Microturbulence simulation in general geometry---A short note

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Magnetic field Representation

The GTC code employs a toroidal magnetic coordinates (ψ, θ, ζ) to represent the electromagnetic fields and plasma profiles, where ψ is the poloidal magnetic flux, θ is the poloidal angle and ζ is the toroidal angle. The equilibrium magnetic field can be represented either in the covariant form

$$\mathbf{B}_0 = g\nabla\zeta + I\nabla\theta + \delta\nabla\psi, \tag{1}$$

Or in the contravariant form

$$\mathbf{B}_0 = q\nabla\psi \times \nabla\theta + \nabla\zeta \times \nabla\psi. \tag{2}$$

For most interesting cases, the toroidal current g and poloidal current I, is merely a function of ψ, i.e., $g = g(\psi), I = I(\psi)$. Therefore, the jacobian of this magnetic coordinate system is

$$J^{-1} \equiv \nabla\psi \times \nabla\theta \cdot \nabla\zeta = \frac{B_0^{\ 2}}{gq + I}. \tag{3}$$

Laplacian operator and Geometric tensor

The Laplacian operator plays a central role in computing perturbed electromagnetic fields. In this section, we study how to discretize the Laplacian operator in the magnetic coordinates.

In a magnetic coordinate system, the Laplacian can be expressed as

$\nabla^2 f = \frac{1}{J} \frac{\partial}{\partial \xi^\alpha} \left(J\nabla\xi^\alpha \cdot \nabla\xi^\beta \frac{\partial}{\partial \xi^\beta} f \right)$, with $\alpha = 1,2,3$, and $\beta = 1,2,3$, where $\left(\xi^1, \xi^2, \xi^3\right) = (\psi, \theta, \zeta)$ are

coordinates the jacobian $J = (\nabla\psi \cdot \nabla\theta \times \nabla\zeta)^{-1}$. Define a contravariant geometric tensor

$g^{\xi^a \xi^\beta} \equiv \nabla \xi^\alpha \cdot \nabla \xi^\beta$. For an axisymmetric system, the Laplacian can be explicitly expressed as

$$
\begin{aligned}
\nabla^2 f = {}& g^{\psi\psi} \frac{\partial^2 f}{\partial \psi^2} + 2 g^{\psi\theta} \frac{\partial^2 f}{\partial \psi \partial \theta} + g^{\theta\theta} \frac{\partial^2 f}{\partial \theta^2} + g^{\zeta\zeta} \frac{\partial^2 f}{\partial \zeta^2} \\
& + \frac{1}{J} \left(\frac{\partial J g^{\psi\psi}}{\partial \psi} + \frac{\partial J g^{\psi\theta}}{\partial \theta} \right) \frac{\partial f}{\partial \psi} + \frac{1}{J} \left(\frac{\partial J g^{\psi\theta}}{\partial \psi} + \frac{\partial J g^{\theta\theta}}{\partial \theta} \right) \frac{\partial f}{\partial \theta}
\end{aligned}
\tag{4}
$$

In order to compute the above Laplacian, we first need to compute the contravariant geometric tensor $g^{\xi^a \xi^\beta}$. Note that B-splines of magnetic fields provides a covariant form, i.e., $X(\psi,\theta)$ and $Z(\psi,\theta)$, where (X,Z,ζ) forms a cylindrical coordinate system. The covariant geometic tensor $g_{\xi^a \xi^\beta}$ can be obtained by the following formula

$$
g_{\psi\psi} = \left(\frac{\partial X}{\partial \psi} \right)^2 + \left(\frac{\partial Z}{\partial \psi} \right)^2,
\tag{5}
$$

$$
g_{\theta\theta} = \left(\frac{\partial X}{\partial \theta} \right)^2 + \left(\frac{\partial Z}{\partial \theta} \right)^2,
\tag{6}
$$

$$
g_{\psi\theta} = \frac{\partial X}{\partial \psi} \frac{\partial X}{\partial \theta} + \frac{\partial Z}{\partial \psi} \frac{\partial Z}{\partial \theta},
\tag{7}
$$

