Full Radius Electromagnetic Gyrokinetic Turbulence Code

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Abstract. We describe work in progress to formulate a general geometry full radius nonlinear electromagnetic gyrokinetic code to simulate high-n turbulence and transport in tokamaks. The code employs continuum (fluid-like) methods in a 5-dimensional grid space. The code has three modes of operation: (1) flux tube with periodic radial boundary condition (i.e, a high-n ballooning mode representation with $\Delta n \approx 10$) ; (2) a full radius wedge code ($\Delta n \approx 10$) to study profiles shear effects; and (3) a full torus ($\Delta n=1$) code to study coupling to low-n MHD.

GENERAL ATOMICS

Introduction and Motivation

- Gyrokinetic code to contains all physics of low frequency (less than ion cyclotron) plasma turbulence assuming only that the ion gyroradius is less than magnetic field gradient length
  - Nonlinear
  - Electromagnetic and finite β
  - Real tokamak geometry
- Continuum (fluid-like) methods in 5-dimensional space (r, θ, n, ε, λ)
  - Possible advantage over partticle codes: implicit advance of electron parallel motion
- 3-modes of operation:
  - flux-tube or high-n ballooning mode representation BMR $\Delta n=10$ ρ^* -> to be bench-marked with Dorland-Kotchenruther new gyrokinetic flux tude code
  - wedge or full radius $\Delta n=10$ ρ^* small but finite
  - full torus $\Delta n=1$ Global MHD modes
- Why full radius? Shear in the ExB velocity known to have a powerful stabilizing effect. But shear in the diamagnetic velocity can be just as large and cannot be treated at $\rho^* = 0$. Also to quantify *avalanches* and *action at a distance* effects

Coordinate System

- (r, θ, α) r = midplane minor radius flux surface label
  θ = poloidal angle labeling Miller's local MHD equilibrium[1]
  which generalizes infinite aspect ratio circular s-α model with finite aspect ratio, Shafranov shift, ellipticity, and triangularity
  $\alpha = \zeta - \int_0^\theta \hat{q}\, d\theta$ field aligned angle in place of toroidal angle ζ
  $$\hat{q} = \hat{b}\cdot\nabla\zeta / \hat{b}\cdot\nabla\theta,\ \hat{b}\cdot\nabla\alpha = 0,\ \hat{b}\cdot\nabla r = 0,\ q = \int_0^{2\pi} \hat{q}\, d\theta / 2\pi$$
- Fourier decomposition of perturbations: $\phi = \Sigma_n \phi_n(r,\theta)\exp(-in\alpha)$ requires $\phi_n(r,\pi) = \phi_n(r,-\pi)\exp(-in2\pi q)$ where *phase factor* $\exp(-in2\pi q)$ is 1 at singular surfaces
- parallel derivative $\nabla_{||} = (\hat{b}\cdot\nabla\theta)\partial_\theta \Rightarrow (1/Rq)\partial_\theta$
- perpendicular derivatives on *fast* part : $\exp(-in\alpha)$

$$\nabla^f_{\perp y} = -in\nabla\alpha\cdot\hat{b}\times\hat{x} = ik_\theta \eta_q(\theta),$$ where $k_\theta \equiv nq/r$ with $\eta_q(\theta) = (rB/RB_\theta)/q \Rightarrow 1$

$$\nabla^f_{\perp x} = -in\nabla\alpha\cdot\hat{x} = ik_\theta\eta_q(\theta)\eta_k(\theta)$$ $\eta_k(\theta) \Rightarrow \hat{s}\theta - \alpha\sin(\theta)$

- additional *slow* derivatives on $\phi_n(r,\theta)$: $\nabla^S_{\perp y} = (B_t/B_p)(\hat{b}\cdot\nabla\theta)\partial_\theta$

  radial derivative is a mixture of *fast* and *slow*: $\nabla^{fs}_{\perp x} = |\nabla r|\,\partial_r$ $|\nabla r| \Rightarrow 1$

