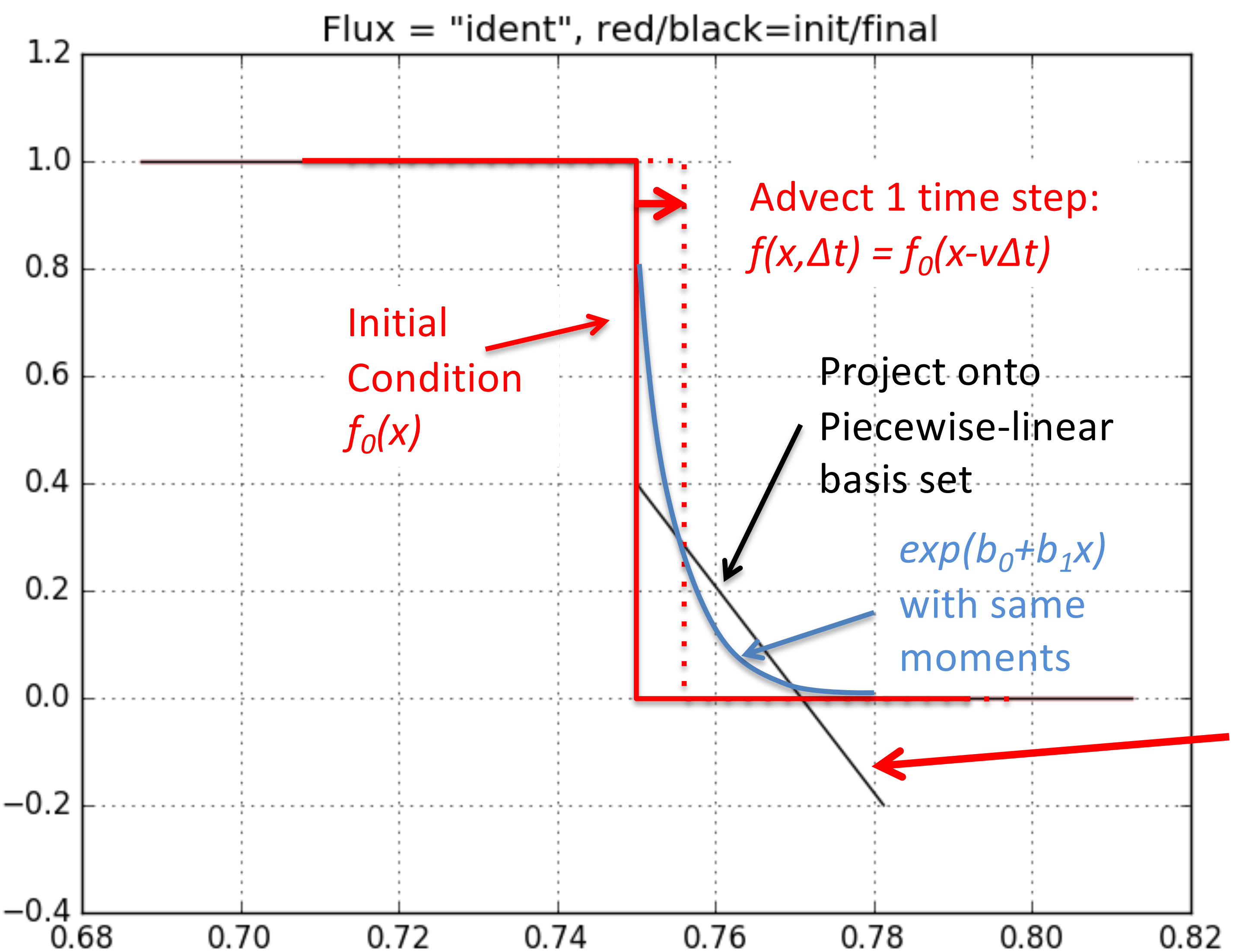


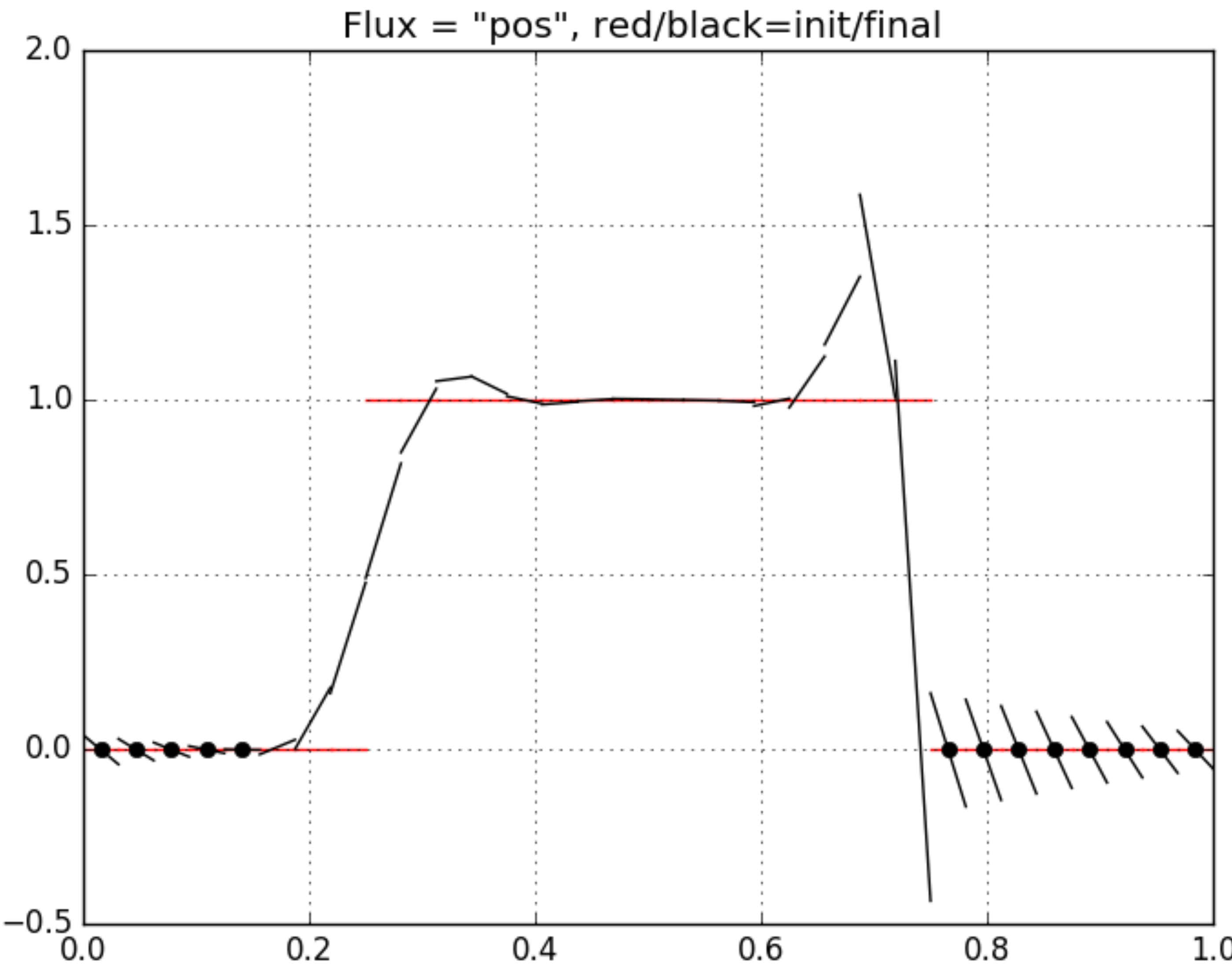
After 1st time step, some of f advects into the left edge of this cell, making the solution in this cell is very steep. Then on the next step a negative f advects into the cell on its right.

