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## Gyrokinetic simulations of turbulence and zonal flows driven by steep profile gradients using a delta-f approach with an evolving background Maxwellian

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# Gyrokinetic simulations of turbulence and zonal flows driven by steep profile gradients using a delta-f approach with an evolving background Maxwellian

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## ABSTRACT

Long global gyrokinetic turbulence simulations are particularly challenging in situations where the system deviates strongly from its initial state and when fluctuation levels are high, for example, in strong gradient regions. For particle-in-cell simulations, statistical sampling noise accumulation from large marker weights due to large deviations from the control variate of a delta-f scheme makes such simulations often impractical. An adaptive control variate in the form of a flux-surface-averaged Maxwellian with a time-dependent temperature profile is introduced in an attempt to alleviate the former problem. Under simplified collisionless physics, this adaptive delta-f scheme is shown to reduce noise accumulation in the zonal flows and the simulated heat flux in a quasi-steady turbulent state. The method also avoids the collapse of the signal-to-noise ratio, which occurs in the standard non-adaptive scheme, and, therefore, allows one to reach numerically converged results even with lower marker numbers.

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## I. INTRODUCTION

The success of magnetic fusion research relies heavily on its accurate modeling by computer simulations. In the most promising reactor configuration, the tokamak, plasma is confined by magnetic fields in a toroidal vacuum chamber. A complete description of the plasma involves simulating regions of the core, edge, the scrape-off layer, and plasma–wall interaction.

To simulate fusion plasmas, many methods exist, which can be categorized by the physical assumptions made. The latter are usually dictated by the physical process of the plasma volume. This work focuses on simulating turbulence in the core and edge transitioning region. Specifically, the gyrokinetic particle-in-cell (PIC) method<sup>1–5</sup> is used. The gyrokinetic formalism<sup>6–8</sup> reduces the number of phase space variables from six to five, approximating the dynamics of plasma particle trajectories by gyrorings bound to evolving gyrocenters. The reduction in dynamics implies a timescale separation between the fast cyclotron motion and the fluctuation time scales typically involved in

turbulent processes. Using Monte Carlo sampling, the PIC method begins by representing an initial distribution function f as a collection of numerical particles (in fact the gyrocenters) called "markers," each having its respective weight. Each marker is then integrated along its characteristic through time.

For plasma core simulations, it is often the case that f does not deviate significantly (not more than a few percent) from its initial state  $f_0$  over characteristic time scales of micro-stabilities and turbulent processes. This allows one to split the distribution function into a stationary analytic control variate<sup>5,9,10</sup>  $f_0$  and a time-dependent deviation part  $\delta f$ , which is represented by numerical markers. This approach is referred to as the delta-f PIC method and is to be contrasted with the full-f PIC scheme, which represents the whole f in terms of markers. The gain in noise reduction of the delta-f scheme relies on the reduced variance of the marker weights, providing that the assumption  $|\delta f|/|f_0| \ll 1$  for some definition of the norm is met.





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However, the plasma edge involves steep profile gradients and low-density levels, which often leads to conditions with fluctuation levels as large as the background such that the assumption of the delta-f scheme will not be met. One could fall back to the full-f scheme, which entails using high marker numbers to achieve similar low noise levels as the delta-f scheme in the core. As marker numbers typically need to be at least at the order of 10 per grid cell for an adequate simulation of the core of a medium-sized tokamak plasma, like that of the Tokamak a Configuration Variable (TCV) at EPFL,<sup>11</sup> larger marker numbers per grid cell may exceed the computational limits of most computers, even more so for particularly large plasma volumes like that of ITER. In order to still possibly retain some advantage of the delta-f scheme, one could also evolve  $f_0$ , albeit at a longer timescale than that of the fluctuating  $\delta f$ . This approach has for example been suggested in references.<sup>12-14</sup> This work explores the implications of a specific implementation of this approach. Namely, to have a time-evolving background by constraining  $f_0$  to be a flux-surface-dependent Maxwellian which is furthermore time-dependent via its evolving temperature profile. It will be shown that this adaptive control variate scheme is always effective in reducing the statistical sampling noise, especially in situations where turbulence saturation is controlled by the zonal flow shearing rate. At the time of writing, a similar work<sup>15</sup> is being done as a followup to Ref. 14.

Another source of statistical sampling noise is due to "weightspreading"<sup>12,16</sup> as a result of the implementation of collision operators using a Langevin approach. However, this problem will not be addressed in this work as collisions are not considered. Though the collision-less limit is valid when simulating core plasmas, which are weakly collisional, collisions are important when simulating plasma edge, the same region in which the adaptive delta-f scheme just mentioned could be useful.

This paper is organized as follows. A brief presentation of the slab-like model considered in the GKengine code used in this study is made in Sec. II. The numerical methods are then discussed in Sec. III, in particular, the adaptive delta-f PIC scheme, which is the main focus of this paper. This is followed in Sec. IV by a discussion of the profiles<sup>17</sup> and parameters used to demonstrate the feasibility and utility of the scheme. Various aspects of noise reduction involving the adaptive scheme are discussed, in turn, with key diagnostics explained as they appear. This paper concludes with a discussion on the effectiveness of the adaptive scheme in high-flux and high-fluctuation level scenarios achieved by tuning the flux-surface-averaged (f.s.a.) potential term  $\langle \phi \rangle$  of the quasi-neutrality equation. As this work is a contribution toward the development of the tokamak edge/scrape-off-layer (SOL) code PICLS,<sup>18</sup> this tuning emulates edge conditions when simulating slab ITG-driven turbulence subject to strong zonal shear flow stabilization.

#### II. PHYSICAL MODEL

All simulations carried out in the frame of this work are run with the GK engine code, <sup>19,20</sup> which solves for the distribution function f of the single kinetic singly charged Z=1 ion species via the gyrokinetic equation

where *S* is a general source term t The electrons on the other hand are assumed to be adiabatic. A review of such a scenario is given for example in Ref. 21. The left-hand side of Eq. (1) reads<sup>8</sup>

df

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \left\{ \frac{\partial}{\partial t} + \frac{\mathrm{d}\vec{R}}{\mathrm{d}t} \cdot \nabla_{\vec{R}} + \frac{\mathrm{d}\nu_{\parallel}}{\mathrm{d}t} \frac{\partial}{\partial\nu_{\parallel}} + \frac{\mathrm{d}\mu}{\mathrm{d}t} \frac{\partial}{\partial\mu} \right\} f, \qquad (2)$$

with f function of the 5D gyrocenter phase space coordinates  $(\vec{R}, v_{\parallel}, \mu)$ . Specifically,  $\vec{R} = [X, Y, Z]$  is the gyrocenter real space position,  $v_{\parallel}$  its parallel velocity, and  $\mu$  its magnetic moment, given by  $\mu = m_i v_{\perp}^2 / 2B$ , with  $m_i$  is the ion mass,  $v_{\perp}$  its gyrating velocity, and B the strength of the local magnetic field  $\vec{B} = B\hat{b}$ , with  $\hat{b}$  its direction. Two further assumptions are made. First, the geometry we considered is that of sheared-slab in a spatial 3D domain that spans  $(x, y, z) \in [0, L_x] \times [0, L_y] \times [0, L_z]$ , where the Cartesian coordinates (x, y, and z) can be related to the radial, poloidal, and toroidal directions, respectively, in a tokamak system. Periodic boundary conditions are thus imposed in the y and z directions, which span  $L_y = \pi a$  and  $L_z = 2\pi R_0$ , respectively, with a the minor radius and  $R_0$  the major radius. Figure 1 illustrates the sheared magnetic field, given by

$$\vec{B}(x) = B_y(x)\mathbf{e}_y + B_z\mathbf{e}_z, = B_z \left[\frac{L_y}{L_z q(x)}\mathbf{e}_y + \mathbf{e}_z\right],$$
(3)

where q(x) is the safety factor profile. The second assumption is that all fluctuations considered are electrostatic. Under these simplifications, the evolution of gyrocenter phase space coordinates is governed by<sup>20</sup>

$$\frac{d\vec{R}}{dt} = v_{\parallel}\hat{b} + \frac{\mu}{eB_{\parallel}^{\star}}\hat{b} \times \nabla B + \frac{1}{B_{\parallel}^{\star}}\hat{b} \times \nabla \tilde{\phi};$$

$$\frac{dv_{\parallel}}{dt} = -\frac{e}{m_{i}}\hat{b} \cdot \nabla \tilde{\phi};$$

$$\frac{d\mu}{dt} = 0.$$
(4)

Here, *e* is the ion charge,  $B_{\parallel}^{\star} = B[1 + m_i B_y^{\prime} B_z v_{\parallel} / (eB^3)]$ ,  $\phi$  the electric potential, and  $\overline{\cdot}$  the gyro-averaging operator, given by

$$\tilde{\phi}(\vec{R},\mu) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\alpha \, \phi(\vec{R}+\vec{\rho_L}(\mu,\alpha)),$$



FIG. 1. The sheared-slab magnetic geometry [see Eq. (3)] used in this work.

with  $\vec{\rho}_L$  the Larmor vector with radius  $\rho_L = \sqrt{2m_i\mu/B}$ , and  $\alpha$  the gyrophase. The set of Eq. (4) is nonlinear as these equations depend on the self-consistent electrostatic potential  $\phi(x, y, z)$  satisfying the quasi-neutrality equation with Z = 1,

$$\frac{e n_{e0}}{T_e} (\phi - \langle \phi \rangle) - \nabla_{\perp} \cdot \left( \frac{m_i n_{i0}}{e B^2} \nabla_{\perp} \phi \right) \\
= \int d\alpha d^3 R d\nu_{\parallel} d\mu \left\{ \frac{B_{\parallel}^{\star}}{m_i} f(\vec{R}, \nu_{\parallel}, \mu, t) \delta\left[\vec{R} + \vec{\rho}_L(\mu, \alpha) - \vec{r}\right] \right\} - n_{e0}, \quad (5)$$

where  $n_{i0}$  is the background ion gyrocenter density, and  $n_{e0}$  and  $T_e$  are the background electron density and temperature profiles, respectively, satisfying a local Maxwellian distribution due to the adiabatic assumption. Here, the  $B_{\parallel}^*/m_i$  term represents the Jacobian for the coordinate transformation from particle variables  $(\vec{r}, \vec{v})$  to gyrocenter variables  $(\vec{R}, v_{\parallel}, \mu)$ , and  $\langle \cdot \rangle$  is the flux-surface-averaging operator defined by

$$\langle \phi \rangle(x) = \frac{1}{L_y L_z} \int_0^{L_y} \mathrm{d}y \int_0^{L_z} \mathrm{d}z \, \phi(x, y, z)$$

Looking at Eq. (5), the first term on the left-hand side represents the linearized adiabatic electron response and the second term represents the ion polarization density in the long wavelength approximation  $k_{\perp}\rho_{th} \ll 1$ , with  $\rho_{th}$  the thermal ion Larmor radius, which together with the right-hand side representing the ion density fluctuation.