  Ballooning Mode Representation(BMR) retains only the fast derivatives

Normalizing Units

- Te(0) and ne(0) for temperature and density
  a = r of last closed flux surface for length
  $c_{s0} = [T_e(0)/M_i]^{1/2}$ for velocity
  a/c_{s0} for time
  $|e|\phi/T_e(0) = \hat{\phi}$ and $(c_{s0}/c)|e|A/T_{e0} = \hat{A}$ for potentials

- $g = \hat{g}(r,\theta,\hat{\varepsilon},\lambda,\sigma)n_e(0)F_M$ for non-adiabatic distribution function

  $\hat{\varepsilon} = \varepsilon/T, \lambda = \mu/\varepsilon, \sigma = \mathrm{sgn}(v_{||})$ and since (ε,μ) are the constants of motion

  $\partial_r \hat{g} = n_e(0)F_M D_r \hat{g}$ where $D_r \hat{g} = \partial_r \hat{g} + \partial_r \lambda \partial_\lambda + (\hat{\varepsilon}/L_T)\partial_{\hat{\varepsilon}} \hat{g} - [(\hat{\varepsilon} - 3/2)/L_T]\hat{g}$

  Note all terms beyond $\partial_r \hat{g}$ are small O(ρ^*) dropped in BMR limit.

- Parameters: the central ρ^* $[\rho_{s0} = c_{s0}/(eB_0/M_i c)]$, Debye length λ_{D0}, and electron beta β_{e0}.

- The gyro average $\langle\phi\rangle = \Sigma_n \exp(-in\alpha)\langle\phi\rangle_n$ expand the arguments of $\langle\phi\rangle_n$ to first order $\rho_\perp/r$, so that $\langle\phi\rangle_n = \oint d\alpha_g/2\pi \exp(-in\bar{\rho}_\perp \cdot \nabla\alpha)\phi_n(r + \bar{\rho}_\perp \cdot \nabla r, \theta + \bar{\rho}_\perp \cdot \nabla\theta)$.

  As a first approximation the *slow* $\bar{\rho}_\perp \cdot \nabla\theta$ can be neglected.

Gyrokinetic Equations

- **Poisson's Equation:** $-\lambda_{D0}^2 \nabla^2 \hat{\phi} = \sum_s \iint z\left[-(z\hat{n}/\hat{T})\hat{\phi} + \langle g \rangle\right]$,

- **Ampere's Law:** $-\rho_{s0}^2 \nabla^2 \hat{A}_{\|} = (\beta_{e0}/2) \sum_s \iint z\hat{v}_{\|} \langle \hat{g} \rangle$,

  where the phase space integral $\iint \Rightarrow \Sigma_\sigma \pi^{-3/2} \int_0^\infty d\hat{\varepsilon}\hat{\varepsilon}^{1/2} \exp(-\hat{\varepsilon})(\pi/2) \int_0^{1/B} d\lambda B/(1-\lambda B)$.

- **Nonlinear Gyrokinetic Equation [2,3] :** $\partial_{\hat{t}} \hat{g} + \hat{v}_{\|}(\hat{b} \cdot \hat{\nabla}\theta)\partial_\theta \hat{g} = z\hat{n}/\hat{T}\partial_{\hat{t}} \langle \hat{U} \rangle$
  $$-i\omega_E(-(z\hat{n}/\hat{T})\langle \hat{U} \rangle + \langle g \rangle) + i\varpi_D \hat{g} - i\hat{n}\varpi_* \langle \hat{U} \rangle + \left\{\langle \hat{U} \rangle, \hat{g}\right\} - \left\{\hat{g}, \langle \hat{U} \rangle\right\} + C\hat{g},$$

  where "hat" quantities are normalized, and $U = \hat{\phi} - \hat{v}_{\|} \hat{A}_{\|}$ **is the effective potential.**

- **The low-n MHD rule of neglecting** $A_\perp$ **while forcing the curvature drift to equal the grad-B drift is very good even for high-n.**

