Particle Closures IMP

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CEMM Meeting

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Background

- For some time, community interest in δf algorithm w. evolving background
  - Chang, Callen – CEL
  - Held – Parallel closures
  - Barnes, Sovinec, Nystrom, Nebel, … – QIP
  - Cohen, *et al.* – collisional electron model
  - Bruner, Valeo, Krommes – collisional physics
  - Peoble, Parker – Kinetic MHD
- Present interest on closure algorithms
  - CEMM
  - Integration initiative

Problems, Problems

- Growing weight problem
- Synchronization between particles and moments
- Constraint moment errors
- Choosing one closure scheme over another
  - Even particle moments preferred
  - Conservation laws?
  - Consistent treatment of fluctuations

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Solutions, Solutions

- Use only 1st 2 moment equations
  - Closure is 2nd order moment (stress)
  - Check energy conservation
- Particle representation enforces constraint moments
- Use particular velocity $\mathbf{w} = \mathbf{v} - \mathbf{u}$

IMP Algorithm

- Fluid equations
  - Quasineutral, no displacement current
  - Electrons are massless fluid (extensions possible)

$$en\left(\mathbf{E}+\mathbf{u}\times\mathbf{B}\right)=\mathbf{J}\times\mathbf{B}-\nabla P_e$$

$$\frac{Dn}{Dt}+n\nabla\bullet\mathbf{u}=0$$

$$\frac{\partial P_e}{\partial t}+\mathbf{u}_e\bullet\nabla P_e+\Gamma_e P_e\nabla\bullet\mathbf{u}_e=0$$

$$\mathbf{u}_e=\mathbf{u}-\frac{\mathbf{J}}{en}$$

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IMP Algorithm

- Fluid equations
  - Ions are massive, collisionless, kinetic species
  - Use ion (actually total) fluid equations w. kinetic closure

$$Mn\frac{D\mathbf{u}}{Dt} = Mn\mathbf{g} + \mathbf{J}\times\mathbf{B} - \nabla P_e - \nabla \bullet \overleftrightarrow{\mathrm{P}}_i$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla\times\mathbf{E};\ \mathbf{J} = \frac{1}{\mu_0}\nabla\times\mathbf{B}$$

$$\frac{\partial f}{\partial t} + \mathbf{v}\bullet\frac{\partial f}{\partial \mathbf{x}} + \frac{e}{M}\left(\mathbf{F} + \mathbf{v}\times\mathbf{B}\right)\bullet\frac{\partial f}{\partial \mathbf{v}} = 0$$

$$\overleftrightarrow{\mathrm{P}}_i = M\int d\mathbf{w} f \mathbf{w}\mathbf{w};\ \mathbf{w} = \mathbf{v} - \mathbf{u}$$

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IMP Algorithm

- δf particle closure algorithm
  - Background is fixed T with n, $\mathbf{u}$ evolving
  - Particle advance uses particular velocity $\mathbf{w}$ (*very important*)

$$f = \bar{f} + \tilde{f};\ \bar{f} = \frac{n}{\left(\sqrt{2\pi}\,\bar{v}_T\right)^3} e^{-w^2/2\bar{v}_T^2}$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{w} + \mathbf{u}$$

$$\frac{d\mathbf{w}}{dt} = \frac{e}{M}\mathbf{w}\times\mathbf{B} - \mathbf{w}\bullet\frac{\partial\mathbf{u}}{\partial\mathbf{x}} + \bar{v}_T^2\frac{1}{n}\frac{\partial n}{\partial\mathbf{x}} - \tilde{\mathbf{A}}$$

$$-\frac{\nabla\bullet\overleftrightarrow{\mathrm{P}}_i}{Mn} = -\frac{k_B\bar{T}\nabla n}{Mn} + \tilde{\mathbf{A}};\ \tilde{\mathbf{A}} = -\frac{1}{n}\nabla\bullet\int d\mathbf{w}\tilde{f}\mathbf{w}\mathbf{w}$$

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IMP Algorithm

$$\frac{1}{1-\tilde{\omega}}\frac{d\tilde{\omega}}{dt} = \nabla \bullet \mathbf{u} - \frac{1}{\bar{v}_T^2}\left(\mathbf{ww} : \frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{w} \bullet \tilde{\mathbf{A}}\right)$$

$$\tilde{\omega} = \tilde{f} / f$$

- Note:
  - (perturbation) $\mathbf{E}$ does not enter closure directly
  - There is some kind of symmetry between $\tilde{\omega}$ advance and $\tilde{\mathbf{A}}$
  - $\tilde{\omega}$ evolution is an implicit equation

