Numerical Solution of the Gyrokinetic Poisson Equation in *TEMPEST*

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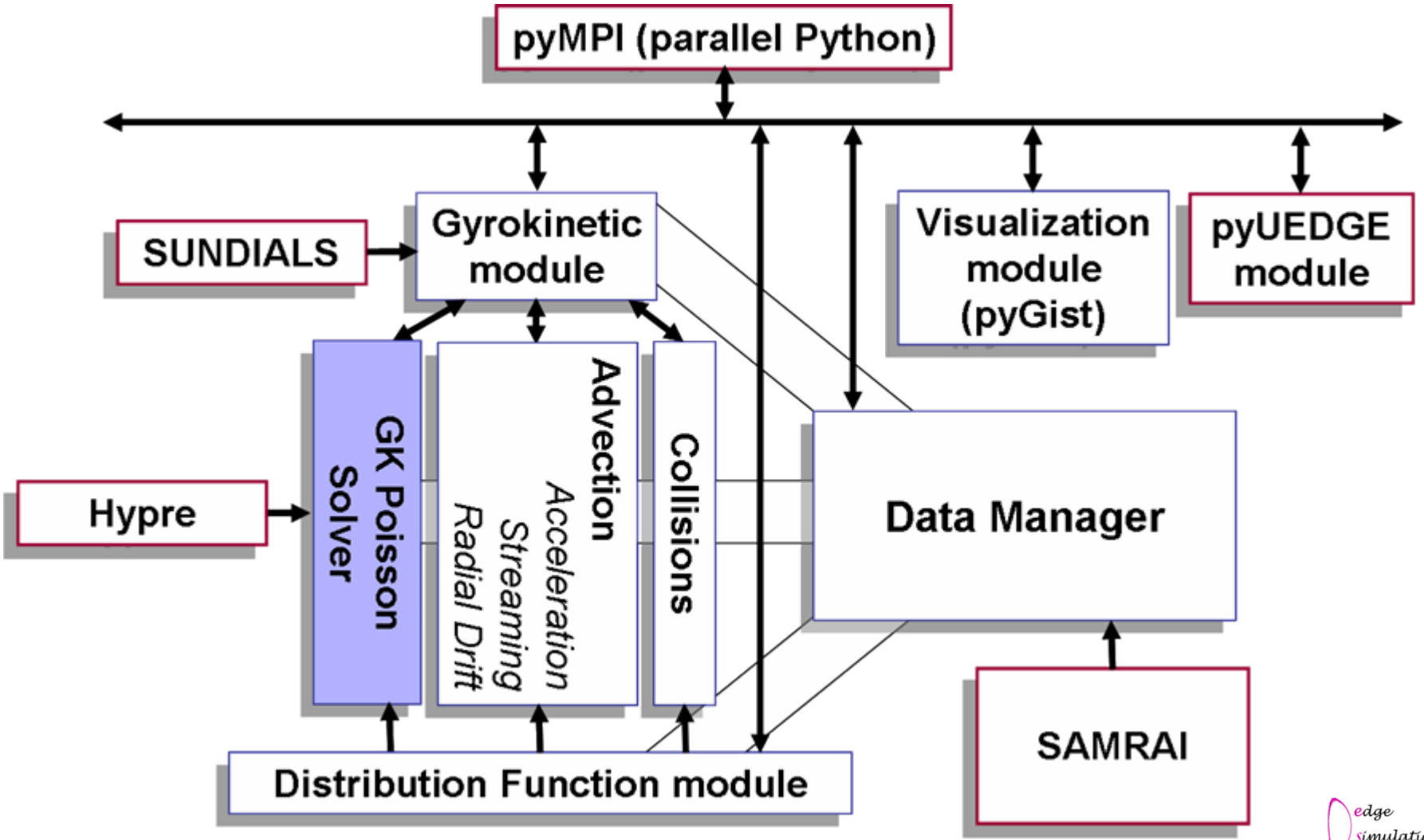
The *TEMPEST* edge simulation infrastructure includes a gyrokinetic Poisson solver



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The gyrokinetic Poisson equation

Poisson Equation: $$\varepsilon_0 \nabla^2 \Phi(\mathbf{x},t) = e\left(n_e(\mathbf{x},t) - \sum_i Z_i n_i(\mathbf{x},t) \right)$$ i = ion species index

