Challenges in Gyrokinetic Numerical Algorithms

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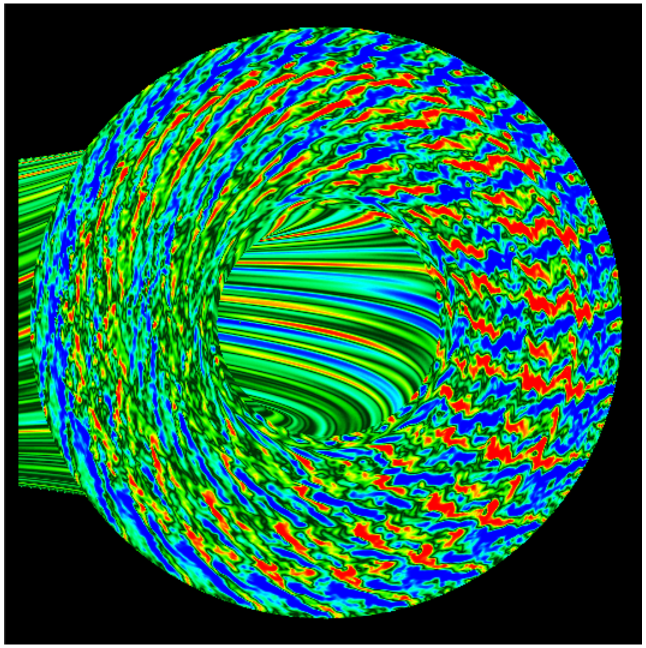

Waltz, Candy, et al, General Atomics

IPAM UCLA Conference

Multiscale Process in Fusion Plasmas

1/11/2005

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Challenges in Gyrokinetic Numerical Algorithms

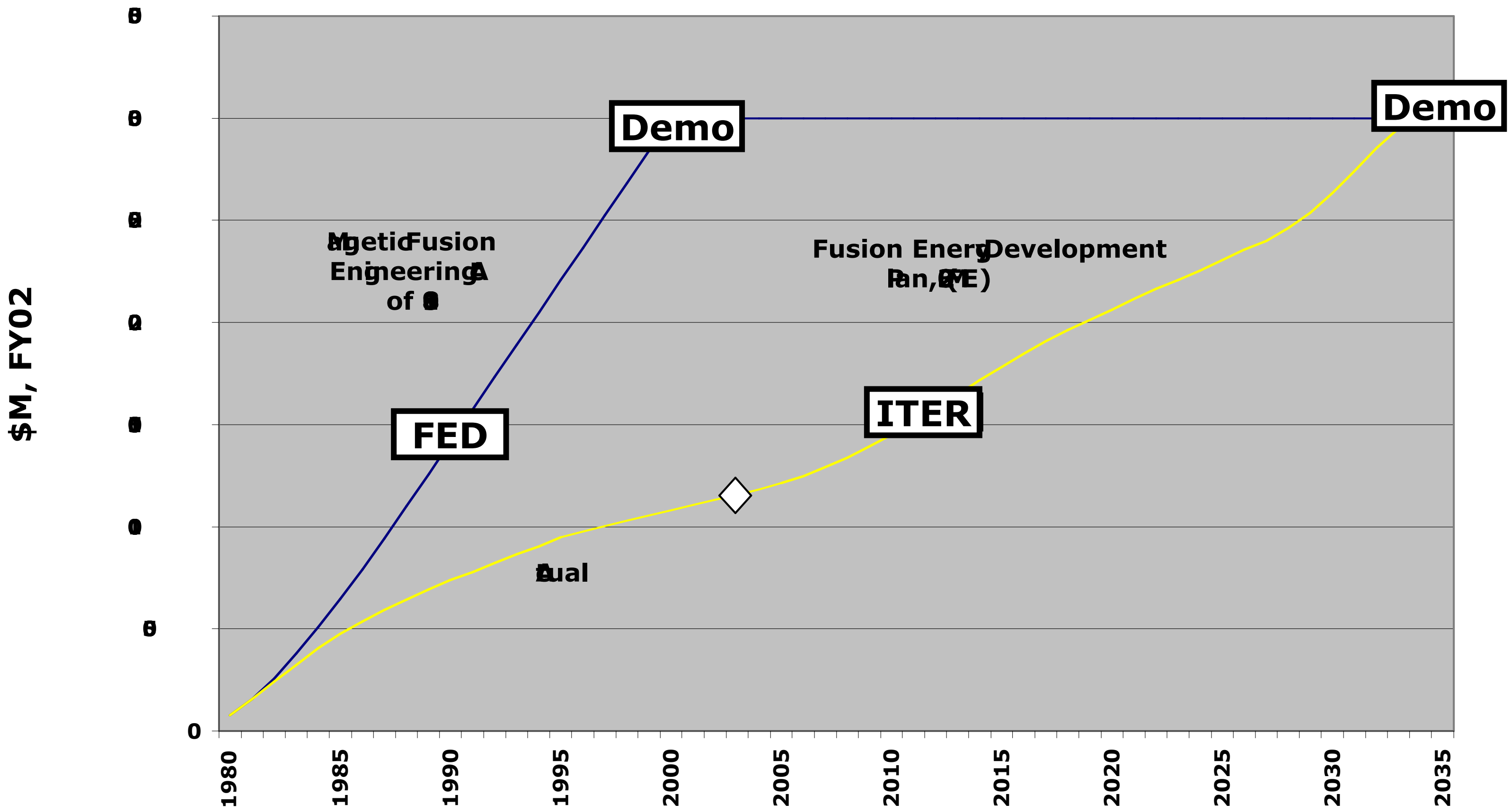
- Motivation: progress being made in fusion, better understanding could help too

- Paradigm gyrokinetic problem: Alfven waves
- A stability limit on a gyrokinetic ADI algorithm

- Kotschenreuther's trick for fast implicit solves
- Are there faster iterative methods? (particularly useful for extending to higher collisionality edge plasmas or including large scale ExB shear?)

