Direct Numerical Analysis of fundamental gyrokinetic turbulence dynamics

DNA SOLVER MANUAL

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2nd January, 2013

CONTENTS

CHAPTER 1

INTRODUCTION TO DNA

SECTION 1.1

KINETIC SLAB ITG MODEL

1.1.1 INITIAL GYROKINETIC EQUATIONS

We begin with the gyrokinetic equations described in Ref. [1] and immediately apply the adiabatic electron approximation, and unsheared slab geometry. Using an unsheared slab eliminates the curvature and trapping terms, so that the starting point for this derivation is the gyrokinetc equation,

$$\frac{\partial f}{\partial t} = \mathcal{L}[f] + \mathcal{N}[f], \tag{1.1}$$

with the linear and nonlinear operators defined as follows:

$$\mathcal{L}[f] = -\left[\omega_n + \omega_T\left(v_{||}^2 + \mu - \frac{3}{2}\right)\right] F_0 i k_y J_0(\lambda)\phi - \sqrt{2} v_{||}\left(\partial_z f + F_0 \partial_z J_0(\lambda)\phi\right) + C(f), \tag{1.2}$$

and

$$\mathcal{N}[f] = \sum_{\vec{k}'_\perp} \left(k'_x k_y - k_x k'_y\right) J_0(\lambda)\phi_{\vec{k}'_\perp} f_{\vec{k}_\perp - \vec{k}'_\perp}, \tag{1.3}$$

where $\omega_n = L_{ref}/L_n$, $\omega_T = L_{ref}/L_T$, $F_0 = \pi^{-3/2} e^{-v_{||}^2 - \mu}$, C represents a collision operator, J_0 is the zeroth-order Bessel function representing a gyroaverage, $\lambda = \sqrt{2\mu} k_\perp$, and the parallel scale length is set to L_{ref}. The gyrocenter distribution function, $g_{k_x,k_y}(z, v_{||}, \mu)$, is a function of three spatial and two velocity coordinates, but these dependencies will not be explicitly noted at this time. The normalization is as in Ref. [1] (see pgs. 28-30), with $m_{ref} = m_{0i}$, $q_i = q_e$, $B_{ref} = B_0$, $n_{ref} = n_{0i}$, and $T_{ref} = T_{0i}$. Note that this normalization produces $v_{Ti} \to \sqrt{2}$.

The field equation for the electrostatic potential is,

$$\phi_{k_x,k_y} = \frac{\int J_0(\lambda) g dv_{||} d\mu + \tau \langle\phi\rangle_{FS} \delta_{k_y,0}}{\tau + [1 - \Gamma_0(b)]}, \tag{1.4}$$

where τ is the ratio of ion to electron temperature, $\Gamma_0(x) = I_0(x) e^{-x}$, $I_0(x)$ is the zeroth order modified Bessel function, $b_i = k_\perp^2$, and the flux-surface averaged potential is,

$$\langle\phi\rangle_{FS} = \frac{\pi \langle \int J_0(\lambda) g dv_{||} d\mu \rangle_{FS}}{[1 - \Gamma_0(b)]}. \tag{1.5}$$

Cases with and without the flux-surface-averaged potential term will be considered, but the term will be kept in this document for the purpose of completeness.

1.1.2 FLR EFFECTS

We wish to reduce the model to one velocity dimension by operating on the gyrokinetic equation with a μ-integral: $\pi \int_0^\infty [X] d\mu$. This requires a treatment of the gyroaverage operators. The gyroaverages in the linear operator can be calculated analytically since additional μ dependecies enter only in the form of,

$$\int_0^\infty J_0(\sqrt{2\mu}k_\perp)e^{-\mu}d\mu, \tag{1.6}$$

and,

$$\int_0^\infty \mu J_0(\sqrt{2\mu}k_\perp)e^{-\mu}d\mu. \tag{1.7}$$

These can be calculated by considering the Taylor series of the zeroth order Bessel function,

$$J_0(x) = \sum_{n=0}^{\infty} \frac{1}{(n!)^2}\left(\frac{ix}{2}\right)^{2n}. \tag{1.8}$$

Applying the appropriate integrals to this expansion, the following identities are determined,

$$\int_0^\infty J_0(\sqrt{\mu}k_\perp)e^{-\mu}d\mu = e^{-b/2}, \tag{1.9}$$

and

$$\int_0^\infty \mu J_0(\sqrt{2\mu}k_\perp)e^{-\mu}d\mu = e^{-b/2}\left(1 - b/2\right), \tag{1.10}$$

where $b \equiv k_\perp^2$.