And $g_{\theta\psi} = g_{\psi\theta}, g_{\zeta\zeta} = X^2$. Using the identity $g_{\xi^a \xi^\beta} g^{\xi^\beta \xi^\gamma} = \delta_\alpha^\gamma$, we can find the transformation from the covariant to contravariant geometric tensor.

$$
\begin{bmatrix} g^{\psi\psi} & g^{\psi\theta} & 0 \\ g^{\theta\psi} & g^{\theta\theta} & 0 \\ 0 & 0 & g^{\zeta\zeta} \end{bmatrix} = \begin{bmatrix} g_{\theta\theta} & -g_{\psi\theta} & 0 \\ -g_{\theta\psi} & g_{\psi\psi} & 0 \\ 0 & 0 & \Delta/g_{\zeta\zeta} \end{bmatrix} \frac{1}{\Delta},
\tag{8}
$$

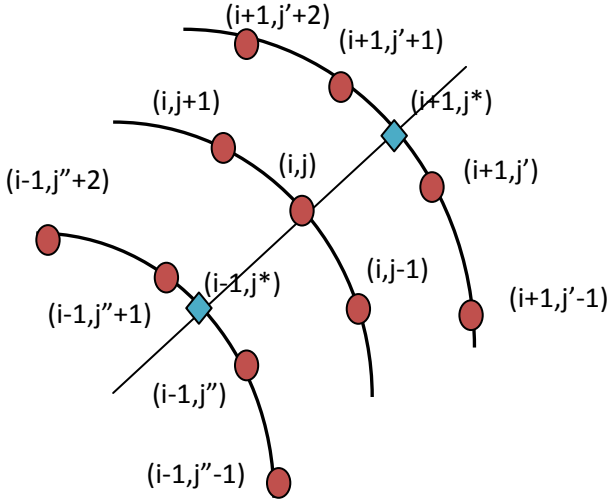With the determinant $\Delta = g_{\psi\psi} g_{\theta\theta} - g_{\theta\psi} g_{\psi\theta}$.

The field aligned coordinate (ψ,θ_0,ζ_0) is employed in the GTC code, where $\theta_0 = \theta - \zeta/q$ and $\zeta_0 = \zeta$. Then the Laplacian in this new coordinate system becomes

$$\nabla^2 f = g^{\psi\psi}\frac{\partial^2 f}{\partial\psi^2} + 2g^{\psi\theta}\frac{\partial^2 f}{\partial\psi\partial\theta_0} + g^{\theta\theta}\frac{\partial^2 f}{\partial\theta_0^2} + g^{\zeta\zeta}\left(\frac{\partial}{\partial\zeta_0} - \frac{\partial}{q\partial\theta_0}\right)^2 f$$
$$+\frac{1}{J}\left(\frac{\partial Jg^{\psi\psi}}{\partial\psi} + \frac{\partial Jg^{\psi\theta}}{\partial\theta_0}\right)\frac{\partial f}{\partial\psi} + \frac{1}{J}\left(\frac{\partial Jg^{\psi\theta}}{\partial\psi} + \frac{\partial Jg^{\theta\theta}}{\partial\theta_0}\right)\frac{\partial f}{\partial\theta_0}. \tag{9}$$

Therefore, using the fact the perpendicular scale length is much shorter than the parallel scalar length, the perpendicular Laplacian can be obtained from the preceding equation:

$$\nabla_\perp^2 f = g^{\psi\psi}\frac{\partial^2 f}{\partial\psi^2} + 2g^{\psi\theta}\frac{\partial^2 f}{\partial\psi\partial\theta_0} + \left(g^{\theta\theta} + g^{\zeta\zeta}/q^2\right)\frac{\partial^2 f}{\partial\theta_0^2}$$
$$+\frac{1}{J}\left(\frac{\partial Jg^{\psi\psi}}{\partial\psi} + \frac{\partial Jg^{\psi\theta}}{\partial\theta_0}\right)\frac{\partial f}{\partial\psi} + \frac{1}{J}\left(\frac{\partial Jg^{\psi\theta}}{\partial\psi} + \frac{\partial Jg^{\theta\theta}}{\partial\theta_0}\right)\frac{\partial f}{\partial\theta_0} \tag{10}$$

