Extension of Discontinuous Galerkin Algorithms to Preserve Locality of Parallel Gyrokinetic Dynamics

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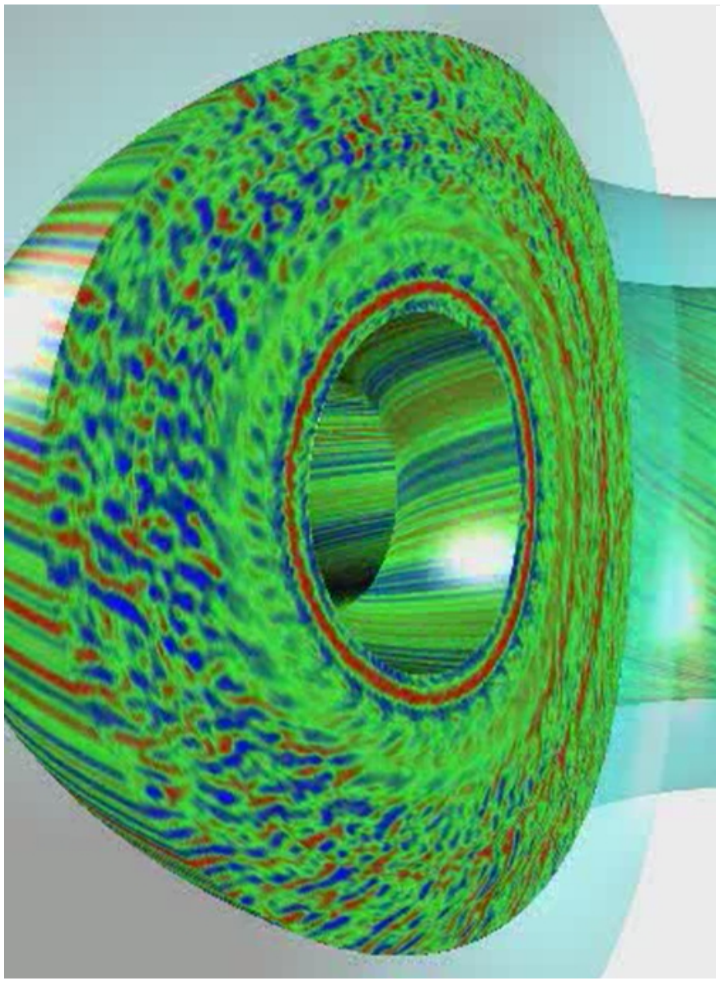
Advanced Algorithms / DG May Help With Challenge of Edge Plasma Turbulence

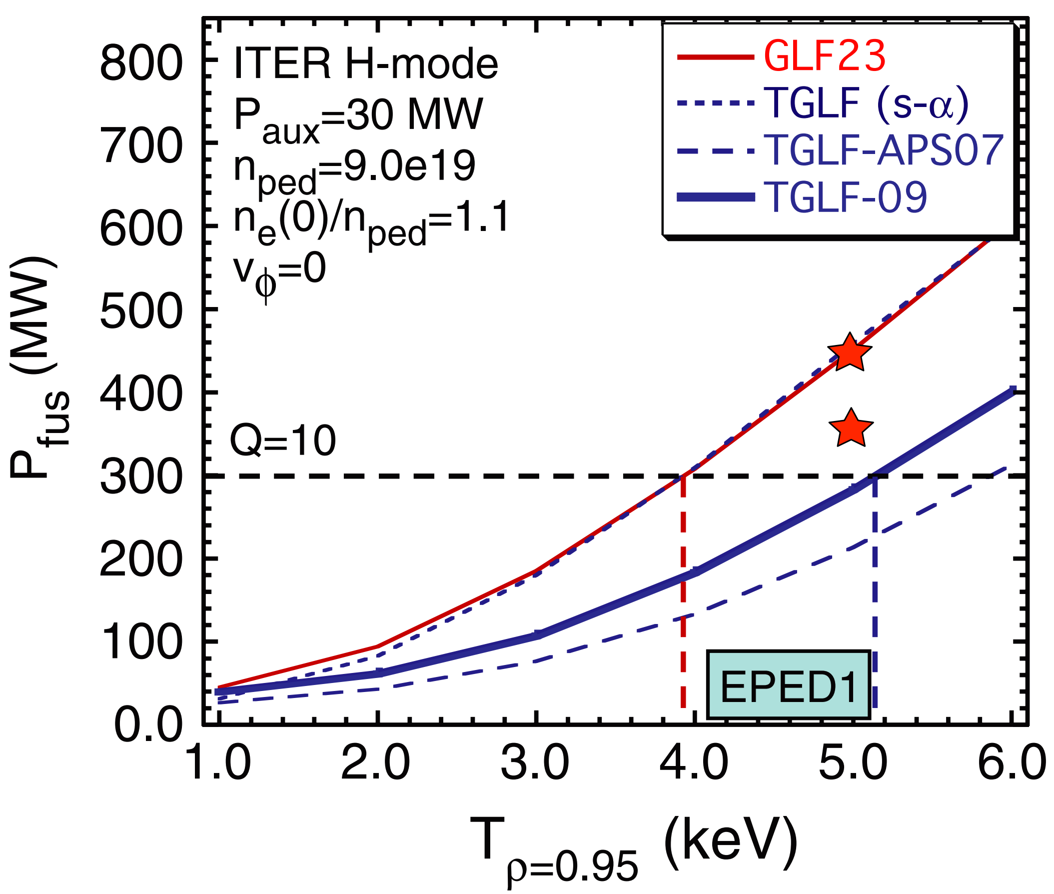


GYRO simulation, Candy & Waltz 2006

Significant success in fusion research in 5D gyrokinetic simulations of turbulence in the core region of tokamaks using continuum/Eulerian algorithms (such as GENE (Jenko et al.) GYRO (Candy & Waltz)). Different than PIC/Lagrangian algorithms, these are “Vlasov codes” with grids in velocity space, spectral & other advanced algorithms. (Always useful to have independent algorithms to cross-check. Different algorithms may be best for different problems.)