First place where f goes <0 is leading edge, Here is solution after 1 time step



After 1st time step, some of f advects into the left edge of this cell, making the solution in this cell is very steep. Then on the next step a negative f advects into the cell on its right.

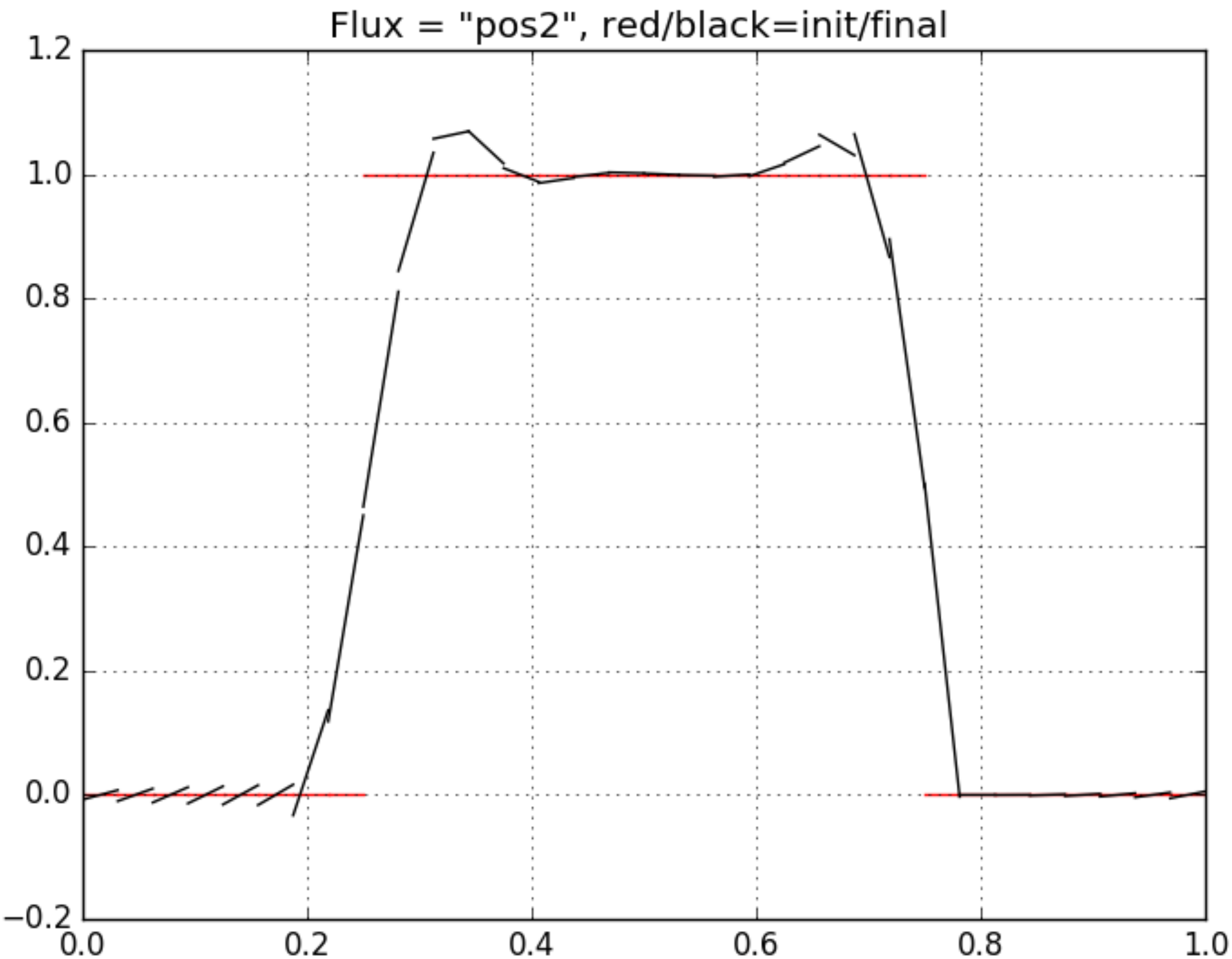
To avoid negative f going into a cell, restrict extrapolation to cell boundary $f_L >= 0$. BAD!