Next we study how to discretize the preceding perpendicular Laplacian. In the GTC code, we use an unstructured mesh to ensure the roughly equal grid size in the radial and poiloidal direction. The mesh is uniform in the θ_0 coordinate and nonuniform in the ψ coordinate. In order to evaluate the Laplacian numerically in Eq. (**Error! Reference source not found.Error! Reference source not found.**), we need to discretize the following five operators: $\frac{\partial}{\partial\theta_0}, \frac{\partial}{\partial\psi}, \frac{\partial^2}{\partial\psi^2}, \frac{\partial^2}{\partial\psi\partial\theta_0}$ and $\frac{\partial^2}{\partial\theta_0^2}$. Since the grid size in the θ_0 is uniform, we can apply a simple spatial central algorithm to discretize $\frac{\partial}{\partial\theta_0}$ to the second order accuracy.

$$\left(\frac{\partial f}{\partial \theta_0}\right)_{i,j} = \frac{f_{i,j+1} - f_{i,j-1}}{2(\Delta\theta_0)_i},$$ (11)

Where i is the index label for ψ, j is the index lable for θ_0, as shown in Fig. 2.

(i,j)

Then we discretize $\dfrac{\partial}{\partial\psi}$ to obtain

$$\left(\frac{\partial f}{\partial \psi}\right)_{i,j} = w_2 \frac{f_{i+1,j*} - f_{i,j}}{h_2} + w_1 \frac{f_{i,j} - f_{i-1,j*}}{h_1},$$ (12)

With $h_1 = \psi_i - \psi_{i-1}$, $h_2 = \psi_{i+1} - \psi_i$, and $w_2 = h_1/(h_1 + h_2)$, $w_1 = h_2/(h_1 + h_2)$. The value of $f_{i+1,j*}$ can be evaluated using the neighboring four points on the same flux surface ψ_{i+1}, as shown in Fig. 1, to the second order of accuracy:

$$f_{i+1,j*} = w_{i+1}f_{i+1,j'+1} + \lambda_{i+1}f_{i+1,j'} + \frac{\lambda_{i+1}w_{i+1}}{2}[w_{i+1}f_{i+1,j'+1} +$$
$$\lambda_{i+1}f_{i+1,j'} - \frac{1}{3}(1+w_{i+1})f_{i+1,j'+2} - \frac{1}{3}(1+\lambda_{i+1})f_{i+1,j'-1}]$$ (13)

Where $w_{i+1} = (\theta - \theta_{i+1,j'})/\Delta\theta_{i+1}$, and $\lambda_{i+1} = 1 - w_{i+1}$. A similar expression can be found for the value $f_{i-1,j*}$.

We continue to discretize $\dfrac{\partial^2}{\partial\theta_0\partial\psi}$ to obtain

$$\left(\frac{\partial^2 f}{\partial \theta_0 \partial \psi}\right)_{i,j} = \left(\frac{w_1}{h_1} - \frac{w_2}{h_2}\right)\frac{f_{i,j+1} - f_{i,j-1}}{2\Delta\theta_i} + \frac{w_2}{h_2}\frac{\partial f_{i+1,j*}}{\partial \theta_0} - \frac{w_2}{h_2}\frac{\partial f_{i-1,j*}}{\partial \theta_0}$$ (14)

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Using four neighboring points in the same flux surface, we can obtain

$$
\frac{\partial f_{i+1,j*}}{\partial \theta_0} = \frac{1}{2\Delta\theta_{i+1}} [\lambda_{i+1}\left(f_{i+1,j'+1} - f_{i+1,j'-1}\right) + w_{i+1}\left(f_{i+1,j'+2} - f_{i+1,j'}\right) +
$$
$$
\frac{1}{3}\left(1 - 3\lambda_{i+1}w_{i+1}\right)\left(f_{i+1,j'-1} - 3f_{i+1,j'} + 3f_{i+1,j'+1} - f_{i+1,j'+2}\right)]
$$
(15)