The gyroaverage operator in the Poisson equation is approximated by assuming that the $v_\perp$ dependence of the perturbed distribution function is Maxwellian (i.e., of the form $e^{-\mu}$), in which case the Poisson equation is modified only by an exponential factor as follows,

$$\phi_{k_x,k_y} = \frac{\int e^{-k_\perp^2/2} g dv_{||} + \tau\langle\phi\rangle_{FS}\delta_{k_y,0}}{\tau + [1 - \Gamma_0(b)]}. \tag{1.11}$$

This is the same assumption used in Ref. [3]. For a discussion of the limitations of this approximation, see Ref. [4]. For our purposes, these limitations are not of critical importance as we only need some reasonable mechanism to provide stabilization of high-$k_\perp$ modes.

Including these FLR effects produces the following operators,

$$\mathcal{L}[g] = -\left[\omega_n + \omega_T\left(v^2 - \frac{1}{2} - \frac{b}{2}\right)\right]F_0 i k_y e^{-b/2}\phi - \sqrt{2}v\left(\partial_z g + F_0 e^{-b/2}\partial_z\phi\right) + C(g), \tag{1.12}$$

and

$$\mathcal{N}[g] = \sum_{k'_\perp}\left(k'_x k_y - k_x k'_y\right)e^{-k'^2_\perp/2}\phi_{k'_\perp}g_{k_\perp - k'_\perp}, \tag{1.13}$$

where $v \equiv v_{||}$, $g(v)$ has only parallel velocity dependence, and the background distribution function is now $F_0 \equiv \pi^{-\frac{1}{2}}e^{-v^2}$.

1.1.3 HERMITE REPRESENTATION

Now we would like to transform the equations into a basis of Hermite polynomials. The basis functions are $H_n(v)e^{-v^2}$, where H_n are the Hermite polynomials,

$$H_n(x) = \frac{(-1)^n e^{x^2}}{(2^n n! \sqrt{\pi})^{\frac{1}{2}}} \frac{d^n}{dx^n} e^{-x^2}, \tag{1.14}$$

so that the expansion of the distribution function is,

$$g(v) = \sum_{n=0}^{\infty} \hat{g}_n H_n(v) e^{-v^2}. \tag{1.15}$$

The orthogonality relation for Hermite polynomials is,

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = \delta_{n,m}, \tag{1.16}$$

so that the Hermite coefficients can be extracted by integrating over v,

$$\hat{g}_n = \int_{-\infty}^{\infty} g(v) H_n(v) dv. \tag{1.17}$$

In order to transform the equations to the Hermite basis, we exploit the orthogonality relation and operate on the gyrokinetic equation,

$$\int_{-\infty}^{\infty} \left[\frac{\partial g}{\partial t} = \mathcal{L}[g] + \mathcal{N}[g] \right] H_n(v) dv. \tag{1.18}$$

We will use the following relations to evaluate the relevant expressions:

$$H_0(x) = \pi^{-\frac{1}{4}}, \tag{1.19}$$

$$H_1(x) = \sqrt{2}\pi^{-\frac{1}{4}} x, \tag{1.20}$$

$$H_2(x) = \frac{2x^2 - 1}{\sqrt{2}\pi^{\frac{1}{4}}}, \tag{1.21}$$

and

$$\sqrt{2} x H_n(x) = \sqrt{n+1} H_{n+1}(x) + \sqrt{n} H_{n-1}(x). \tag{1.22}$$

We need to evaluate terms which include the following integrals:

$$\int_{-\infty}^{\infty} v^2 F_0(v) H_n(v) dv = \int_{-\infty}^{\infty} \pi^{-\frac{1}{4}} \left[\frac{H_2}{\sqrt{2}} + \frac{H_0}{2} \right] e^{-v^2} H_n(v) dv = \frac{\pi^{-\frac{1}{4}}}{2} \left[\sqrt{2}\delta_{n,2} + \delta_{n,0} \right], \tag{1.23}$$

$$\int_{-\infty}^{\infty} v F_0(v) H_n(v) dv = \int_{-\infty}^{\infty} \frac{\pi^{-\frac{1}{4}}}{\sqrt{2}} H_1(v) H_n(v) e^{-v^2} dv = \frac{\pi^{-\frac{1}{4}}}{\sqrt{2}} \delta_{n,1}, \tag{1.24}$$

and,

$$\int_{-\infty}^{\infty} F_0(v) H_n(v) dv = \pi^{-\frac{1}{4}} \delta_{n,0}. \tag{1.25}$$

We also need to treat the term,

$$vg = \sum_{n=0}^{\infty} \hat{g}_n e^{-v^2} \left[\sqrt{\frac{n+1}{2}} H_{n+1} + \sqrt{\frac{n}{2}} H_{n-1} \right], \tag{1.26}$$

which becomes in the Hermite representation,

$$\int_{-\infty}^{\infty} vg(v) H_n(v) dv = \left(\frac{n}{2}\right)^{\frac{1}{2}} \hat{g}_{n-1} + \left(\frac{n+1}{2}\right)^{\frac{1}{2}} \hat{g}_{n+1}. \tag{1.27}$$

With these results (Eqns. 1.23-1.25, 1.27) we can rewrite the gyrokinetic equation in the Hermite basis,

$$\frac{\partial \hat{g}_n}{\partial t} = \mathcal{L}[\hat{g}_n] + \mathcal{N}[\hat{g}_n], \tag{1.28}$$

with the following linear and nonlinear operators:

$$\begin{aligned} \mathcal{L}[\hat{g}_n] = &\frac{\omega_T i k_y}{\pi^{\frac{1}{4}}} \frac{k_\perp^2}{2} e^{-b/2} \phi \delta_{n,0} - \frac{\omega_n i k_y}{\pi^{\frac{1}{4}}} e^{-b/2} \phi \delta_{n,0} - \frac{\omega_T i k_y}{\sqrt{2}\pi^{\frac{1}{4}}} e^{-b/2} \phi \delta_{n,2} \\ &- \left[\left(\frac{n}{2}\right)^{\frac{1}{2}} \partial_z \hat{g}_{n-1} + \left(\frac{n+1}{2}\right)^{\frac{1}{2}} \partial_z \hat{g}_{n+1} \right] - \pi^{-\frac{1}{4}} e^{-b/2} \partial_z \phi \delta_{n,1} + C(\hat{g}_n), \end{aligned} \tag{1.29}$$

and

$$\mathcal{N}[\hat{g}_n] = \sum_{k'_\perp} \left(k'_x k_y - k_x k'_y \right) e^{-k'^2_\perp/2} \phi_{k'_\perp} \hat{g}_{n, k_\perp - k'_\perp}. \tag{1.30}$$

1.1.4 COLLISION OPERATOR

The Lenard-Bernstein collision operator has a particularly simple representation in the Hermite basis. In direct velocity space the collision operator is,

$$C[g] = \nu g + \nu v \partial_v g + \frac{1}{2} \nu \partial_v^2 g. \tag{1.31}$$

Using Eqn. 1.22, along with the following identity,

$$H'_n = \sqrt{2n} H_{n-1}, \tag{1.32}$$

the collision operator can be expressed in the Hermite basis. This procedure reveals the Hermite polynomials to be eigenfunctions of the Lenard-Bernstein collision operator,

$$C[\hat{g}_n] = -\nu n \hat{g}_n. \tag{1.33}$$

1.1.5 FIELD EQUATION IN THE HERMITE REPRESENTATION

The field equation also has a simple form in the Hermite representation. The velocity space integral reduces to the $n = 0$ contribution of the distribution function,