In order to simulate physics under strong profile gradients in quasi-steady state, heat sources are implemented to clamp ion temperature  $T_i$  at profile edges to prevent relaxation below critical gradients. This Krook-like source  $S_h$  with associated relaxation rate  $\gamma_h(x)$  is stationary and radially dependent, maintaining over time the high and low ends of the  $T_i$  profile of the initial background distribution function  $f_0(t = 0)$ . Particle sources are not needed as there is no density profile relaxation. The assumed adiabatic electron response indeed enables no particle transport. Therefore, an additional correction term  $S_{h,corr}$  to  $S_h$  is included to conserve density, along with parallel momentum  $v_{\parallel}$ .

Furthermore, it is shown<sup>22</sup> that the inclusion of a Krook-like noise control operator  $S_m$  with uniform relaxation rate  $\gamma_n$  (usually taken to be a few percent of the maximum linear growth rate), which relaxes to a (possibly time-dependent) reference distribution  $f_n$ , is important in PIC simulations to achieve a converged quasi-steady state at long simulation times. A corresponding correction term  $S_{n,corr}$  is also included to conserve density, parallel momentum  $v_{\parallel}$ , and energy  $v^2$ .

Taken together, considering Eqs. (2) and (4), Eq. (1) is expanded to

$$\begin{cases} \frac{\partial}{\partial t} + \frac{d\vec{R}}{dt} \cdot \nabla_{\vec{R}} + \frac{d\nu_{\parallel}}{dt} \frac{\partial}{\partial\nu_{\parallel}} \end{cases} f \\ = -\gamma_h(x)(f - f_0(t=0)) + S_{h,\text{corr}} - \gamma_n(f - f_n) + S_{n,\text{corr}}. \quad (6) \end{cases}$$

#### **III. NUMERICAL METHODS**

#### A. Delta-f scheme with adaptive control variate

The solution method of the GKengine employs the delta-f PIC scheme, which splits the ion distribution *f* into an unperturbed background part  $f_0$ , and a perturbed part  $\delta f_{\cdot}^{5,10}$  Namely,

$$f = f_0 + \delta f. \tag{7}$$

 $\delta f$  therefore represents the deviation component of f, including in particular fluctuations. The rationale for the splitting of f is that  $f_0$  acts as a control variate.<sup>9</sup> As long as  $|\delta f|/|f| \ll 1$ , that is, as long as the system does not deviate too much from a known  $f_0$ , the scheme reduces sampling noise. However, processes involving large profile gradients and high fluctuation amplitudes will result in f deviating far from its initial background  $f_0$ . Therefore, in order to reduce sampling noise in a delta-f scheme, we now allow the control variate  $f_0$  to be a timedependent local Maxwellian. Specifically,

$$f_{0} = f_{M}(R, v_{\parallel}, \mu, t),$$
  
=  $\frac{n_{i0}(X)}{[2\pi T_{i0}(X, t)/m_{i}]^{3/2}} \exp\left\{-\frac{m_{i}v_{\parallel}^{2}/2 + \mu B(X)}{T_{i0}(X, t)}\right\},$  (8)

with  $T_{i0}$  the background ion temperature profile. Note that the profiles of  $n_{i0}$  and  $T_{i0}$  are spatially only functions of the "radial" variable. The time dependence of  $f_0$  appears only through  $T_{i0}$ , which is governed by an *ad hoc* relaxation equation<sup>12</sup> of the form

$$\frac{\partial}{\partial t} \left( \frac{3}{2} n_{i0}(x) T_{i0}(x, t) \right) = \alpha_E \left\langle \int \mathrm{d}\nu_{\parallel} \mathrm{d}\mu \frac{2\pi B_{\parallel}^*}{m_i} \delta f\left( \frac{m_i \nu_{\parallel}^2}{2} + \mu B \right) \right\rangle, \tag{9}$$

where  $\alpha_E$  is the relaxation rate, which is a constant numerical parameter. The left-hand side of Eq. (9) represents the variation in time of the background kinetic energy density  $E_{kin0}(x, t)$  related to  $f_{0}$ .

$$E_{kin0}(x,t) = \frac{3}{2}n_{i0}(x)T_{i0}(x,t),$$
(10)

with

and

$$T_{i0}(x,t) = T_{i0}(x,0) + \delta T_{i0}(x,t)$$

$$\delta E_{kin0}(x,t) = \frac{3}{2}n_{i0}(x)\delta T_{i0}(x,t).$$

Here,  $\delta E_{kin0}(x, t)$  and  $\delta T_{i0}(x, t)$  are the deviations of the background ion kinetic energy density and temperature profiles from their initial states  $E_{kin0}(x, 0)$  and  $T_{i0}(x, 0)$ , respectively.

Finally, let us explicate the contributions from  $f_0$  and  $\delta f$  to the gyrodensity on the right-hand side of the quasi-neutrality equation, Eq. (5). Assuming the gyrodensity associated with  $f_0(t = 0)$  verifies quasi-neutrality

$$\int \mathrm{d}^{3}R\mathrm{d}\alpha\mathrm{d}\nu_{\parallel}\mathrm{d}\mu \, \frac{B_{\parallel}^{\star}}{m_{i}}f_{0}(\vec{R},\nu_{\parallel},\mu,0)\delta\left[\vec{R}+\vec{\rho}_{L}(\mu,\alpha)-\vec{r}\right]=n_{e0},$$

Equation (5) becomes

$$\begin{aligned} &\frac{en_0}{T_e}(\phi - \langle \phi \rangle) - \nabla_{\perp} \cdot \left(\frac{m_i n_0}{eB^2} \nabla_{\perp} \phi\right) \\ &= \int d^3 R d\alpha d\nu_{\parallel} d\mu \, \frac{B_{\parallel}^{\star}}{m_i} \delta \left[\vec{R} + \vec{\rho}_L(\mu, \alpha) - \vec{r}\right] \\ &\times \left[ f_0(\vec{R}, \nu_{\parallel}, \mu, t) - f_0(\vec{R}, \nu_{\parallel}, \mu, 0) + \delta f(\vec{R}, \nu_{\parallel}, \mu, t) \right]. \end{aligned}$$
(11)

Here, the electron density  $n_{e0}$  has been approximated to the ion background density  $n_{i0}$ , both denoted by  $n_0$ . The perpendicular gradient  $\nabla_{\perp} \approx \nabla_{pol} = \mathbf{e}_x \partial_x + \mathbf{e}_y \partial_y$  has been approximated to the gradient in the (x, y) plane (corresponding to the poloidal plane in a tokamak) due to the fact that micro-instabilities align along field lines and assuming  $B_y/B_z = L_y/(L_zq(x)) \ll 1$ . Since  $f_0$  has an analytic form, the integral involving  $f_0$  terms are calculated using Gauss–Laguerre and Gauss–Chebyshev quadratures for the  $\mu$  and  $\alpha$  integrations, respectively. Convergence of this scheme is detailed in Appendix. For this work, we use 30 quadrature points for each of these dimensions. The  $v_{\parallel}$  integration on the other hand can be integrated analytically.