These continuum codes are highly optimized for core region of tokamaks (nested magnetic surfaces, simple b.c., small amplitude fluctuations). Major extensions or new code needed to handle the edge region. Advanced algorithms (variations of discontinuous Galerkin, sub-grid models in phase space) could help with additional challenges of edge region. Continuum algorithms strengths for edge turbulence include their low noise and demonstrated capability of handling fully electro-magnetic fluctuations.

Fusion Motivation: Need comprehensive simulations of edge turbulence, because predicted fusion performance is a strong function of edge temperature

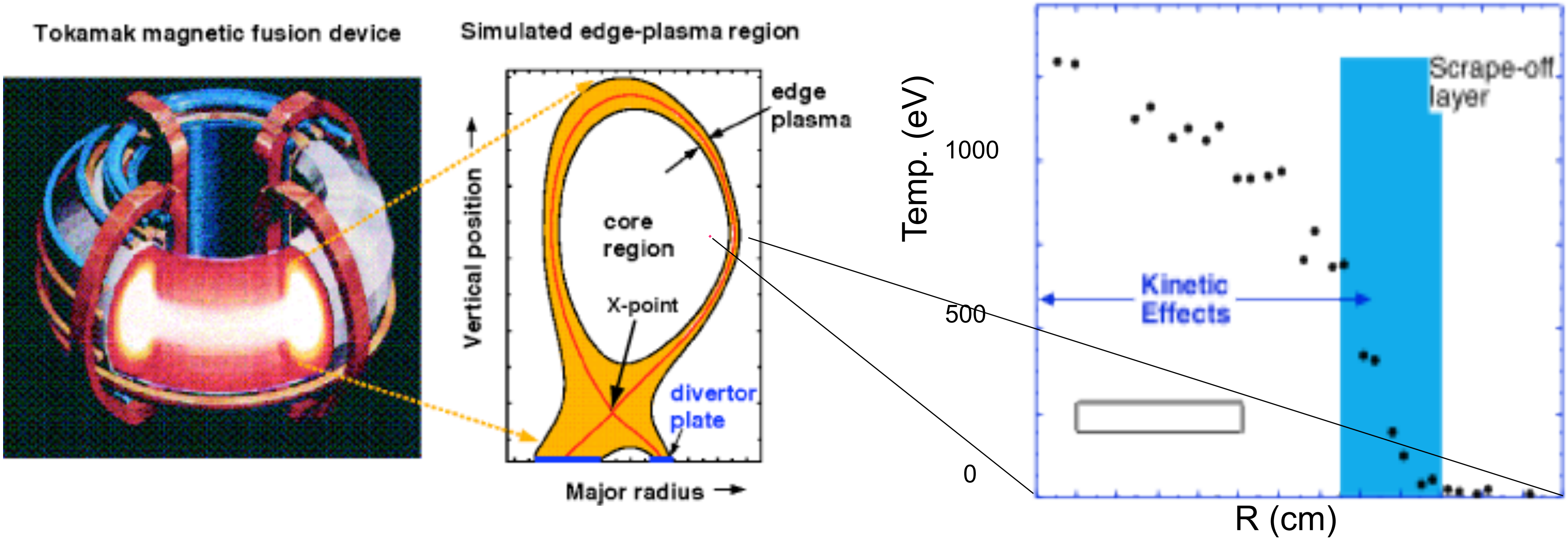


Need to understand and predict power threshold for H-mode transport barrier formation, height of the pedestal, spontaneous rotation mechanisms, ways to suppress ELMs, improvements with lithium walls.

Hard problem, but tractable: continuum gyrokinetic codes very successful in understanding tokamak core, but need extension to handle additional complexities of edge turbulence: large amplitude fluctuations, separatrix and open/closed field lines, ...

Kinsey et al. Nucl. Fus. 2011 http://stacks.iop.org/NF/51/083001

Edge region very important



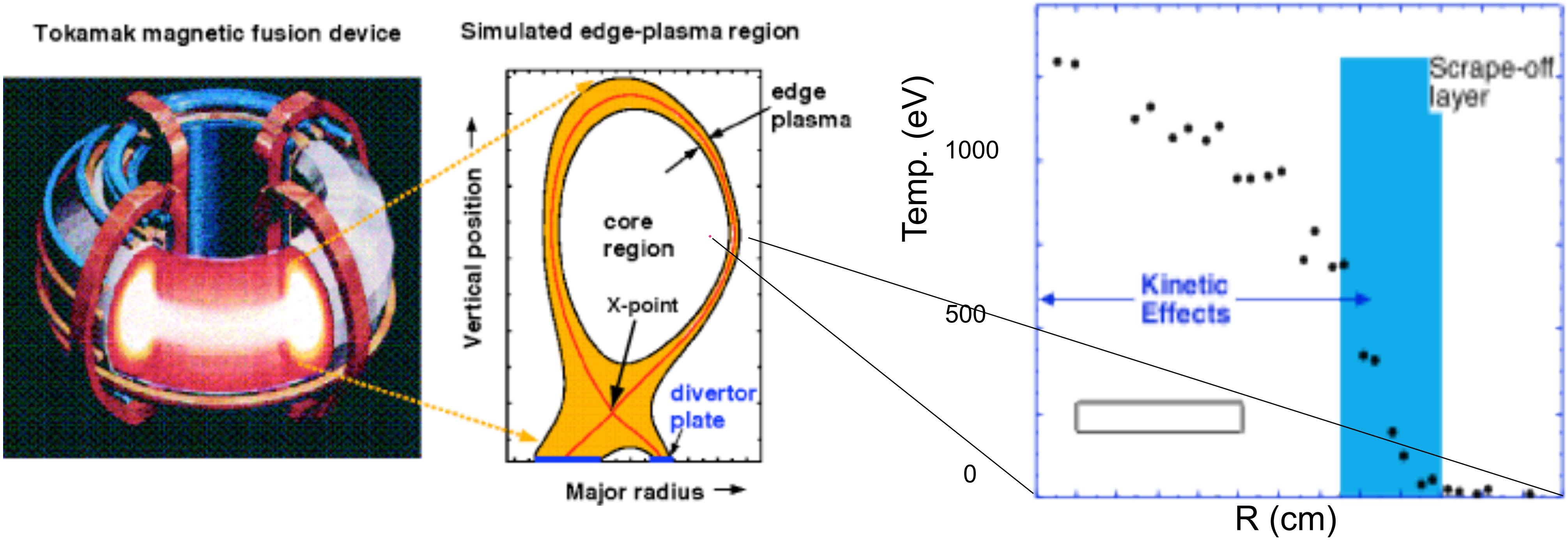
Edge pedestal temperature profile near the edge of an H-mode discharge in the DIII-D tokamak. [Porter*2000*]. Pedestal is shaded region.