$$\int g dv_{||} = \int \sum_{n=0}^{\infty} \hat{g}_n H_n(v) e^{-v^2} dv = \pi^{\frac{1}{4}} \hat{g}_0, \tag{1.34}$$

so that the field equation is,

$$\phi_{k_x,k_y} = \frac{q_i n_{0i} \pi^{\frac{1}{4}} e^{-k_\perp^2/2} \hat{g}_0 + \tau \langle \phi \rangle_{FS} \delta_{k_y,0}}{\tau + \frac{q_i^2 n_{0i}}{T_{0i}} \left[1 - \Gamma_0(b)\right]}, \tag{1.35}$$

where the flux-surface-averaged potential is,

$$\langle \phi \rangle_{FS} = \frac{\pi^{\frac{1}{4}} \langle e^{-k_\perp^2/2} \hat{g}_0 \rangle_{FS}}{\left[1 - \Gamma_0(b)\right]}. \tag{1.36}$$

1.1.6 FOURIER REPRESENTATION IN THE PARALLEL DIRECTION

We also wish to implement a Fourier representation in the parallel coordinate,

$$g(z) = \sum_{k_z=-\infty}^{\infty} \hat{g}_{k_z} e^{ik_z z}, \tag{1.37}$$

so that the Fourier coefficients are defined,

$$\hat{g}_{k_z} = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(z) e^{-ik_z z} dz. \tag{1.38}$$

With this Fourier representation, parallel derivatives in the linear operator simply reduce to multiplication by ik_z, and another summation is introduced in the nonlinearity so that the final equations are as follows:

$$\frac{\partial \hat{g}_{n,k_z}}{\partial t} = \mathcal{L}[\hat{g}_{n,k_z}] + \mathcal{N}[\hat{g}_{n,k_z}], \tag{1.39}$$

with the following linear and nonlinear operators:

$$\begin{aligned} \mathcal{L}[\hat{g}_{n,k_z}] = &\frac{\omega_T i k_y}{\pi^{\frac{1}{4}}} \frac{k_\perp^2}{2} e^{-k_\perp^2/2} \phi_{k_z} \delta_{n,0} - \frac{\omega_n i k_y}{\pi^{\frac{1}{4}}} e^{-k_\perp^2/2} \phi_{k_z} \delta_{n,0} - \frac{\omega_T i k_y}{\sqrt{2}\pi^{\frac{1}{4}}} e^{-k_\perp^2/2} \phi_{k_z} \delta_{n,2} \\ &- \frac{i k_z}{\pi^{\frac{1}{4}}} e^{-k_\perp^2/2} \phi_{k_z} \delta_{n,1} - i k_z \left[\sqrt{n} \hat{g}_{n-1,k_z} + \sqrt{n+1} \hat{g}_{n+1,k_z}\right] - \nu n \hat{g}_{n,k_z}, \end{aligned} \tag{1.40}$$

and

$$\mathcal{N}[g] = \sum_{k'_\perp} \left(k'_x k_y - k_x k'_y\right) e^{-k'^2_\perp/2} \phi_{k'_\perp} g_{k_\perp - k'_\perp}. \tag{1.41}$$

1.1.7 SUMMARY EQUATIONS

The time evolution of the distribution function is,

$$\frac{\partial \hat{g}_n}{\partial t} = \mathcal{L}[\hat{g}_n] + \mathcal{N}[\hat{g}_n], \tag{1.42}$$

with the following linear and nonlinear operators:

$$\begin{aligned} \mathcal{L}[\hat{g}_n] = &\frac{\omega_T i k_y}{\pi^{\frac{1}{4}}} \frac{k_\perp^2}{2} e^{-k_\perp^2/2} \phi \delta_{n,0} - \frac{\omega_n i k_y}{\pi^{\frac{1}{4}}} e^{-k_\perp^2/2} \phi \delta_{n,0} - \frac{\omega_T i k_y}{\sqrt{2}\pi^{\frac{1}{4}}} e^{-k_\perp^2/2} \phi \delta_{n,2} \\ &- \frac{i k_z}{\pi^{\frac{1}{4}}} e^{-k_\perp^2/2} \phi \delta_{n,1} - i k_z \left[\sqrt{n} \hat{g}_{n-1} + \sqrt{n+1} \hat{g}_{n+1}\right] - \nu n \hat{g}_n, \end{aligned} \tag{1.43}$$

and

$$\mathcal{N}[g] = \sum_{\mathbf{k}'} \left(k'_x k_y - k_x k'_y\right) e^{-k'^2_\perp/2} \phi_{\mathbf{k}'} g_{\mathbf{k}-\mathbf{k}'}. \tag{1.44}$$