#### **B.** Numerical discretization

Under the PIC scheme,  $\delta f$  is represented by markers and is given by

$$\delta f = \frac{1}{2\pi} \sum_{p}^{N_{p}} \frac{w_{p}(t)}{B_{\parallel}^{\star}/m_{i}} \delta \Big[ \vec{R} - \vec{R}_{p}(t) \Big] \delta \big[ v_{\parallel} - v_{\parallel p}(t) \big] \delta \big[ \mu - \mu_{p}(t) \big],$$
(12)

where the denominator represents the same Jacobian as in Eq. (5),  $N_p$  is the total number of markers, and  $w_p(t)$  and  $(\vec{R}_p(t), v_{\parallel p}(t), \mu_p(t))$  are the weight and the phase space position in gyrocenter variables at time *t* of the marker with index *p*, respectively. All markers are initialized in phase space using Hammersley sequences<sup>23</sup> and are time-integrated using a fourth-order Runge–Kutta scheme.<sup>20</sup>

Under the delta-f scheme, with reference to the discussion leading to Eq. (6), the *f* conservation term, the heat source  $S_{h}$  and noise control  $S_n$  operators with their corresponding corrections are implemented consecutively. The control variate is the chosen reference function for  $S_n$ ,  $f_n = f_0$ . Designating  $f_{00} = f_0(t = 0)$ , Eq. (6) is split into three equations

$$\frac{\mathrm{d}\delta f^{(0)}}{\mathrm{d}t} = -\frac{\mathrm{d}f_0}{\mathrm{d}t},\tag{13}$$

$$\frac{\mathrm{d}\delta f^{(1)}}{\mathrm{d}t} = -\gamma_h(x)(f_0(t) - f_{00} + \delta f^{(0)}) + S_{h,\mathrm{corr}},\tag{14}$$

$$\frac{\mathrm{d}\delta f^{(2)}}{\mathrm{d}t} = -\gamma_n \delta f^{(1)} + S_{n,\mathrm{corr}},\tag{15}$$

with  $\delta f^{(0)}(t) = \delta f(t)$ , and  $\delta f^{(2)}$  is assigned to  $\delta f$  once these equations are solved. Equations (13)–(15) are discretized by multiplying by the phase space volume  $\Omega_p$  associated with the marker with index p, which remains constant along characteristics due to the collisionless physics under study, and are each integrated over the full time step  $\Delta t$  considered for integrating the marker trajectories. Equation (13) is first solved using the "direct- $\delta f$  approach."<sup>13</sup>

Focusing on Eqs. (14) and (15), let us denote  $(1, v_{\parallel}, v^2)$  to represent the density, parallel velocity, and energy moments, respectively. Then, the terms  $S_{h,corr}$  and  $S_{n,corr}$  are the corrections that are necessary to ensure that  $\delta f$  conserves  $(1, v_{\parallel})$  and  $(1, v_{\parallel}, v^2)$  with respect to  $S_h$  and  $S_n$ , respectively. Indeed, these different conservations motivate the consecutive implementation of Eq. (6). The correction term  $S_{corr}$  of either  $S_{h,corr}$  or  $S_{n,corr}$  is expressed as<sup>22</sup>

$$S_{\text{corr}} = \sum_{c} g_c(x) f_0(x, v_{\parallel}, \mu, t) G_c, \qquad (16)$$

where  $c \in \{0, 1, 2\}$ , and  $G_c \in \{1, v_{\parallel}, v^2\}$ , terms of which are included when their conservation is required. Here,  $f_0$  is the control variate, which is the adaptive background local Maxwellian, Eq. (8). Here, we demonstrate the implementation of the heat source. Since Eq. (16) is time-independent within a time step, Eq. (14) is first analytically integrated over  $\Delta t$  to give the *p*-indexed marker weight change

$$\Delta w_p = (e^{-\gamma_{hj}\Delta t} - 1) \times \left[ w_p + \Omega_p (f_0 - f_{00})_p - \frac{\Omega_p f_{0p}}{\gamma_{hj}} (g_{0j} + g_{1j} \nu_{||p}) \right],$$

where  $f_{0p}$  is a shorthand for  $f_0$  evaluated at the phase point  $(\vec{R}, v_{\parallel}, \mu)$  of the marker with index p, the subscript j represents the profile evaluation at the center of the jth radial bin of width  $\Delta x$ , and having made use of the relation  $\Omega_p \delta f_p = w_p$ . Then, simultaneous conservation of  $(1, v_{\parallel})$  in each jth radial bin leads to the 2-by-2 linear system with which the coefficients  $g_{0j}$  and  $g_{1j}$  are to be solved

$$\begin{split} &\sum_{x_p \in \begin{bmatrix} x_j, x_j + \Delta x \end{bmatrix}} \Omega_p f_{0p} \begin{bmatrix} 1 & v_{\parallel p} \\ v_{\parallel p} & v_{\parallel p}^2 \end{bmatrix} \begin{bmatrix} g_{0j} \\ g_{1j} \end{bmatrix} \\ &= \sum_{x_q \in \begin{bmatrix} x_j, x_j + \Delta x \end{bmatrix}} \gamma_{hj} \begin{bmatrix} \Omega_q (f_0 - f_{00})_q + w_q \\ \Omega_q (f_0 - f_{00})_q v_{\parallel q} + w_q v_{\parallel q} \end{bmatrix} \end{split}$$

The implementation of the noise control operator, Eq. (15), is done analogously, which involves a 3-by-3 linear system due to the simultaneous conservation of  $(1, v_{\parallel}, v^2)$ .

Finally, under the adaptive scheme, the term on the right-hand side of Eq. (13) now includes the change in  $f_0$  associated with the background ion temperature  $T_{i0}(x, t)$  adaptation, which is derived via the background ion internal energy density deviation  $\delta E_{kin0}(x, t)$  of Eq. (10). This field is represented with finite element cubic B-spline basis functions  $\Lambda_i(x)$ ,

$$\delta E_{kin0}(x,t) = \frac{3}{2} n_{i0}(x) \delta T_{i0}(x,t) = \sum_{k} \xi_{k}(t) \Lambda_{k}(x).$$
(17)

The time-dependent coefficients  $\xi_k(t)$  are obtained by first projecting Eq. (9) on the same B-spline basis functions. Combining Eqs. (9), (10), (12), and (17), the time derivatives  $\dot{\xi}_k(t)$  are retrieved by back-solving

$$\sum_{k} \dot{\xi}_{k}(t) M_{kj} = \alpha_{E} \sum_{p}^{N_{p}} w_{p} \Lambda_{j}(X_{p}) \left( \frac{m_{i} v_{\parallel p}^{2}}{2} + \mu_{p} B(X_{p}) \right), \quad (18)$$

where  $M_{kj} = \int_0^{L_x} dx \Lambda_k(x) \Lambda_j(x)$  are the mass matrix elements, with  $\xi_k(0) = 0, \forall k$  as initial condition.

The terms in the parenthesis of Eq. (18) motivate the adaption of  $E_{kin0}$  as it is the  $v^2$ -moment of the distribution function, contrary to  $T_{i0}$ , which is a derived measure, that is,  $2E_{kin0}/3n_{i0}$ . Having solved Eq. (18) for  $\xi(t)$ , these coefficients are then integrated in time by applying a first-order accurate forward Euler scheme with fixed time step  $N_{\alpha}\Delta t$ , where  $N_{\alpha}$  is a user-defined fixed integer. We have

$$\alpha_E N_{\alpha} \Delta t \le 2, \tag{19}$$

for all simulations performed in this paper. Violation of Eq. (19) has shown to lead to numerical instability.

Obviously, marker weights  $w_p$  need to be adapted if the background distribution  $f_0$  is adapted as a result of applying Eqs. (17) and (18). In the following lines of this section, let  $\Delta$  represent the change before and after the adaptation of  $f_0$ . Then, invoking the invariance of the total distribution f, from Eq. (7) one obtains

$$0 = \Delta f_0 + \Delta \delta f \iff \Delta \delta f = -\Delta f_0,$$

and after evaluating this relation at a marker position and multiplying by  $\Omega_{p_{i}}$ 

$$\Delta w_p = -\Omega_p \Delta f_{0p}, \qquad (20)$$

having made use of  $\Delta \Omega_p = 0$ .

#### **IV. PROFILES AND SIMULATION PARAMETERS**

Let the normalized radial coordinate be  $s = x/L_x \in [0, 1]$ . Then, the profiles representing the initial unperturbed ion and electron background densities,  $n_0$ , as well as their temperatures  $T_{i0}$  and  $T_{e0}$ , respectively, are parameterized by three parameters given by the amplitude A, the normalized absolute maximum logarithmic gradient  $\bar{\kappa}$ , and the slope half-width  $\bar{\Delta}$ . For  $s \in [0, 0.5]$ , such a profile g(s) is given explicitly by

$$g(s;\kappa,\Delta) = \begin{cases} A \exp\left(\frac{2\bar{\kappa}\bar{\Delta}}{3}\right) & 0 \le s < s_0 - \bar{\Delta}, \\ A \exp\left[-\bar{\kappa}(s-s_0) + \frac{\bar{\kappa}(s-s_0)^3}{3\bar{\Delta}^2}\right] & |s-s_0| \le \bar{\Delta}, \\ A \exp\left[-\frac{2\bar{\kappa}\bar{\Delta}}{3}\right] & s_0 + \bar{\Delta} < s \le 0.5. \end{cases}$$

$$(21)$$

Note that this definition ensures that g(s) and  $\frac{dg}{ds}$  are both continuous. At the reference radial position  $s = s_0$ , it has a value of A, and its parabolic normalized logarithmic gradient peaks at this same point with value  $\bar{\kappa}$ .

The heat source radial profile  $\gamma_h$  is parameterized by the amplitude  $A_{h}$ , and the half-widths  $\overline{\delta}_c$  and  $\overline{\delta}_s$  of the clamp maximum and edge-slope regions, respectively, with  $\overline{\delta}_c \geq \overline{\delta}_s$ . This profile for  $s \in [0, 0.5]$  is given explicitly by

$$\gamma_{h}(s;\bar{\delta}_{c},\bar{\delta}_{s}) = \begin{cases} A_{h} & 0 \leq s < \bar{\delta}_{c} - \bar{\delta}_{s}, \\ \frac{A_{h}}{2} \left[ 1 - \frac{3}{2} \left( \frac{s - \bar{\delta}_{c}}{\bar{\delta}_{s}} \right) + \frac{1}{2} \left( \frac{s - \bar{\delta}_{c}}{\bar{\delta}_{s}} \right)^{3} \right] & |s - \bar{\delta}_{c}| \leq \bar{\delta}_{s}, \\ 0 & \bar{\delta}_{c} + \bar{\delta}_{s} < s \leq \frac{1}{2} - (\bar{\delta}_{c} + \bar{\delta}_{s}), \\ \frac{A_{h}}{2} \left[ 1 + \frac{3}{2} \left( \frac{s - (1/2 - \bar{\delta}_{c})}{\bar{\delta}_{s}} \right) - \frac{1}{2} \left( \frac{s - (1/2 - \bar{\delta}_{c})}{\bar{\delta}_{s}} \right)^{3} \right] & \left| s - \left( \frac{1}{2} - \bar{\delta}_{c} \right) \right| \leq \bar{\delta}_{s}, \\ A_{h} & \frac{1}{2} - (\bar{\delta}_{c} - \bar{\delta}_{s}) < s \leq 0.5. \end{cases}$$

$$(22)$$

The noise control profile is uniform and is parameterized by as single parameter  $\gamma_n = A_n$ .

