Accuracy of momentum and gyrodensity transport equations in global gyrokinetic PIC simulations

Ben F McMillan, Peter Hill[1], Laurent Villard, Thibaut Vernay[2], Alberto Bottino[3]

[1]*Centre for Fusion, Space and Astrophysics, Department of Physics, University of Warwick, CV4 7AL, Coventry UK*

[2]*Centre de Recherches en Physique des Plasmas, Association Euratom-Confédération Suisse, Ecole Polytechnique Fédérale de Lausanne, PPB, 1015 Lausanne, Switzerland.*

[3]*Max Planck Institut für Plasmaphysik, Boltzmannstr. 2, D-85748 Garching, Germany*

Abstract

In control-variate PIC simulations, as used to model microturbulence in the tokamak core, a consequence of the splitting of the background and perturbed parts via $f = f_0 + \delta f$ is that analytical transport relations for the relevant fluxes and moments are only conserved in the large marker number limit. However, the analytic transport equations allow the error to be written explicitly in terms of the sampling of the background distribution. This immediately allows estimates of the consistency of momentum transport in control-variate PIC simulations. We then demonstrate numerically that global gyrokinetic simulations reproduce these transport equations as expected with sufficient accuracy to determine the slow evolution of global scale profiles.

Introduction

PIC-based simulations of plasma are a well-established technique for simulating the microturbulence which typically dominates transport in tokamaks. These simulations take advantage of the conservation of the distribution function along the collisionless particle trajectories, and sample the distribution function at a set of positions, so that the Vlasov advection problem is translated into an equation of motion for a set of markers. To reduce the sampling errors in PIC simulations, control variates are used, so that only the fluctuating components of the distribution function need to be evaluated with Monte-Carlo sampling, and in combination with noise-control techniques, this is highly effective as a path to low-noise simulations.

Particle conservation and satisfaction of the integral form of the local particle transport equation is immediately guaranteed for conventional PIC simulations, but this is no longer the case when control variates are used, and the particle weights are a function of time, as a result of computing background quantities f_0 analytically. However, we still have

$$0 = \frac{\partial}{\partial t} \int dZJf + \frac{\partial}{\partial R} \int dZJf \tag{1}$$

and with the decomposition $f \to f_0 + \delta f$, and a decomposition the trajectories into the perturbed and unperturbed parts, R_0 and R_1 respectively, we find

$$\frac{\partial}{\partial t}\int dZJ\delta f + \frac{\partial}{\partial R}\int dZJ[\delta f(\dot{R}_0+\dot{R}_1)+f_0\dot{R}_1] = -\frac{\partial}{\partial t}\int dZJ f_0 - \frac{\partial}{\partial R}\int dZJ f_0\dot{R}_0, \quad (2)$$

where f_0 and δf are evaluated using Monte-Carlo sums at the marker positions. The right hand side is zero analytically when f_0 is chosen to be a time-independent equilibrium of the unperturbed system, but is only guaranteed to converge to zero in a PIC simulation as the number of markers $\to \infty$.

The second term on the RHS of eq. 2 is largely oscillatory, and the first term dominates. To estimate the error in integrals of f_0, let us consider markers which are initially uniformly distributed, but are displaced randomly in radial position by a normally distributed amount with RMS amplitude σ (velocities are unchanged). The markers are distributed on a periodic domain $r \in [-0.5, 0.5]$, to sample a Maxwellian PDF $f(r,v)$. If $f(r,v) = f(v)$, the expected error in the Fourier spectrum of the Monte-Carlo error is

$$< u_k >^2 = \sum(\Omega_i f_i)^2 \left\{1 - e^{\sigma^2 k^2/4}\right\} \quad (3)$$

where Ω_i is the phase space volume associated with each marker. This expression tends to zero for small σk and to the usual $1/N$ result for large marker displacements. When the marker distribution is Gaussian, thus proportional to the particle distribution, this sum reduces to n^2/N, but will be larger by some constant factor for non-Maxwellian marker loadings.

