Time step choice in Gkeyll kinetic solvers

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Note: this is merely a description of the state of things, not to be taken as the ideal approach, and open to modification.

Gkeyll solves Vlasov and gyrokinetic equations, whose collisionless terms can be written as

$$\frac{\partial f_s}{\partial t} + \nabla_{\mathbf{z}} \cdot \boldsymbol{\alpha} f_s = 0 \tag{1}$$

at least for collisionless electrostatic gyrokinetics. Here f_s is the distribution function of species s, $\mathbf{z}$ is the phase-space coordinate, and $\boldsymbol{\alpha}$ is the phase-space advection velocity. Specifically, these $\mathbf{z}$ and $\boldsymbol{\alpha}$ in Gkeyll are:

$$\begin{aligned}
&\text{Vlasov-Poisson:} && \mathbf{z} = (\mathbf{x}, \mathbf{v}), && \boldsymbol{\alpha} = \left(\mathbf{v}, \frac{q_s}{m_s}(\mathbf{E} + \mathbf{v}\times\mathbf{B})\right) \\
&\text{Gyrokinetics (electrostatics):} && \mathbf{z} = \left(\mathbf{R}, v_\parallel, \mu\right), && \boldsymbol{\alpha} = \left(\dot{\mathbf{R}}, \dot{v_\parallel}\right)
\end{aligned} \tag{2}$$

where q_s and m_s are the species charge and mass, $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic field (may have contributions from those produced by the plasma and external fields), $\mathbf{R}$ is the guiding center position, $v_\parallel$ the velocity parallel to the magnetic field, $\mu = m_s v_\perp^2/(2B)$ the adiabatic moment, and the gyrokinetic guiding center velocities are

$$\begin{aligned}
\dot{\mathbf{R}} &= \frac{\mathbf{B}^*}{B_\parallel^*} v_\parallel + \frac{\hat{\mathbf{b}}}{q_s B_\parallel^*} \times \left(\mu \nabla B + q_s \nabla\phi\right), \\
\dot{v_\parallel} &= -\frac{\mathbf{B}^*}{m_s B_\parallel^*} \cdot \left(\mu\nabla B + q_s\nabla\phi\right).
\end{aligned} \tag{3}$$

1 Collisionless CFL constraint on Δt

We integrate equation 1 with explicit methods that have a maximum time step Δt in order for the time integration to remain stable. This maximum Δt is set by a Courant-Friedrichs-Lewy (CFL) condition, which for a 1D avection equation $\partial_t f + \partial_x(vf) = 0$, is

$$\Delta t_{\max} \leq C \min\left(\frac{\Delta x}{v}\right) = \frac{C}{\max\left(\omega_{\mathrm{CFL}}\right)}, \tag{4}$$

where C is an $O(1)$ factor that depends on the spatial discretization and the time integration method, and v is some advection velocity in a grid with cell length Δx. There is lots of ambiguity in equation 4, however, especially for a multidimensional discontinuous Galerkin (DG) code. Despite such ambiguities, solvers in Gkeyll essentally compute the Δt from the relation

$$\Delta t = \Delta t_{\max} \leq \texttt{cflFrac} \cdot \frac{C}{\max_{i=1}^{N}\left(\omega_{\mathrm{CFL},i}\right)} \tag{5}$$

with, for example, $C = 1$ for integration with SSP-RK3 and the maximum of the CFL frequency ($\omega_{\mathrm{CFL},i}$) computed amongst all our N cells in phase space. The user has the option to make the time step smaller by providing an additional cflFrac factor in the input file.

The Δt calculation thus mostly comes down to how we compute the CFL frequencies, $\omega_{\mathrm{CFL},i}$ in every cell. In Gkeyll we have settled for a couple of options, which differ between the Vlasov and gyrokinetic solvers.

1.1 Vlasov's $\omega_{\mathrm{CFL},i}$

In a Vlasov simulation with cdim configuration space dimensions and vdim velocity space dimensions (pdim = cdim+vdim) using a polynomial basis of order p, the CFL frequency is computed as

$$\omega_{\mathrm{CFL},i} = (2p+1)\left[\sum_{d=1}^{\texttt{cdim}} \frac{\max(|v_{d,i}|)}{\Delta z_d} + \sum_{d=\texttt{cdim}+1}^{\texttt{pdim}} \frac{\alpha_{d,i}|_{\mathbf{z}=\mathbf{z}_i}}{\Delta z_d}\right]. \tag{6}$$

In this relation Δz_d is the cell length in the d^{th} direction. The term proportional to the d-component of the velocity in the i^{th} cell, $v_{d,i}$, arises from advection in configuration space. The term proportional to the d-component of the acceleration in the i^{th} cell evaluated at the cell center, $\alpha_{d,i}|_{\mathbf{z}=\mathbf{z}_i}$, arises from advection in velocity space.