Get unphysical result! The mean f still goes (slightly) negative in some cells. But worse is that slopes go wild, get very large. Slopes are so steep that there is no realizable f(x) that has the same moments and remains positive.

If you first observe this in a 5D code, give up for a while because it's hard to diagnose and just use the older method that was more diffusive.

Also enforcing extrapolation $f_L < f_0 / (v\Delta t/\Delta x)$ ensures avg $f_0 > 0$, but slopes still unphysical



How can slopes get so large? (Have to *enhance* the flux, not limit it.)

How can the slope become unphysically too large? Consider the simple case of a cell with nothing flowing into it ($f_{j-1/2} = 0$), and solve the equations only for the outflow. Then can show

$$df_0/dt = -vf_{j+1/2}/\Delta x$$

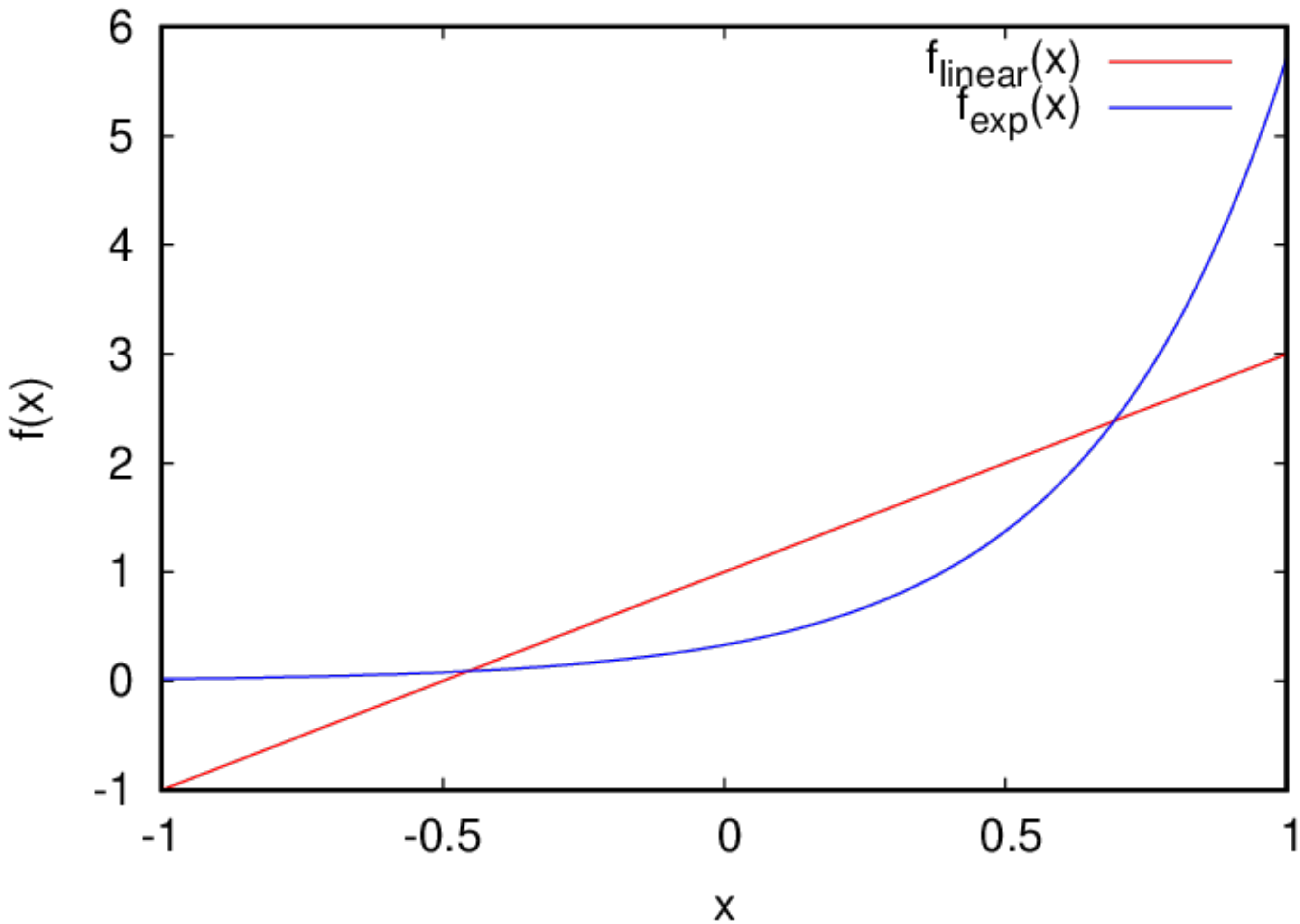
$$df_1/t = -3vf_{j+1/2}/\Delta x + 6vf_0/\Delta x$$