Based on this caclulation, we can estimate the saturated late time error, once the markers are fully mixed over the transport time; for weak flows of order of the drift velocities the error in momentum transport is comparable to the total flow, so such simulations would be challenging. For intermediate flows in a reactor-scale device, of a few percent of the Mach velocity, the relative error will be small.

Electrostatic, collisional simulations with no source operators were performed with standard CYCLONE parameters using the code NEMORB[1] to examine numerical convergence, and check that the sampling error in f_0 agreed with expectations: these matched well, and scaled correctly.

Toroidal Momentum equation

A toroidal momentum equation for the numerical system, analogous to the the momentum conservation relations in Ref. [2] beginning from their Equation 73 is

$$-\frac{\partial}{\partial t}\left\langle \frac{1}{c}\mathbf{P}\cdot\nabla A_\varphi \right\rangle + \frac{\partial}{\partial t} < f p_z b_\varphi > + \frac{\partial}{\partial V} < f p_z b_\varphi \dot{V} > + \left\langle f\frac{\partial H}{\partial t}\right\rangle = \frac{e}{c}\frac{\partial A_\varphi}{\partial V}\frac{\partial}{\partial t}\int_0^V f_0 dV'. \quad (4)$$

This formulation is valid for the code NEMORB, where FLR terms[3] need to be carefully included. We note that the approximation $< \nabla\phi > \rightarrow \nabla < \phi >$, used originally in NEMORB also needs to be relaxed to obtain accurate momentum conservation.

As with the density transport equation, terms can be split into contributions which are used to diagnose momentum in the code, and those which are zero in the converged simulation limit, so that the error in the numerical transport equation can be directly evaluated. Note that, unlike in the density equation, there is an error term on the RHS of eq. 4 involving the radial integral of the background distribution, leading to a non-local error in toroidal momentum transport. This term arises because spurious density sources (which cannot be written as a divergence of a flux) at a particular radial position lead to an outward electric field between this radius and the edge, and an associated toroidal flow component.

Convergence of density and toroidal momentum diagnostics

For marker numbers of $2 \times 10^8, 1 \times 10^9$, and 1.6×10^{10} the relative RMS errors in the time-and-space integrated momentum transport equation are $0.102, 0.069$ and 0.0083, and in the gyrodensity transport errors are $1.1, 0.52$, and 0.10 respectively. 2D plots of the time-integrated fluxes are shown in figure 1.

At $t = 15a/c_s$, the Signal-to-Noise Ratio (SNR), as defined in reference [1, 4], is around 600 and 30 for the 16e9 simulation and 1e9 simulation respectively. Typically, we require a SNR of at least 10 to ensure reasonable convergence of the heat flux and large-scale flows; however the large scale flow pattern is well converged even for the simulation with the fewest markers where the SNR criterion is marginal. Reduction in noise is of course visible in plots of certain quantities, like potential on the poloidal cross section and shearing rates. Qualitatively, the main difference is the GAM levels seen near the edge converge to close to zero as the marker number is increased: this is in agreement with the expectation that localised unphysical density perturbations can drive GAMs across the simulation domain. For the case with fewest markers, unphysical GAMs are driven at roughly 10% of the maximum flow level in the turbulent region.

References

[1] S. Jolliet, A. Bottino, P. Angelino, R. Hatzky, T.M. Tran, B.F. McMillan, O. Sauter, K. Appert, Y. Idomura, and L. Villard. A global collisionless PIC code in magnetic coordinates. *Computer Physics Communications*, 177:409–425, 2007.

[2] B. Scott and J. Smirnov. Energetic consistency and momentum conservation in the gyrokinetic description of tokamak plasmas. *Physics of Plasmas*, 17:112302, 2010.