- Need sufficiently high pedestal temperature for core to get to fusion temperatures

- Periodic instabilities in edge region can dump outer ~5-10% of plasma onto divertor plates. Might be manageable, or divertor erodes, melts?

- Is there a way to use breaking of up-down symmetry in tokamaks (or “stellarator symmetry” in quasi-symmetric stellarators) and enhance spontaneous flows (to reduce turbulence)?

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.

Major extensions to gyrokinetic codes needed to handle additional complications of edge region of tokamaks (& stellarators):

> open & closed field lines, steep gradients near beta limit, electric & magnetic fluctuations, strong shear-flow layers, steep-gradients and large amplitude fluctuations, positivity constraints, wide range of collisionality, non-axisymmetric RMP coils, plasma-wall interactions, strong sources and sinks in atomic physics.

A new code with these capabilities will also be more robust for a wider range of astrophysics applications.

Exploring Several Advanced Algorithms

Will explore several advanced algorithms, including some of our own ideas:

- extension of DG to preserve separability of GK Poisson solver and conservation properties

- DG-FV hybrids and other advances in limiters to minimize numerical diffusion

- subgrid models for higher-dimensional phase-space, guided by other subgrid models and Landau-fluid experience, to make code more robust on coarse grid.

- Maxwellian-weighted basis functions for v-space (while preserving conservation properties) to improve robustness on course grids.

Certain types of DG have excellent conservation properties even at coarse velocity resolution. Numerical diffusion only along contours of constant energy, thus preserving energy conservation!

Goal: a robust code capable of running very quickly at coarse velocity space resolution while preserving all conservation laws of gyro-fluid/fluid equations and giving fairly good results. Can occasionally turn up velocity resolution for rigorous convergence tests.