To avoid spurious marker build-up at the radial domain boundaries for long-time simulations with large  $\kappa$  under Dirichlet boundary conditions  $\phi(s = 0) = \phi(s = 1) = 0$ , all radial profiles are mirrored about s = 0.5, and periodic boundary conditions are imposed. Examples of such profiles, along with heat source and noise control operator profiles, are shown in Fig. 2. Henceforth, only profiles from the left half will be shown, that is, for  $s \in [0, 0.5]$ .

The GK-engine code works in units such that time and speeds are normalized to  $\Omega_c^{-1} = m_i/eB(s_0)$  and  $c_s = \sqrt{T_e(s_0)/m_i}$  (Z=1), representing the inverse ion cyclotron frequency and ion sound speed at  $s_0 = 0.25$ , respectively, which together give the ion sound Larmor radius  $\rho_s = c_s/\Omega_c$  for units of length. The magnetic and potential fields are normalized to  $B_z$ , and  $T_{e0}(s_0)/e$ , respectively. To simulate slab-ITG instabilities, we use the major and minor radii values of  $R_0 = 243.5\rho_s$  and  $a = 66.4\rho_s$ . The spatial domain is  $L_x = 2a$  for an *x*-periodic profile,  $L_y = \pi a$  and  $L_z = 2\pi R_0$ . The grid-cell number for  $\phi$  is  $(N_x, N_y, N_z) = (256, 512, 128)$ . The time step used here is  $\Delta t = 20\Omega_c^{-1} = 0.15L_x/c_s$ . The safety factor is given by q(s) = 1.25 $+12s^2$  for the half-domain  $s \in [0.0, 0.5]$  and mirrored in the other half-domain. All normalized parameters describing profiles are converted to physical units via a multiplication/division by  $L_x$ . The initial profile gradients used in this paper are  $\bar{\kappa}_n = 0.8$  and  $\bar{\kappa}_{TI} = \bar{\kappa}_{Te} = 8.0$ , with  $\bar{\kappa}_n = |d \log n(s_0)/ds|$ , so that  $\eta_i(s_0) = \bar{\kappa}_{Ti}/\bar{\kappa}_n = 10$ . This value corresponds to a peak value of  $T_i$  logarithmic gradient of  $|d \log T_i(s_0)/dx| = 4.0/a$ , that is,  $R_0/L_T = 14.6$ . The radial profile



**FIG. 2.** Symmetrized profiles used for this work. Blue: initial (solid) and typical final (dashed)  $T_{i}$ . Red: heat  $\gamma_{h}$  (solid) and noise control  $\gamma_{n}$  (dashed).

widths for  $n_0$  and  $T_{i0}$  are  $\bar{\Delta}_n = 0.3$  and  $\bar{\Delta}_{Ti} = 0.15$ , respectively, and  $T_{e0}(x) = T_{i0}(x, t = 0)$ . The maximum values  $A_h$  and  $A_n$  of the profiles for heat source  $\gamma_h$ , and noise control  $\gamma_m$  are at 100% and 3% of the maximum linear growth rate, respectively, which is found to be  $\gamma_{max} = 1.169 \times 10^{-3} \Omega_c = 0.155 c_s / L_x$  for these values of gradient, as shown in Fig. 3. The radial parameters of  $\gamma_h$  are  $(\bar{\delta}_c, \bar{\delta}_s) = (0.025, 0.025)$ . The control variate at initial time is taken to be the initial background  $f_0 = f_M(t = 0)$ .

For the toroidal, we chose to resolve modes in the range of  $[n_{\min}, n_{\max}] = [0, 32]$ , and poloidal modes *m* determined by the fieldaligned Fourier-filter  $|nq(s) + m| \leq \Delta m$ , with  $\Delta m = 5$ .<sup>24</sup> All simulations are initialized with  $f_{00} + \delta f(t = 0)$ . The initial background is taken to be  $f_{00} = f_{M0}$ , where  $f_{M0} = f_M(\vec{R}, v_{\parallel}, \mu, 0)$ .  $\delta f(t = 0)$  represents a density perturbation of amplitude  $10^{-4}$  and toroidal mode number n = 7 corresponding to the strongest growing linear mode. The poloidal modes initialized are those within the field-aligned filter at  $s = s_0$ , that is,  $|12q(s_0) + m| \leq 5$ .

Unless otherwise stated, all cases are run with  $N_p = 256$ M and adaptive background cases consider the relaxation rate  $\alpha_E = 1.92\gamma_{\text{max}}$ . The number of time steps after which the background temperature profile is adapted via Eq. (9) is set to  $N_{\alpha} = 10$  for all cases.

#### V. RESULTS

#### A. Marker convergence

Characteristic of all simulations is a turbulent burst in the initial phase of the simulation ( $0 < c_s t/L_x < 300$ ) represented by a spike in the radially averaged heat flux  $q_H$  and diffusitivity  $\chi_H$  expressed by

$$\chi_H(t) = \left\langle \left| \frac{q_H(x,t)}{n_{i0}(x) \frac{\partial T_i(x,t)}{\partial x}} \right| \right\rangle_x$$

 $\chi_H$  is represented in gyro-Bohm units, and  $\chi_{GB} = \rho_s^2 c_s / L_x$  with reference to the radial position of steepest initial profile gradient, that is,  $s = s_0$ . All radial averaging in this paper is done outside the heat source profile of Eq. (22), namely,  $s \in [0.025, 0.475] \cup [0.525, 0.975]$ .



**FIG. 3.** Linear studies: maximum growth rate of linear modes as a function of each toroidal mode number *n*, for normalized ion temperature logarithmic gradient  $a|d \log T_i/dx| = 4.0$  and  $(d \log T_i/dx)/(d \log n/dx) = 10$ . The poloidal mode number *m* is radially dependent and is determined by the Fourier filter.

Figure 4 shows how turbulence is quenched for the non-adaptive cases by increasing zonal flow shearing rate  $\omega_{E \times B}$ . The latter is estimated by

$$\omega_{E\times B} = \frac{1}{B} \frac{d^2 \phi_{00}}{dx^2},$$
(23)

where  $\phi_{mn}(x)$  is, in general, the Fourier component of the electrostatic field corresponding to poloidal (y) mode m and toroidal (z) mode n,  $\phi_{00}(x)$  thus being the zonal component. As can be seen in Fig. 4(b), the very significant rise in  $|\omega_{E\times B}|$  for non-adaptive simulations is dependent on the number of markers,  $N_p$ , and is thus of numerical origin. We note that even though the rise is reduced by increasing  $N_p$ , the simulation is far from having converged even for the largest  $N_p = 512M$  considered. We interpret the rise in  $|\omega_{E\times B}|$  as resulting from the statistical sampling noise accumulation in the zonal components,



**FIG. 4.** Time traces of the radially averaged absolute value of (a) heat diffusivity  $\chi_H$  and (b) zonal flow shearing rate  $\omega_{E \times B}$ , for various marker numbers, considering the non-adaptive and adaptive cases. The adaptive rate is set to  $\alpha_E = 1.92\gamma_{max}$  where applicable. A moving time-averaging window of half-width  $c_s t/L_x = 10$ , which is equivalent to  $\gamma_{max}t = 1.6$ , has been implemented.

which are not physically damped.<sup>25</sup> As expected, the accumulated noise is highest for the case with lowest  $N_p$ . Corresponding un-physically large  $\omega_{E\times B}$  levels lead to large-eddy shearing and reduced transport. The time of  $\chi_H$  collapse is correlated with  $|\omega_{E\times B}|$ , reaching a value comparable to  $3\gamma_{\max}L_x/c_s$ ; thus, the sequence of rises of  $\omega_{E\times B}$  in Fig. 4(b) corresponds to the sequence of falls of  $\chi_H$  in Fig. 4(a) for the three non-adaptive cases. On the other hand, for the adaptive case, the converged results show that  $\omega_{E\times B}$  increases at a much slower rate with time, resulting in a somewhat longer sustained flux. One notes that these converged fluxes nonetheless ultimately drop to zero as seen in Fig. 4(a).

To further confirm that low marker numbers lead to an increase in zonal  $\omega_{E\times B}$  levels due to noise accumulation, Fig. 5(a) shows the radially averaged absolute value of  $\omega_{E \times B}$  at the initial time t = 0 against marker number Np. All simulations are initialized with a density perturbation defined as including only  $n \neq 0$  Fourier modes. Despite that, due to the finite and random marker number representation of  $\delta f$ , there is a resulting spurious finite zonal,  $(m, n) = (0, 0), \omega_{E \times B}$ profile, whose amplitude increases with decreasing number of markers as  $\sim 1/\sqrt{N_p}$ , as expected due to statistical sampling error. The magnitude of the corresponding zonal flow shearing rate  $\omega_{E\times B}$  is then further increased at every time step. Thus, lower marker numbers lead to larger noise accumulation in  $\omega_{E \times B}$  with time, which leads to Fig. 5(b) for end-time values of  $\omega_{E \times B}$ . Assuming linear increment, Fig. 5 indicates that the rate of increase in  $\omega_{E \times B}$  is  $d\omega_{E \times B}/dt \approx 2.12$  $\times 10^{-3} c_s^2 / L_r^2$  for  $N_p = 256$  M. For non-adaptive cases, the general trend of lower zonal  $E \times B$  shearing with increasing  $N_p$  is apparent. The endtime  $\omega_{E\times B}$  value is expected to plateau at higher  $N_p$  values, but this limit is not reached for the maximum marker number considered, Np = 512M. This converged value would represent the zonal  $\omega_{E\times B}$ derived from the physics of the problem, and not the result of the accumulation of noise. On the other hand, the adaptive cases show much lower and similar end-time  $\omega_{E\times B}$  values throughout all  $N_p$  values considered in the different simulations.