The ion species number density is the sum of gyrophase-independent and gyrophase-dependent parts:

$$n_i(\mathbf{x},t) = \overline{n}_i(\mathbf{x},t) + \hat{n}_i(\mathbf{x},t)$$

Gyroaveraged gyrocenter density:

$$\overline{n}_i(\mathbf{x},t) \equiv \int f_i(\mathbf{R}, \mathrm{v}_\parallel, \mu, t)\delta(\mathbf{R} - \mathbf{x} + \rho) B_\parallel^* d\mathbf{R} d\mathrm{v}_\parallel d\mu d\theta$$

Polarization density (long wavelength limit $k_\perp \rho << 1$)

$$\hat{n}_i(\mathbf{x},t) \equiv \frac{m_i c^2}{eB^2} \nabla_\perp \cdot (\overline{n}_i \nabla_\perp \Phi)(\mathbf{x},t)$$

Normalizations:

Densities, temperatures, field, masses scaled by reference values $n_0, \underbrace{T_0, B_0, m_0}$

Potential scaled by T_0 / e

$\Rightarrow$ Reference gyroradius ρ_0

Lengths scaled by ρ_0 and a reference parallel scale length $L_\parallel$

Normalized GK Poisson equation:

$$\frac{\rho_0^2}{2B(\mathbf{x},t)^2} \nabla_\perp \cdot \left[\left(\sum_i m_i \overline{n}_i(\mathbf{x},t) \right) \nabla_\perp \varphi(\mathbf{x},t) \right] + \lambda_D^2 \nabla^2 \Phi(\mathbf{x},t) = n_e(x,t) - \sum_i Z_i \overline{n}_i(\mathbf{x},t)$$

λ_D = Debye length scaled by $L_\parallel$

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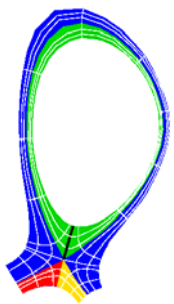
Mapping physical to flux coordinates introduces spatially varying coefficients into the GK Poisson operator

Physical domain

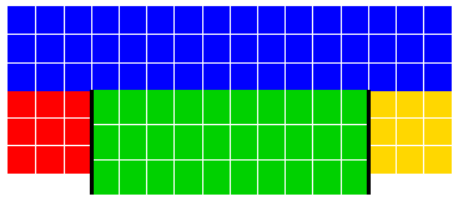


mapping

$\mathbf{x}=\boldsymbol{J}(\psi,\theta,\zeta)$

Computational domain

Flux surface label ψ



Poloidal angle θ

Metric factors arise in the GK Poisson differential terms, for example:

$$\nabla_\perp\cdot\left(\beta(x)\nabla_\perp\right)\longrightarrow\frac{1}{J}\left[\frac{\partial}{\partial\psi}\left(JJ_{11}\beta\frac{\partial}{\partial\psi}\right)+\frac{\partial}{\partial\psi}\left(JJ_{12}\beta\frac{\partial}{\partial\theta}\right)+\frac{\partial}{\partial\theta}\left(JJ_{21}\beta\frac{\partial}{\partial\psi}\right)+\frac{\partial}{\partial\theta}\left(JJ_{22}\beta\frac{\partial}{\partial\theta}\right)-\frac{1}{B}\frac{\partial}{\partial\theta}\left(\frac{\beta}{JB}\frac{\partial}{\partial\theta}\right)\right]$$

where $J\equiv\left(\nabla\psi\times\nabla\theta\cdot\nabla\zeta\right)^{-1}$ $\quad J_{11}\equiv\left|\nabla\psi\right|^2$ $\quad J_{12}\equiv J_{21}\equiv\nabla\psi\cdot\nabla\theta$ $\quad J_{22}\equiv\left|\nabla\theta\right|^2$