- The curvature drift operator which acts only on $\hat{g}$ is

$$\hat{\varpi}_D = -iz\hat{T}(2/R_0)\rho_{s0}(B_0/B)\{C(\theta,\hat{\varepsilon},\lambda)\ [inq/\hat{r}]\ + S(\theta,\varepsilon,\lambda)\ [i(nq/\hat{r})\eta_k + (|\nabla r|/\eta_q)D_{\hat{r}}]\}\ .$$

where C is the cosine-like normal curvature, S the sine-like geodesic curvature [1]

- The diamagnetic term is $\varpi_* = -i(B_0/B_{unit})\rho_{s0}[inq/\hat{r}][1/\hat{L}_n + 1/\hat{L}_T(\hat{\varepsilon}-3/2)]$.

- The E×B equilibrium rotation frequency is $\hat{\omega}_E = -i(B_0/B_{unit})\partial_{\hat{r}}\hat{\Phi}_0\rho_{s0}\,[inq/\hat{r}]$.

- The nonlinear term $\{X,Y\} \equiv \sum_{n',n''=n-n'} (B_0/B_{unit})\rho_{s0}\left[in''q/\hat{r}\right]X_{n''}\left[\partial_r + i(n'q/\hat{r})\eta_k\eta_q/|\nabla r|\right]Y_{n'}$,

- We define $[inq/\hat{r}] \equiv inq/\hat{r} + (B_t/B)(\hat{R}q/\hat{r})(\hat{b}\cdot\hat{\nabla}\theta)\partial_\theta$. $\quad B_{unit} = B_0\rho d\rho/rdr$

The nq/r terms are *fast* and the ∂_θ terms are *slow*. where again we use D_r when ∂_r acts on g.

- C is the pitch angle scattering operator.

Numerical Methods

- Electron parallel motion term $Lg = v_{\|}(\hat{b}\cdot\nabla\theta)\partial_\theta g$ is much faster than drift frequencies we are trying to follow, hence need an implicit method which solves for the fields U simultaneously with the advance of g

- Gyrokinetic equation can be differenced in a time-centered fashion $M \equiv z\hat{n}/\hat{T}$

  $[1/\Delta t + \delta L]g(t+\Delta t) = (M/\Delta t)\langle U\rangle(t+\Delta t)H(t) = S_g(t)$ where information at time t is given by

  $H(t) = [1/\Delta t - (1-\delta)L]g(t) - (M/\Delta t)\langle U\rangle(t) + E(t)$, and E explicit terms: 2nd line of equation.

- The Green's function $G = (1/\Delta t + \delta L)^{-1}$ is discretized by 2-point θ-derivatives centered at j + 1/2

  G is diagonal in the radial grid, and must account for bouncing , and the *phase factor* on passing .

  $g(t+\Delta t)_j = \Sigma_j G_{jj'}[(M/\Delta t)\langle U\rangle(t+\Delta t)]_{j'+1/2} + \{\{g(t)\}\}_j$ where $\{\{g(t)\}\}_j = \sum_{j'} G_{jj'} H(t)_{j'+1/2}$

- Source for the Poisson equation : $S_{\phi j}(t) = \Sigma_s \iint z^s \langle\{\{g^s(t)\}\}\rangle_j$

$$- \lambda_{s0}^2 \nabla^2 \phi_j(t+\Delta t) - \Sigma_s z^s \{-M^s \phi_j(t+\Delta t) + \iint \langle \Sigma_{j'} G^s_{jj'} [(M^s/\Delta t) \langle U(t+\Delta t)\rangle]_{j'+1/2} \rangle\} = S_{\phi j}(t)$$

and a similar equation for Ampere's law combine to an implicit field equation solver

$$\overline{\mathrm{M}}\vec{V}(t+\Delta t) = \vec{S}(t) \qquad \text{for } \vec{V} = \{\phi, A_{||}\}.$$

- Since the gyroaveraging essentially spans all radii m, $M_{jj', mm'}$ is a full matrix inverted to get field response matrix R. $R_{jj', mm', ff'}$ and $G_{m, n, s, e, l, jj'}$ [or it' s tridiagonal equivalent for $(1/\Delta t + \delta L)$] are computed once and stored.