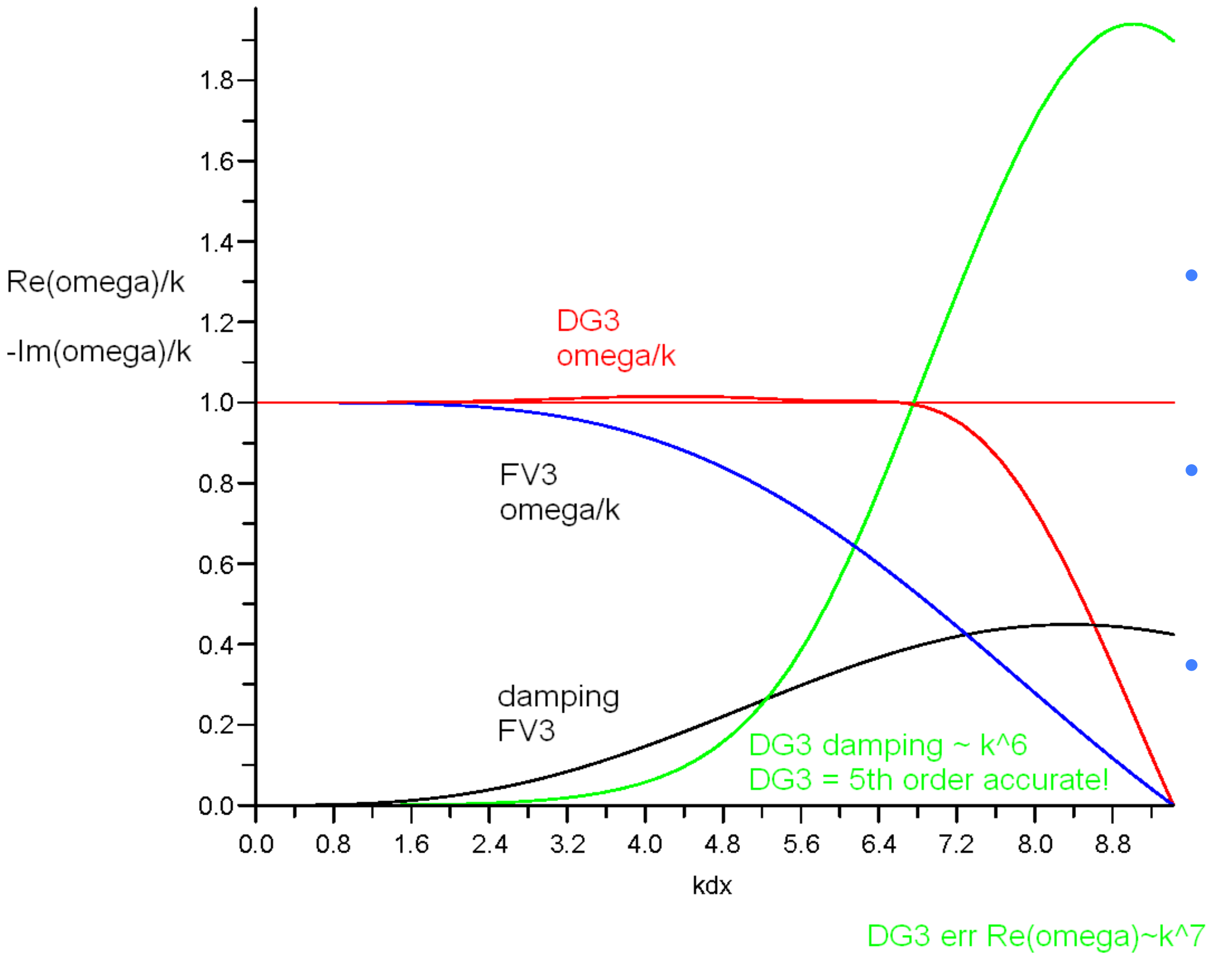
DG Algorithm Motivation

- Discontinuous Galerkin (DG) algorithms: hot topic in CFD & Applied Math in recent years. (Cockburn & Shu JCP 1998, ~500 citations)
- Recent plasma studies using DG include: Heath, Gamba, Morrison, Michler (JCP 2012), Ayuso, Carrillo, and C.-W. Shu (2012), Cheng, Gamba, Morrison; Rossmanith, Johnson, and Seal.
- DG combines key advantages of Finite Element (low-phase error, high accuracy, flexible geometry) with Finite Volume algorithms (limiters to preserve positivity/monotonicity --> avoid unphysical overshoots, locality --> parallelizes well).
- Positivity-preserving limiters important for plasma edge with large amplitude fluctuations.
- DG has excellent conservation properties for Hamiltonian systems, low noise, low dissipation.
- DG Computational efficiency:
  - Finite Volume algorithms: interpolate p points to get p'th order accuracy
  - DG algorithms: interpolate p points to get 2p-1 order accuracy
  - tradeoffs: high-order methods reduce memory-access/FLOP ratio, but need upwinding at cell boundaries for limiters to avoid artificial oscillations and dissipate small scales. Optimum around 3rd-5th order?
- Edge/pedestal gyrokinetic turbulence very challenging, 5D, problem, not yet solved. Benefits from all tricks we can find: Factor of 2 reduction in resolution --> 64x speedup.

DG Algorithm Motivation(part 2):

- DG key idea: generalize Finite Volume methods to keep track not only of the cell average, but also the weights of higher order polynomials in each cell.
- DG Basis functions localized within each cell, no overlap with adjacent cells. Relaxing continuity avoids implicit solve of standard Finite Elements. (Continuity can be restored during interpolations from adjacent cells to cell face, with limiters if desired)
- Variant of DG (Liu and Shu 2000, Bernsen 2006) can conserve both quadratic invariants (energy and enstrophy/entropy) of Poisson bracket for Hamiltonian systems if centered fluxes are used. Upwind fluxes still preserves energy conservation. (Energy errors only from time step algorithm: converges quickly for small Δt, or could use symplectic algorithm in the future.)
- Momentum conservation not exact, but independent of velocity resolution and converges rapidly with spatial and time resolution.
- Implication: can run quickly on a coarse velocity grid and still satisfy key conservation laws.
- New Idea: A key to success of Finite-Volume Piecewise Parabolic Method is that it reverts to centered, undamped, 4th order accuracy in smooth regions, adding numerical dissipation only near the grid scale. Similarly, could relax original upwind DG to be centered in smooth regions. Similar to hybrid DG/FV method found independently: Dumbser, Balsara, Toro JCP 2008.

DG has low phase error and low damping



DG quite efficient:

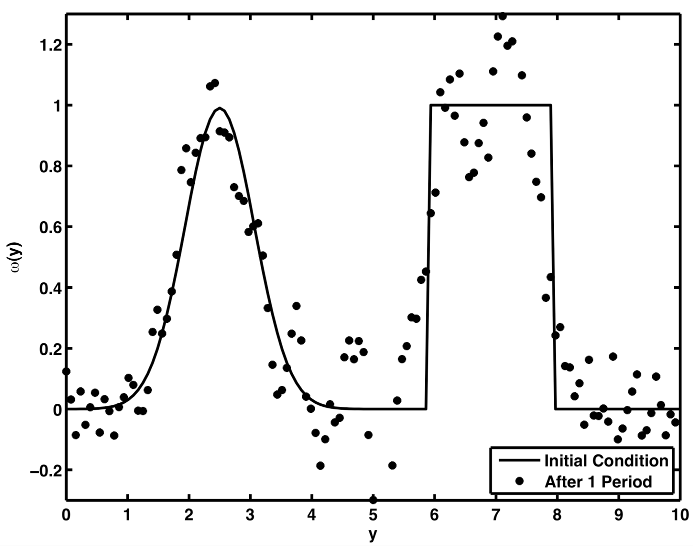
- Finite Volume: p point interpolation --> p order accuracy (PPM: 4 points -> 4th order)
- DG: p points per cell with optimal non-uniform spacing for Gaussian integration --> 2p-1 accuracy
- (For our problems p~2-3 probably optimal...)

Comparison of linear dispersion relation ω/k for passive advection with exact $\omega/k=1$, for FV3 (Finite Volume method with parabolic reconstructions) and DG3 (Discontinuous Galerkin with piecewise parabolic basis functions). Grid spacing for DG3 3 times coarser than for FV3, $\Delta x_{DG} = 3\,\Delta x_{FV}$, so they have roughly comparable amounts of memory, CPU work, and maximum Nyquist limit on the wavenumber.