The mapped GK Poisson equation thus takes the form:

$$\sum_{j=1}^{3}\alpha^{(j)}(\psi,\theta)\left(\frac{\partial}{\partial\psi}\mathbf{F}^{(j)}+\frac{\partial}{\partial\theta}\mathbf{G}^{(j)}\right)=n_e(\psi,\theta)-\sum_i Z_i\bar{n}_i(\psi,\theta)$$

where

$$\mathbf{F}^{(j)}\equiv\left(a^{(j)}(\psi,\theta)\frac{\partial}{\partial\psi}+b^{(j)}(\psi,\theta)\frac{\partial}{\partial\theta}\right)\Phi(\psi,\theta)\qquad\mathbf{G}^{(j)}\equiv\left(c^{(j)}(\psi,\theta)\frac{\partial}{\partial\psi}+d^{(j)}(\psi,\theta)\frac{\partial}{\partial\theta}\right)\Phi(\psi,\theta)$$

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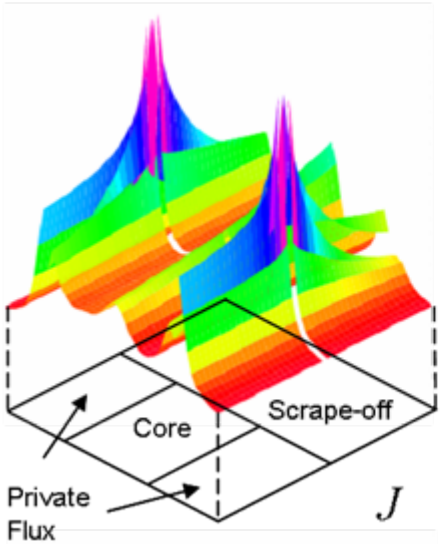
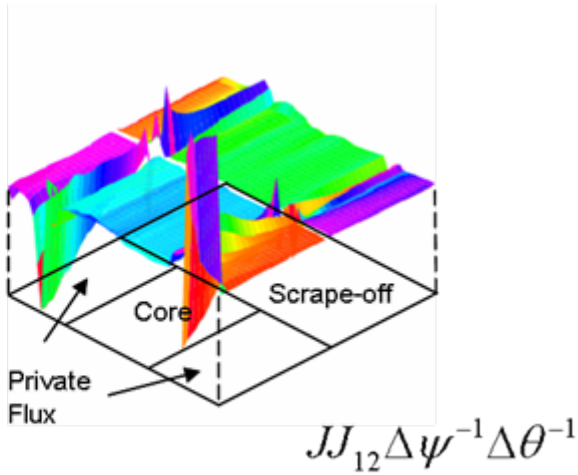
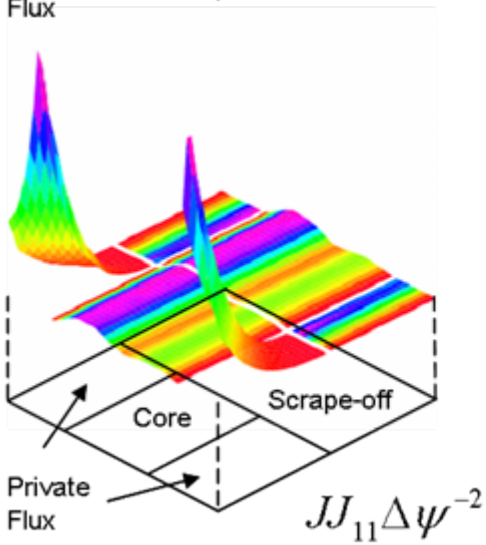
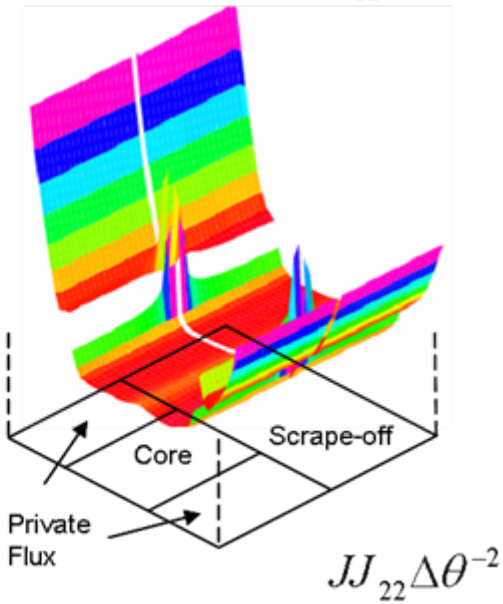
The coefficients arising from the metric factors and meshing are highly anisotropic









