The Gyrokinetic Regime
Geometry
Velocity Space
Linear How-To
Units
Non-Linear Issues
Miscellany
Primary concerns when setting up nonlinear runs:

1. Simulation domain size, resolution and aspect ratio
2. Implicitness parameters
3. Timing
4. “Magic” numbers of parallel processes
Simulation Domain Size

- Size of simulation along the field is basically fixed, with $-\pi < \theta < \pi$. I do not recommend using nperiod > 1 for non-linear runs. It is physically acceptable but computationally prohibitive.

- Size of box in perpendicular direction set by either $y_0$ or $L_y$ in the kt_grids_box_parameters namelist.

- Size of box in $\alpha$ (or $y$) direction is $L_y = 2\pi y_0$. 
Radial Domain Size

- Size of simulation in radial direction is affected by magnetic shear $\hat{s}$, $L_y$ and $J_{\text{twist}}$.


- In a nutshell:
  \[
  \frac{L_x}{L_y} = \frac{J_{\text{twist}}}{2\pi \hat{s}} \quad \left( L_x = \frac{y_0 J_{\text{twist}}}{\hat{s}} \right)
  \]

- Optimal choice of $J_{\text{twist}}$ is not known in general. Recommended choice: $j_{\text{twist}} = 2\pi \hat{s}$. Corresponds to roughly square simulation domain at outboard midplane.
Boundary Conditions

- Triply-periodic twist&shift boundary conditions In `dist_fn_knobs` namelist, set `boundary_option = 'linked'`

- Results in different $\theta_0$’s ($k_\rho$’s) being linearly coupled together

- In axisymmetric geometry, coupling only occurs among radial wavenumbers with the same poloidal wavenumbers.

- To understand which modes are coupled, use

$$k_x \equiv -k_y \hat{s} \theta_0$$

for modes with finite $k_y$. 
Twisted Domain

- Simple bracket form of nonlinear term valid in general geometry

\[ \{\chi, h\} = \frac{\partial \chi}{\partial \rho} \frac{\partial h}{\partial \alpha} - \frac{\partial \chi}{\partial \alpha} \frac{\partial h}{\partial \rho} \]

can be evaluated with standard de-aliased pseudo-spectral algorithm.

- Derivatives evaluated in transform space, multiplication carried out in real space.

- Requires rectangular domain in \((\rho, \alpha)\) coordinates.
Twisted Domain

- Given $L_x$ and $L_y$, also require $n_x$ and $n_y$ to fully specify domain.

- Because of FFT’s, $n_x$ and $n_y$ (in the `kt_grids_box_parameters` namelist) should have prime factors from the set \{2, 3, 5\} although any value is allowed. Alternative choices just reduce the performance.

- De-aliasing implies a particular relationship between the numbers of $k_x$ and $k_y$ modes in the calculation (Orszag 2/3 rule)
Why Pseudo-Spectral?

1. “Exponentially convergent” derivatives. Compare with finite difference:

\[
\frac{\partial f}{\partial x} \sim \frac{f(x + h) - f(x - h)}{2h} + O(h^2)
\]

\[
\frac{\partial f}{\partial x} \sim \frac{-f(x + 2h) + 8f(x + h) - 8f(x - h) + f(x - 2h)}{12h} + O(h^4)
\]

Pseudo-spectral is much better: error in \(\frac{\partial f}{\partial x} \sim O(h^N)\) at fixed \(h\) but

\[
\text{error} \sim O\left(\left(\frac{1}{N}\right)^N\right)
\]

since \(h\) decreases as \(N\) increases.
Pseudo-Spectral Advantages

2. At fixed accuracy, pseudo-spectral is memory minimizing.

- To resolve a function with 1% accuracy, spectral requires $N/2$ (compared to non-spectral scheme with $N$ points)
- GS2 is spectral in $\rho$, $\alpha$, $E$, $\lambda$, implying $\sim$ factor of 16 savings.
In detail, GS2 uses (with standard Fortran integer arithmetic rules):

\[ n_{aky} = \frac{n_y - 1}{3} + 1 \quad \text{and} \quad n_{theta0} = 2 \left( \frac{n_x - 1}{3} \right) + 1 \]

- The number of \( k_x \) modes is equal to \( n_{theta0} \).

- The value of \( \theta_0 \) for a given mode can be calculated:

\[ \theta_0 = \frac{k_x}{\hat{s}k_y} \]

for \( k_y \neq 0 \). For the \( k_y = 0 \) modes (\( \sim \) the zonal flows), use \( \theta_0 = 2\pi/(\hat{s}L_x k_y) \).
Potential Gotchas

- At a given $k_y$, different $k_x$ modes are coupled by the twist & shift boundary conditions if their $\theta_0$ values differ by integer multiples of $2\pi$. Each connection adds a $2\pi$ segment of the eigenfunction.

- If the linear eigenfunctions are extended along the field line, then the nonlinear run should have enough resolution in the $x$ (i.e., $\rho$) direction to permit sufficient connections to resolve it.

- Operationally, linear runs with grid_option = 'box' in the kt_grids_knobs namelist should give the same results as linear runs with any other grid option.
Recommendations

- Foregoing typically requires $n_x > n_y$. A rule of thumb to use is $n_x \sim 3n_y$. Key is to do linear checks to look for spuriously fast-growing modes. Time-consuming, but better than wasting a nonlinear run.

- For nonlinear runs, in the `dist_fn_species_knobs_i` namelists, recommend setting `fexpr = 0.45` and `bakdif = 0.05`.

- Use restart capabilities for nonlinear runs. Need to set `save_for_restart = T` in the `gs2_diagnostics_knobs` namelist and provide a restart file name with `restart_file` in the `init_g_knobs` namelist.
Restart Recommendations

- For restarted runs, use `delt_option = 'check_restart'` in the `knobs` namelist

- Also, set `ginit_option = 'many'` in the `init_g_knobs` namelist

- In general, can use restarts for many purposes. It is wise to save the restart files before re-doing run.
How long is long enough?

- Open question!