The potential field  $\phi$  of Eq. (11) is solved by first projecting it onto the B-spline basis  $\Lambda_{ijk}(\vec{r}) = \Lambda_i(x)\Lambda_j(y)\Lambda_k(z)$  followed by taking the Discrete Fourier transform of spline indices in the *y* and *z* directions, thus representing the discretized equation in terms of poloidal *m* and toroidal *n* mode numbers together with the spline index *i* related to the remaining radial dimension *x*.<sup>26</sup> By gyrokinetic ordering arguments,<sup>24</sup> one can apply on the projected right-hand side of Eq. (11) a centered band filter  $\mathscr{F}_1$  in (m, n)-space keeping only keeping modes satisfying  $|m + nq(x)| < \Delta m = \text{constant}$ , as the physically relevant, that is,  $k_{\parallel}\rho_{th} \ll 1$ , modes, which are nearly field aligned and constitute the signal. Here,  $k_{\parallel} = 2\pi (m + nq)/(L_z q)$  is the wavevector component along  $\vec{B}$ . The region  $\mathscr{F}_2$  consists of two bands, each on either side of  $\mathscr{F}_1$ , is defined to represent physically strongly damped modes. Any finite levels of modes in  $\mathscr{F}_2$  are thus assumed to provide a measure of the noise level. Estimates of the signal and noise levels are thus, respectively, provided by

$$\text{signal} = \frac{\sum_{i} \sum_{(m,n) \in \mathscr{F}_{1}} |b_{i}^{(m,n)}|^{2}}{\sum_{i} \sum_{(m,n) \in \mathscr{F}_{1}} 1}, \quad \text{noise} = \frac{\sum_{i} \sum_{(m,n) \in \mathscr{F}_{2}} |b_{i}^{(m,n)}|^{2}}{\sum_{i} \sum_{(m,n) \in \mathscr{F}_{2}} 1}.$$
(24)

Here,  $\Sigma_i$  sums over all radial indices of spline amplitude  $b_i^{(m,n)}$  of the right-hand side. The latter is expressed by

$$egin{aligned} &b_i^{(m,n)} = \sum_{j=0}^{N_y-1} \sum_{k=0}^{N_y-1} \exp\left[-2\pi \mathrm{i}\left(rac{mj}{N_y} + rac{nk}{N_z}
ight)
ight] \ & imes \left\{\int \mathrm{d}^3R\mathrm{d}lpha \mathrm{d} 
u_{\parallel} \mathrm{d} \mu rac{B_{\parallel}^{\star}}{m_i} \Lambda_{ijk}ig[ec{R} + ec{
ho}_L(\mu, lpha)ig] \ & imes ig[f_0(ec{R}, 
u_{\parallel}, \mu, t) - f_0(ec{R}, 
u_{\parallel}, \mu, 0)ig] \ & imes \sum_p w_p \int \mathrm{d}lpha \Lambda_{ijk}ig[ec{R}_p + ec{
ho}_L(\mu_p, lpha)ig] 
ight\}. \end{aligned}$$

It should be noted that what we call "signal" here also includes the discretization noise present within the filter.<sup>27</sup> Nonetheless, these measures provide a practical estimate of the signal-to-noise ratio (SNR).

From Fig. 6(a), non-adaptive cases start from high SNR values and gradually drop to their respective lowest point after the initial burst  $c_s t/L_x \sim 300$ .  $N_p$  is reflected in the maximum of SNR values for each case, which latter seem to scale as  $1/N_p$ . The adaptive cases follow a similar trend, but do not fall as low. From past works,<sup>22,27</sup> the ruleof-thumb SNR threshold of 10 is a value above which results can be deemed reliable. Therefore, we can see that only the adaptive cases

**FIG. 5.** Radial averaged absolute value of the zonal flow shearing rate  $\omega_{E\times B}$  at (a) initial time  $c_{\rm s}t/L_{\rm x}=0$  and (b) end-time  $c_{\rm s}t/L_{\rm x}=753$ , as a function of the inverse square root of marker number  $N_p$ . The adaptive case (orange) adapts at a rate  $\alpha_E=1.92\gamma_{\rm max}$ . All simulations are initialized with perturbations with toroidal mode  $n\neq 0$ .



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**FIG. 6.** Signal-to-noise ratio (SNR) time traces for signal (a) including and (b) excluding, the (m, n) = (0, 0) mode, for increasing marker number  $N_{\rho}$ , and considering both the non-adaptive (solid line) and adaptive (dashed line) cases.

with  $N_p = 256$  M, 512 M meet this criterion throughout the whole simulation. All SNR values eventually rise with time, with the non-adaptive case at  $N_p = 128$  M rising the quickest. This reflects the noise accumulation in the physically undamped zonal component. Indeed, by subtracting the zonal component from the signal, Fig. 6(b) shows that the non-adaptive case with  $N_p = 128$  M gives the lowest SNR value throughout the simulation. Thus, for this set of parameters, only the results from the adaptive case with  $N_p = 256$  M or  $N_p = 512$  M may be deemed reliable.

Figures 7 and 8 show the f.s.a. profiles at the end of the simulations for the zonal flow shearing rate  $\omega_{E\times B}$ , the ion temperature  $\langle T_i \rangle$ relative deviation  $(\langle T_i \rangle - T_{i0})/T_{i0}$ , and its logarithmic gradient for different total number Np of markers, under the non-adaptive and adaptive cases, respectively. It should be noted that the maximum relative deviation value for  $T_i$  of around 60% in Fig. 7(a) for the nonadaptive cases challenges the  $\delta f$  assumption of  $|\delta f|/|f_0| \ll 1$ . For the adaptive case in Fig. 8(a) however, the relative deviation of  $\langle T_i \rangle$  from the adapted background temperature  $T_{i0}(t)$ , which remains low at all times, qualifies. One notes that the adaptive cases in fact resulted in f.s.a.  $T_i$  profiles with a larger deviation of 100%, from its initial state, as shown in Fig. 8(b). This shows that the adaptive scheme appears to allow for simulations with more accurate profile evolution in the case of large deviations, not afforded by the standard scheme. One notes also the development of strong  $T_i$  gradients at s = 0.05, just outside the heat source for the non-adaptive case (see Fig. 7). This is suspected to be related to spurious marker accumulation by error in drift calculation, whose magnitude reduces with increasing  $N_p$ . Under the adaptive scheme, this problem does not occur.

#### B. Adaptive control variate and noise control

Tentatively, two mechanisms contribute to the improvement of SNR with the adaptive scheme: (a) the adapted  $f_0(t)$  as a good control variate; (b) the noise control operator  $S_n$  of the non-adapted scheme, which tends to bring back f toward the initial distribution  $f_{00}$ , whereas in the adapted scheme it tends to relax f toward the time-evolved  $f_0$ , which is closer to the time-averaged f, especially at late times. To study the relative importance of the adaptive scheme and the noise control, we varied in this section the control variate  $f_0$ , both in the framework of the adaptive delta-f scheme, Eq. (7), and in the reference function  $f_n$  of the noise control operator, that is,



**FIG. 7.** F.s.a. profiles at quasi-steady state averaged over a time interval of  $c_s t/L_x \in [1030, 1130]$  for various marker numbers  $N_p$  under the non-adaptive scheme for the ion temperature (a) relative deviation with respect to background and its (b) logarithmic gradient, and the (c) zonal flow shearing rate.



**FIG. 8.** F.s.a. profiles at quasi-steady state averaged over a time interval of  $c_s t/L_x \in [1030, 1130]$  for various marker numbers  $N_p$  under the adaptive scheme with adaptive rate  $\alpha_E = 1.92\gamma_{max}$  for the ion temperature (a) relative deviation with respect to adapted background, (b) relative deviation with respect to background at initial time t=0, its (c) logarithmic gradient, and the (d) zonal flow shearing rate.

$$S_n = -\gamma_n (f - f_n).$$

All simulations begin with  $f = f_{M0} + \delta f(t = 0)$ , where  $\delta f(t = 0)$  represents a small perturbation and the control variate  $f_0$  is taken to be  $f_M$  [see Eq. (8)]. By choosing different  $f_0$  and  $f_m$ , four different adaptive scenarios can be constructed, depending on whether the adaptive scheme is used [ $f_0 = f_{M0}$  or  $f_0 = f_M(t)$ ] and whether adaptive noise control scheme is used [ $f_n = f_{M0}$  or  $f_n = f_M(t)$ ]. Below, except for scenario 3,  $f_M(t)$  adapts via  $T_{i0}$  from Eq. (8) according to Eq. (9).