- The "Explicit E " terms can be handled in different ways. The terms local in θ or with $\partial/\partial\theta$ can be added to the implicit parallel operator. The other parts can be done with "split steps".

We expect the split step for nonlinear terms to be done explicitely but the split step for the $D_{\hat{r}}$ radial derivative terms in the geodesic curvature apparently must be done implicitly (see below)

Reduction to Ballooning Mode Space and First Results

- **An important first step is to recover the BMR using the periodic boundary condition**

$\phi_n(\theta, r_s + \Delta r/2) = \phi_n(\theta, r_s - \Delta r/2)$ n_{max} -> ∞ and ρ_{s0} -> 0 $\rho_{s0}(n_{max} q/r) \approx 1$

slow **terms become negligible compared to the *fast* terms.**

- **BMR is a Fourier transform:** $\phi_n(\theta, r_s + x) = \Sigma_{k_x} \bar{\phi}_{n,k_x}(\theta) \exp(i k_x x)$ $-\infty < \theta < \infty$.

Fourier label: $k_x = \hat{s} k_\theta (\theta_0 + 2\pi p)$ **where** $k_\theta = nq(r_s)/r_s$ **so** $\sum_{k_x} \Rightarrow \sum_{\theta_0} \sum_{p}$

p is the "image index" which runs over all integers

$\theta_0 \in [-\pi, \pi)$ **is the discretized "ballooning angle label"**

Periodicity requires BMR space functions : $\bar{\phi}_{n,\theta_0,p}(\theta - 2p\pi) = \bar{\phi}_{n,\theta_0,0}(\theta) \exp[inq(r_s) 2\pi p x]$.

Equivalent to the *phase factor* in real space (r,θ) : $\phi_n(\pi, r_m) = \phi_n(-\pi, r_m) \exp[-2\pi n q(r_m)]$

which transforms to the *continuity* condition : $\bar{\phi}_{n,\theta_0,p+1}(-\pi) = \bar{\phi}_{n,\theta_0,p}(\pi)$

• To get finite grids ballooning modes must be localized in θ , for example -3π to 3π.

Hence only first images p = ±1 need be retained.

If we place the highest $J_* - 1$ image retained at half the Nyquist wave number (4 radial grids per wavelength), then

$\delta r / \rho_{s0} = 1/[2 J_* \hat{s} (k_\theta^{ref} \rho_{s0})] = (\Delta_s / \rho_{s0})/(2 J_*)$ where Δ_s is the singular surfaces spacing.

Note that $N_r = 2 l_* J_*$ where $l_* (\theta_0 / 2\pi) = 0, 1, .2 ... (l_* - 1)$.
We take $k_\theta^{ref} \rho_{s0} = 0.5$ is highest fully resolved with $k_\theta^{\max} \rho_{s0} = 1.0$

For nonlinear runs we expect $l_* = 40$ and $J_* = 2$ to suffice or a box of $160/(2\hat{s})$ gyrolengths ρ_{s0}

These gyrolengths can be concentrated over a distance with no significant profile variation or eventually over the full radius.

Must use a spectral technique to evaluate radial derivatives and gyroaverages.