Similar expressions can be written for $\dfrac{\partial f_{i-1,j*}}{\partial \theta_0}$ .Finally we deal with the operator $\dfrac{\partial^2}{\partial\psi^2}$.

$$
\left(\frac{\partial^2 f}{\partial\psi^2}\right)_{i,j} = \frac{2}{h_1 h_2}\left(w_1 f_{i-1,j*} + w_2 f_{i+1,j*} - f_{i,j}\right)
$$
(16)

Where $f_{i+1,j*}$ can be evaluated by the four point interpolation using Eq. (13). Similar expression can be found for $f_{i-1,j*}$.

Poisson solver in the general geometry

The gyrokinetic poisson equation for perturbed electrostatic potential, suitable for the particle simulation, is formulated as following

$$
\frac{Z_i^2 e n_{0i}}{T_i}\left(\delta\phi - \delta\tilde{\phi}\right) = Z_i \delta\bar{n}_i(x) - \delta n_e(x)
$$
(17)

For the electrostatic case, the electron is dominated by adiabatic response. Therefore, it is convenient to write $\delta n_e(x) = \delta_e n_{e0} e \delta\phi / T_e + \delta n_e^{(1)}$, where $\delta_e = 1 - magnetic$, with $magnetic = 0$ for electrostatic case and $magnetic = 1$ for electromagnetic case. So we obtain the following gyrokinetic poisson equation:

$$
\left(\frac{Z_i^2 e n_{i0}}{T_i} + \frac{e n_{e0}}{T_e}\delta_e\right)\delta\phi - \frac{Z_i^2 e n_{i0}}{T_i}\delta\tilde{\phi} = Z_i\delta\bar{n}_i - \delta n_e^{(1)}
$$
(18)

There are two approaches to solve for $\delta\tilde{\phi}$, the n-point average or Pade approximation. The n-point average method is illustrated in Ref [Lin 95] and improved by Wang Zhixuan's notes. In the n-point average method, we can use iterative solver for the electrostatic case. For the electromagnetic case, the

Petsc solver has to be invoked. The Pade approximation needs further elucidation.

$$\delta\tilde{\phi} = \frac{-\rho_i^2 \nabla_\perp^2 \delta\phi}{1 - \rho_i^2 \nabla_\perp^2 \delta\phi} \tag{19}$$

Suppose a scale separation between equilibrium scale and perturbed scale, the gyrokinetic poisson equation Eq. (18) can be rewritten as

$$\left[\delta_e \frac{n_{e0}}{T_e} - \left(\frac{Z_i^2 n_{i0}}{T_i} + \delta_e \frac{n_{e0}}{T_e} \right) \rho_i^2 \nabla_\perp^2 \right] \delta\phi = \left(1 - \rho_i^2 \nabla_\perp^2 \right) \left(Z_i \delta\bar{n}_i - \delta n_e^{(1)} \right) \tag{20}$$

For this Pade approximation, we invoke Petsc solver for either electrostatic or electromagnetic case.

The poisson solver and Laplacian related subroutines in the current GTC are listed in the following table.

Poisson Solver

	ipade=0 n-point average for $\tilde{\phi}$	ipade=1 Finite diff. for $\tilde{\phi}$	Set ipad in setup.F90
Magnetic=0	iterative poisson solver	Petsc Pade-poisson solver	*For ipade=1, requires idiagonal=1 in sub lap2pestc;*
Magnetic=1	Petsc poisson solver	Petsc Pade-poisson solver	*Automatically enforce the source n=0 for inner and outer flux surfaces*

Laplacian

Set laplacian locally	ilaplacain=0 n-point average	ilaplacian=1 Finite difference
$n = \nabla^2 \phi$	Call laplacian_petsc() (set magnetic=1)	Call laplacian()
$\phi = \left(\nabla^2\right)^{-1} n$ (not used in the current GTC)	call petsc_solver (set magnetic=1), valid in long wave-length limit	*Set idiagonal=0 in sub lap2pestc* call lapmat_pssolver