Preservation of Zero Velocity Divergence in a High-Order, Mapped-Grid, Finite-Volume Discretization of a Gyrokinetic System

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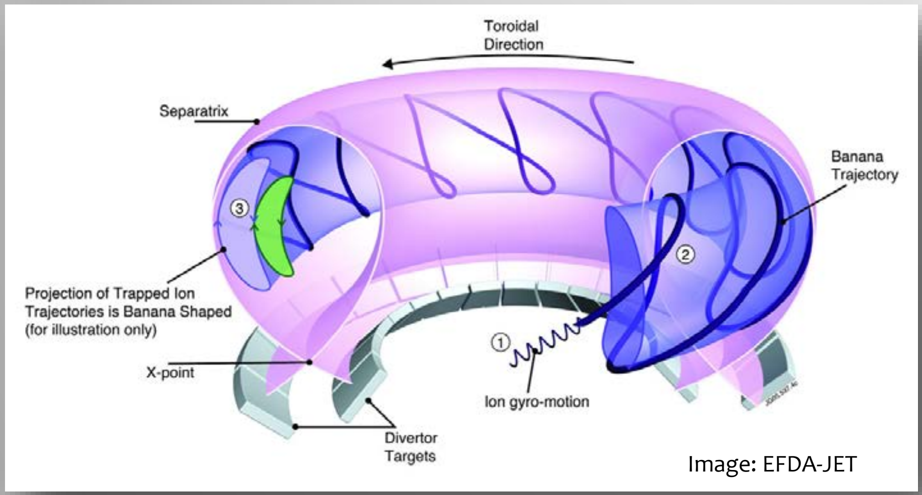
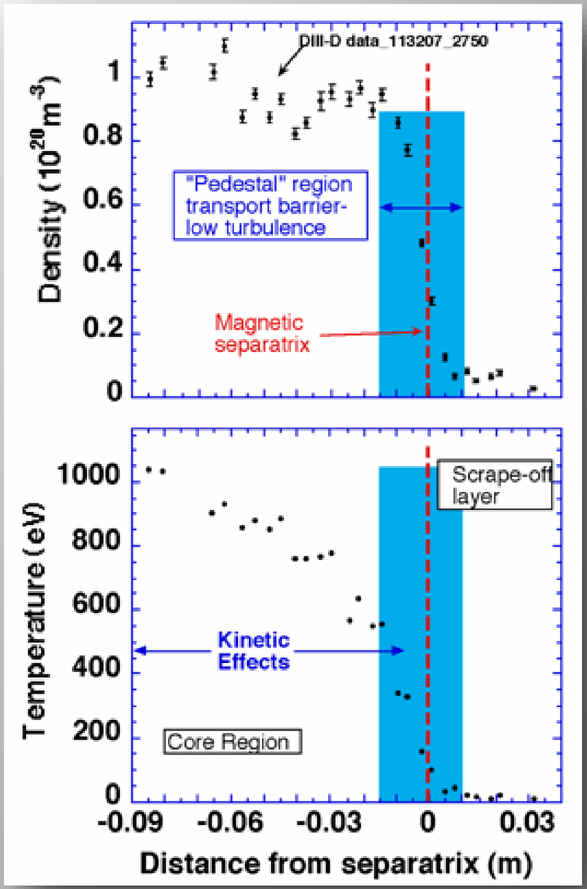
Simulation of the edge plasma region of a tokamak fusion reactor requires a kinetic model





- Radial width of the "pedestal" region is comparable to particle orbits
- Mean-free path is comparable to the temperature variation scale length along field lines

The edge pedestal density (ne) and temperature (Te) profiles near the edge of an H-mode discharge in the DIII-D tokamak. The horizontal scale is distance from nominal boundary of the plasma at R= 2.34m [from G.D. Porter, et al., Phys. Plasmas 7 (7), 3663 (Sept. 2000)].