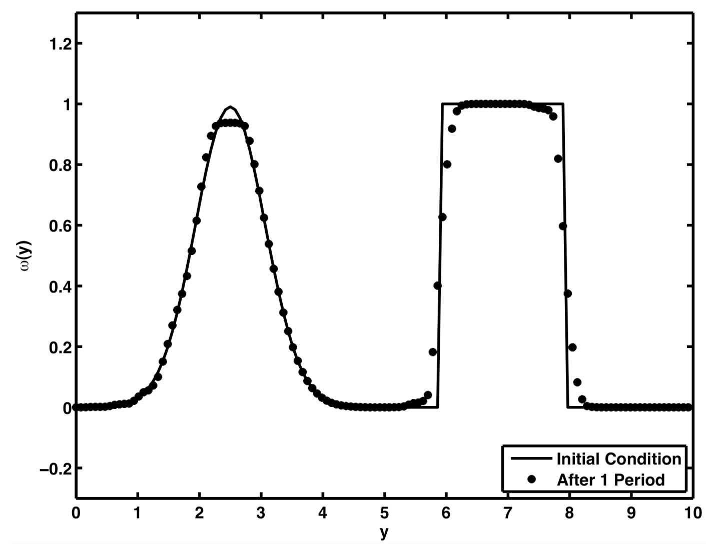
DG3 can do quite well in linear wave propagation tests, with very low phase errors. (Here the flux at the boundaries was tuned, adding some additional dissipation and lowering the phase error.)

Recent advances in limiters avoid clipping

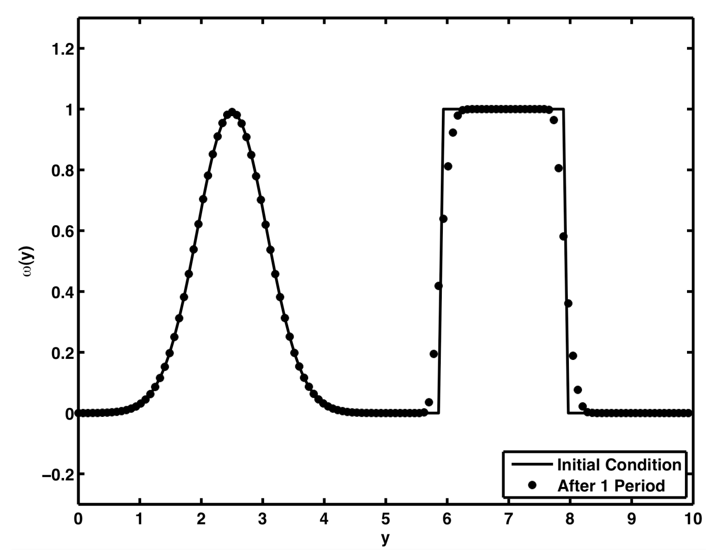
Arakawa Algorithm (std algorithm for conserving quadratic invariants of Poisson Bracket)



Standard PPM4



New XPPM



- Simple 1D advection test: $\partial f/\partial t + v\, \partial f/\partial x = 0$ solution (points) should overlay initial condition (line)
- Recent advances in limiters for Finite-Volume interpolations (Colella-Sekora 08, Suresh-Hyunh 97) eliminates clipping at smooth extrema (being used in Edge Simulation Laboratory code).
- A version of DG can combine excellent energy conservation properties of Arakawa with improved limiters that minimize numerical diffusion
- Important in edge plasma to avoid negative density overshoots.

Peterson Hammett (2012)

Initial 2D Tests for Poisson Bracket Problems

Ammar Hakim wrote initial DG code and implemented a range of 1D and 2D tests.

Many physics problems can be written in terms of Poisson bracket because of Hamiltonian structure (ExB flow, gyrokinetics, full Vlasov Eq.). Useful paradigm test problem: Incompressible 2-D Euler equations (similar to ExB advection and Hasegawa-Mima Eq. for drift waves):