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The GK Poisson equation is discretized using centered differencing

Consider a uniform grid with cells indexed by (k,m) of size $(\Delta\psi_k, \Delta\theta_m)$. We average the GK Poisson equation over each cell and apply the divergence theorem

$$\frac{1}{\Delta\psi_k \Delta\theta_m}\sum_{j=1}^{3}\overline{\alpha}_{k,m}^{(j)}\left(F_{k+1/2}^{(j)} - F_{k-1/2}^{(j)} + G_{m+1/2}^{(j)} - G_{m-1/2}^{(j)}\right) = \frac{1}{\Delta\psi_k \Delta\theta_m}\int_{\psi_{k-1/2}}^{\psi_{k+1/2}}\int_{\theta_{m-1/2}}^{\theta_{m+1/2}}\left(n_e(\psi,\theta) - \sum_i Z_i \overline{n}_i(\psi,\theta)\right)d\psi d\theta$$

$$F_{k\pm1/2,m}^{(j)} \equiv \int_{\Gamma_{k\pm1/2}}\left(a^{(j)}(\psi_{k\pm1/2},\theta)\frac{\partial}{\partial\psi} + b^{(j)}(\psi_{k\pm1/2},\theta)\frac{\partial}{\partial\theta}\right)\Phi(\psi_{k\pm1/2},\theta)d\theta$$

$$G_{k,m\pm1/2}^{(j)} \equiv \int_{\Gamma_{m\pm1/2}}\left(c^{(j)}(\psi,\theta_{m\pm1/2})\frac{\partial}{\partial\psi} + d^{(j)}(\psi,\theta_{m\pm1/2})\frac{\partial}{\partial\theta}\right)\Phi(\psi,\theta_{m\pm1/2})d\psi$$

$$\overline{\alpha}_{k,m}^{(j)} \equiv \frac{1}{\Delta\psi_k \Delta\theta_m}\int_{\psi_{k-1/2}}^{\psi_{k+1/2}}\int_{\theta_{m-1/2}}^{\theta_{m+1/2}}\alpha^{(j)}(\psi,\theta)d\psi d\theta$$

where $\Gamma_{k\pm1/2}$ and $\Gamma_{m\pm1/2}$ are the faces of cell (k,m). The fluxes $F^{(j)}_{k\pm1/2,m}$ and $G^{(j)}_{k,m\pm1/2}$ are discretized using standard second-order differencing, e.g.,

$$F_{k+1/2,m}^{(j)} = \Delta\theta_m\left[a^{(j)}(\psi_{k+1/2},\theta_m)\frac{\Phi_{k+1,m} - \Phi_{k,m}}{\Delta\psi_{k+1/2}} + b^{(j)}(\psi_{k+1/2},\theta_m)\frac{\Phi_{k+1,m+1} + \Phi_{k,m+1} - \Phi_{k+1,m-1} - \Phi_{k,m-1}}{2(\Delta\theta_{m+1/2} + \Delta\theta_{m-1/2})}\right]$$

where the $\Phi_{k,m}$ are the values of Φ at cell centers and

$$\Delta\psi_{k+1/2} \equiv (\Delta\psi_k + \Delta\psi_{k+1})/2 \qquad \Delta\theta_{m\pm1/2} \equiv (\Delta\theta_m + \Delta\theta_{m\pm1})/2$$

with appropriate modifications at physical boundaries for Dirichlet or Neumann boundary conditions. This discretization results in a 9 point stencil in 2D and a 27 point stencil in 3D.

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The GK Poisson equation is solved self-consistently with the gyrokinetic equations as a differential algebraic system in *TEMPEST*