The Estimated Development Cost for Fusion Energy is Essentially Unchanged since 1980

Cumulative Funding

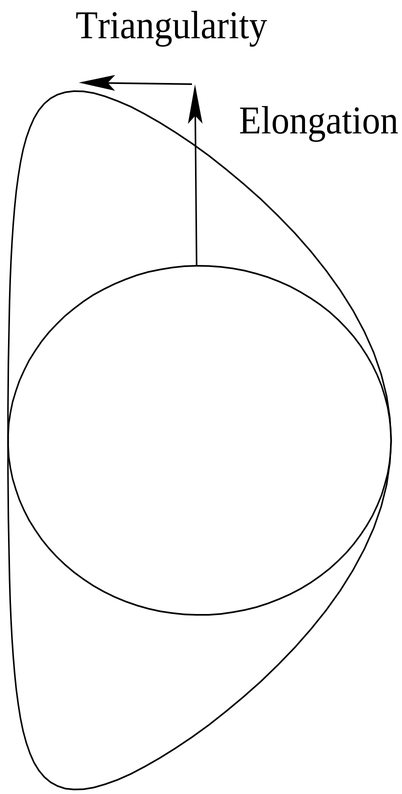


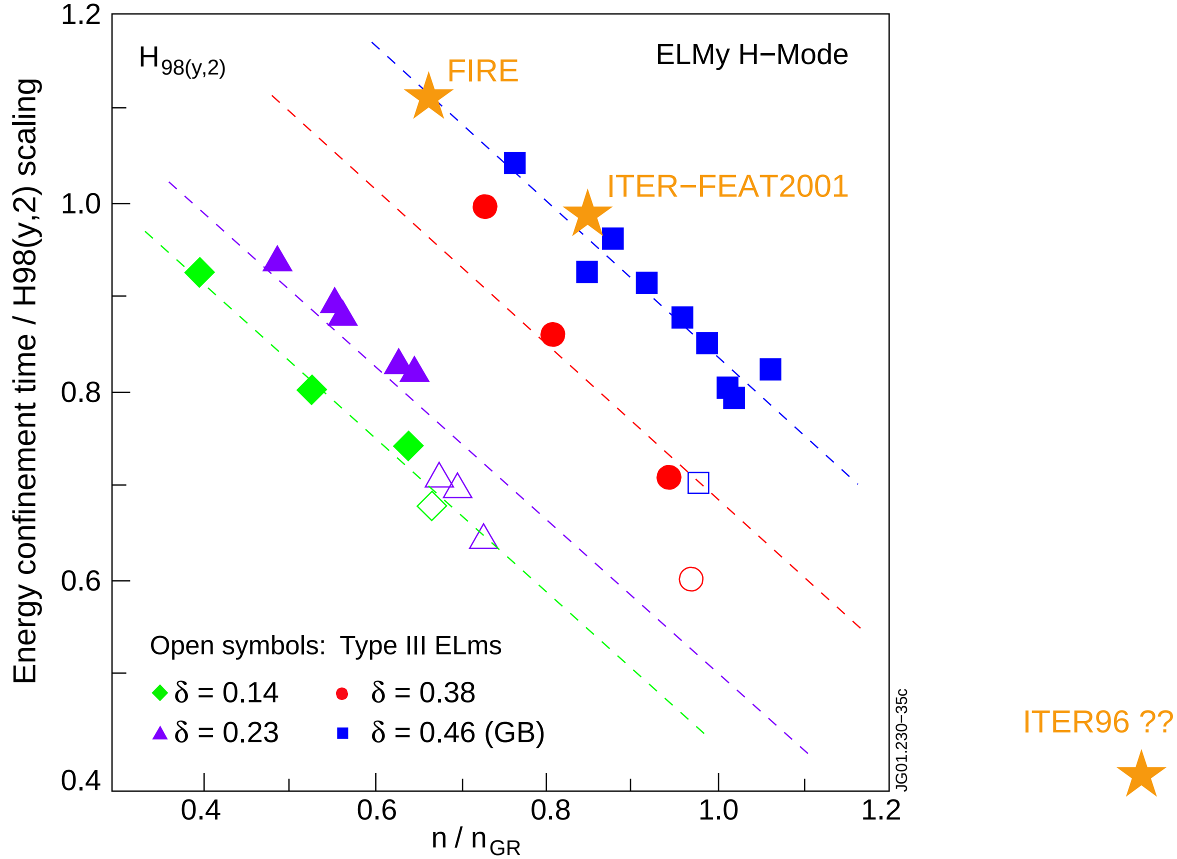
On budget,
if not on time.

$30B development cost tiny compared to >$100 Trillion energy needs of 21st century and potential costs of global warming. Still 40:1 payoff after discounting 50+ years.

R. Goldston, PPPL

New Reactor Designs Much Better than 1996 ITER





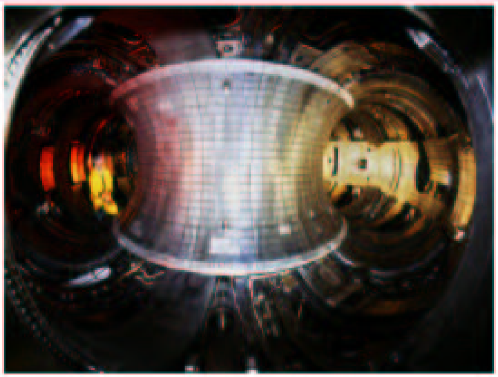
Confinement degrades if density too large relative to empirical Greenwald density limit $n_{Gr} = I_p /(\pi a^2)$, but improves with higher triangularity.