Continuum gyrokinetic models describe the advection of distribution functions in 5D phase space

Gyrokinetic Vlasov equation:

$$\frac{\partial (B_{\|}{}^* f)}{\partial t} + \nabla_{\mathbf{R}} \cdot \left(\dot{\mathbf{R}} f \right) + \frac{\partial}{\partial v_{\|}} \left(\dot{v}_{\|} f \right) = 0$$

where

$f(\mathbf{R}, v_{\|}, \mu, t)$	species distribution function
$\mathbf{R}$	gyrocenter spatial coordinate
$v_{\|}$	parallel velocity
$\mu = \frac{1}{2} m v_{\perp}^2 / B$	magnetic moment

Gyrokinetic models remove the gyromotion phase and frequency, reducing the phase space dimension from 6 to 5

The phase space velocity

$$\dot{\mathbf{R}} \equiv v_{\|} \mathbf{B}^* + \frac{\rho_L}{Z} \mathbf{b} \times \mathbf{G}$$

$$\dot{v}_{\|} \equiv -\frac{1}{m} \mathbf{B}^* \cdot \mathbf{G}$$

$$\mathbf{G} \equiv Z \nabla_{\mathbf{R}} \Phi + \frac{\mu}{2} \nabla_{\mathbf{R}} B$$

$$\mathbf{B}^* \equiv \mathbf{B} + \rho_L \frac{m v_{\|}}{Z} \nabla_{\mathbf{R}} \times \mathbf{b}$$

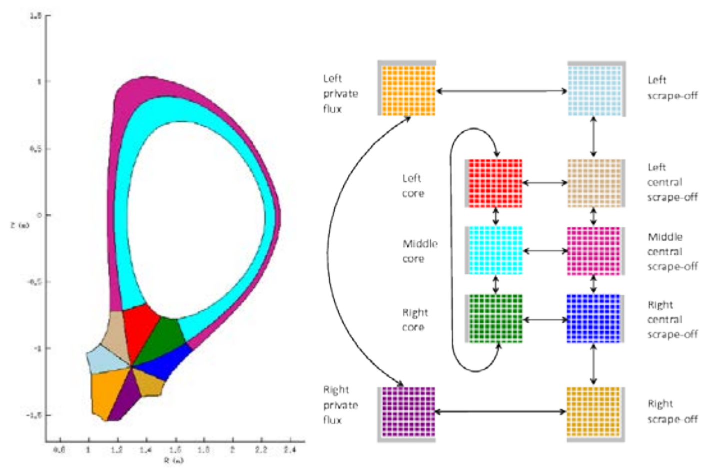
$$B_{\|}{}^* \equiv \mathbf{b} \cdot \mathbf{B}^*$$

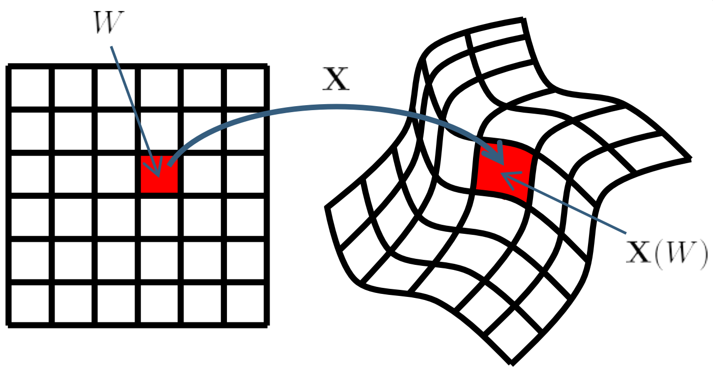
is divergence-free:

$$\nabla_{\mathbf{R}} \cdot \left(\dot{\mathbf{R}} \right) + \frac{\partial}{\partial v_{\|}} \left(\dot{v}_{\|} \right) = 0$$

This is a 4D condition

We discretize the gyrokinetic system using a high-order, mapped-multiblock, finite-volume approach





$$\mathbf{X} \equiv \mathbf{X}(\xi), \quad \mathbf{X} : [0,1]^D \rightarrow \Omega \subset \mathbf{R}^D$$

$$\int_{\mathbf{X}(W)} \nabla_{\mathbf{X}} \cdot \mathbf{F} d\mathbf{x} = \sum_{d=0}^{D-1} \sum_{\alpha=0,1} (-1)^{1+\alpha} \int_{V_d^\alpha} (\mathbf{N}^T \mathbf{F})_d d\mathbf{V}_{\xi}$$

$$\frac{1}{h^{D-1}} \int_{V_d^\alpha} (\mathbf{N}^T \mathbf{F})_d d\mathbf{V}_\xi \equiv \sum_{s=1}^{D} \langle N_d^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \langle F^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} + \frac{h^2}{12} \sum_{s=1}^{D} \left(\mathbf{G}_0^{\perp,d} \langle N_d^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \right) \cdot \left(\mathbf{G}_0^{\perp,d} (\langle F^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}) \right) + O(h^4)$$

$$\int_{\mathbf{X}(W)} \nabla_{\mathbf{X}} \cdot (\mathbf{u} f) \, d\mathbf{x} = \sum_{d=0}^{D-1} \sum_{\alpha=0,1} (-1)^{1+\alpha} \int_{V_d^\alpha} (\mathbf{N}^T \mathbf{u})_d d\mathbf{V}_{\xi} \int_{V_d^\alpha} f d\mathbf{V}_{\xi} + \text{h.o.c.}$$

P. Colella, M. R. Dorr, J. A. F. Hittinger and D. F. Martin, "High-order, Finite-Volume Methods in Mapped Coordinates," J. Comput. Phys. 230, pp. 2952-2976 (2011).