Constraint Moments

- Satisfy constraints by shaping particle in both $\mathbf{x}$ and $\mathbf{w}$

$$\int d\mathbf{w}\ \bar{f}_T \tilde{\omega} = \int d\mathbf{w}\ \bar{f}_T \mathbf{w} \tilde{\omega}$$

$$\bar{f}_T(\mathbf{w}) \equiv \frac{e^{-w^2/2\bar{v}_T^2}}{\left(2\pi \bar{v}_T^2\right)^{3/2}}$$

$$\tilde{\omega}(\mathbf{x},\mathbf{w}) \equiv \sum_p W_p \tilde{\omega}_p s(\mathbf{x}-\mathbf{x}_p) s_w(\mathbf{w}\ ,\mathbf{w}_p)$$

$$\int d\mathbf{w}\ \bar{f}_T s_w = 0 = \int d\mathbf{w}\ \bar{f}_T \mathbf{w}\, s_w$$

$$s_w = \delta + correction$$

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Constraint Moments

- Using Hermite polynomials, find

$$s_w(\mathbf{w}\ ,\mathbf{w}_p) = \delta - \bar{f}_T(\mathbf{w}_p)\left(1 + \frac{\mathbf{w}\ \bullet \mathbf{w}_p}{\bar{v}_T^2}\right)$$

- Projection of weight equation is then

$$\frac{1}{1-\tilde{\omega}_p}\frac{d\,\tilde{\omega}_p}{dt} = \int d\mathbf{w}\, s_w(\mathbf{w}\ ,\mathbf{w}_p)\left[\nabla \bullet \mathbf{u} - \frac{1}{\bar{v}_T^2}\left(\mathbf{ww} : \frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{w} \bullet \tilde{\mathbf{A}}\right)\right]$$

$$= \left(\nabla \bullet \mathbf{u} - \frac{1}{\bar{v}_T^2}\mathbf{ww} : \frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right)\Bigg|_p$$

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Symmetry Leads to Energy Integral

$$\frac{d}{dt}\int d\mathbf{x}\left(\frac{Mnu^2}{2}+Mn\phi+\frac{B^2}{2\mu_0}+\frac{P_e}{\Gamma_e-1}+M\,\bar{v}_T^2\,n\log n\right)$$

$$=M\int d\mathbf{x}n\mathbf{u}\bullet\tilde{\mathbf{A}}$$

Usual fluid w. isoT ions **Interchange w. closure**

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Symmetry Leads to Energy Integral

$$\ldots$$

$$= M \int d\mathbf{x} n \mathbf{u} \bullet \tilde{\mathbf{A}}$$

$$= M\, C_n \bar{v}_T^2 \sum_p W_p \frac{d}{dt}\left[\log\left(1-\tilde{\omega}_p\right)+\tilde{\omega}_p\right] \approx -\frac{d}{dt}\frac{M\, C_n \bar{v}_T^2}{2}\sum_p W_p \tilde{\omega}_p^2$$

Usual fluid w. isoT ions **Closure energy**

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Symmetry Leads to Energy Integral

$$\int d\mathbf{x}\left(\frac{Mnu^2}{2}+Mn\phi+\frac{B^2}{2\mu_0}+\frac{P_e}{\Gamma_e-1}+M\,\bar{v}_T^2\,n\log n\right)$$
$$-M\,C_n\bar{v}_T^2\sum_p W_p\left[\log\left(1-\tilde{\omega}_p\right)+\tilde{\omega}_p\right]=\boldsymbol{\mathcal{E}}=const.$$

$$-M\,C_n\bar{v}_T^2\sum_p W_p\left[\log\left(1-\tilde{\omega}_p\right)+\tilde{\omega}_p\right]\approx\frac{M\,C_n\bar{v}_T^2}{2}\sum_p W_p\,\tilde{\omega}_p^2=$$
$$\boldsymbol{\mathcal{E}}\text{-}\int d\mathbf{x}\left(\frac{Mnu^2}{2}+Mn\phi+\frac{B^2}{2\mu_0}+\frac{P_e}{\Gamma_e-1}+M\,\bar{v}_T^2\,n\log n\right)<\boldsymbol{\mathcal{E}}$$

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Symmetry Leads to Energy Integral

- r.m.s. of particle weights absolutely bounded
- Stability comparison theorem
  - Kinetic system more stable than isoT ion fluid system
  - But only for marginal mode at zero frequency
- This is absolutely the most important point!