Compared to original 1996 ITER design, new ITER-FEAT 2001 and FIRE designs can operate at significantly lower density relative to Greenwald limit, in part because of stronger plasma shaping (higher triangularity and elongation).

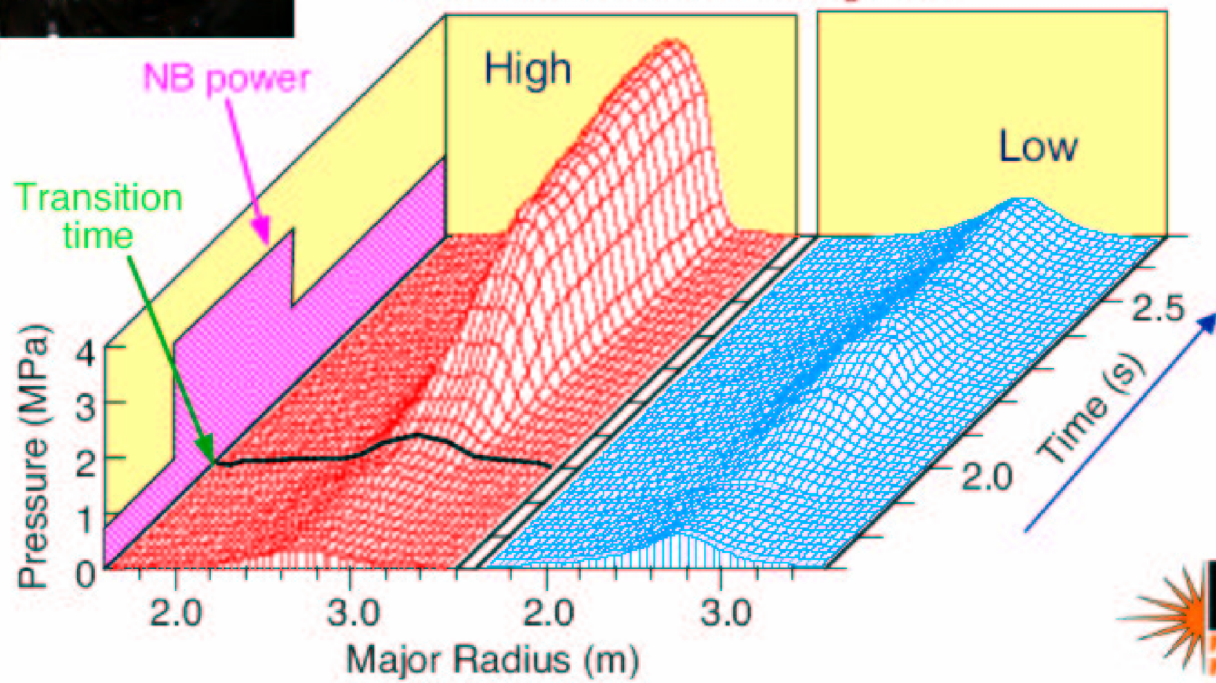
JET data from G. Saibene, EPS 2001, J. Ongena, PPCF 2001. Seen in other tokamaks also.

Fascinating Diversity of Regimes in Fusion Plasmas. What Triggers Change? What Regulates Confinement?

TFTR



- Two regimes with very different confinement for similar initial conditions and neutral beam heating
- Access depends on plasma heating and reducing current density on axis
- Can we attribute a difference in turbulence to these two different confinement regimes?



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The 5D Nonlinear Integro-Differential Gyrokinetic Equation

$$\boxed{\left(\frac{d}{dt} + \mathrm{v}_{\parallel}\vec{b}\cdot\nabla + i\omega_d + C\right)h = \left(i\omega_{*T} + \frac{Z_s e F_M}{T_s}\frac{\partial}{\partial t}\right)\chi}$$

$$\gamma = \frac{k_{\perp}\mathrm{v}_{\perp}}{\Omega_s}$$

The fields are represented by: $\chi \equiv \left(J_o(\gamma)(\Phi - \frac{\mathrm{v}_{\parallel}}{c}A_{\parallel}) + \frac{J_1(\gamma)}{\gamma}\frac{m_s \mathrm{v}_{\perp}^2}{Z_s e}\frac{\delta B_{\parallel}}{B}\right)$

The total time derivative contains the nonlinear term, i.e. $\frac{dh}{dt} = \frac{\partial h}{\partial t} + \frac{c}{B}\{\chi, h\}$

The self-consistent electromagnetic field fluctuations are computed from the gyrokinetic Poisson-Ampere Equations:

$$\boxed{\nabla_{\perp}^2\Phi = 4\pi\sum_s Z_s e\int d^3\mathrm{v}\left(\frac{-Z_s e F_M}{T_s}\Phi + J_0(\gamma)h\right)}$$

$$\boxed{\nabla_{\perp}^2 A_{\parallel} = -\frac{4\pi}{c}\sum_s Z_s e\int d^3\mathrm{v}\left(\mathrm{v}_{\parallel}J_0(\gamma)h\right)}$$

$$\boxed{\frac{\delta B_{\parallel}}{B} = -\frac{4\pi}{B^2}\sum_s\int d^3\mathrm{v}\left(m_s \mathrm{v}_{\perp}^2\frac{J_1(\gamma)}{\gamma}h\right)}$$

Alfven waves in a Simple Limit of Gyrokinetic Eq.