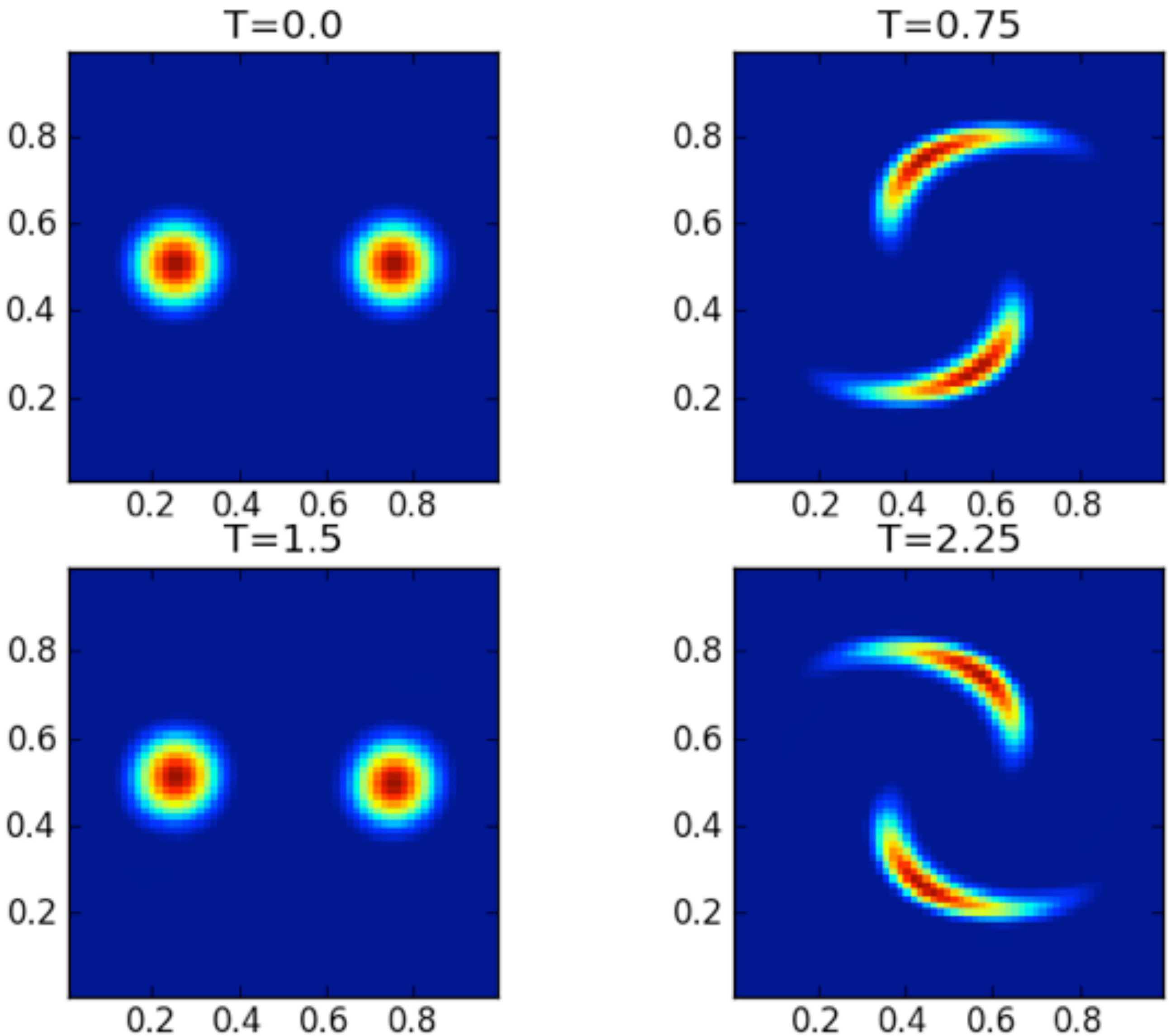
$$\begin{aligned}\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\vec{v}\rho) \\ &= -\hat{z} \times \nabla\phi \cdot \nabla\rho \qquad\qquad \nabla_\perp^2 \phi = -\rho \\ &= -[\phi, \rho] \ \ (+\text{viscosity term})\end{aligned}$$

Verified DG discretization for ρ and continuous Galerkin for ϕ exactly preserves both quadratic invariants of Poisson bracket (energy and enstrophy/entropy) for central fluxes, like Arakawa method. Even with upwind fluxes, still have energy conservation (proved in 2000, 2006). Neat trick, implies numerical diffusion is effectively only along contours of constant energy.

More complicated: extension to 1x+1v Vlasov equation (parallel gyrokinetics) with quasineutrality (with adiabatic electrons: $\phi = n_i$). Invented 2 algorithms that preserve energy conservation. Method (1) projects onto continuous basis functions but couples different toroidal planes. Method (2) allows discontinuous potential and keeps gyrokinetic Poisson solver local at each toroidal angle.