"harmonic derivative" is defined such that for any of the N_r allowed k_x's of the simulation box,

$$[\partial_r]_H \exp(ik_x x) = (ik_x)\exp(ik_x x)$$

This results in radial derivative and gyroaverageing operators which connect <u>all</u> N_r gridpoints.

$$[\partial_r]_H \phi_m(\theta) = \sum_{m'=-N_r/2}^{m'=N_r/2-1} H_{m,m'}\phi_m(\theta) \quad \text{and} \quad \langle \phi(\theta) \rangle_m = \sum_{m'=-N_r/2}^{m'=N_r/2-1} W_{m,m'}\phi_m(\theta)$$

The electrons can pose a problem in r-space since the Landau damping layer is impractical to resolve without a 100-fold increase in J_*

$$\Delta_e/\rho_{s0} = (Rq/\hat{s})(\omega/\omega_*)(m_e/2M_i)^{1/2} << \delta r/\rho_{s0} = 1/[2J_*\hat{s}(k_\theta^{\max}\rho_{s0})]$$

If any grid is within a distance Δ_e of a singular surface, it will over-weight the $k_{||} = 0$ passing electron dynamics. The BMR avoids this by forcing 0 boundary conditions at the extended angle $\theta=\pm 3\pi$ which <u>properly</u> [5] nullifies $k_{||} = 0$ contribution, since its true weight is only $\Delta_e/\delta r$ [5] .

Varying the position of the singular surface so it falls on a grid point or midway between grid points, can result in as much as a 10% variation in the growth rate.

Must use an implicit method for the radial (harmonic) derivative component of geodesic curvature

split R-step : $\sum_{m'} (1_{mm'} - (i/2)dt\varpi_{Dr} H_{mm'})\bar{g}_{m'} = \sum_{m'} (1_{mm'} + (i/2)dt\varpi_{Dr} H_{mm'})g_{m'}$

or $\bar{g}_m = \sum_{m'=-N_r/2}^{m'=N_r/2-1} G^R_{mm'} g_{m'}$; $g_m \Rightarrow \bar{g}_m$

The gyroaverage Wmm' and split R-step $G^R_{mm'}$ matices are diagonally dominant (cyclic) cornered

and it is much better to use pointers $m' = m'(m, \Delta m = m' - m)$ to write in "banded form", e.g

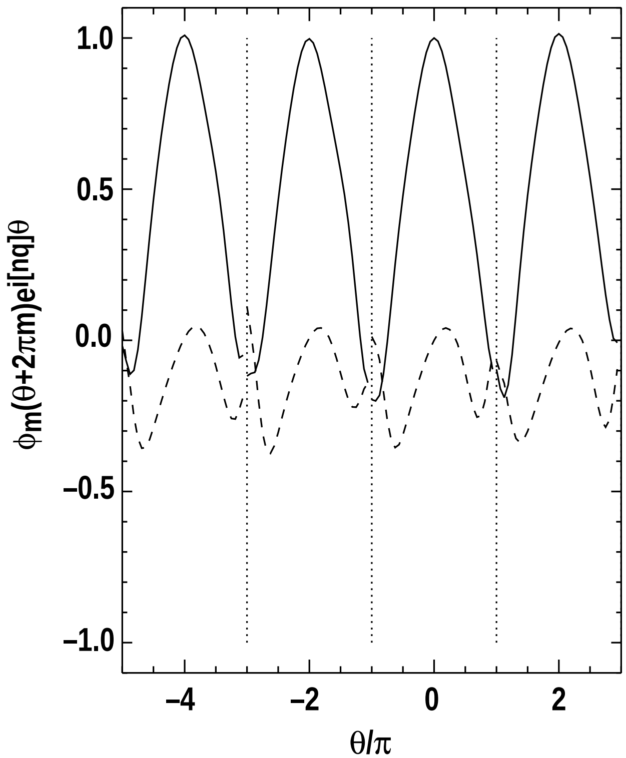
$\bar{g}_m = \sum_{\Delta m=-N_b}^{\Delta m=N_b^u} G^R_{m\Delta m} g_{mm'}$ $N_b \le N_r/2$ [$N_b^u = \min(N_b, N_r/2-1)$]

Linear illustration with $I_* = 1$ and $J_* = 2$, adiabatic electron, electrostatic, $\hat{s} - \alpha$ circular case :