IMP2 Implementation

- 2D, Cartesian
- TE polarization
  - $\mathbf{B}$ normal to simulation plane $\left(k_{\parallel} = 0\right)$
  - $\mathbf{E}$ in plane
- Linearized, 1D equilibrium
- Uniform T

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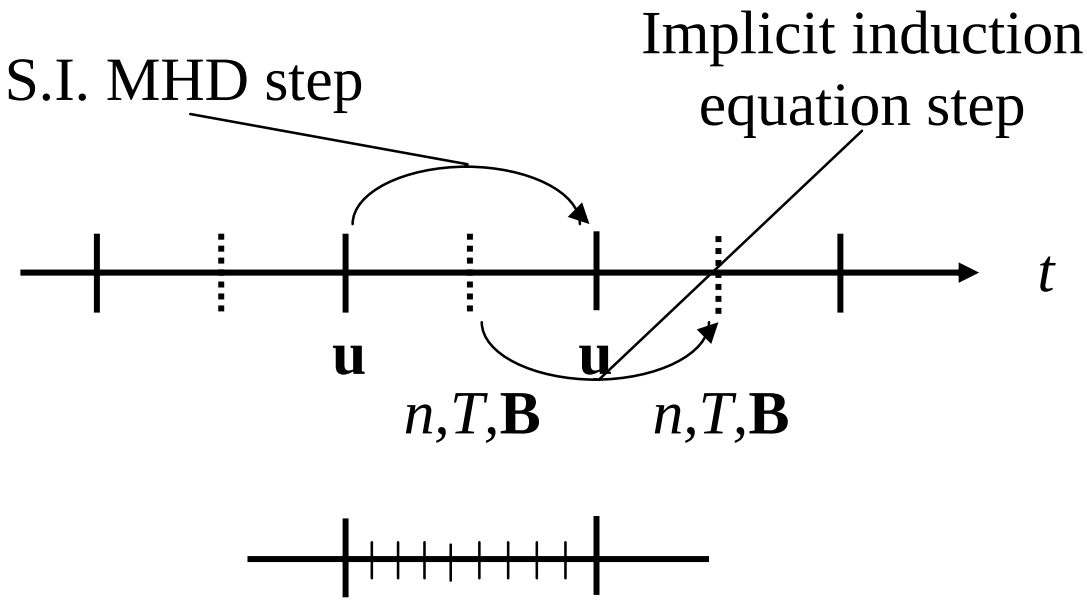
Time Centering



Leap-frog particle substeps give orbit averaged $\tilde{\mathbf{A}}$

Particles use average of $\mathbf{u}$ (depends on $\mathbf{A}$, so need iterate)

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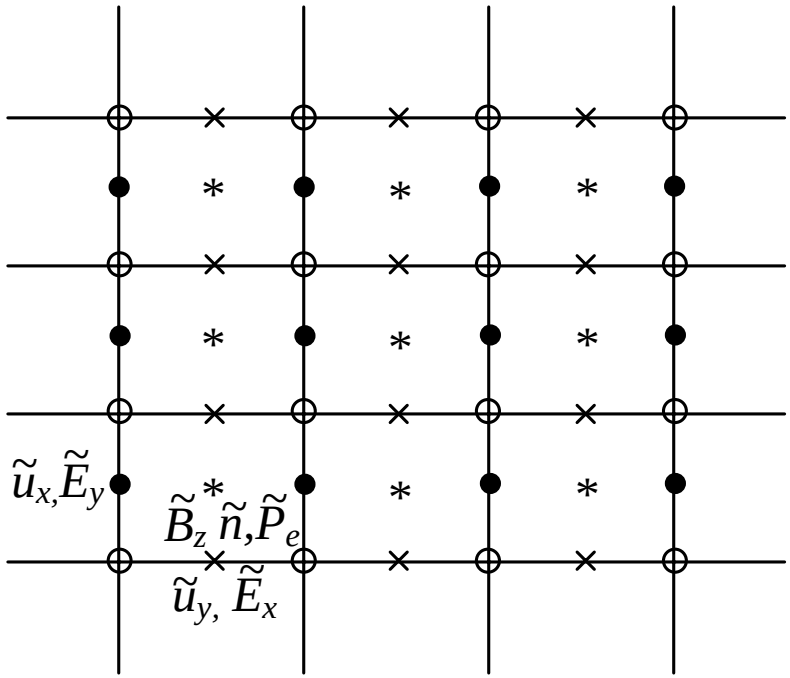
Space Differencing