Key: The phase space velocity can be written as a skew symmetric tensor divergence plus a divergence-free term

$$\mathbf{u} \equiv (\dot{\mathbf{R}}, \dot{v}_\parallel) = \tilde{\mathbf{u}} + \hat{\mathbf{u}}$$

$$\dot{\mathbf{R}} \equiv v_\parallel \mathbf{B}^* + \frac{\rho_L}{Z}\mathbf{b}\times\mathbf{G}$$

$$\dot{v}_\parallel \equiv -\frac{1}{m}\mathbf{B}^*\cdot\mathbf{G}$$

$$\mathbf{G} \equiv Z\nabla_{\mathbf{R}}\Phi + \frac{\mu}{2}\nabla_{\mathbf{R}}B$$

$$\mathbf{B}^* \equiv \mathbf{B} + \rho_L\frac{mv_\parallel}{Z}\nabla_{\mathbf{R}}\times\mathbf{b}$$

$$B_\parallel{}^* \equiv \mathbf{b}\cdot\mathbf{B}^*$$

Define

$$(x_0, x_1, x_2, x_3) = (v_\parallel, \mathbf{R})$$

$$\mathbf{B} = \nabla_{\mathbf{R}}\times\mathbf{A} \qquad p \equiv \rho_L\left(\phi + \frac{\mu B}{2Z}\right).$$

$$\tilde{\mathbf{u}}_j \equiv \sum_{j'=0}^{3}\frac{\partial\zeta_{j,j'}}{\partial x_{j'}}, \qquad 0\le j\le 3,$$

$$\begin{aligned}
\zeta_{i,i} &= 0, && 0\le i\le 3,\\
\zeta_{0,j} &= -v_\parallel(\mathbf{b}\times\nabla_{\mathbf{R}}p)_j, && 1\le j\le 3,\\
\zeta_{1,2} &= v_\parallel\left(\mathbf{A} + \frac{mv_\parallel\rho_L}{Z}\mathbf{b}\right)_3 &&\\
\zeta_{1,3} &= -v_\parallel\left(\mathbf{A} + \frac{mv_\parallel\rho_L}{Z}\mathbf{b}\right)_2 &&\\
\zeta_{2,3} &= v_\parallel\left(\mathbf{A} + \frac{mv_\parallel\rho_L}{Z}\mathbf{b}\right)_1 &&\\
\zeta_{i,j} &= -\zeta_{j,i}, && 0\le j< i\le 3.
\end{aligned}$$

$$\hat{\mathbf{u}}_j \equiv -\delta_{0,j}\frac{Z}{m\rho_L}\mathbf{B}\cdot\nabla_{\mathbf{R}}p, \qquad 0\le j\le 3.$$

$$\nabla\cdot\hat{\mathbf{u}} = -\frac{Z}{m\rho_L}\partial_{v_\parallel}\mathbf{B}\cdot\nabla_{\mathbf{R}}p = 0$$

Evaluation of the normal velocity integrals yields a zero divergence via telescoping cancellation

Defining the 2-form

$$\boldsymbol{\omega} \equiv \zeta_{3,2} dx_0 \wedge dx_1 + \zeta_{1,3} dx_0 \wedge dx_2 + \zeta_{2,1} dx_0 \wedge dx_3 + \zeta_{3,0} dx_1 \wedge dx_2 + \zeta_{0,2} dx_1 \wedge dx_3 + \zeta_{1,0} dx_2 \wedge dx_3,$$

the exterior derivative

$$d\boldsymbol{\omega} = \widetilde{u}_3 \, dx_0 \wedge dx_1 \wedge dx_2 - \widetilde{u}_2 \, dx_0 \wedge dx_1 \wedge dx_3 + \widetilde{u}_1 \, dx_0 \wedge dx_2 \wedge dx_3 - \widetilde{u}_0 \, dx_1 \wedge dx_2 \wedge dx_3$$

satisfies

$$\int_{V_d^\alpha} (\mathbf{N}^T \tilde{\mathbf{u}})_d d\mathbf{V}_\xi = (-1)^{d+1} \int_{V_d^\alpha} \mathbf{X}^*(d\boldsymbol{\omega})$$