The equation for the electrostatic potential is,

$$\phi_{k_x,k_y} = \frac{\pi^{\frac{1}{4}} e^{-k_\perp^2/2} \hat{g}_0 + \frac{T_{0i}}{T_{0e}} \langle\phi\rangle_{FS} \delta_{k_y,0}}{\frac{T_{0i}}{T_{0e}} + [1 - \Gamma_0(b)]}, \tag{1.45}$$

where the flux-surface-averaged potential is,

$$\langle\phi\rangle_{FS} = \frac{\pi^{\frac{1}{4}} e^{-k_\perp^2/2} \hat{g}_{0,k_z=0}}{[1 - \Gamma_0(b)]}. \tag{1.46}$$

$\Gamma_0(x) = I_0(x)e^{-x}$, $I_0(x)$ is the zeroth order modified Bessel function, and $b_i = k_\perp^2$.

It is also useful to have the expression for the nonlinearity in direct space so that this term can be treated numerically with pseudo-spectral methods:

$$\mathcal{N}[\hat{g}_n(x,y,z)] = \partial_y \bar{\phi} \partial_x g - \partial_x \bar{\phi} \partial_y g. \tag{1.47}$$

SECTION REFERENCES

[1] F. Merz, Ph.D. Thesis, Universität Münster, (2008).

[2] A. Banon Navarro, P. Morel, M. Albrecht-Marc, D. Carati, F. Merz, T. Grler, and F. Jenko, Physics of Plasmas **18**, 092303 (2011).

[3] T.-H. Watanabe and H. Sugama, Physics of Plasmas **11**, 1476 (2004).

[4] W. Dorland and G. W. Hammett, Phys. Fluids B **5**, 812.

SECTION 1.2

QUANTITIES OF INTEREST

1.2.1 HEAT FLUX

The heat flux is the spatial average of the radial $E \times B$ advection of the pressure fluctuation,

$$Q \equiv \langle \tilde{p}\tilde{v}_{E,r} \rangle = -\frac{\int dxdydz \left(\tilde{p}\partial_y \bar{\phi}/B_0\right)}{L_x L_y L_z}. \tag{1.48}$$

This can be transformed into Fourier space using Parseval's theorem,

$$Q = -\sum_{k_x,k_y,k_z} \tilde{p}^* i k_y e^{-k_\perp^2/2} \phi / B_0. \tag{1.49}$$

The pressure fluctuation must also be transformed into the Hermite representation:

$$\tilde{p} \equiv \int dv v^2 g = \frac{\pi^{1/4}}{\sqrt{2}} \hat{g}_2 + \frac{\pi^{1/4}}{2} \hat{g}_0. \tag{1.50}$$

The $\hat{g}_0$ component drops out of the $\vec{k}$ sum for the heat flux so that the final expression is,

$$Q = -\frac{\pi^{1/4}}{\sqrt{2}B_0} \sum_{k_x,k_y,k_z} i k_y e^{-k_\perp^2/2} \phi \hat{g}_2^*. \tag{1.51}$$

1.2.2 ENERGETICS

The energy equation for this system can be derived (in analogy with the energetics [2] for the gyrokinetic equations) by operating with,

$$E[X] \equiv Re\left[\int_{-\infty}^{\infty} \left(\frac{g}{F_0} + e^{-k_\perp^2/2}\phi\right)^* X dv\right]. \tag{1.52}$$

In the remainder of this section the notation signifying the real part of the expression will be suppressed.