The gyrokinetic system is expressed in residual form

$$\left.\begin{aligned}
&\dot{F}_i + \vec{v}_d \cdot \nabla_\perp F_i + \left(\vec{v}_{\parallel i} + v_{Banos}\right)\nabla_\parallel F_i + \left[q\frac{\partial\langle\Phi_0\rangle}{\partial t} + \bar{\mu}\frac{\partial B}{\partial t} - \frac{qB}{B^*}\bar{v}_\parallel \nabla_\parallel \langle\delta\Phi\rangle - q v_d^0 \cdot \bar{\nabla}\langle\delta\Phi\rangle \right]\frac{\partial F_i}{\partial E_0} - C(F_i, F_i) = 0 \\
&\frac{\rho_s^2}{2B^2}\nabla_\perp \cdot \left[\left(\sum_i m_i N_i\right)\nabla_\perp \varphi\right] + \lambda_D^2 \nabla^2 \varphi - n_e + \sum_i Z_i \left(N_i + \frac{\rho_s^2 m_i}{2B^2 e}\nabla_\perp^2 p_{\perp,i}\right) = 0 \\
&n_e - \frac{\langle Z_i n_i\rangle}{\langle \exp(\Phi/T_e)\rangle}\exp(\Phi/T_e) = 0
\end{aligned}\right\} \quad R(F_\alpha, \dot{F}_\alpha, \Phi, n_e) = 0$$

and solved by the IDA (Implicit Differential Algebraic) integrator using variable-order, variable-step backward difference formulas. At the nth time step, we solve

$$G(y^n) \equiv G(F_\alpha^n, \Phi, n_e) \equiv R(F_\alpha^n, h_n^{-1}\sum_{i=0}^{k}\sigma_{n,i}F_\alpha^{n-i}, \Phi^n, n_e^n) = 0$$

to a prescribed tolerance using an approximate Newton iteration $J(y_{m+1}^n - y_m^n) = -G(y_m^n)$

where

$$J = \begin{pmatrix} J_{11} & J_{12} & 0 \\ J_{21} & J_{22} & -I \\ J_{31} & J_{32} & I \end{pmatrix} \approx \frac{\partial G}{\partial y} = \frac{\partial R}{\partial y} + \frac{\sigma_{n,0}}{h_n}\frac{\partial R}{\partial \dot{y}}$$

The Generalized Minimum Residual (GMRES) algorithm is used to solve the preconditioned system

$$PJ(y_{m+1}^n - y_m^n) = -PG(y_m^n)$$

which in turn requires the approximate solution of systems of the form

$$Pz \equiv \begin{pmatrix} \frac{\sigma_{n,0}}{h_n}I & 0 & 0 \\ 0 & J_{22} & -I \\ 0 & J_{32} & I \end{pmatrix}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix} \equiv r$$

The key step in solving this system is therefore the solution of the subsystem

$$(J_{22} + J_{32})z_2 = r_1 + r_2$$

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A subspace decomposition is employed in the preconditioned Krylov solution of the GK Poisson system with adiabatic electrons

GK Poisson with adiabatic electron model:

$$\rho^2\nabla_\psi^2\Phi + Z_i n_i - \frac{\langle Z_i n_i\rangle_j}{\langle \exp(\Phi/T)\rangle_j}\exp(\Phi/T) = 0$$

where

$$\langle u\rangle_j = \sum_k w_{j,k}\, u(\psi_j,\theta_k) \qquad w_{j,k} \equiv \frac{\frac{h(\psi_j,\theta_k)\Delta\theta}{B_p(\psi_j,\theta_k)}}{\sum_{k'=1}^{N}\frac{h(\psi_j,\theta_{k'})\Delta\theta}{B_p(\psi_j,\theta_{k'})}}$$

and j = flux surface index

As described above, the application of the Jacobian preconditioner involves the approximate solution of the system:

$$(J_{22}+J_{23})z = (\rho^2\nabla_\psi^2 - L)z = r$$

where

$$L \equiv \mathrm{diag}_j\left[N_j\left(I - e w_j^T D_j\right)\right]$$

$$D_j \equiv \frac{1}{\langle \exp(\Phi/T)\rangle_j}\mathrm{diag}\left[\exp(\Phi_{j,k}/T)\right]$$

$$N_j \equiv \frac{\langle Z_i n_i\rangle_j}{T} D_j$$

$$e \equiv (1,\ldots,1)^T \qquad w_j \equiv (w_{j,1},\ldots,w_{j,N})^T$$

Problem: L is a singular operator

If ρ is small (i.e., the radial dimension spans many gyroradii), the coefficient matrix for the Jacobian system

$$(\rho^2\nabla_\psi^2 - L)z = r$$

is nearly singular, which causes Krylov methods (e.g., conjugate gradient) to converge poorly