Applying Stokes' theorem

$$\int_{V_d^\alpha} \mathbf{X}^*(d\boldsymbol{\omega}) = \int_{V_d^\alpha} d(\mathbf{X}^* \boldsymbol{\omega}) = \sum_{d' \neq d} \sum_{\beta=0,1} (-1)^{d'+1+\beta} \int_{A_{d,d'}^{\alpha,\beta}} \mathbf{X}^* \boldsymbol{\omega}.$$

evaluation of the pullbacks yields

$$\int_{\mathbf{X}(W)} \nabla_{\mathbf{X}} \cdot \tilde{\mathbf{u}} \, d\mathbf{x} = \sum_{d=0}^{3} \sum_{\alpha=0,1} (-1)^{1+\alpha} \int_{V_d^\alpha} (\mathbf{N}^T \mathbf{u})_d f d\mathbf{V}_\xi$$

$$= \sum_{d=0}^{3} \sum_{d' \neq d} \sum_{\alpha=0,1} \sum_{\beta=0,1} (-1)^{d+d'+\alpha+\beta+1} \int_{A_{d,d'}^{\alpha,\beta}} \mathbf{X}^* \boldsymbol{\omega}$$

$$= 0$$

The face normal velocity integrals are metric-free and almost discretely exact

Mapping to axisymmetric configuration coordinates

$$x_0 = v_{\parallel}(\xi_0),$$
$$x_1 = R(\xi_1,\xi_2)\cos(\xi_3),$$
$$x_2 = R(\xi_1,\xi_2)\sin(\xi_3),$$
$$x_3 = Z(\xi_1,\xi_2)$$

and assuming axisymmetric fields:

$$\int_{V_0^\alpha} (\mathbf{N}^T\mathbf{u})_0 d\mathbf{V}_\xi = \sum_{\beta=0,1} (-1)^\beta \left(Q_{0,2}^{\alpha,\beta} - Q_{0,1}^{\alpha,\beta} \right) + \widehat{U}^\alpha$$

$$\int_{V_1^\alpha} (\mathbf{N}^T\mathbf{u})_1 d\mathbf{V}_\xi = \sum_{\beta=0,1} (-1)^\beta \left(Q_{0,1}^{\alpha,\beta} - Q_{1,2}^{\alpha,\beta} \right),$$

$$\int_{V_2^\alpha} (\mathbf{N}^T\mathbf{u})_2 d\mathbf{V}_\xi = \sum_{\beta=0,1} (-1)^\beta \left(Q_{1,2}^{\alpha,\beta} - Q_{0,2}^{\alpha,\beta} \right)$$

$$\int_{V_3^\alpha} (\mathbf{N}^T\mathbf{u})_3 d\mathbf{V}_\xi = 0$$

$$Q_{0,1}^{\alpha,\beta} \equiv -2\pi\rho_L (RB)_{tor} \left[\eta_0 \int_{\xi_2^0}^{\xi_2^1} \left(\frac{1}{B}\frac{\partial\phi}{\partial\xi_2} \right)_{\xi_1=\xi_1^\beta} d\xi_2 + \frac{\eta_1}{2Z} \ln \frac{B(\xi_1^\beta,\xi_2^1)}{B(\xi_1^\beta,\xi_2^0)} \right]$$

$$Q_{0,2}^{\alpha,\beta} \equiv -2\pi\rho_L (RB)_{tor} \left[\eta_0 \int_{\xi_1^0}^{\xi_1^1} \left(\frac{1}{B}\frac{\partial\phi}{\partial\xi_1} \right)_{\xi_2=\xi_2^\beta} d\xi_1 + \frac{\eta_1}{2Z} \ln \frac{B(\xi_1^1,\xi_2^\beta)}{B(\xi_1^0,\xi_2^\beta)} \right]$$

$$Q_{1,2}^{\alpha,\beta} \equiv -2\pi \left(\eta_2\Psi + \eta_3 \frac{m\rho_L}{Z}\frac{(RB)_{tor}}{B} \right)_{\xi_1=\xi_1^\alpha,\xi_2=\xi_2^\beta}$$