This can be applied in the Hermite representation by noting that,

$$\int_{-\infty}^{\infty} \left(\frac{g}{F_0} + e^{-k_\perp^2/2}\phi\right)^* f dv = \sum_n \left(\pi^{1/2}\hat{g}_n + \pi^{1/4} e^{-k_\perp^2/2}\phi\delta_{n,0}\right)^* f_n, \tag{1.53}$$

where the Hermite expansions of g and f are as follows,

$$g(v) = \sum_{n=0}^{\infty} \hat{g}_n H_n(v) e^{-v^2}. \tag{1.54}$$

Operating on the distribution function produces the energy quantity,

$$E = \frac{1}{2}\sum_n |\hat{g}_n|^2 \pi^{1/2} + \frac{1}{2}\phi^* e^{-k_\perp^2/2} \hat{g}_0 \pi^{1/4}, \tag{1.55}$$

which for $k_y \neq 0$ reduces to,

$$E = \frac{1}{2}\sum_n |\hat{g}_n|^2 \pi^{1/2} + \frac{1}{2} D(k_\perp^2) |\phi|^2, \tag{1.56}$$

where $D(k_\perp^2) = \frac{1}{\tau+1-\Gamma_0(b)}$. The energy evolution equation is produced by operating on each term on the RHS of Eq. 1.43 as will be outlined below. By summing over all $\vec{k}$, one can extract the non-vanishing terms which define the sources and sinks of the system.

The density gradient, ω_n, term in the energy equation is proportional to $ik_y\hat{g}_0\phi$. Since $\hat{g}_0$ is proportional to ϕ, this term drops out when summed over $\vec{k}$ due to the reality constraint.

The temperature gradient term produces the energy drive,

$$Q = -\frac{\pi^{1/4}}{\sqrt{2}}\omega_T i k_y e^{-k_\perp^2/2}\hat{g}_2^*\phi. \tag{1.57}$$

The parallel electric field has two terms–one proportional to $ik_z|\phi|^2$ which vanishes when summed over $\vec{k}$ and another term,

$$-\pi^{1/4} i k_z \hat{g}_1^* e^{-k_\perp^2/2}\phi, \tag{1.58}$$

which will be shown to cancel with quantities in the phase-mixing term.

The phase mixing term produces two results, $-ik_z\pi^{1/4}e^{-k_\perp^2/2}\phi^*\hat{g}_1$, which cancels with the term in expression 1.58, and additional terms,

$$\sum_n \pi^{1/2}(-ik_z)\left[\sqrt{n}\hat{g}_n^*\hat{g}_{n-1} + \sqrt{n+1}\hat{g}_n^*\hat{g}_{n+1}\right], \tag{1.59}$$

which cancel in the sum over n. This cancellation can be seen, e.g., by considering the expressions in 1.59 for $n = m-1$ and $n = m$. The $\sqrt{n+1}\hat{g}_n^*\hat{g}_{n+1}$ term for $n = m-1$ cancels exactly with the $\hat{g}_n^*\hat{g}_{n-1}$ term for $n = m$. In other words, the phase-mixing term transfers energy in a conservative linear cascade through velocity space. Numerically this is violated only at $n = n_{max}$ where the Hermite representation is truncated and thus well-behaved energetics is only expected with sufficient velocity space resolution.

Finally, the collision term provides the energy sink of the system,

$$C = -\pi^{1/2}\sum_n \nu n\left|\hat{g}_n\right|^2. \tag{1.60}$$

The final energy equation is,

$$\frac{\partial E}{\partial t} = \sum_{\vec{k}}\left[\frac{\pi^{1/4}}{\sqrt{2}}\omega_T i k_y e^{-k_\perp^2/2}\hat{g}_2^*\phi - \pi^{1/2}\sum_n \nu n\left|\hat{g}_n\right|^2\right]. \tag{1.61}$$

1.2.3 Nonlinear Energy Transfer

Fill in some explanation:

$$T_{n,k,k'} = -\pi^{1/2}(k_x' k_y - k_x k_y')\hat{g}_{n,k}^*\bar{\phi}_{k-k'}\hat{g}_{n,k'} \tag{1.62}$$

$$T_{\phi,k,k'} = \pi^{1/4}(k_x' k_y - k_x k_y')\bar{\phi}_k^*\bar{\phi}_{k'}\hat{g}_{0,k-k'} \tag{1.63}$$