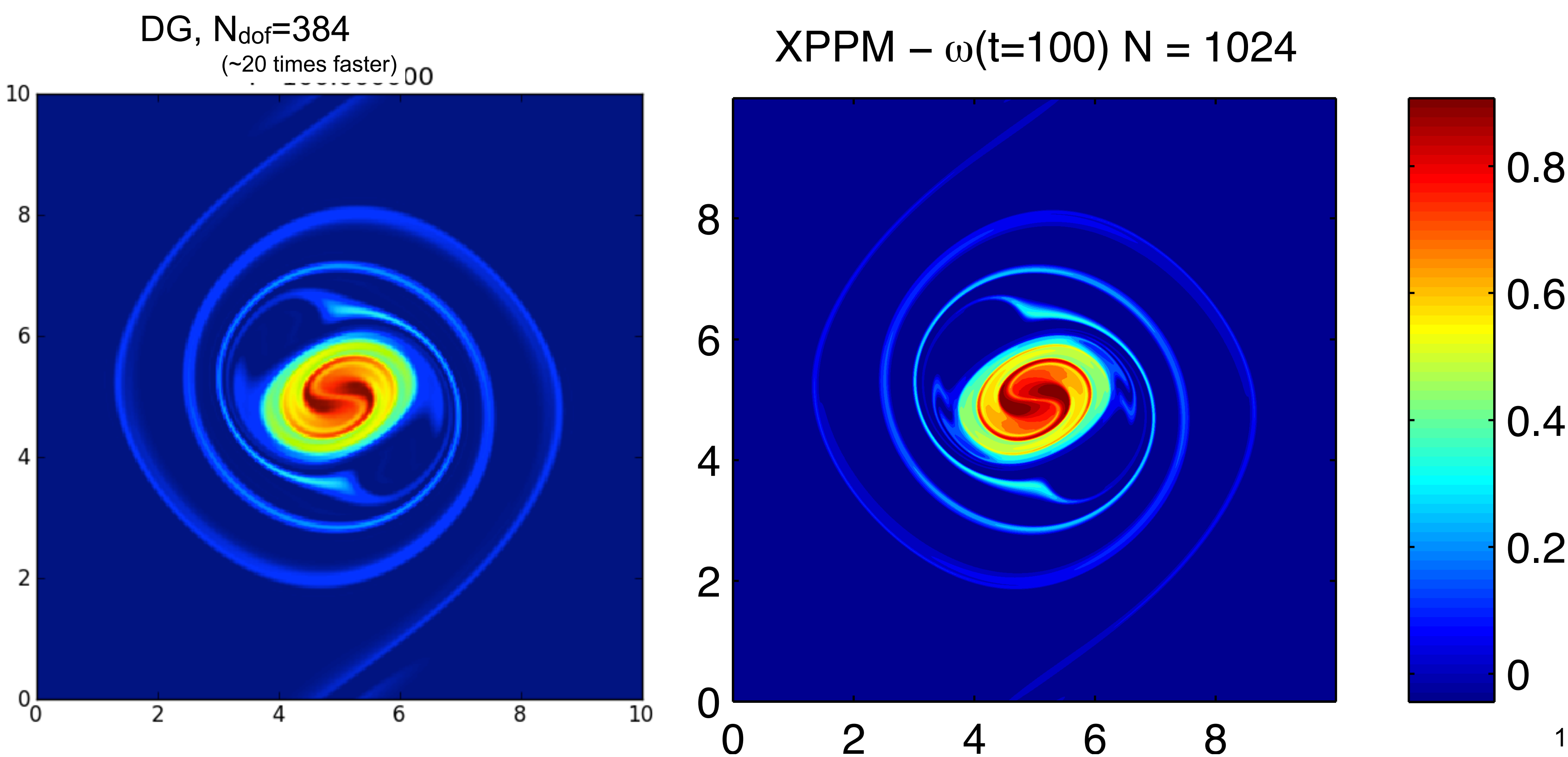
Successful 2D passive advection tests

- Passive advection in specified sheared-flow field (32x32 cells, piecewise cubic DG), reproduces initial condition with very little distortion



Successful benchmark on 2D Vortex Merger Problem

- Ammar Hakim: successfully benchmarked his new 2D DG code with finite-volume code
  - Standard finite-volume / finite-difference interpolate *p* uniform points to get *p* order accuracy. But DG with *p* non-uniform points per cell has higher *2p-1* order accuracy.
  - Comparison between
    - DG with 128 cells/direction & 3 points/(cell/direction) (N_{dof} = 384, 5th order accurate, ν=0)
    - 4th-order accurate XPPM finite-volume code, N=1024 cells/direction, Re=10^5



Progress To Date (Since January)

- Initial code written, carrying out various 1D and 2D tests
- 2D tests of properties of algorithm for both perpendicular and parallel dynamics in gyrokinetics:
  - 2D incompressible hydrodynamics like ExB nonlinearity in gyrokinetics
  - 1x-1v Vlasov equation: ion acoustic wave with adiabatic electrons (becomes ITG instability in higher dimensions) like parallel dynamics in gyrokinetics
- 2D vortex merger and other 2D problems cross-checked with other codes
- Linear and nonlinear Landau damping tested.
- Conservation and high-order convergence properties of DG algorithms confirmed: Excellent conservation even on a coarse velocity grid:
  - Particle and Energy conservation exact (except for small time step errors)
  - Momentum conservation not exact, but converges with finer spatial grid and Δt, independent of velocity grid
- implemented simplified Lenard-Bernstein diffusion-drag collision operator. Conserves particles, momentum, and energy. (can upgrade to more complete operator later.) Plan to use as kernel of a hyper-collision operator for a subgrid model.

Vlasov Eq. for ion dynamics with adiatic electrons & quasineutrality

(models parallel dynamics of gyrokinetics)

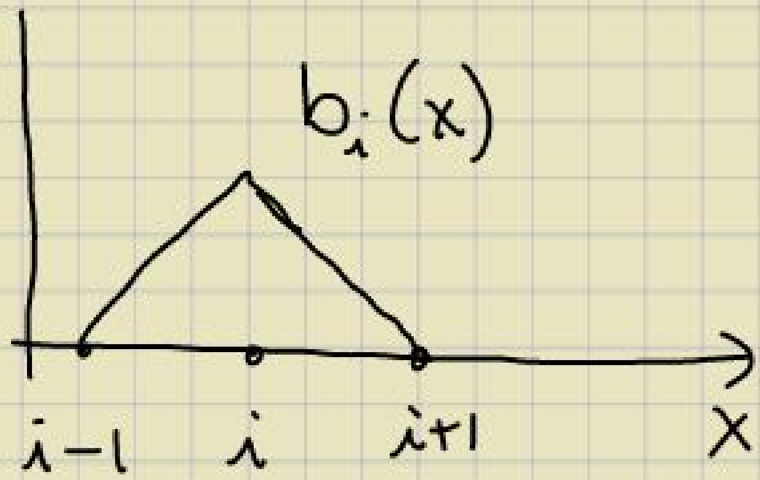
$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(v f) - \frac{\partial}{\partial v}\left(\frac{\partial \phi}{\partial x} f\right) = 0$$

$$\phi = \int dv f - n_{e0} = n - n_{e0}$$

Two ways to solve this & conserve energy:

① Use finite element / weak form of quasineutrality, projecting on to best fit of continuous basis functions. Then Shu's proof of energy conservation follows. But makes quasineutrality eq. nonlocal.

Example, with tent basis functions:



$$\langle b_i \phi \rangle = \langle b_i \, RHS \rangle$$

$$\frac{1}{6}\phi_{i-1} + \frac{2}{3}\phi_i + \frac{1}{6}\phi_{i+1} = S_i$$

requires matrix inversion

For GK quasineutrality Eq. $\nabla_\perp^2 \phi \approx S(\underset{\sim}{x})$
(with ion polarization term)
this would couple together into a single large 3D inversion problem.