Solution: Decompose the linear solve to avoid the operator null space

Since $w_j^T e = 1$, the operator

$$P \equiv \mathrm{diag}_j\left(e w_j^T\right)$$

is a projection onto the null space N(L) of L:

$$P^2 = \mathrm{diag}_j\left(e w_j^T e w_j^T\right) = \mathrm{diag}_j\left(e w_j^T\right) = P$$

$$LP = \mathrm{diag}_j\left[\left(I - e w_j^T D_j\right) e w_j^T\right] = 0$$

$$PL = \mathrm{diag}_j\left[e w_j^T D_j\left(I - e w_j^T D_j\right)\right] = 0$$

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A subspace decomposition is employed in the preconditioned Krylov solution of the GK Poisson system with adiabatic electrons

Use P to decompose the Jacobian preconditioner system into N(L) and N(L)$^{\perp}$:

$$P\left(\rho^2\nabla_\psi^2 - L\right)\left[Pz + (I-P)z\right] = P\,r$$
$$(I-P)\left(\rho^2\nabla_\psi^2 - L\right)\left[Pz + (I-P)z\right] = (I-P)r$$

Assuming P and $\rho\nabla_\perp^2$ commute:

$$\rho^2\nabla_\psi^2 Pz = Pr$$
$$\left(\rho^2\nabla_\psi^2 - L\right)(I-P)z = (I-P)r$$

The equation

$$\rho^2\nabla_\psi^2 Pz = Pr$$

is a tridiagonal system that can be solved directly.

Since the actual gyrokinetic Poisson operator is more complicated than the radial Laplacian assumed here, which commutes with the projection P, a poloidally averaged approximation is used instead.

Since L is the sum of a diagonal and rank-one matrix, the solution of the system

$$\left(\rho^2\nabla_\psi^2 - L\right)(I-P)z = (I-P)r$$

is given by*

$$(I-P)z_1 = A^{-1}(I-P)r - \beta A^{-1}u$$

where

$$A \equiv \rho^2\nabla_\psi^2 - \mathrm{diag}_j N_j \qquad \beta = \frac{v^T A^{-1} b}{1 + v^T A^{-1} u}$$
$$u \equiv \left(N_1 e, \ldots, N_M e\right)^T \qquad v^T \equiv \left(w_1^T D_1, \ldots, w_M^T D_M\right)$$

Since $-A$ is symmetric and positive definite, approximations of the vectors $A^{-1}(I-P)r$ and $A^{-1}u$ are obtained using a preconditioned conjugate gradient algorithm.

*Sherman-Morrison formula: For a general matrix A and vectors u and v:

$$\left(A + uv^T\right)^{-1} = A^{-1} - \alpha A^{-1} u v^T A^{-1}, \quad \alpha = \frac{1}{1 + v^T A^{-1} u}$$

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The block-multigrid-preconditioned conjugate gradient solve is performed using solvers from the *Hypre* library

In each GMRES iteration, the key step is the solution of the linear system:

$$\left(J_{22}+J_{32}\right)z_2=\left\{\sum_{j=1}^{3}\alpha^{(j)}\left[\frac{\partial}{\partial\psi}\left(a^{(j)}\frac{\partial}{\partial\psi}+b^{(j)}\frac{\partial}{\partial\theta}\right)+\frac{\partial}{\partial\theta}\left(c^{(j)}\frac{\partial}{\partial\psi}+d^{(j)}\frac{\partial}{\partial\theta}\right)\right]-\frac{\langle Z_i n_i\rangle}{T_e\langle\exp(\Phi/T_e)\rangle}\exp(\Phi/T_e)\right\}z_2=r_1+r_2$$

Since the coefficient matrix is symmetric and negative definite, this system is solved using a preconditioned conjugate gradient (PCG) solver. The PCG solver and preconditioners are provided by the *Hypre* library using the "semi-structured interface".

Preconditioners: block Gauss-Seidel with PFMG or SMG in each block

- Blocks: the logically distinct regions: core, scrape-off, private flux
- SMG (Schaffer semicoarsening multigrid): Uses a combination of semi-coarsening, line-relaxation and operator-based interpolation
- PFMG: Similar to SMG, but uses pointwise smoothing instead of plane smoothing

These solvers are specifically designed for robustness and efficiency in solving linear systems resulting from the discretization of operators with widely varying coefficients.