1.2 The gyrokinetic ω_{CFL}

The CFL frequency in every cell is evaluated differently in the gyrokinetic solver. We instead use a function that depends on the advection speeds at quadrature points on the surfaces of a cell. For this reason we introduce a set of $N_{q,d}$ Gauss-Legendre quadrature points on the surface orthogonal to the d-direction whose coordinates are $\mathbf{z}_{q,d}$. The CFL frequency in the gyrokinetic solver is then computed using

$$\omega_{\text{CFL},i} = \frac{2p+1}{2^{\texttt{pdim}}} \sum_{d=1}^{\texttt{cdim}+1} \frac{2}{\Delta z_d} \sum_{q=1}^{N_{q,d}} \left[\frac{1}{2} \left(|\alpha_{d,i}| - \alpha_{d,i} \right) |_{\mathbf{z}_{q,d}^{\text{left}}} + \frac{1}{2} \left(|\alpha_{d,i}| + \alpha_{d,i} \right) |_{\mathbf{z}_{q,d}^{\text{right}}} \right]. \tag{7}$$

The notation $\mathbf{z}_{q,d}^{\text{left}}$ and $\mathbf{z}_{q,d}^{\text{right}}$ is used to indicate that the coordinate in the d-direction is evaluated at the left or right boundary of the cell. **For example**, for the $d = \texttt{cdim}+1$ terms in the first sum of equation 7, the advection speeds are evaluated at

$$\begin{aligned} \mathbf{z}_{q,d}^{\text{left}} &= (\mathbf{R}_q, v_{\parallel i-1/2}, \mu_q), \\ \mathbf{z}_{q,d}^{\text{right}} &= (\mathbf{R}_q, v_{\parallel i+1/2}, \mu_q), \end{aligned} \tag{8}$$

i.e. the gyrocenter position R and the adiabatic moment μ are evaluated at the quadrature points on the $v_\parallel$ surface of the i^{th} cell.

2 Collisional CFL

The CFL constraint from collisions follows the ideas in previous sections, but depend on the form of the collision operator. At the moment we only have BGK and Dougherty (LBO) collisions, so we deal with this below.

2.1 BGK collisions

The BGK operator, regardless of whether it is used for Vlasov or gyrokinetic simulations, has the form

$$\frac{df_s}{dt} = \sum_r \nu_{sr} \left(f_{M,sr} - f_s \right), \tag{9}$$

with the sum running over the species other than s, ν_{sr} being the collision frequency of species s colliding with species r, and $f_{M,sr}$ the Maxwellian this operator relaxes f_s to. In this case the CFL frequency is simply

$$\omega_{\text{CFL},i} = \sum_r \nu_{sr,i}, \tag{10}$$

i.e. the sum of the collision frequencies evaluated at the center of the cell.

2.2 Dougherty (LBO) collisions

The LBO, whether for Vlasov or gyrokinetics, uses cell centered values to compute the CFL. This means that for the **Vlasov** LBO

$$\frac{df}{dt} = \sum_r \nu_{sr} \nabla_{\mathbf{v}} \cdot \left[(\mathbf{v} - \mathbf{u}_{sr}) f_s + v_{tsr}^2 \nabla_{\mathbf{v}} f_s \right] \tag{11}$$

the CFL frequency is

$$\omega_{\text{CFL},i} = \sum_{d=1}^{\texttt{vdim}} \frac{2}{\Delta v_d} \left[C_{\text{adv},p} \left(2p+1 \right) \left| \sum_r \nu_{sr,i} v_{d,i} - \sum_r \nu_{sr,i} u_{sr,d,i} \right| + C_{\text{diff},p} \frac{2}{\Delta v_d} \left(p+1 \right)^2 \sum_r \nu_{sr,i} v_{tsr,i}^2 \right], \tag{12}$$

and we take $C_{\text{adv},p} = C_{\text{diff},p} = 1$, although $C_{\text{adv},p}$ should really be 1.2 for $p = 2$ (see M. Francisquez, et al. Nucl. Fusion 60 (2020) 096021, section 4.1).

The **gyrokinetic** LBO on the other hand

$$\frac{df}{dt} = \sum_r \nu_{sr} \left\{ \frac{\partial}{\partial v_\parallel} \left[\left(v_\parallel - u_{\parallel sr} \right) f_s + v_{tsr}^2 \frac{\partial f_s}{\partial v_\parallel} \right] + \frac{\partial}{\partial \mu} \left(2\mu f_s + \frac{2m_s}{B} v_{tsr}^2 \mu \frac{\partial f_s}{\partial \mu} \right) \right\} \tag{13}$$

uses the CFL frequency

$$\begin{aligned} \omega_{\text{CFL},i} = &\frac{2}{\Delta v_\parallel} \left[C_{\text{adv},p} \left(2p+1 \right) \left| \sum_r \nu_{sr,i} v_\parallel - \sum_r \nu_{sr,i} u_{\parallel sr,i} \right| + C_{\text{diff},p} \frac{2}{\Delta v_\parallel} \left(p+1 \right)^2 \sum_r \nu_{sr,i} v_{tsr,i}^2 \right] \\ &+ \frac{2}{\Delta \mu} \left[2C_{\text{adv},p} \left(2p+1 \right) \sum_r \nu_{sr,i} \mu_i + C_{\text{diff},p} \frac{2}{\Delta \mu} \left(p+1 \right)^2 \frac{2m_s}{B_i} \sum_r \nu_{sr,i} v_{tsr,i}^2 2\mu_i \right]. \end{aligned} \tag{14}$$

3 Other Δt considerations

- In simulations with multiple species the max function in equation 5 is over the species. That is, we search for the maximum over the phase-space grids of very species.
- The CFL frequencies from various terms are (assumed to be) additive. For example, in simulations with collisionless and collisional terms, we simply add their respective CFL frequencies: $\omega_{\mathrm{CFL},i} = \omega_{CFL,i}^{\mathrm{collisionless}} + \omega_{CFL,i}^{\mathrm{collisional}}$.
- There are likely improvements that can be made, e.g. making sure we resolve the (electrostatic) shear Alfvén wave frequency (ω_H in electrostatics, Ω_A in electromagnetics).
- Boundary conditions can have an impact on stability of time integration. We have not accounted for this.