Differentiating $\bar{x} = f_1/(3f_0)$ then gives:

$$\frac{d\bar{x}}{dt} = v\left(2 - (1-\bar{x})\frac{f_{j+1/2}}{f_0}\right)$$

As $\bar{x}$ approaches 1, $\bar{x}$ will continue to grow and will exceed the physical limit, unless $f_{j+1/2}$ is *enhanced* over a linear extrapolation. This is different than most limiters, which would *reduce* the extrapolation.

Linear reconstruction with $f_{lin}(x)<0$ some places not necessarily bad, a realizable f(x) can exist that has the same moments.



In our earlier work, we were overly restrictive and required

$$f_{lin}(x) = f\_0 + f\_1\ x > 0$$

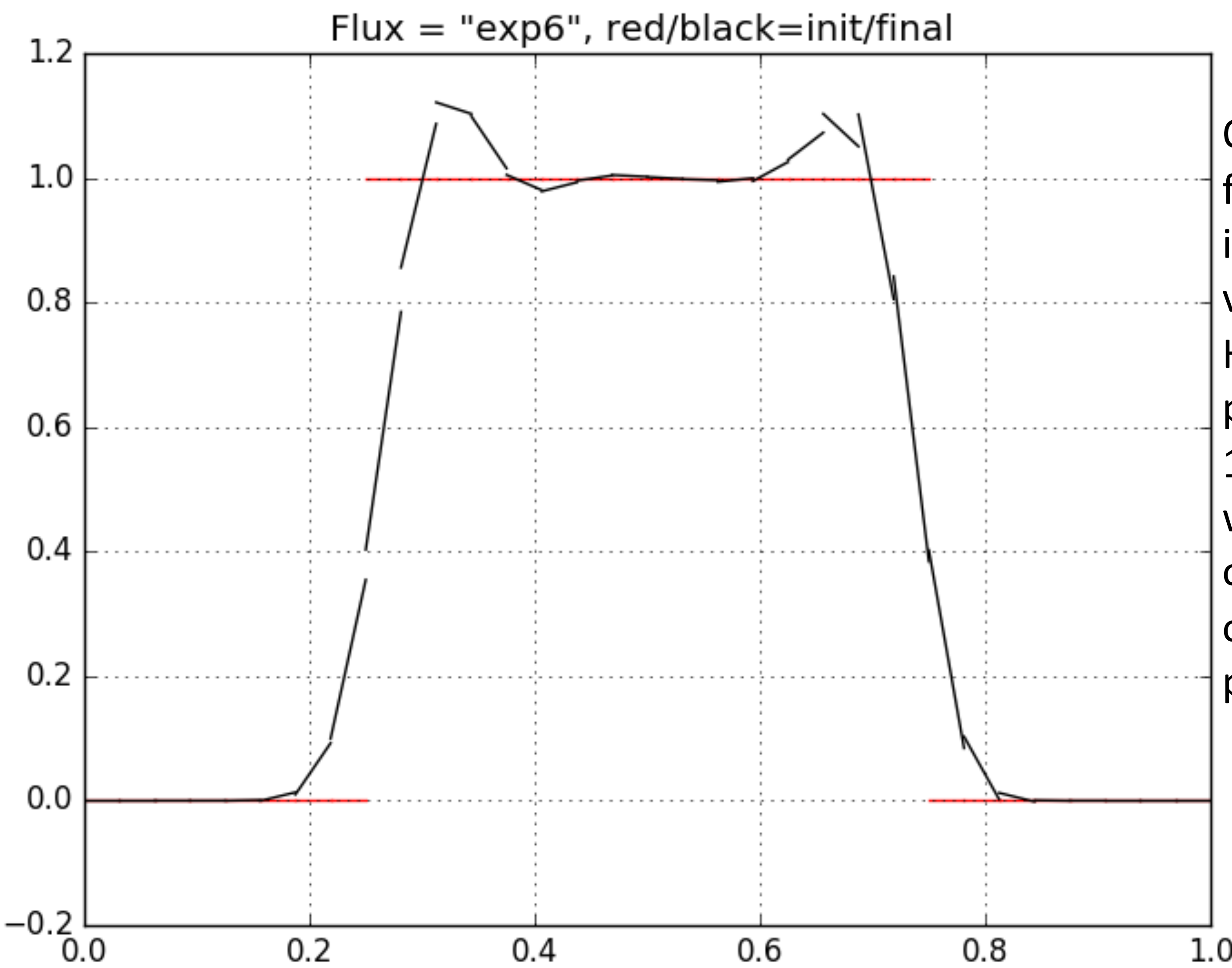
for all x in the cell. But even if $f_{lin}(x) < 0$ in some places, there can be an equivalent exponential reconstruction

$$f(x) = c \exp(\text{ beta } x)$$

with the same moments but that is >0 everywhere.