- non-adaptive δf scheme, non-adaptive f<sub>n</sub>, labeled (no, no)
   (f<sub>0</sub>, f<sub>n</sub>) = (f<sub>M0</sub>, f<sub>M0</sub>).
- 2. adaptive  $\delta f$  scheme, non-adaptive  $f_n$ , labeled (yes, no) •  $(f_0, f_n) = (f_M(t), f_{M0}).$
- 3. non-adaptive  $\delta f$  scheme, adaptive  $f_n$ , labeled (no, yes)
- $(f_0, f_n) = (f_{M0}, f_M(t)),$
- $f_n = f_0(t)$  is adaptive according to

$$\frac{\partial}{\partial t} \left( \frac{3}{2} n_{i0} T_{i0} \right) = \alpha_E \left\langle \int d\nu_{\parallel} d\mu \frac{2\pi B_{\parallel}^{\star}}{m_i} \left[ \delta f - (f_M(t) - f_{M0}) \right] \right\rangle, \quad (25)$$

- the adaptive scheme is run in the background to update  $f_n = f_M(t)$ , but the control variate  $f_0 = f_{M0}$  remains time-independent.
- 4. adaptive  $\delta f$  scheme, adaptive  $f_n$  labeled (yes, yes)
  - $(f_0, f_n) = (f_M(t), f_M(t)).$

Viewing the adaptive scheme as essentially a means to reduce noise, considering the different scenarios described allows one to determine which strategy is the most effective in this respect. Figure 9 shows the effect of different adaptive scenarios on the simulation results. The adaptation of  $f_0$  and/or  $f_n$  for the different scenarios is done at the same rate  $\alpha_E$ . It can be seen that the full adaptive scheme with adaptive  $f_0$  and  $f_n$  [scenario (yes, yes)], implying weight transfer from  $\delta f$  to  $f_0$  of Eq. (20) and noise control only on the fluctuating part  $\delta f$ , respectively, is necessary for effective noise control, as indicated by a reasonably high SNR value and a zonal flow shearing rate  $\omega_{E\times B}$  value that does not increase indefinitely. For scenario (yes, no) with only the adaptive  $f_0$ , noise control is effective only at an early stage when f is close to  $f_{M0}$ . As the former deviates away from the latter,  $S_n$  acts as a weak source, thus enlarging the  $\delta f$  component. The larger the portion of f that is represented by markers, the more noise accumulates. The weak improvement of scenario (no, yes), which is the standard delta-f scheme with a time-dependent reference function  $f_n = f_M(t)$ , indicates that the improvement from weight transfer from  $\delta f$  to  $f_0$  far outweights an adaptive  $S_n$ .

Noise can also be approached from the standard deviation of the f.s.a. weights  $\sigma_{w_2}$  as shown in Fig. 10. Based on this measure, the full adaptive scheme (yes, yes) once again gives the best results, with low values of  $\sigma_w$  right after the burst at around  $c_s t/L_x = 150$ . One can see that  $\sigma_w$  as already plateaued for the non-adaptive case (no, no), whereas for the case (yes, no), the  $S_n$  acting as weak source continues to relax the distribution toward that at initial time. This is proved to be the case when see that a lower  $\alpha_E$  value gives a smaller yet increasing  $\sigma_w$  value. Finally, the scenario (no, yes) with an adaptive noise control is able to continuously decrease  $\sigma_w$  values, but these values remain high after the burst, which may affect the results at late times.

A note on the inclusion of the  $f_0(t) - f_0(t = 0)$  term in Eq. (11) is in order. While cases studied in this paper do not involve a timedependent background density, with reference to the full adaptive scheme [scenario (yes, yes)] described above, the exclusion of this extra term leads to a lower heat diffusivity and a 17% increase in the zonal flow shearing rate at quasi-steady state, which in turn resulted in a lower final ion temperature deviation. Nonetheless, similar improvement in SNR and local f.s.a. weight standard deviation has been observed.

#### C. Noise control strength and adaptive rate variations

The purpose of the conservative noise control is to reduce the weight standard deviation at the expense of introducing numerical diffusion, thus affecting the validity of the simulation by adding artificial damping on the main instability drive and zonal flows. From Figs. 11(a) and 11(b), it can be seen that at a larger  $\gamma_n$  value, both  $\chi_H$  and  $\omega_{E\times B}$  values are lower. Therefore, its amplitude  $\gamma_n$  should be adjusted just high enough to maintain a good SNR value throughout the simulation, taken in this work to be 10. Figure 11(c) shows that  $\gamma_n = 0.03\gamma_{\text{max}}$  for the adaptive case is just enough, and it is this value of  $\gamma_n$  that is used in all other sections of the paper. For the non-adaptive case, it is seen that a high  $\gamma_n$  value only postpones the eventual decrease in SNR, implying that noise control alone is insufficient to prevent simulations being drowned in noise. Finally, the reduced weight standard deviation is shown in Fig. 11(d). It is shown that  $S_n$  alone is insufficient to control noise to acceptable levels, while the

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**FIG. 9.** Diagnostics under four different adaptive scenarios (see description in text) for the radially averaged absolute (a) heat diffusivity  $\chi_H$  and (b) zonal flow shearing rate  $\omega_{E \times B}$ , and the signal-to-noise (SNR) ratio with signal (c) including and (d) excluding the (m, n) = (0, 0) mode. Marker number set to  $N_p = 256$ M, and adaptive rate to  $\alpha_E = 1.92\gamma_{max}$  where applicable. A moving time-averaging window of half-width  $c_s t/L_x = 10$  has been implemented.



**FIG. 10.** Local f.s.a. weight standard deviation  $\sigma_w$  through time under four different adaptive scenarios (see description in text), illustrated with the cases of (a) (no, no), (b) (no, yes) with  $\alpha_E = 1.92\gamma_{\text{max}}$ , (c) (yes, no) with  $\alpha_E = 1.92\gamma_{\text{max}}$ , (d) (yes, no) with  $\alpha_E = 0.12\gamma_{\text{max}}$ , and (e) (yes, yes) with  $\alpha_E = 1.92\gamma_{\text{max}}$ .  $\sigma_w$  is defined by  $\sqrt{\sum_{p \in i} w_p^2 / N_i - (\sum_{p \in i} w_p / N_i)^2}$ , with  $N_i = N_p / N_x$  the average number of markers of the *i*th radial bin, taken to be uniform for all bins. Marker number set to  $N_p = 256$ M. All figures share the same color scale.



**FIG. 11.** Diagnostics for various noise control strength  $\gamma_n$  considering both the non-adaptive and adaptive cases, for the radially averaged absolute (a) heat diffusivity  $\chi_H$  and (b) zonal flow shearing rate  $\omega_{E \times B}$ , and the (c) signal-to-noise (SNR) ratio with signal excluding the (m, n) = (0, 0) mode, and the (d) sum of f.s.a. weight standard deviation. Marker number set to  $N_p = 256$  M. The sum of f.s.a. weight standard deviation is calculated by summing the standard deviations of f.s.a. weights from each radial bin, and multiplying by the sum by  $L_x/N_x$ .

adaptive scheme is able to do so even in the presence of minimal noise control relaxation rate  $\gamma_n$ .

Turning now to the choice of the adaptive rate  $\alpha_E$ , from Eqs. (9)

second velocity moment of the f.s.a.  $\delta f$  to the control variate, in this case,  $f_0 = f_M(t)$ . Figure 12 shows that the maximum relative deviation of  $T_i$  from its time evolved adapted profile  $T_{i0}(x, t)$  is lower with higher values of  $\alpha_E$ . Also, the decrease in the relative deviation after the



FIG. 12. Time evolution of f.s.a. ion temperature relative deviation from its time-evolved adapted  $T_{i0}(t)$ ,  $(\langle T_i \rangle(\mathbf{x}, t) - T_{i0}(\mathbf{x}, t))/T_{i0}(t)$  under various adaptive rates  $\alpha_{E}$ . Marker number set to  $N_p = 256$  M. (a)  $\alpha_E = 0.00\gamma_{max}$  (b)  $\alpha_E = 0.03\gamma_{max}$  (c)  $\alpha_E = 0.12\gamma_{max}$  (d)  $\alpha_E = 0.48\gamma_{max}$  (e)  $\alpha_E = 1.92\gamma_{max}$ .

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initial burst is faster with increasing  $\alpha_E$ . More specifically, Figs. 13(a) and 13(b) show that for  $\alpha_E = 0.12\gamma_{\text{max}}$  or higher, the simulation under given parameters is sufficient in terms of low zonal flow shearing rate  $\omega_{E\times B}$  and high enough SNR values, respectively. Therefore, under the parameters studied in this paper, any  $\alpha_E$  value satisfying  $\alpha_E > 0.12\gamma_{\text{max}}$  and Eq. (19) gives results with the lowest noise accumulation.

#### D. Adjusting the f.s.a. potential term

In sheared-slab geometry with adiabatic electrons on the magnetic surfaces, ITG turbulence is strongly suppressed by zonal flows, resulting in a quasi-steady state with relatively low heat fluxes. In a real tokamak, much stronger heat fluxes and large relative fluctuation amplitudes are present in the plasma edge. In order to emulate such a



**FIG. 13.** Time traces of the (a) radially averaged absolute zonal shearing rate  $\omega_{E\times B}$  and the (b) signal-to-noise ratio (SNR) with signal excluding the (m, n) = (0, 0) mode, with varying adaptation rates  $\alpha_{E}$ . Marker number set to  $N_{p} = 256$ M.

situation but staying in slab geometry, the f.s.a. potential term  $\langle \phi \rangle$  of the adiabatic electron response of Eq. (11) is tuned by defining a multiplicative parameter  $\lambda$ ,

$$\begin{aligned} \frac{en_0}{T_e}(\phi - \lambda\langle\phi\rangle) &- \nabla_{\perp} \cdot \left(\frac{m_i n_0}{eB^2} \nabla_{\perp}\phi\right) \\ &= \int \mathrm{d}^3 R \mathrm{d}\alpha \mathrm{d}\nu_{\parallel} \mathrm{d}\mu \frac{B_{\parallel}^*}{m_i} \delta\left[\vec{r} - (\vec{R} + \vec{\rho}_L(\mu, \alpha))\right] \\ &\times \left[f_0(\vec{R}, \nu_{\parallel}, \mu, t) - f_0(\vec{R}, \nu_{\parallel}, \mu, 0) + \delta f\right]. \end{aligned}$$
(26)

With  $\lambda = 0.00$ ,<sup>28,29</sup> the electrons respond adiabatically in all directions, that is, not only in the magnetic surface, but also radially. This results in much lower  $E \times B$  flows and thus higher turbulent heat fluxes.