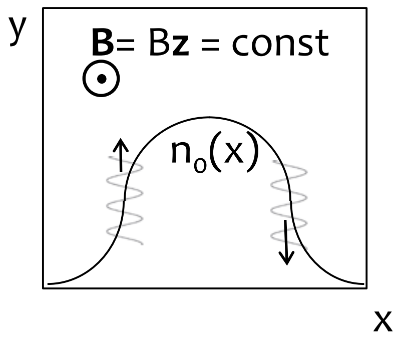
$$\widehat{U}^\alpha \equiv \frac{1}{m}\int_{\xi_1^0}^{\xi_1^1}\int_{\xi_2^0}^{\xi_2^1} \mathbf{B}\cdot\left(Z\mathbf{E} - \frac{\mu}{2}\nabla B \right) J d\xi_1 d\xi_2$$

$$\eta_0 \equiv v_{\parallel}(\xi_0)$$
$$\eta_1 \equiv v_{\parallel}(\xi_0)\mu$$
$$\eta_2 \equiv (v_{\parallel}^2(\xi_0^1) - v_{\parallel}^2(\xi_0^0))/2$$
$$\eta_3 \equiv (v_{\parallel}^3(\xi_0^1) - v_{\parallel}^3(\xi_0^0))/3$$

$$J \equiv 2\pi R \left(\frac{\partial R}{\partial\xi_1}\frac{\partial Z}{\partial\xi_2} - \frac{\partial R}{\partial\xi_2}\frac{\partial Z}{\partial\xi_1} \right)$$

This formulation also enables the stable high-order integration of drift waves

2D slab model (d/dz = 0):



Model equations:

$$\frac{\partial n}{\partial t} + \nabla \cdot \left(c \frac{\mathbf{b} \times \nabla \phi}{B} n \right) = 0$$

$$e\phi / T_e = \delta n / n_0$$

Perturbative, analytic solution:

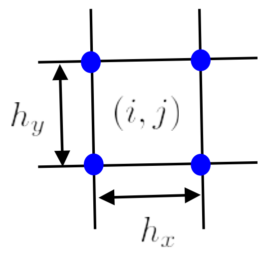
$$\frac{\partial}{\partial t}\delta n - \left(\frac{cT_e}{eBn_0} \frac{dn_0}{dx} \right) \frac{\partial}{\partial y} \delta n = 0$$

Von Neumann analysis of centered differencing applied to

$$\frac{\partial}{\partial t}\delta n - \frac{\partial}{\partial x}\left(\frac{c}{B} n_0(x) \frac{\partial \phi}{\partial y} \right) + \frac{\partial}{\partial y}\left(\frac{c}{B} n_0(x) \frac{\partial \phi}{\partial x} \right) = 0,$$

yields the explicit integration stability requirement:

$$\frac{1}{h_x}\left(\left.\frac{\partial \phi}{\partial y}\right|_{i+1/2,j} - \left.\frac{\partial \phi}{\partial y}\right|_{i-1/2,j} \right) + \frac{1}{h_y}\left(\left.\frac{\partial \phi}{\partial x}\right|_{i,j+1/2} - \left.\frac{\partial \phi}{\partial x}\right|_{i,j-1/2} \right) = 0,$$

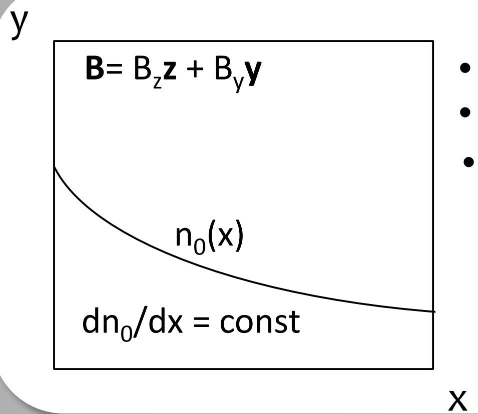


This is a requirement of nodal potential cancellation that is

- satisfied by second-order centered diverencing
- *not* satisfied by fourth-order centered differencing
- satisfied by the new formulation (at any order)

Note: This is not a zero velocity divergence issue!