- Use Yee mesh, w. velocity with $\mathbf{B}$



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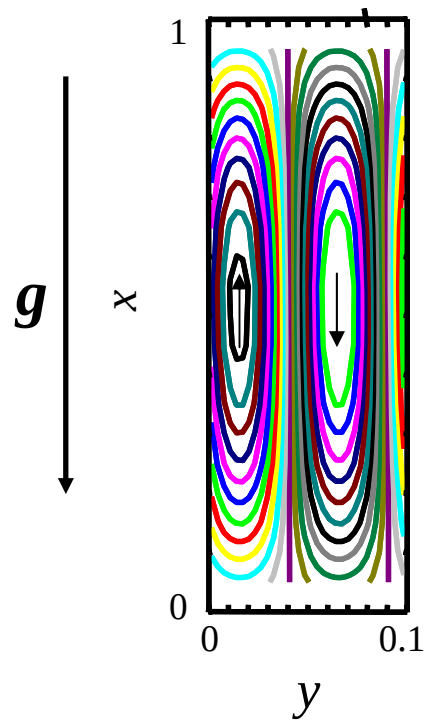
G-Mode Tests

- Following Roberts, Taylor, Schnack, Ferraro, Jardin, …



Contours of u_x for Roberts-Taylor G-mode

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G-Mode Tests

- Two series
  - Low β Hall stabilized – with and w/o closure
  - High β gyro-viscous stabilized (Hall turned off)
- Numerical parameters
  - N_x x N_y = 30 x 16
  - 9 – 25 particles/cell
  - Typically 100 particle steps/fluid step

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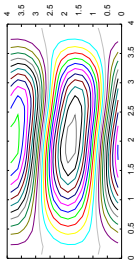
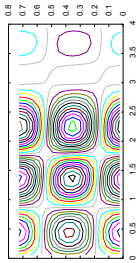
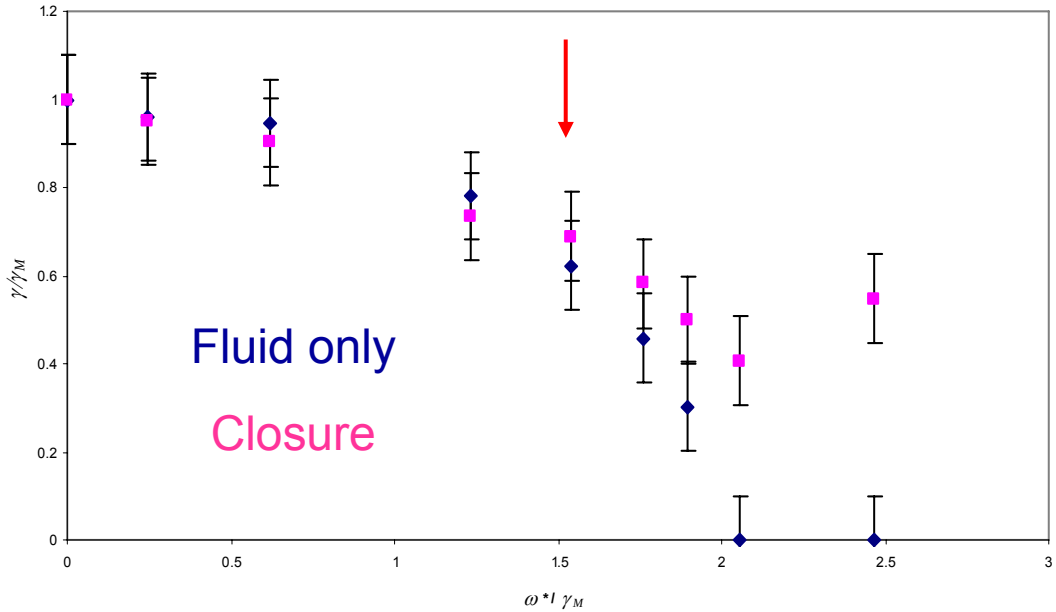
G-Mode Tests



Perturbed density





- Low β
  - $\beta = 0.02$
  - B = 6.0 T
  - n = 2. x 10^{20} m^{-3}
  - g = 1. x 10^{12} m/s^2
  - L_n = 120 m
  - T = 8.94 keV
  - ρ = 2.28 mm
- Arrow marks $k\rho$ = 0.15