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(2) Discovered alternative algorithm:
allow discontinuous ϕ but conserve energy by carefully treating δ-function electric fields at cell boundaries.
Keeps quasineutrality equation local.
GK quasineutrality $\nabla_\perp^2 \phi = S(\underset{\sim}{x})$
remains a set of <u>uncoupled</u> 2D Poisson problems.

Illustrate discontinuous ϕ algorithm

Simplest possible DG: piecewise const. ϕ & f with upwind fluxes. ($v>0$ for simplicity.)

$$\frac{\partial f_{ij}}{\partial t} + v_j \frac{(f_{ij} - f_{i-1,j})}{\Delta x} - \frac{1}{\Delta x \Delta v}\int_{i,j+\frac{1}{2}} dx \, \frac{\partial \phi}{\partial x} f + \frac{1}{\Delta x \, \Delta v}\int_{i,j-\frac{1}{2}} dx \, \frac{\partial \phi}{\partial x} f = 0$$

Missing factor of 1/(Delta x) in this expression: (GWH/Mandell 2018.02.01)

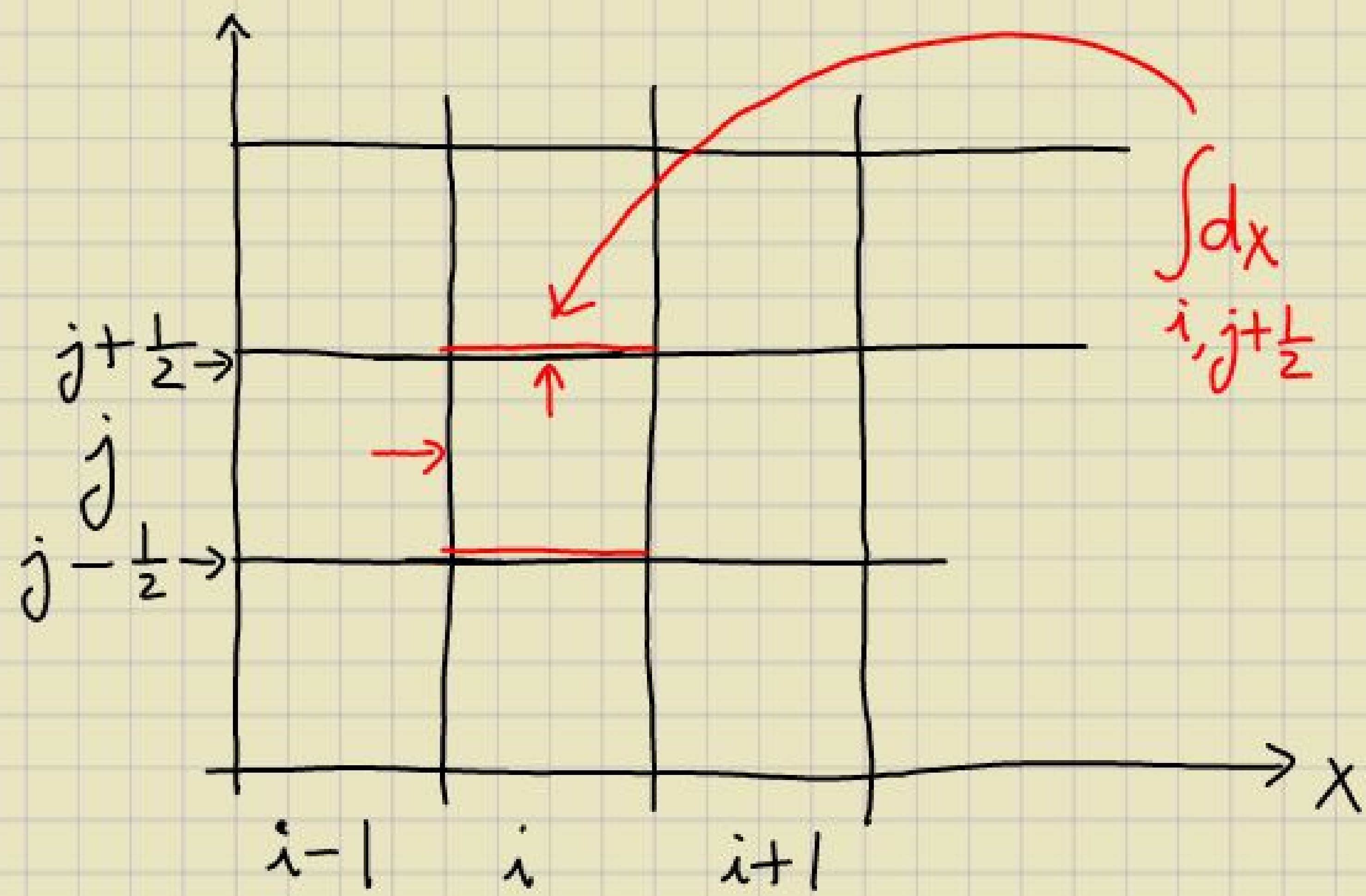
$$-\frac{1}{\Delta v}(\phi_i - \phi_{i-1})\left(f_{i-\frac{1}{2},j+\frac{1}{2}} - f_{i-\frac{1}{2},j-\frac{1}{2}}\right)$$

Can show

$$f_{i-\frac{1}{2},j+\frac{1}{2}} = H(-(\phi_i - \phi_{i-1}))\, f_{i-1,j} + H(\phi_i - \phi_{i-1}) f_{i-1,j+1}$$

conserves total energy!

$$W = \sum_i \Delta x \sum_j \Delta v \langle v^2 \rangle_j f_{ij} + \sum_i \Delta x \frac{1}{2}\phi_i^2$$


$\int dx$
$i, j+\frac{1}{2}$
$j+\frac{1}{2}$
j
$j-\frac{1}{2}$
x
$i-1$
i
$i+1$


$\phi(x)$
x
$i-1$
i
$i+1$