This velocity discretization has enabled the high-order verification of collisionless (universal) drift instability

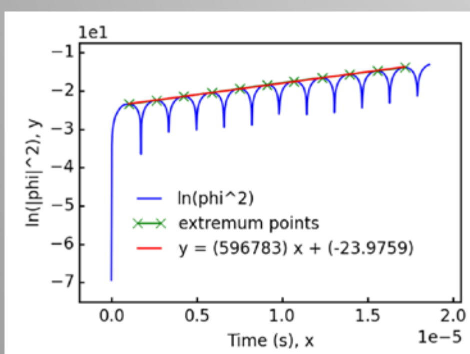


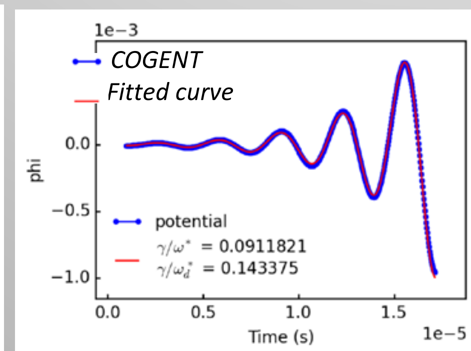
- *2D slab geometry (d/dz=0), B is uniform*
- *Drift-kinetic electrons and ions (Z_i=1)*
- *Long wavelength limit of gyro- Poisson equation*
  - Periodic BC in y-direction
  - Zero Dirichlet BC in x-direction

$$\frac{\partial f_\alpha}{\partial t} + \frac{B_y}{B}\frac{\partial}{\partial y}(v_\parallel f_\alpha) + \frac{c}{B}\frac{\partial}{\partial x}([\mathbf{b}\times\nabla\phi]f_\alpha) - \frac{q_\alpha}{m_\alpha}\frac{B_y}{B}\frac{\partial}{\partial v_\parallel}\left(\frac{\partial\phi}{\partial y}f_\alpha\right) = 0$$

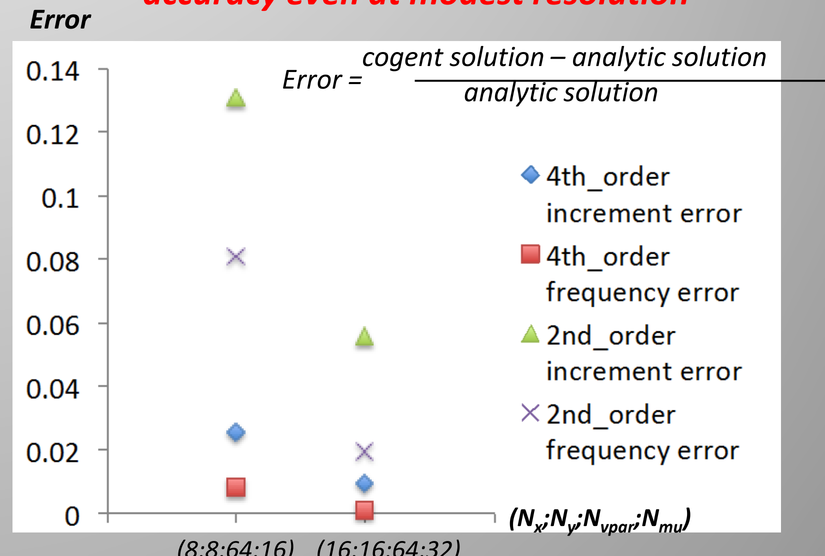
$$\nabla_\perp\left(\frac{c^2 m_i n_i}{eB^2}\nabla_\perp\phi\right) = 2\pi B\int\left(\frac{f_e}{m_e} - \frac{f_i}{m_i}\right)dv_\parallel d\mu$$

Cogent results are post-processed to obtain increment (γ) and frequency (ω)





4th-order scheme yields significantly improved accuracy even at modest resolution



<u>Simulations parameters</u>: $m_i = 2m_p$, $m_e = 0.01m_p$, $T_e=T_i$=400eV, $L_x=L_y$=0.8 cm, B_z=3 T, B_y=0.01 T, $dn=10^{-5}\sin(2\pi y/L_y)\sin(\pi x/L_x)$, $n_0=\exp(-x/4L_x)$; $k_y\rho_i=1$, $k_y (B_y/B_z)V_{Te}=2.2\omega^*$, $\omega^*= ck_yT_e/L_n eB$

This divergence-free velocity formulation is now a key part of our COGENT edge plasma code

- Solves the gyrokinetic Vlasov-Poisson system in
  - 4D axisymmetric edge geometry spanning both sides of the separatrix
  - 5D slab geometry
- Electron vorticity model
- Multiple collision operators, including fully nonlinear Fokker-Planck
- Multiple high-order flux options (WENO5, UW3, UW5, centered)
- Built on Chombo AMR framework
- Arbitrary decomposition of configuration and phase space
- Implicit-explicit time integration (next talk)