For high frequency waves, ignore parallel ion motion.
For $k_\perp \rho_e$ <<1, gyrokinetic eq. for electrons reduces to drift-kinetic eq.:

$$\frac{\partial F}{\partial t} + (\mathrm{v}_\| \hat{b} + \mathrm{v}_{\mathrm{ExB}}) \cdot \nabla F + \frac{q}{m} E_\| \frac{\partial F}{\partial \mathrm{v}_\|} = 0$$

$$E_\| = -\hat{b} \cdot \nabla \Phi - \frac{1}{c} \frac{\partial A_\|}{\partial t}$$

Linearize $F=F_{max}+f$, use Ampere's Law & Quasineutrality (w/ polarization):

$$k_\perp^2 A_\| = -\frac{4\pi}{c} e \int d^3\mathrm{v} f_e \mathrm{v}_\|$$

$$\int d\mathrm{v} f_e = n_{i,pol} = -(1 - \Gamma_0(k_\perp^2 \rho_i^2)) n_{i0} \frac{e\Phi}{T_i}$$

$$\approx -\frac{k_\perp^2 \rho_i^2}{1 + k_\perp^2 \rho_i^2} n_{i0} \frac{e\Phi}{T_i}$$

polarization density & current related:

$$\frac{\partial n_{pol}}{\partial t} = -\nabla \cdot (n_{i0} \vec{\mathrm{v}}_{pol}) = \nabla \cdot (n_{i0} \frac{1}{\Omega_{ci}} \frac{c}{B} \frac{\partial E_\perp}{\partial t})$$

Alfven waves in a Simple Gyrokinetic Limit (cont.)

Density moment of drift kinetic eq.:

$$\frac{\partial n_e}{\partial t} = -\frac{\partial}{\partial z}(n_{e0} u_\parallel)$$

$$-k_\perp^2 \rho_s^2 n_{e0} \frac{\partial}{\partial t}\frac{e\Phi}{T_e} = -k_\perp^2 \frac{c}{4\pi e}\frac{\partial}{\partial z} A_\parallel$$

$k_\perp^2$ cancel. Combine with $E_\parallel=0$ to get $\omega^2=k_\parallel^2 v_A^2$. Or combine with parallel momentum moment of drift kinetic equation

$$m_e n_e \frac{\partial u_{\parallel e}}{\partial t} = -\frac{\partial p_e}{\partial z} - e n_e E_\parallel$$

with eq. of state $p_{e1} = \Gamma\, n_{e1}\, T_{e0}$, and Pade approx. $\Gamma_0 = 1/(1+k_\perp^2\, \rho_i^2)$ to get kinetic Alfven wave:

$$\omega^2 = k_\parallel^2 v_A^2 \frac{1 + k_\perp^2(\rho_i^2 + \Gamma \rho_s^2)}{1 + k_\perp^2 c^2/\omega_{pe}^2}$$

Simple Limit of Gyrokinetic Equation (dimensionless, electrostatic)

$$\frac{\partial f(z,\mathrm{v},t)}{\partial t} = -\mathrm{v}\frac{\partial f}{\partial z} + \mathrm{v}\frac{\partial \Phi}{\partial z} F_M$$

$$k_\perp^2 \Phi = -\int d\mathrm{v}\, f$$

Requires implicit treatment for high frequency, irrelevant waves $\omega^2 = k_z^2 / k_\perp^2$

Simple ADI algorithm for gyrokinetics

$$\frac{\partial f(z, \mathrm{v}, t)}{\partial t} = -\mathrm{v}\frac{\partial f}{\partial z} + \mathrm{v}\frac{\partial \Phi}{\partial z} F_M \qquad k_\perp^2 \Phi = -\int d\mathrm{v}\, f$$

$$\frac{f^{n+1/2} - f^{n}}{\Delta t/2} = -\mathrm{v}\frac{\partial f^{n+1/2}}{\partial z} + \mathrm{v} F_M \frac{\partial \Phi^{n}}{\partial z}$$

$$\frac{f^{n+1} - f^{n+1/2}}{\Delta t/2} = -\mathrm{v}\frac{\partial f^{n+1/2}}{\partial z} + \mathrm{v} F_M \frac{\partial \Phi^{n+1}}{\partial z}$$

$$k_\perp^2 \Phi^{n+1} = -\int d\mathrm{v}\, f^{n+1}$$

Easy to invert operators, but found stability limit $\Delta t\ k_{\|}/k_\perp = \Delta t\ \omega < 2$