CHAPTER 2

CORE COMPONENTS FILES OF DNA

SECTION 2.1

SUBROUTINES IN FILE: CC_COMM.F90

This file contains the subroutines responsible for accessing the MPI communication environment. The subroutines contained in this file and their main function are:

- `init_comm`: starts the MPI communication environment
- `comm`: nothing necessary right now for only v parallelization
- `finalize_mpi`: terminates the MPI communication environment

SECTION 2.2

DNA INPUT NAMELISTS

2.2.1 PHYSICAL_PARAMETERS

`nu [real]`: collision frequency (normalized to v_{ti}/R).

`omt [real]`: temperature gradient scale length R/L_{ti}.

`omn [real]`: density gradient scale length R/L_n.

`Ti0Te [real]`: ratio of background ion to electron temperature.

2.2.2 NUMERICAL_PARAMETERS

`kxmin [real]`: minimum radial wavenumber.

`kymin [real]`: minimum binormal wavenumber.

`kzmin [real]`: minimum parallel wavenumber.

`nkx0 [integer]`: number of radial wavenumbers. Note that the code directly calculates the wavenumbers $k_x = 0$ through $k_{x,\text{max}} =$(`nkx0`$-1)\times$`kxmin`. The negative k_x modes are implicitly defined via the reality constraint.

`nky0 [integer]`: number of binormal wavenumbers, including positive and negative wavenumbers.

`nkz0 [integer]`: number of parallel wavenumbers, including positive and negative wavenumbers.

`nv0 [integer]`: number of Hermite polynomials.

`hyp_x [real]`: prefactor for radial hyperdiffusion.

`hyp_y [real]`: prefactor for binormal hyperdiffusion.

`hyp_z [real]`: prefactor for parallel hyperdiffusion.

`hyp_v [real]`: prefactor for hyper-collisions.

`hypx_order [integer]`: order of radial hyperdiffusion.

`hypy_order [integer]`: order of binormal hyperdiffusion.

`hypz_order [integer]`: order of parallel hyperdiffusion.

`hypv_order [integer]`: order of hyper-collisions.

`hyp_conv [real]`: prefactor for a Krook-like term acting on the $k_z = 0$, $n = 0$ part of the distribution function (where n is the Hermite number). The net prefactor is `hyp_conv`$\times$`nu`, so that setting this equal to one extends the minimum collisionality to $k_z = 0$, $n = 0$. This part of the distribution function is otherwise often subject to slow growth over the course of a simulation.

`num_v_procs [integer]`: number of processors. Note that the code is only parallelized over the Hermite coordinate at this time.

`courant [real]`: courant factor for the nonlinear time step adaptation.

2.2.3 DIAGNOSTICS

`diagdir [character]`: output directory.

`istep_ffm [integer]`: parameter defining how frequently to activate diagnostics calculating ϕ^2 and the heat flux summed over all coordinates. This data is output to the file 'ffm.dat.' As with all of the following '`istep`' parameters, the diagnostic is activated every `istep`-th time step.

`istep_energy3d [integer]`: parameter defining how frequently to activate diagnostics calculating the three dimensional free energy, energy drive, collisional dissipation and any dissipation from artificial hyperdiffusion. This data is output to the file 'energy3d.dat.'

`istep_energy [integer]`: parameter defining how frequently to activate diagnostics calculating the total value of various energy-related quantities–1. the 'entropy' part of the free energy, 2. the electrostatic part of the free energy, 3. total RHS of the free energy evolution equation, 4. free energy drive, 5. collisional dissipation, 6. hypercollisional dissipation, 7. dissipation via other artificial hyperdiffusion, 8. nonlinear contribution to the energy equation (should be extremely small), 9. calculated time derivative of the free energy. This data is output to the file 'energy3d.dat.'

`istep_hermite [integer]`: parameter defining how frequently to activate diagnostics calculating the free energy as a function of Hermite polynomial, summed over all spatial coordinates. This data is output to the file 'energy_hermite.dat.'