Hypre documentation and software available at: www.llnl.gov/CASC/linear_solvers/

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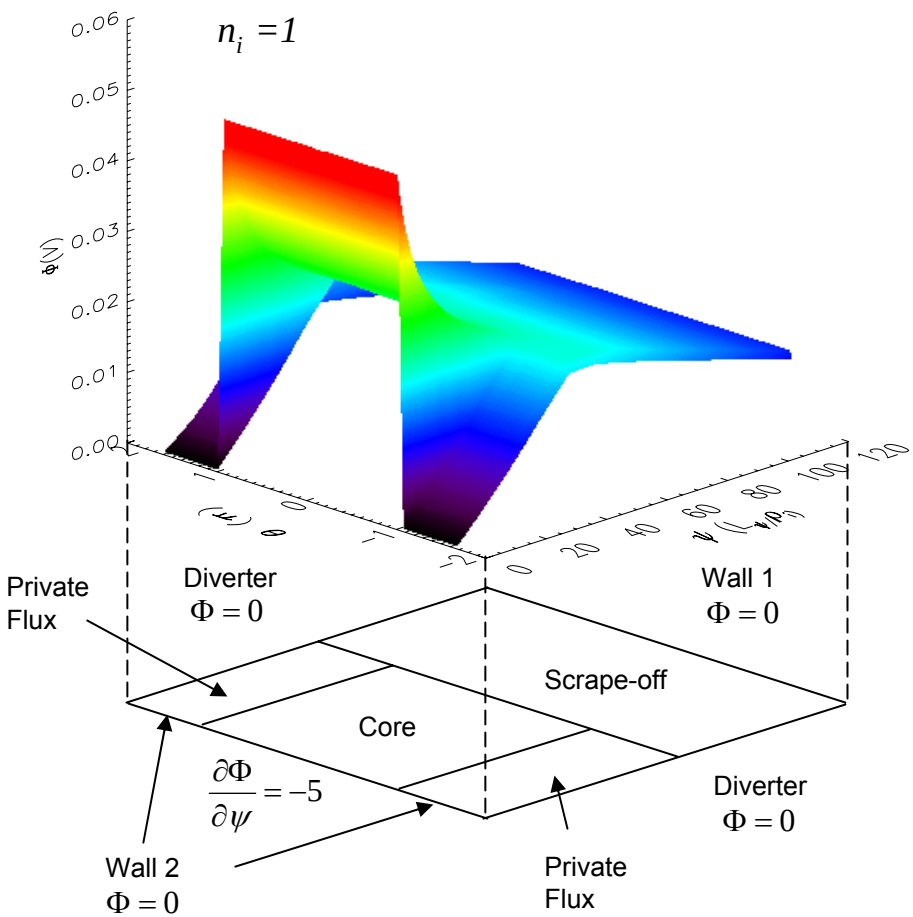
Example calculation on a diverter geometry



Calculation of initial condition in DIII-D poloidal slice

Nonlinear convergence criteria:

$$R\left\| y_k - y_{k-1} \right\|_{WRMS} < 0.1\varepsilon_{LE}$$

$$\left\| v \right\|_{WRMS} \equiv \left[\frac{1}{N} \sum_{1}^{N} \left(v_i / w_i \right)^2 \right]^{1/2} \qquad w^i \equiv 10^{-3} \left| y^i \right| + 10^{-6}$$

R = dynamic convergence rate estimate

ε_{LE} = local error test tolerance

PCG relative residual tolerance = 10^{-3}

40 radial cells x 50 poloidal cells = 2000 spatial unknowns

Total number of Newton iterations	**5**
Total number of GMRES iterations	**11**
Average number of PCG iterations per preconditioner application	**10**