Numerical Instabilities in Gyrokinetic ADI algorithm

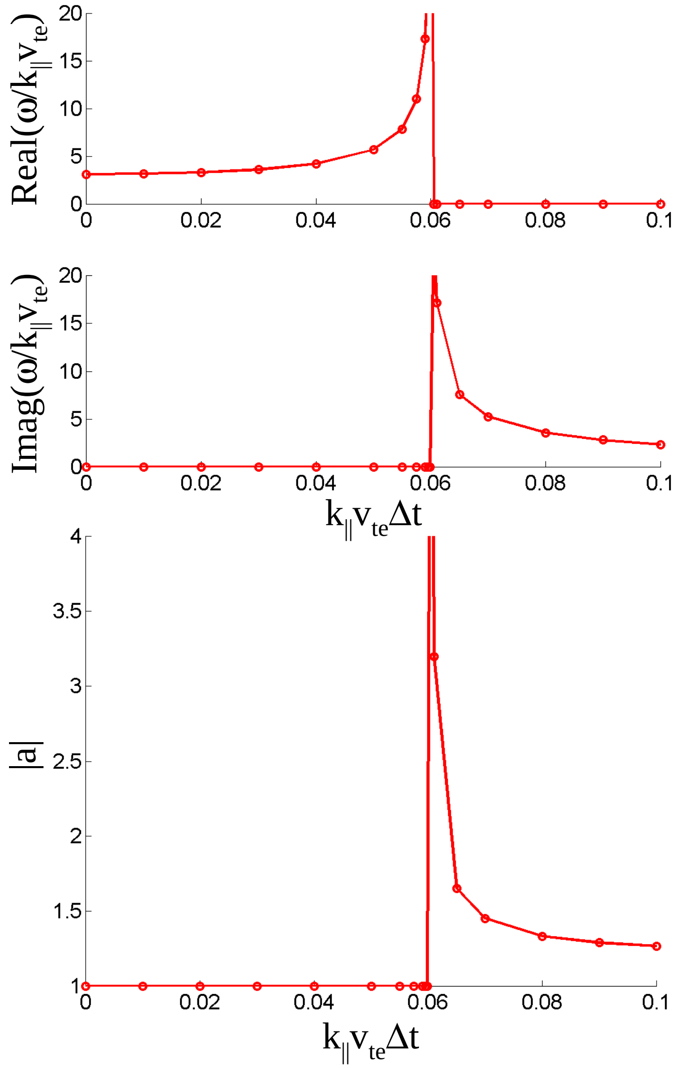
Even when extended to the electromagnetic case with $A_{||} \neq 0$, which slows down the waves to have $\omega = k_{||} << k_{||}/k_{\perp}$, still find numerical instability if $\Delta t\, k_{||}/k_{\perp} > 2$.   (E.A. Belli & G.W. Hammett, sub. to Comp. Phys. Comm.)

Usually think of ADI algorithms as being at least robust and absolutely stable, even if splitting errors cause accuracy problems. But here we found an instability.

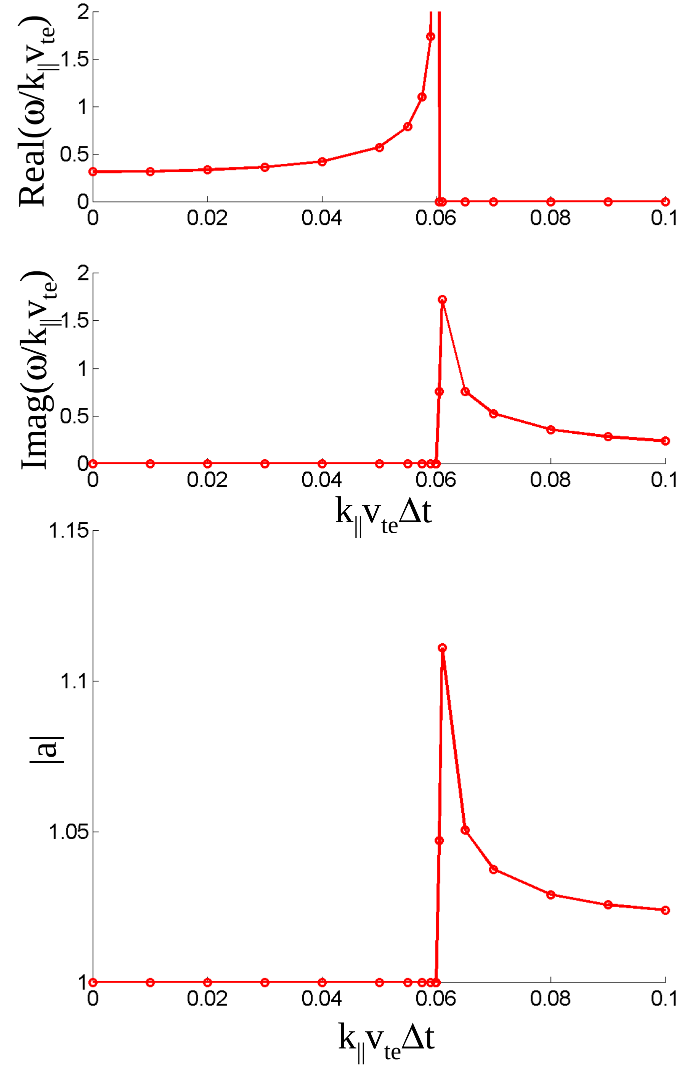
We find that the ADI algorithm is numerically unstable for $\Delta t/2 > |k_\perp \rho_s / k_\| v_{te}|$ in both the low and high $(\beta_e/2)(m_i/m_e)$ regimes.

Mode frequency & amplitude vs. time step for the kinetic Alfven wave at $k_\perp \rho_s$=0.03.

$(\beta_e/2)(m_i/m_e)$ = 0.1



$(\beta_e/2)(m_i/m_e)$ = 10



A Simple Illustration of the Numerical Difficulties of the ADI algorithm

The Landau-fluid approx to the kinetic eqn:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial u}{\partial z} - \frac{\partial A_{\parallel}}{\partial z} \qquad k_{\perp}^{2}\Phi = -\rho$$

$$\frac{\partial u}{\partial t} = -\frac{\partial P}{\partial z} + \frac{\partial \Phi}{\partial z} \qquad \left(k_{\perp}^{2} + \hat{\beta}\right)A_{\parallel} = -\hat{\beta} u$$

$$\frac{\partial P}{\partial z} = \Gamma \frac{\partial \rho}{\partial z} + \nu \left|k_{\parallel}\right| u$$

Fourier transform in space:

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho \\ u\end{pmatrix} = \begin{pmatrix} 0 & -ik_{\parallel} \\ -i\Gamma k_{\parallel} & -\nu\left|k_{\parallel}\right| \end{pmatrix}\begin{pmatrix}\rho \\ u\end{pmatrix} + \begin{pmatrix} 0 & ik_{\parallel}\hat{\beta}/(k_{\perp}^{2}+\hat{\beta}) \\ -ik_{\parallel}/k_{\perp}^{2} & 0 \end{pmatrix}\begin{pmatrix}\rho \\ u\end{pmatrix} \Rightarrow \boxed{\frac{\partial \vec{y}}{\partial t} = \overline{\overline{P}}\,\vec{y} + \overline{\overline{E}}\,\vec{y}}$$

Apply the ADI algorithm:

$$\frac{\vec{y}^{\,n+1/2} - \vec{y}^{\,n}}{\Delta t/2} = \overline{\overline{P}}\vec{y}^{\,n+1/2} + \overline{\overline{E}}\vec{y}^{\,n}$$

$$\frac{\vec{y}^{\,n+1} - \vec{y}^{\,n+1/2}}{\Delta t/2} = \overline{\overline{P}}\vec{y}^{\,n+1/2} + \overline{\overline{E}}\vec{y}^{\,n+1}$$

$$\Rightarrow \boxed{\vec{y}^{\,n+1} = \left(1 - \frac{\Delta t}{2}\overline{\overline{E}}\right)^{-1}\left(1 + \frac{\Delta t}{2}\overline{\overline{P}}\right)\left(1 - \frac{\Delta t}{2}\overline{\overline{P}}\right)^{-1}\left(1 + \frac{\Delta t}{2}\overline{\overline{E}}\right)\vec{y}^{\,n}}$$

ES: E is not diagonalizable & $E^n=0$, $n>1$

EM: eigenvalues of E are purely real ($\pm\,|k_{\parallel}/k_{\perp}|[\beta/(k_{\perp}^{2}+\beta)]^{1/2}$)

Direct Implicit Solve Expensive

$$\frac{\partial f(z,\mathrm{v},t)}{\partial t} = -\mathrm{v}\frac{\partial f}{\partial z} + \mathrm{v}\frac{\partial \Phi}{\partial z}F_M \qquad\qquad k_\perp^2 \Phi = -\int d\mathrm{v}\, f$$

Combine into standard ODE form:

$$\frac{\partial f}{\partial t} = \mathbf{A} f \qquad = -\mathrm{v}\frac{\partial f}{\partial z} - \mathrm{v}F_M \frac{\partial}{\partial z}\frac{1}{k_\perp^2}\int d\mathrm{v}\, f$$

Integro-differential equation. **A** *not* very sparse. Very inefficient to use directly.

F = N_z N_v vector ~ 500 x 200 ~ 10^5
A = (N_z N_v) x (N_z N_v) matrix
Direct implicit solve: (N_z N_v) x (N_z N_v) matrix problem

Kotschenreuther trick: 2 N_v calls to N_z x N_z tridiagonal solver
1 dense N_z x N_z matrix solve

Kotschenreuther et al.., Comp. Phys. Comm. 1995

Kotschenreuther Trick For Fast, Exact Implicit Solve

Illustrate with simple uncentered, implicit time, upwind space, explicit source S:

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = -\mathrm{v}\frac{f_j^{n+1} - f_{j-1}^{n+1}}{\Delta z} + \mathrm{v}F_M \frac{\Phi_{j+1}^{n+1} - \Phi_{j-1}^{n+1}}{2\Delta z} + S_j^n$$

$$\begin{aligned}
k_\perp^2 \Phi_j^{n+1} &= -\int d\mathrm{v}\, f_j^{n+1}\left[\Phi^{n+1}\right] \\
&= -\int d\mathrm{v}\left\{ f_j^{n+1}[0] + \frac{\delta f_j^{n+1}}{\delta \Phi_m^{n+1}} \Phi_m^{n+1} \right\} \\
&= -\int d\mathrm{v}\, f_j^{n+1}[0] - \mathbf{M}_{j,m}\Phi_m^{n+1} \\
(k_\perp^2 \mathbf{1} + \mathbf{M})\Phi^{n+1} &= -\int d\mathrm{v}\, f_j^{n+1}[0]
\end{aligned}$$

Response matrix $M_{j,m}$ measures charge induced at position j in response to potential perturbation at position m. Requires N_z solves of kinetic equation, but only has to be computed once (unless Δt changes).

Kotschenreuther et al.., Comp. Phys. Comm. 1995

Alternative Iterative Implicit Solve

Kotschenreuther's algorithm works fairly well, factoring a hard problem exactly Into two simpler problems. But there is overhead. Are there ways to do better? Response matrix $\mathbf{M}_{j,m}$ requires N_z solves of kinetic equation, but only has to be computed once (unless Δt changes).

If we have a good approximation $\hat{\mathbf{M}}$, can use a simple iterative method, or use it as a preconditioner for an iterative Krylov solver.

$$k_\perp^2 \Phi_j^{n+1} = -\int d\mathrm{v}\, f_j^{n+1}[0] - \mathbf{M}_{j,m}\Phi_m^{n+1}$$

$$(k_\perp^2 \mathbf{1} + \hat{\mathbf{M}}_{j,m})\Phi_m^{n+1,p+1} = -\int d\mathrm{v}\, f_j^{n+1}[0] - (\mathbf{M}_{j,m} - \hat{\mathbf{M}}_{j,m})\Phi_m^{n+1,p}$$

$$(k_\perp^2 \mathbf{1} + \hat{\mathbf{M}}_{j,m})\Phi_m^{n+1,p+1} = -\int d\mathrm{v}\, f_j^{n+1}[\Phi^{n+1,p}] + \hat{\mathbf{M}}_{j,m}\Phi_m^{n+1,p}$$

Kotschenreuther et al.., Comp. Phys. Comm. 1995

A numerical preconditioner was developed based on insight from the Pade approximations.