`istep_gout [integer]`: parameter defining how frequently to output the entire distribution function. This data is output to the file 'gout.dat.'

`istep_nlt [integer]`: parameter defining how frequently to activate nonlinear energy transfer diagnostics.

`istep_eshells [integer]`: parameter defining how frequently to activate energy diagnostics formulated in terms of $k_\perp$ shells.

`min_shell_width [integer]`: parameter for determining the $k_\perp$ shells.

`istep_real [integer]`: parameter defining how frequently to enforce the reality constraint on $k_x = 0$ modes.

`istep_fmom3d [integer]`: parameter defining how frequently to activate diagnostics calculating the three dimensional electrostatic potential and pressure fluctuations. This data is output to the file 'fmom3d.dat.'

`istep_gamma [integer]`: parameter defining how frequently to calculate the growth rate for linear initial-value simulations.

`istep_schpt [integer]`: parameter defining how frequently to write a security checkpoint in case the simulation stops unexpectedly.

`output_nlt_n [integer]`: flag for calculating nonlinear transfer functions for various Hermite polynomials.

`istep_gk [integer]`: parameter defining how frequently to output the distribution function for certain wavenumbers. This is useful if memory constraints limit the frequency at which the entire distribution function can be output.

`gk_ky_index [integer]`: index defining the k_y mode for a k_z scan associated with `istep_gk`.
`gk_kz_index [integer]`: index defining the k_z mode for a k_y scan associated with `istep_gk`.

2.2.4 FLAGS

`nonlinear [logical]`: 'T' denotes a nonlinear simulation.
`calc_dt [logical]`: 'T' activates calculation of the initial time step. Otherwise `dt_max` must be set.
`comp_type [character]`: 'IV' activates initial value computation, 'EV' activates eigenvalue computation.
`checkpoint_read [logical]`: 'T' activates a checkpoint read as an initial condition in case of restarts. Additional data output will be appended to existing files.
`etg_factor [real]`: factor determining the adiabatic response for $k_y = 0$ modes. `etg_factor`=0.0 defines to an 'ETG' simulation, and `etg_factor`=1.0 defines to an 'ITG' simulation.

2.2.5 EIGENSOLVE

`n_ev [logical]`: number of eigenvalues to solve for (maximum is `nv0`).
`left_ev [logical]`: 'T' activates calculation of the left eigenvectors.
`kxmax0 [real]`: maximum k_x wavenumber. Whatever is input is overwritten and the correct value is output in the resulting parameters.dat file. This is then used in post-processing diagnostics.
`kymax0 [real]`: maximum k_y wavenumber (not including the Nyquist wavenumber). Whatever is input is overwritten and the correct value is output in the resulting parameters.dat file. This is then used in post-processing diagnostics.
`kzmax0 [real]`: maximum k_z wavenumber (not including the Nyquist wavenumber). Whatever is input is overwritten and the correct value is output in the resulting parameters.dat file. This is then used in post-processing diagnostics.

2.2.6 INITIAL_VALUE

`max_itime [integer]`: maximum number of time steps before termination of the simulation.
`max_walltime [integer]`: maximum walltime before termination of the simulation.
`max_time [real]`: maximum time in R/v_{ti} before termination of the simulation.
`dt_max [real]`: initial time step. The time step will be calculated automatically if `calc_dt`=T, and will be automatically adapted in the nonlinear regime.

CHAPTER 3

EXTRA ELEMENTS FILES OF DNA

SECTION 3.1

SUBROUTINES IN FILE: CC_PERFORMANCE.F90

This file houses the `performance` module that contains subroutines responsible for running various tests.
The subroutines contained in this file and their main function are:

- `performance_compute`: the main performance subroutine that calls all other subroutines depending on the logical performance switches selected.
- `performance_linear`: linear performance test
- `performance_nl`: nonlinear performance test
- `performance_rhs`: rhs performance test
- `performance_par`: parallelisation performance test
- `start_clock`: starts a chronometer
- `end_clock`: end a chronometer