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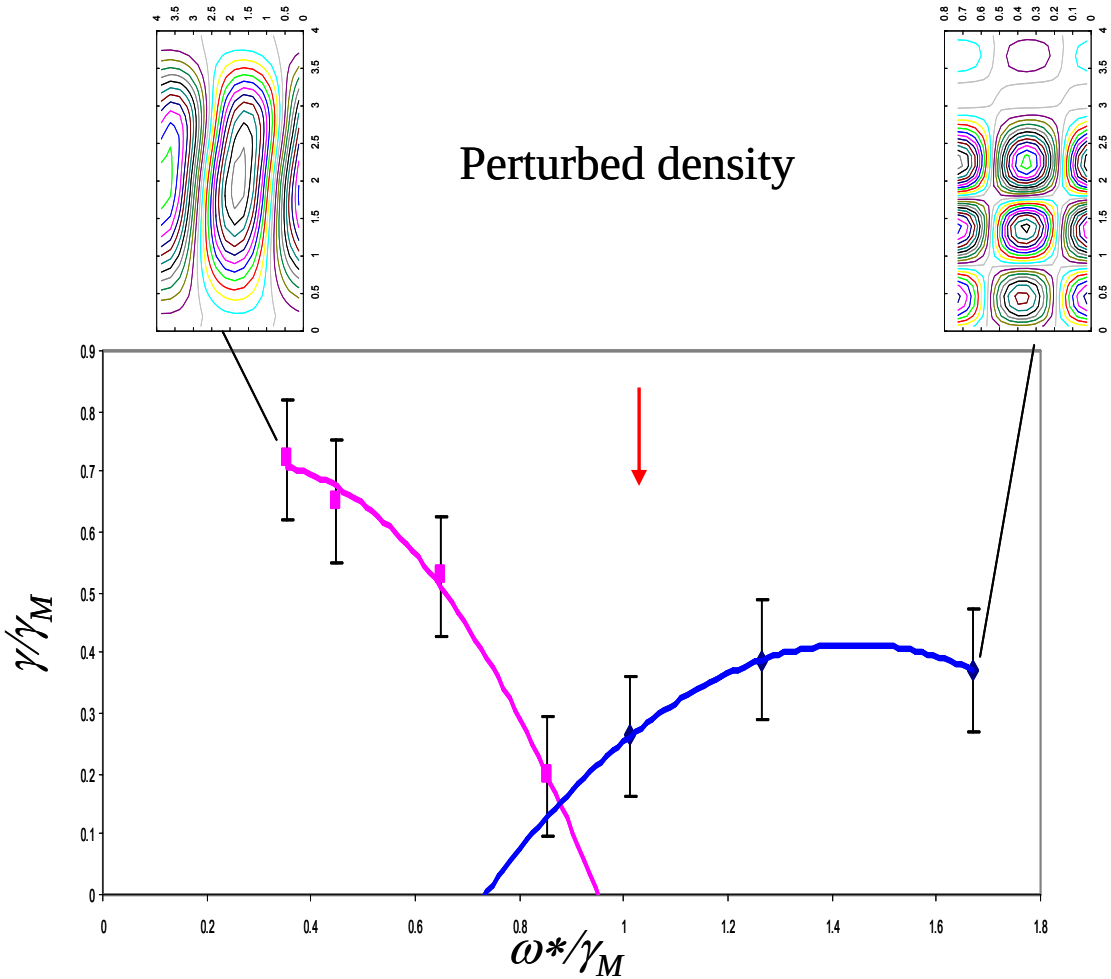
G-Mode Tests



- High β
  - $\beta = 1.0$
  - B = 0.482 T
  - $n = 5.78 \times 10^{19}$ m^{-3}
  - $g = 2.7 \times 10^{8}$ m/s^2
  - $L_n = 10$ m
  - $T = 10$ keV
  - $\gamma/\Omega_i = 2.25 \times 10^{-4}$
  - $\rho = 2.99$ cm
- Arrow marks $k\rho = 0.15$

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G-Mode Tests

- Hall and gyro-viscous stabilization of fundamental G-mode observed
  - Stability seems consistent with Roberts-Taylor, modified by Schnack & Ferraro, Jardin
- New, higher k_x mode observed at $k\rho > 0.2$ or so
  - Drift wave?
  - Present in fluid (+ Braginskii) also?

Conclusions

- New, evolving background δf method developed
  - Use particular velocity
  - Symmetric formulation
  - Energy integral for discrete system
  - Demonstrated consistency with implicit Δt and orbit averaging
- IMP ready for prime time?
  - Check $k_{\|} \neq 0$
  - Integrate with CEMM

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