Figure 14 shows the effect of tuning  $\lambda$  on the heat diffusitivity  $\chi_H$ and zonal shearing rate  $\omega_{E\times B}$ . One can see that fluxes are sustained longer and higher due to a lower zonal flow shearing rate  $\omega_{E\times B}$  from a greater attenuation of  $\langle \phi \rangle$ . This trend also exists for the adaptive cases, though  $\omega_{E\times B}$  levels there are generally low as compared to the nonadaptive cases, see Fig. 14(d). From Fig. 14(b) for the adaptive cases, the value of  $\lambda = 0.95$  seems to be just sufficient to sustain the flux. Therefore, looking at the case of  $\lambda = 0.95$  specifically, Fig. 15 shows that the result trend is similar to that of Fig. 4, albeit with lower levels of  $\omega_{E\times B}$ . Under this tuning, the non-adaptive cases (continuous lines) seem to evolve toward low  $\chi_H$  values at long times, whereas the adaptive cases (dashed lines) are maintained at a higher  $\chi_H$  value as compared to Fig. 4(a). The adaptive cases seem to have converged already with  $N_p = 128M$  markers, whereas the non-adaptive case is still subject to collapse even with  $N_p = 512M$  markers.

Figure 16 shows that  $\lambda$  only affects the SNR values of the nonadaptive cases. Taking the standard non-adaptive case of  $\lambda = 1.00$  as reference, the effect of higher attenuation of  $\langle \phi \rangle$  only delays the eventual collapse of SNR values for each case, except for the case of complete  $\langle \phi \rangle$  suppression, in which high SNR value and sustained flux [see Fig. 14(a)] are achieved. For a fixed value of  $\lambda = 0.95$ , in addition to the delayed fall of SNR values for the non-adaptive cases, Fig. 15(b) reflects the SNR value proportional to  $N_p$  relation, as was already shown in Fig. 6(b). This convergence, instead of  $\sqrt{N_p}$ , is a result of taking the noise as a quadratic measure, see Eq. (24).

We now consider simulations with  $\lambda = 0.95$ , which demonstrated high sustained flux for the adaptive cases for the following analysis. Figure 17 shows that the fixed-time non-zonal  $T_i$  relative deviation across each magnetic surface increases toward the low-end of the  $\langle T_i \rangle$  profile at quasi-steady state. The case with  $\lambda = 0.95$  has relative deviation at least twice that of  $\lambda = 1.00$ , indicating the expected higher levels of turbulence. Since the adaptive scheme implemented in this work adapts its control variate  $T_{i0}$  by its f.s.a. values as shown in Eq. (9), it is not expected to further improve noise reduction for edge plasma simulations involving relative non-zonal deviation much higher than 25%. However, a similar adaptive scheme could still be used for noise control, providing that  $f_0$  is now a function of all spatial dimensions. This would allow for a transfer of non-zonal components of  $\delta f$  to  $f_0$ , though with increased noise levels due to lower  $N_p$  per spatial bin when implementing Eq. (9).

Under the same simulation parameters, Fig. 18 further shows that the relative fluctuation of  $T_i$  evaluated in an end-time window is



**FIG. 14.** Time traces of radial averaged absolute value of heat diffusivity  $\chi_{H_i}$  (a) and (b), and zonal flow shearing rate  $\omega_{E \times B}$ , (c) and (d), for the non-adaptive and adaptive cases, respectively, under various tuning parameter  $\lambda$  [see Eq. (26)]. The adaptive rate is set to  $\alpha_E = 1.92\gamma_{max}$ . A moving time-averaging window of half-width  $c_s t/L_x = 10$  has been implemented. Total number of markers is set to  $N_p = 256$  M.

derived mostly from its non-zonal variations. There, the curves are calculated as follows. Let the *j*th flux tube on flux surface *x* occupy the space

$$(y,z)_j \in \left[ egin{array}{c} B_y(x)z \ B_z \le y - j\Delta y < egin{array}{c} B_y(x)z \ B_z \ \end{array} 
ight] + \Delta y \ 0 \le z < L_z \end{array} 
ight].$$

Visually, these  $N_y$  flux tubes are the straight blue lines of Fig. 1 of y-width  $\Delta y$ , spanning each x = constant plane. The *j*-th flux tube gives the value  $T_i(x, t; j)$ . It is assumed that the plasma reaches thermal equilibrium instantly along the flux tube. Finally, let  $\langle \cdot \rangle_t$  be the averaging in time for  $t \in [t_1, t_2]$ , and  $\langle \cdot \rangle_{f.t.}$  be the flux-tube average on the flux surface *x*, that is,

$$\langle T_i(x,t;j) \rangle_{f.t.} = \frac{1}{N_y} \sum_{j=1}^{N_y} T_i(x,t;j)$$

Then, referring to Fig. 18,

black : 
$$\frac{\sqrt{\langle\langle T_i\rangle^2(x,t)\rangle_t - \langle\langle T_i\rangle(x,t)\rangle_t^2}}{\langle\langle T_i\rangle(x,t)\rangle_t}$$
orange : 
$$\frac{\sqrt{\langle\langle T_i^2(x,t;j)\rangle_{f.t.}\rangle_t - \langle\langle T_i(x,t;j)\rangle_{f.t.}\rangle_t^2}}{\langle\langle T_i(x,t;j)\rangle_{f.t.}\rangle_t}.$$
(27)

For each fixed  $\lambda$ , the relative fluctuation when non-zonal variations are included gives a value at least twice as high as that of the case when only the f.s.a. values are considered. Consistent with Fig. 17, lower  $\lambda$  value gives higher fluctuation levels. These results summarily show that non-zonal fluctuations are dominant at quasi-steady state under current simulation parameters.

In conclusion, simulations using the adaptive scheme are shown to be better than the non-adaptive ones under all scenarios considered.



**FIG. 15.** Time traces of the (a) radially averaged absolute zonal flow shearing rate  $\omega_{E\times B}$ , and the (b) signal-to-noise ratio (SNR) with signal excluding the (m, n) = (0, 0) mode. The tuning parameter is set to  $\lambda = 0.95$ , and the adaptive rate is set to  $\alpha_E = 1.92\gamma_{max}$  where applicable. A moving time-averaging window of halfwidth  $c_s t/L_x = 10$  has been implemented.



**FIG. 16.** Signal-to-noise ratio (SNR) time traces with signal excluding the (m, n) = (0, 0) mode, under various tuning parameter  $\lambda$  [see Eq. (26)] considering the non-adaptive and the adaptive cases. Marker number set to  $N_p = 256$ M, and adaptive rate to  $\alpha_E = 1.92\gamma_{max}$  where applicable.

To further test the advantage gained from the adaptive scheme under high fluctuation level, scenarios would require simulating ITG instabilities in toroidal geometry, which could be done, for example, in the code ORB5.<sup>30</sup> There, toroidal effects naturally results in higher fluxes and fluctuation levels, while zonal flows are an important factor determining the turbulent flux levels.

#### VI. CONCLUSION

In this work, the advantage gained using a simple adaptive control variate for the  $\delta f$  scheme has been demonstrated in cases with high  $T_i$  gradients and simple physics in sheared-slab geometry. The necessary implementation of the boundary conditions and a stationary heat source has been done to further ensure simulations reach quasisteady state in reasonable integration time. The mechanism of the adaptive scheme has been described in detail. Namely, the adaptation of  $T_i$  of the f.s.a. Maxwellian control variate  $f_0 = f_M$  via a relaxation equation, through which a fraction the ion kinetic energy density derived from the marker represented  $\delta f_i$  is periodically transfered to  $f_0$ .

For the cases considered, the adaptive scheme has shown to reduce the ion temperature relative deviation with increasing adaptive rate. Maximum relative deviation of 1% has been achieved from 100%



**FIG. 17.** Time snapshot at  $c_s t/L_x = 2259$  with tuning parameter  $\lambda$  at (a) 1.00 and (b) 0.95, of the ion temperature  $T_i$  relative non-zonal deviation on each magnetic surface, expressed by  $(\delta T_i - \langle \delta T_i \rangle)/\langle T_i \rangle$ , where  $T_i = T_{i0} + \delta T_i$ , integrated over the toroidal *z* direction.  $s_y$  is the normalized poloidal *y* axis. Both quasi-steady-state cases have adaptive rate and marker number set to  $\alpha_E = 1.92\gamma_{\rm max}$  and  $N_p = 256$ M, respectively.

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**FIG. 18.** Relative fluctuation averaged over  $c_s t/L_x \in [1807, 2259]$  of ion temperature  $T_i$  and its f.s.a. profile  $\langle T_i \rangle$ , as measured by its standard deviation over mean, see Eq. (27), for the cases of  $\lambda = 1.00, 0.95$  with adaptive rate  $\alpha_E = 1.92\gamma_{\text{max}}$  and marker number  $N_p = 256$ M.

of the non-adaptive case. Due to spurious increase in the zonal flow shear with time, all non-adaptive cases show an eventual collapse of the heat flux. Under the adaptive scheme, not only is quasi-steady state achieved with non-collapsing heat fluxes, these fluxes have also been achieved using marker numbers as low as 1/4 of that required with the non-adaptive one, allowing for longer unquenched turbulence resulting in higher ion temperature deviation from its initial state. The scheme is further shown to be effective in reducing noise accumulation in the physically undamped zonal flow via the measure of  $\omega_{E\times B}$ . Such noise accumulation is shown to be the result of marker sampling. SNR values of adaptive simulations remain high for long integration times. In contrast, the eventual drop of SNR for the non-adaptive scheme is only postponed by increasing  $N_p$ .