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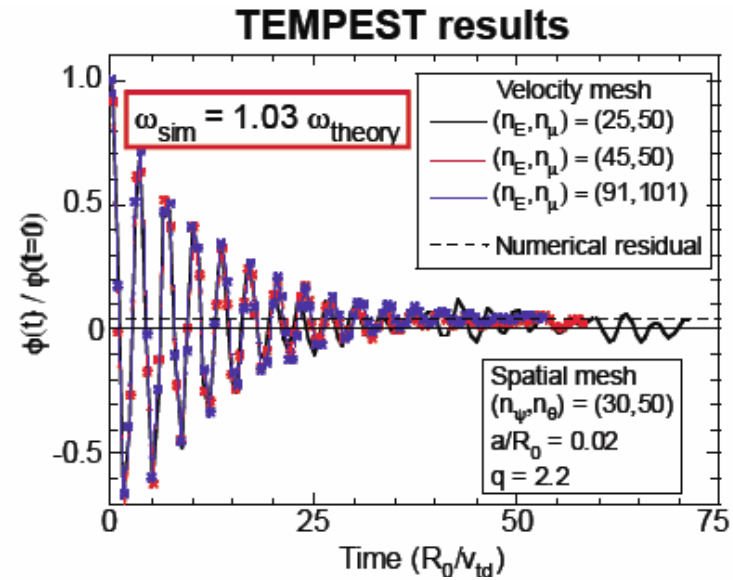
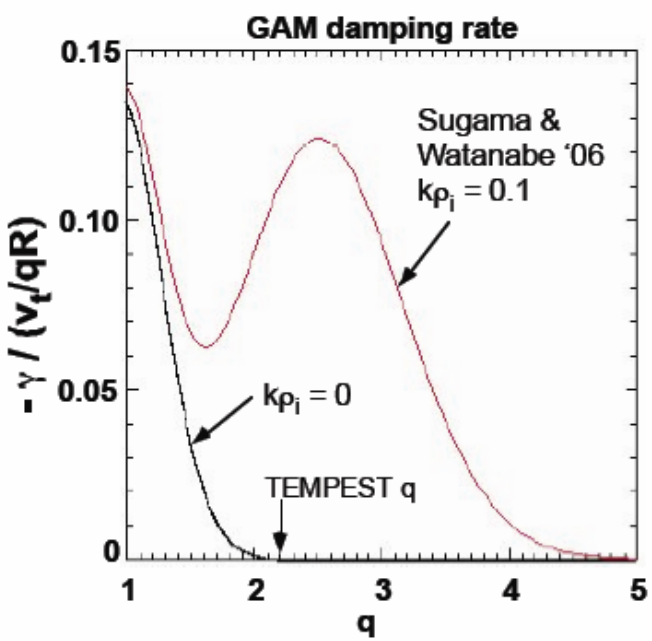
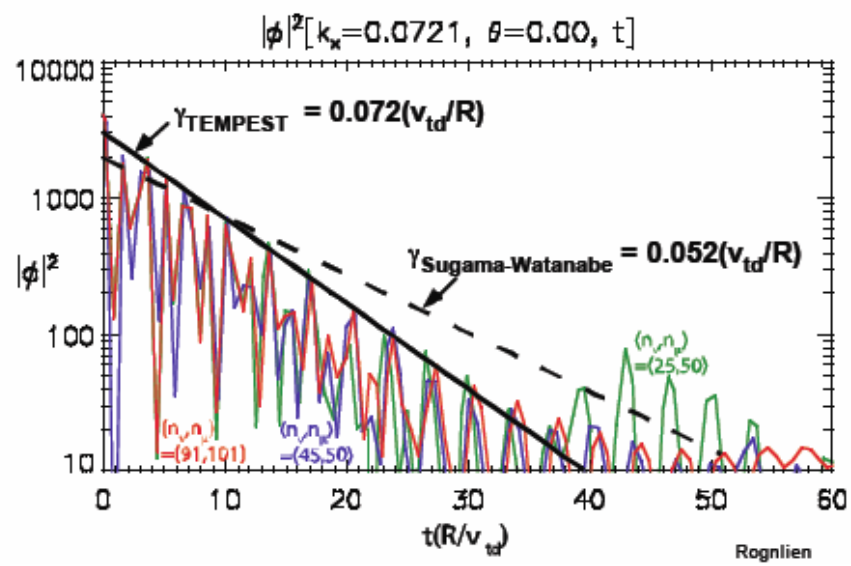
The GK Poisson solver has been used to validate *TEMPEST* on GAM problems

- Initial 2D fixed n_e pertubation cause ions/poten. to relax as GAM
- Sugama, Watanabe show damping sensitive to $k\rho_i$ at large q (bananas)
- TEMPEST example follows the larger damping from finite $k\rho_i$ and q







Rognlien

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