Our first simple numerical approx:

-- compute the exact M_{ij} vs. i for a single value of $j=j_0$

-- assume other values can be calculated by translation

$$\boxed{M_{ij} = M_{i-j+j0,j0}}$$

$\rightarrow$ only nk_x*nk_y*nfields GK-Poisson-Ampere solves are required.
However, in a real tokamak there are some spatial variations.

A new preconditioner was developed based on computing approx values for M_{ij} vs. i at various j simultaneously:

Example Illustration for n_{start} =1 and n_{stride} = 4, nipts = 1:

Set Φ values set for spatial grid pts j = 1, 5, 9, …

+1 0 0 0 -1 0 0 0 +1 0 0 …

Solve for the response row R_i

$M_{11} = R_1$
$M_{21} = R_2$

Extrapolate to get
M_{i1}, i=3,…

$M_{45} = -R_4$
$M_{55} = -R_5$
$M_{65} = -R_6$

Extrapolate to get
M_{i5}, i =1,..3 &
i =7,…

$M_{89} = R_8$
$M_{99} = R_9$
$M_{10,9} = R_{10}$

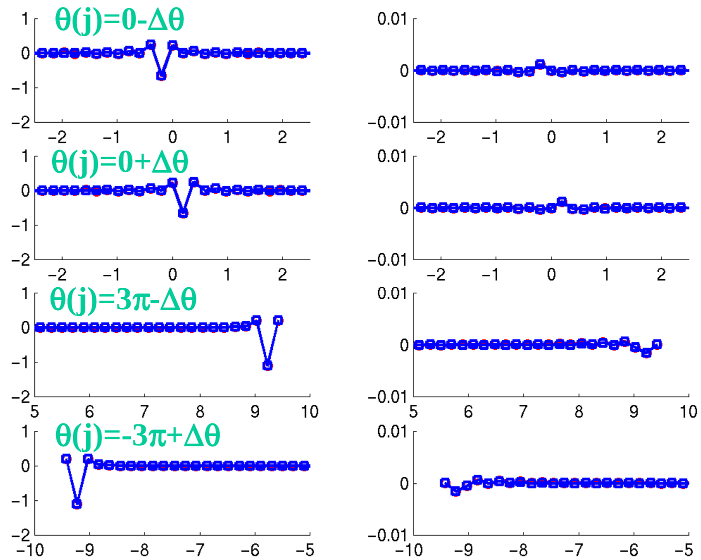
Extrapolate to get
M_{i9}, i=1,..7 &
i=11,…

The approximate response matrices agree well with the exact matrices, even at the boundaries.

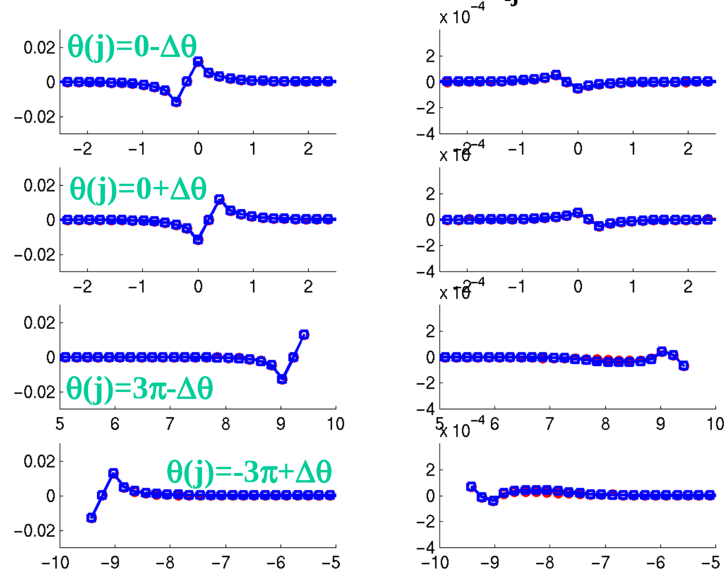
Test case parameters:

1 ion species & GK electrons
Concentric circular geo.
r/a = 0.80
R/a = 3.42
q = 2.03
s = 1.62
$\partial_r R_0$ = -0.14
$\partial_\rho \beta$ = -0.0084
β = 0 (es)
= 1e-3 (em)
a/L_T = 3.15
a/L_n = 1.02
T_i/T_e = 1.0
collisionless

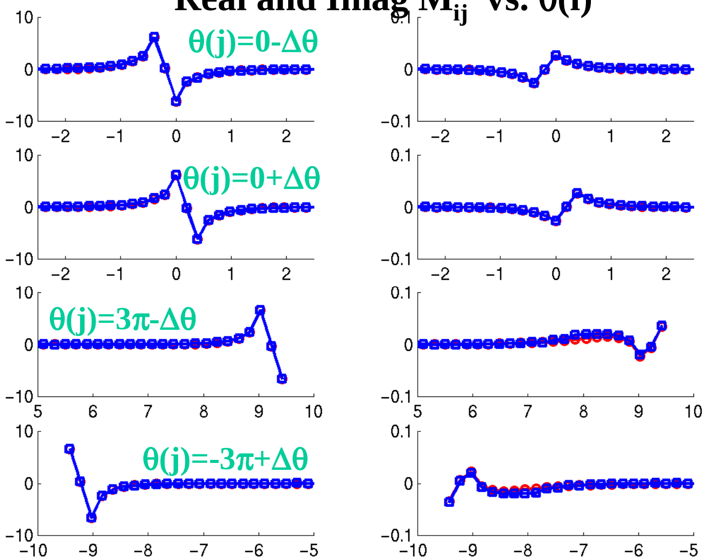
Real and Imag (M_{ij}^1 - δ_{ij} * Γ factor) vs. $\theta(i)$