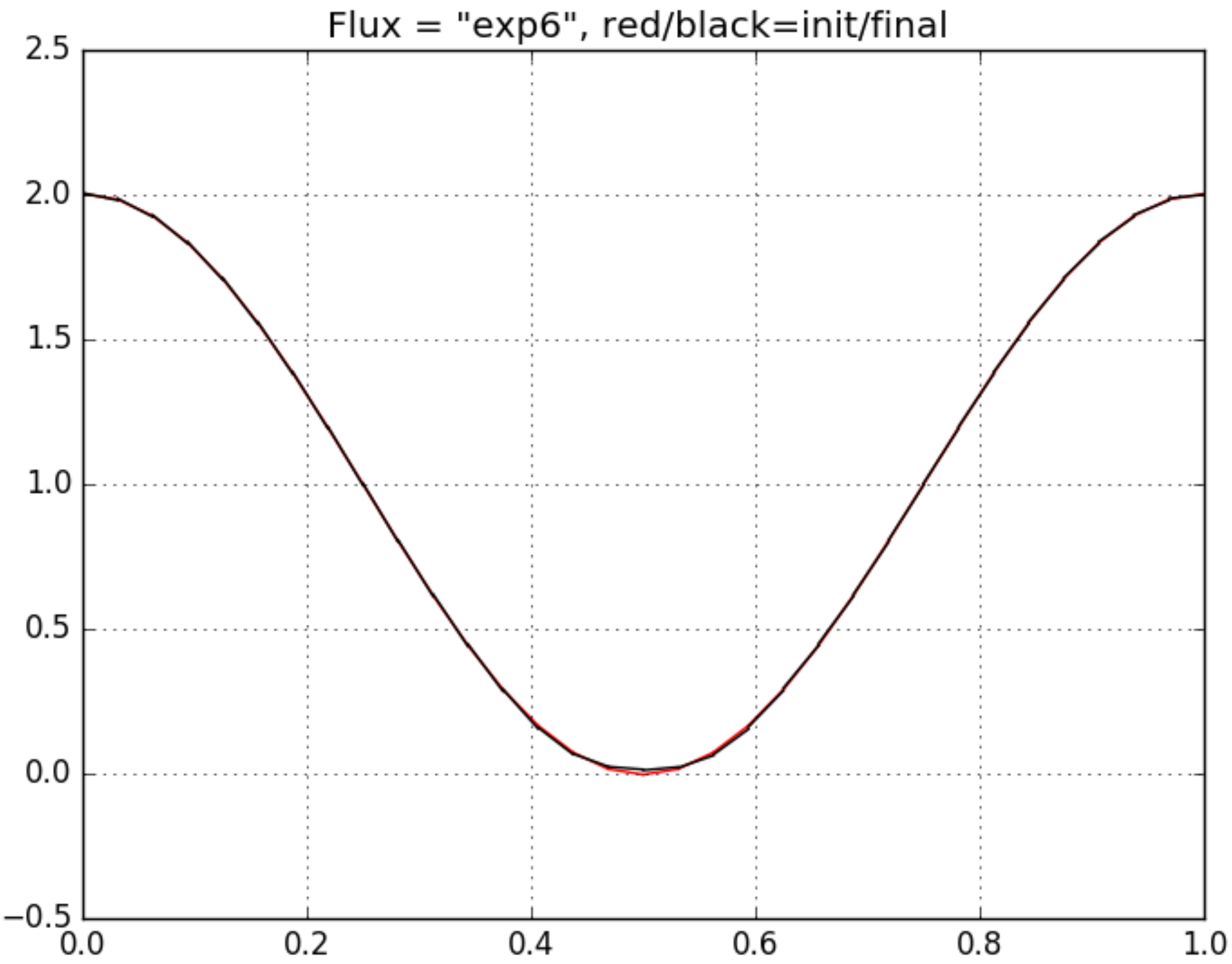
However, this works only as long as <x> = f_1 / (3 f_0) lies within the range -1 < <x> < 1. If the slope to mean ratio is too large, |f_1|/f_0 > 3, then there is no non-negative f(x) with the right moments.

DG with exponential reconstruction completely fixes f<0 problems.



Overshoots away from f=0 can also be improved in the future, using DG variants of the Suresh-Huynh monotonicity-preserving limiters (JCP 1997), perhaps with a weaker “essentially non-oscillatory” goal instead of a strict monotonicity-preserving requirement.

DG with exponential reconstruction continues to work well for smooth solutions.



Implementing exponential reconstruction in DG

To implement exponential reconstructions in this conservative DG form, the only modification to the DG algorithm is in the extrapolation to the boundary terms. I.e., one advances the same set of moment equations in time:

$$\int dx\, b_j \frac{\partial f}{\partial t} = -v\, b_j(x)\hat{f}(x)\Big|_{x_{j-1/2}}^{x_{j+1/2}} + v\int dx\, \frac{\partial b_j}{\partial x} f$$

But now the extrapolation to the boundary, $\hat{f}(x_{j+1/2})$ is based on an exponential function

$$\hat{f}(x) = f_0 \frac{2\beta}{\exp(\beta) - \exp(-\beta)} \exp(\beta x)$$

that reproduces the given moments $f_0 = \langle f \rangle$ and $f_1 = \langle x f(x) \rangle$, where β is a function of $\bar{x} = f_1/(3 f_0)$.