We have then investigated further to determine whether conservative noise control alone would suffice to produce a similar noise reduction advantage. Via a systematic separation of adaptation and noise control, it is shown that the scheme with an adaptive control variate  $f_0 = f_M(t)$ , coupled with a noise control operator  $S_n$  which relaxes f to the same  $f_0$ , gives the best results. Therefore, the former is proved to be more important than the latter in noise control. Moreover, it is shown that further increase in the strength of  $S_n$  not only unphysically damps zonal flows at early times but also is only able to delay the latter's eventual indefinite rise due to noise accumulation. The adaptation of  $f_0$  is therefore shown to be necessary, even with an adaptation rate as low as  $\alpha_E = 0.12\gamma_{max}$ .

To mimic prolonged fluxes and high fluctuation levels not afforded by slab-ITG, the  $\langle \phi \rangle$  term of the adiabatic electron response in the quasi-neutrality equation is attenuated. Such a measure is done to better simulate edge-plasma conditions, despite testing the adaptive scheme in sheared-slab geometry. This work has shown that for slightly attenuated  $\langle \phi \rangle$ , the adaptive scheme exhibited improved noise control as before, for relative fluctuation in  $T_i$  as high as 20%. Such fluctuations are shown to be non-zonal. Therefore, it hints to a more sophisticated  $f_0$ , which extends beyond a f.s.a. function that could prove to be useful for better noise control. Despite that, the adaptive scheme still gives SNR values orders of magnitude higher than that of the non-adaptive scheme, further increasing the credibility of simulated results. To further test the merits of the adaptive scheme, its implementation in a code, which better simulates the plasma edge in toroidal geometry, is required.

The obvious generalization of this adaptive scheme to include a time-dependent background density profile is left for future work. This will involve a similar relaxation equation to that of Eq. (9), with its own relaxation rate parameter  $\alpha_n$ . However, recalculation of the left-hand side of the quasi-neutrality equation, Eq. (5), should also be performed at periodic time intervals to account for the time dependence of the background density. Such an adaptive scheme involving a control variate with both time-dependent background density and temperature profiles could be useful even in the core, for example, in simulating kinetic ballooning, tearing, and internal kink modes. In the presence of fast ions, a time-dependent background density could be useful when simulating Alfvén or energetic particle modes.

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### AUTHOR DECLARATIONS Conflict of Interest

The authors have no conflicts to disclose.

#### **Author Contributions**

Moahan Murugappan: Data curation (lead); Formal analysis (lead); Investigation (lead); Methodology (equal); Software (lead); Validation (lead); Visualization (lead); Writing – original draft (lead). Laurent Villard: Conceptualization (equal); Formal analysis (supporting); Methodology (equal); Supervision (equal); Writing – review & editing (equal). Stephan Hans Rudolf Brunner: Conceptualization (equal); Formal analysis (supporting); Methodology (equal); Supervision (equal); Writing – review & editing (equal). Ben Fynney McMillan: Conceptualization (supporting). Alberto Bottino: Conceptualization (supporting).

#### DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

#### APPENDIX: QUADRATURE POINT CONVERGENCE FOR R.H.S. OF QUASI-NEUTRALITY EQUATION

The aim of this section is to determine the number of quadrature points sufficient to integrate the r.h.s. of Eq. (11), formally written as

$$\delta n_{gd} = \frac{1}{2\pi} \int d^3 R d^3 \nu d\alpha \delta \left[ \vec{R} + \vec{\rho}_L - \vec{r} \right] \delta f(\vec{R}, \nu_{\parallel}, \mu).$$
(A1)

To proceed, we introduce a simple but non-trivial form of  $\delta f$ , so that Eq. (A1) can be solved analytically, namely,

$$\delta f = \frac{\cos{(\xi x)}}{(2\pi T_i/m)^{3/2}} \exp\left[-\frac{mv_{\parallel}^2/2 + \mu B}{T_i}\right], \\ = \frac{\cos{(\xi x)}}{(2\pi)^{3/2}v_{th}^3} \exp\left[-\frac{v_{\parallel}^2 + v_{\perp}^2}{2v_{th}^2}\right],$$
(A2)

with  $v_{th} = \sqrt{T_i/m_i}$  the local thermal velocity,  $\mu = mv_{\perp}^2/2B$ the magnetic moment, and  $\xi$  a constant. To simplify further, we shall assume constant  $T_i$  and B. Furthermore, given that  $B_{\parallel}^*$  $= B[1 + m_i B'_y(x) B_z v_{\parallel}/(eB^3)]$  and all velocity variables  $v_{\parallel}$  and  $v_{\perp}$  are contained in  $\delta f$  and that  $\delta f$  is an even function of  $v_{\parallel}$ , the velocity integration effectively becomes

$$\delta f d^{3} v = \delta f \frac{2\pi B_{\parallel}}{m_{i}} dv_{\parallel} d\mu,$$

$$= \delta f \frac{2\pi B}{m_{i}} dv_{\parallel} d\mu,$$

$$= \delta f 2\pi v_{\perp} dv_{\perp} dv_{\parallel}.$$
(A3)

Inserting Eq. (A2) into Eq. (A1) gives

$$\delta n_{gd}(\vec{r}) = \operatorname{Re}\{I(x)\},\$$

with

$$\begin{split} I(x) &= \int d\alpha \int_{-\infty}^{\infty} \frac{dv_{\parallel} e^{-\frac{v_{\parallel}^2}{2v_{th}^2}}}{\sqrt{2\pi v_{th}^2}} \times \int_{0}^{\infty} \frac{dv_{\perp} v_{\perp} e^{-\frac{v_{\perp}^2}{2v_{th}^2}}}{2\pi v_{th}^2} \exp\left[i\xi(x+\rho_L \sin\alpha)\right], \\ &= e^{i\zeta x} \int d\alpha \frac{1}{2\pi} \int_{0}^{\infty} \frac{dv_{\perp}}{v_{th}} \frac{v_{\perp}}{v_{th}} e^{-\frac{v_{\perp}^2}{2v_{th}^2}} \exp\left(i\xi\rho_{th}\frac{v_{\perp}}{v_{th}}\sin\alpha\right), \\ &= e^{i\zeta x} \int_{0}^{\infty} \frac{dv_{\perp}}{v_{th}} J_0\left(\zeta\rho_{th}\frac{v_{\perp}}{v_{th}}\right) \frac{v_{\perp}}{v_{th}} e^{-\frac{v_{\perp}^2}{2v_{th}^2}}, \\ &= \exp\left[i\xi x - \frac{(\xi\rho_{th})^2}{2}\right], \end{split}$$

where  $\rho_{th} = v_{th}/\Omega$  is the thermal Larmor radius and  $J_0$  is the zeroth-order Bessel function of the first kind.

The evaluation of the field  $\phi$ , which is represented by a B-spline expansion, involves the contraction of the r.h.s. of Eq. (11) with a B-spline element of order p,  $\Lambda^p(\vec{r} - \vec{r}_{ijk}) = \Lambda^p(x - x_i)$  $\Lambda^p(y - y_i)\Lambda^p(z - z_k)$ . Here, the zeroth-order B-spline is defined as

$$\Lambda^0(x) = \begin{cases} 1 & |x| < \Delta x/2, \\ 0 & \text{else}, \end{cases}$$

so that  $\int dx \Lambda^0(x) = \Delta x$ , and the higher order elements by the recurrence relation

$$\Lambda^p(x) = rac{1}{\Delta x} \Lambda^{p-1}(x) * \Lambda^0(x) \qquad p \ge 1,$$

where  $\Delta x$  is the grid size of equidistant points along dimension *x*, and \* stands for convolution. Therefore, we conduct a convergence analysis on the real part of the expression

$$\int d^{3}r \Lambda^{p}(\vec{r} - \vec{r}_{ijk}) \delta n_{gd}(x)$$
  
=  $\Delta y \Delta z \exp\left[i\xi x_{i} - \frac{(\xi\rho_{th})^{2}}{2}\right] \times \int dx \Lambda^{p}(x - x_{i}) e^{i\xi(x - x_{i})},$   
=  $\Delta x \Delta y \Delta z \exp\left[i\xi x_{i} - \frac{(\xi\rho_{th})^{2}}{2}\right] \left[\frac{2}{\xi\Delta x} \sin\left(\frac{\xi\Delta x}{2}\right)\right]^{p}.$  (A4)



**FIG. 19.** Convergence analysis for the (a) x integration with Gauss–Legrendre, (b)  $\alpha$  integration with Gauss–Chebyshev, and (c)  $\mu$  integration with Gauss–Laguerre, quadrature points, respectively, of the  $f_0(t, \vec{R}, v_{\parallel}, \mu) - f_0(0, \vec{R}, v_{\parallel}, \mu)$  term of the r.h.s. of Eq. (11). ( $N_q, N_c, N_l$ ) quadrature points are used for the integration of the dimensions x,  $\alpha$ , and  $\mu$ , respectively. For each of the above cases, the quadrature point number for a dimension is set to vary, while the other two are fixed at either 32 or 64.

In practice, the  $f_0(\vec{R}, v_{\parallel}, \mu, t) - f_0(\vec{R}, v_{\parallel}, \mu, 0)$  term of the r.h.s. of Eq. (11) is calculated using Gaussian quadratures. Specifically, due to the limits of integration for each of the variables,  $N_q$ Legendre points for the *x* integral,  $N_c$  Chebyshev points for the  $\alpha$ integral, and  $N_l$  Laguerre points for the  $\mu$  integral have been used. The convergence study for  $\xi L_x = 32\pi$ , which exceeds the typical wavelength of the integrand for this work, is show in Fig. 19.

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