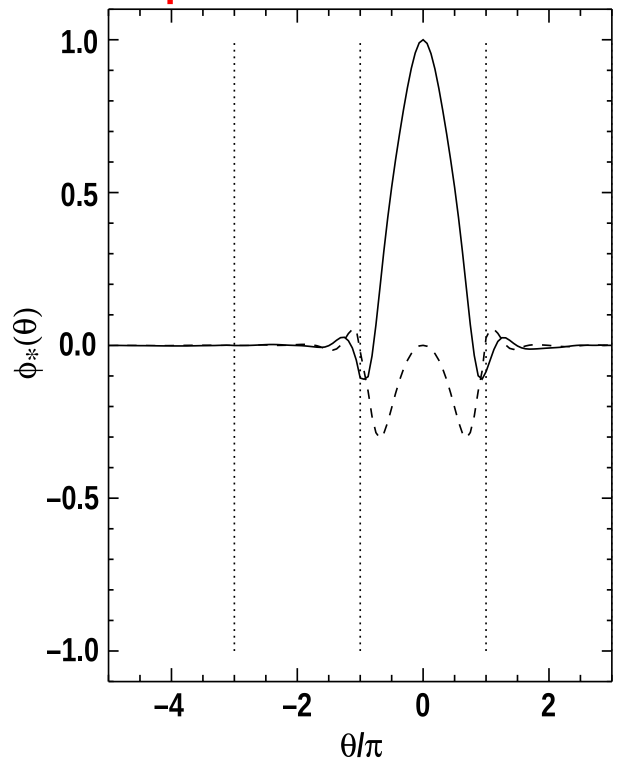
$\hat{s}$ = 0.25, α = 0, q = 2, $1/L_T$ = 6, $1/L_n$ = 1, T_i/T_e = 1, r = 1/2, and R = 1/3.

Using N_r=4 and N_θ =32 on $\theta \in [-\pi, \pi)$ we obtained the preliminary result (ω,γ) = (–0.257,0.312) compared to Kotschenreuther's [4] code (–0.249,0.303) on a $\theta \in [-3\pi, 3\pi]$ ballooning angle space.

Thus we are using 2-dimensions to solve a normally 1-dimensional problem for the BMR.
The added dimension will later allow us to treat the profile effects.



$\phi_m(\theta)$ from (r,θ) -space of code m=-2,-1,0,1



$\phi_p(\theta)$ Fourier reconstruction in ballooning space p=-2,-1,0,1

$$\bar{\phi}_p(\theta) = \sum_{m=-2}^{m=1} (\phi_m(\theta)/4)\exp(-i\pi m p)$$

Computer time and storage with radial grid number N_r scaling

- **Our original aim was to built a radial code which would reproduce *exactly* the BMR flux tube then be expanded to full radius. Using the exact Harmonic derivative operations $H_{mm'}$ and $W_{mm'}$, we found much of the memory required scaled as N_r^2, most of the linear steps as N_r^2, the nonlinear step as N_r^3, and the Matrix M setup time as N_r^3. These are prohibative.**

We have recently learned how to diagonally "band" these diagonally dominate operations for the linear parts and use a modified conservative nonlinearly operation with a 3-pt derivative.

Most all of an *approximate* code (with the exception of the field solve) should scale linearly N_r. BMR code of the same resolution, $N_k = N_r$, has linear part scaling as N_k and nonlinear part as N_k^2. The approximations from banding and be realaxed to test convergence.

- **Banding: $(N_b/N_r) = (11/160)$!!!!**

t_g = $(N_{step}/100)\,(16./N_{proc})\,(N_r/40)^2\ (N_\theta/8)\ N_n\ (N_e/5)\ (N_{pass}+N_\theta)/(5+8)\ N_s$
t_U = $(N_{step}/100)\,(16./N_{proc})\,(N_r/40)^2\ (N_\theta/8)^2\ (N_f)^2\ N_n$

Some bench points from 16ps LUNA assuming 0 communications in sec.