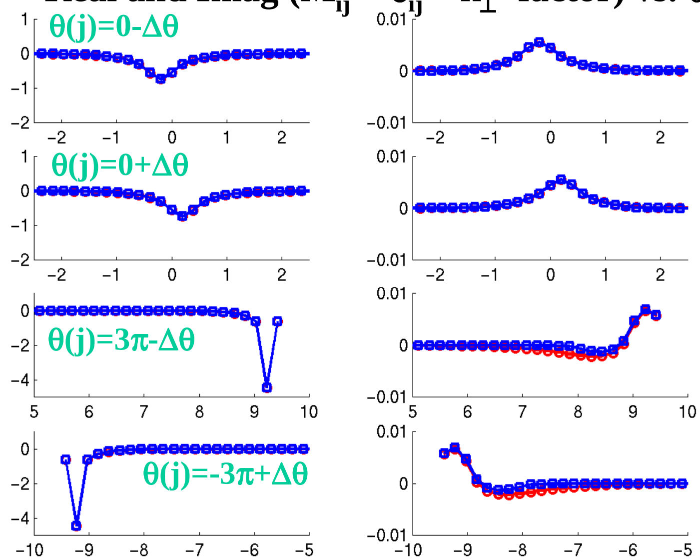
Real and Imag M_{ij}^3 vs. $\theta(i)$



Real and Imag M_{ij}^2 vs. $\theta(i)$



Real and Imag (M_{ij}^4 - δ_{ij} * $k_\perp^2$ factor) vs. $\theta(i)$



Figures are for $k_y\rho_i$=0.1, Δt=0.05
Exact (red)
Approx (blue)

Various initializers & iterative schemes were implemented in GS2.

iteration tol = ¼ ω tol = 2.5e-6	**Δt=0.01**		**Δt=0.05**		**Δt=0.1**	
	Avg. Num iterations/tstep	Avg. Num GK solves/tstep	Avg. Num iterations/tstep	Avg. Num GK solves/tstep	Avg. Num iterations/tstep	Avg. Num GK solves/tstep
Exact Implicit	**1**	**2**	**1**	**2**	**1**	**2**
Iterative implicit at $k_y\rho_i$=0.5:						
Simple iteration simple init →	**2.05** **3.01** **2.11 (em)**	**2.05** **3.01** **2.11 (em)**	**3.06** **4.00** **3.10 (em)**	**3.06** **4.00** **3.10 (em)**	**5.11** **6.04** **5.37 (em)**	**5.11** **6.04** **5.37 (em)**
Steepest Descent	**2.14**	**4.14**	**3.09**	**5.09**	**4.15**	**6.15**
BiConjugate Gradient Stabilized (Bi-CGSTAB)	**1.01**	**5.02**	**1.05**	**5.11**	**2.02**	**7.05**
Generalized Minimal Residual (GMRES)* $n_{restart}$=1→ $n_{restart}$=2→	**2.00** **2.00**	**5.00** **5.00**	**2.94** **2.09**	**5.94** **5.09**	**3.87** **3.00**	**6.87** **6.00**
Iterative implicit at $k_y\rho_i$=0.1:						
Simple iteration simple init →	**2.18** **3.05** **2.77 (em)**	**2.18** **3.05** **2.77 (em)**	**4.40** **7.20** **20.47 (em)**	**4.40** **7.20** **20.47 (em)**	**8.66** **15.29** **not convg (em)**	**8.66** **15.29** **not convg (em)**
Steepest Descent	**2.25**	**4.25**	**3.75**	**5.75**	**5.93**	**7.93**
BiConjugate Gradient Stabilized (Bi-CGSTAB)	**1.01**	**5.02**	**1.60**	**6.21**	**2.63**	**7.73**
Generalized Minimal Residual (GMRES)* $n_{restart}$=1→ $n_{restart}$=2→	**2.98** **2.92**	**5.98** **5.92**	**4.81** **3.99**	**7.81** **6.99**	**8.70** **6.21**	**11.70** **9.21**

Initializers:

linear extrapolation initializer: $\Phi^{n+1,0} = \Phi^n+(\Phi^n-\Phi^{n-1})$

simple initializer: $\Phi^{n+1,0} = \Phi^n$

* Routines adapted from V. Fraysse, et al, CERFACS Technical Report TR/PA/03/3.

Conclusions: Gyrokinetic Algorithms

- Paradigm gyrokinetic problem: Alfven waves
- Numerical instability in a gyrokinetic ADI algorithm

- Kotschenreuther's trick for fast implicit solves
- Are there faster iterative methods? (particularly useful for extending to higher collisionality edge plasmas or including large scale ExB shear?)

Conclusions

I. Studies of Improved Algorithms for Gyrokinetics

- **An iterative implicit scheme based on numerical or analytic approxs of the plasma response has been developed. A numerical preconditioner with a simple iterative scheme was found to work well in the es limit, but a more robust Newton-Krylov solver might be necessary with em dynamics.**
- **Implementation of an ADI algorithm in a gyrokinetic problem was surprisingly found to yield a severe time step restriction for a test problem of a shear kinetic Alfven wave at low $k_\perp \rho_i$ in both the low and high $(\beta_e/2)(m_i/m_e)$ regimes.**

II. Studies of the Effects of Shaping on Plasma Turbulence

- **…**

Future Work:

- **Investigate the numerical stability of other possible partially implicit algorithms.**
- **Continue to explore other numerical improvements, such as higher-order / variable time-stepping explicit treatment of the nonlinear term in GS2.**
- **…**