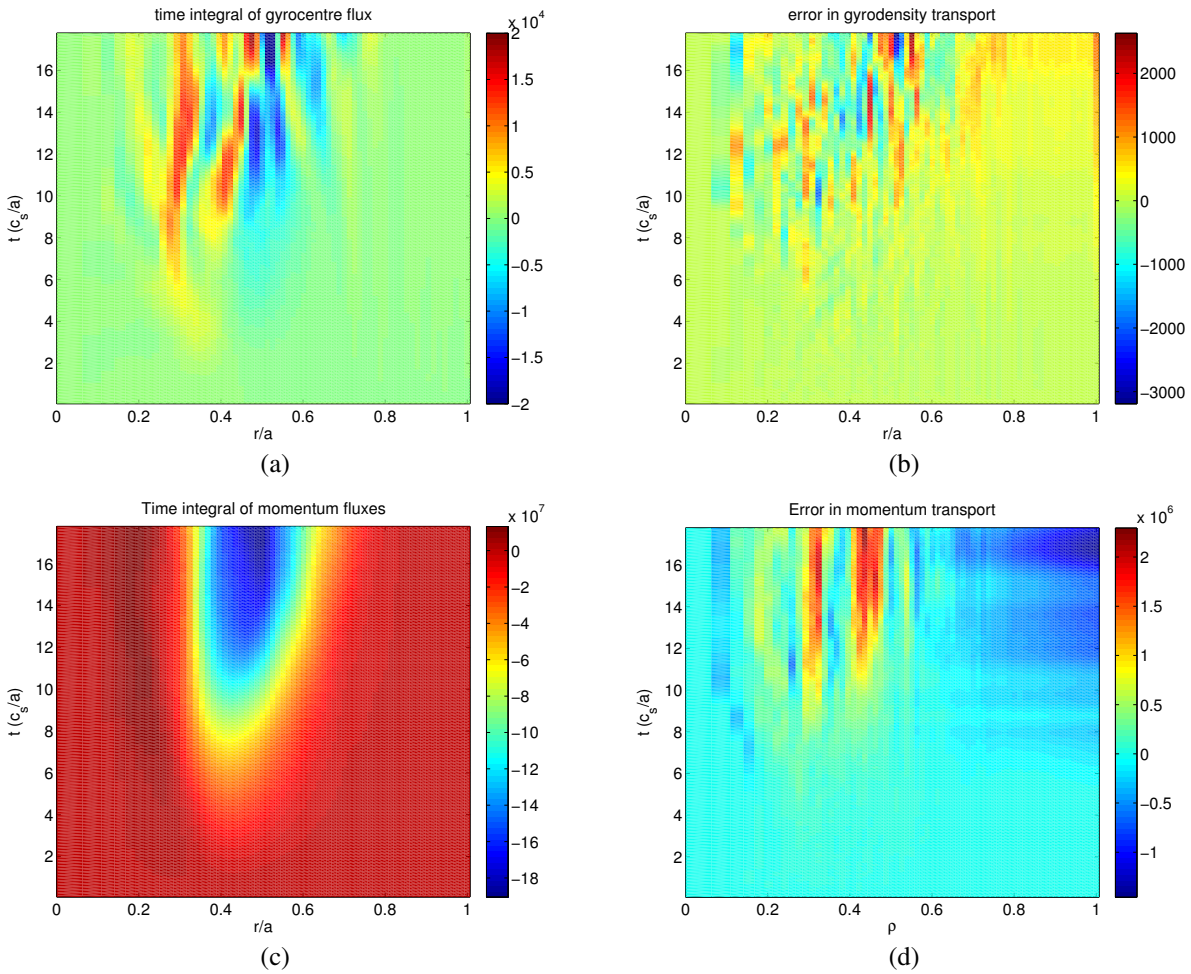

Figure 1: (a) Time integral of gyrodensity flux, and (b) gyrodensity transport error, (time and radial integral of transport equation), (c) Time integral of toroidal momentum flux and (d) momentum transport error, vs. radius and time, using 1.6×10^{10} Markers.).

[3] B F McMillan, P Hill, S Jolliet, T Vernay, L Villard, and A Bottino. Gyrokinetic transport relations for gyroscale turbulence. *Journal of Physics: Conference Series*, 401(1):012014, 2012.

[4] A. Bottino, B. Scott, S. Brunner, B.F. McMillan, T.M. Tran, T. Vernay, L. Villard, S. Jolliet, R. Hatzky, and A.G. Peeters. Global nonlinear electromagnetic simulations of tokamak turbulence. *Plasma Science, IEEE Transactions on*, 38(9):2129–2135, 2010.