$t_{linear} = [\,(3.3+2.7/N_s + 2 + 3.5 + 5.4/N_n)\,(N_b/N_r) + 3.6/(N_r/40)\,] \times t_g + [2.9 + 0.4/(N_\theta/8)/N_f/N_n\,] \times t_U$
$t_{setup} = 160\,(N_r/40)\ (N_b/N_r)^3 / N_s \times t_g$

N_r=160 N_θ = 16 N_n=11 N_e=5 N_{pass}=10 N_s=2 N_f=1 N_{proc} = 256 N_{step}=10000

with banding t_{linear} = 3hrs (1sec/step) t_{setup} very little
without = 40hrs and t_{setup} = 20 hrs.

Almost all storage from gyroaverage Wmm' , split-R step $G^R_{mm'}$ and $R_{jjmm'}$

$2.(1+N_s)\ N_n\ N_e\ (N_{pass}+N_\theta)\ \ (2N_\theta)\ N_r^2 \times (N_b/N_r)\ /\ N_{proc}/10^6$ = 25.5MW /ps with
1.7 MW /ps with banding
$2\ N_n\ N_f(2N_\theta)^2\ N_r^2 \times (N_b/N_r)\ /\ N_{proc}/10^6$ = 2MW (16-32 MW/ps)

- **Conservative nonlinearly operation with a 3-pt derivative**

Schematically: in p-space (BMR k_x-space), the nonlinear term looks like

$$\partial_t \tilde{g}_{np} = \sum_{p'=-J}^{p'=J-1} \sum_{n'=-n_{max}}^{n'=n_{max}} \{(in')(ip'')\tilde{g}_{n'p'}\tilde{\phi}_{n''p''}\} - \{\tilde{g} \Leftrightarrow \tilde{\phi}\} \qquad n''=n-n';\, p''=p-p';\, J=N_r/2$$

This nonlinearly preserves $1/2 \sum_{p=-J}^{p=J-1} \sum_{n=-n_{max}}^{n=n_{max}} |\tilde{g}_{np}|^2$ Back in m-space (real r-space

$\phi_{nm} = \sum_{p=-J}^{p=J-1} \tilde{\phi}_{np} \exp(i\pi mp/J)$ and by Parseval's Theorem, we want to preserve the norm

$1/2 \sum_{m=-J}^{m=J-1} \sum_{n=-n_{max}}^{n=n_{max}} |g_{nm}|^2$. The exact m-space equivalent is a Harmonic derivative $H_{mm'm''}$

$$\partial_t g_{nm} = \sum_{m'=-J}^{m'=J-1} \sum_{m''=-J}^{m''=J-1} \sum_{n'=-n_{max}}^{n'=n_{max}} \{(in')H_{mm'm''}g_{n'm'}\phi_{n''m''}\} - \{g \Leftrightarrow \phi\}$$ scaling as $N_r^3 N_n^2$

However it is possible to write a conservative 3-pt (cyclic) derivative nonlinear term

$$\partial_t g_{nm} = \sum_{n'=-n_{max}}^{n'=n_{max}} \{(in')g_{n'm}(\phi_{n''m+1} - \phi_{n''m+1})/2dr\} - f_{nm}\{g \Leftrightarrow \phi\}$$

$$f_{nm} = (g_{nm+1} + g_{nm-1})/2g_{nm}$$

Progress & Conclusions

- We have how obtained good linear EM agreement with Kotschenreuther's GKS code

- We have found efficient MPI parallelization methods independent of grid size.

- Have EM real geometry linear runs on the 16ps GA Linux Beowulf LUNA and 64ps/128ps low resolution nonlinear runs ES adiabatic-e ITG runs on SDSC -T3E

- The use of banding and conservative 3-pt nonlinear derivative appears to allow almost linear N_r scaling.

- Immediate goals:

__Obtain high resolution saturated nonlinear flux tube run benchmark check with new Dorland-Kotschenreuther code. Show convergence with decreased banding.

__Move to "flux wedge" full radius operation with non-cyclic radial boundary conditions.

References

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