Conservation of total energy and toroidal angular momentum in gyrokinetic particle-in-cell simulations

T. Korpilo[1], J.A. Heikkinen[2], S.J. Janhunen[1], T.P. Kiviniemi[1], S. Leerink[1]

[1] *Aalto University, Euratom-Tekes Association, Espoo, Finland*

[2] *VTT, Euratom-Tekes Association, Espoo, Finland*

Predictive transport simulations of tokamak discharges are continuously improving thanks to increasing computational resources available and to the efforts made in code development. As an example of the progress, a recent work [1] with the Elmfire code demonstrates the ability of global gyrokinetic full f electrostatic particle simulations, including both neoclassical and turbulence physics, to reproduce experimental FT-2 tokamak measurements quantitatively. The validity of such first-principles simulations in a toroidal axisymmetric tokamak configuration requires naturally the conservation of total energy and total toroidal angular momentum, in order to model long-term neoclassical and turbulence physics correctly.

The conservation of energy and toroidal angular momentum in gyrokinetic simulations necessitates the existence of corresponding conservation laws in the underlying theory and the application of numerical methods that realize the conservation laws in practice. For Elmfire, the gyrokinetic formalism in Ref. [2] provides the expressions for total energy K and total toroidal angular momentum L (explicit form given in Ref. [3]) with exact conservation up to the second order in the gyrokinetic expansion for a quasineutral plasma. Therefore, the conservation of these variables is analyzed in Elmfire simulations despite the low-order gyrokinetics may neglect important terms affecting, e.g., the expression for the conserved toroidal angular momentum [4]. The accuracy of the conservation of K and L is determined by the numerical methods applied in Elmfire, as shown in the following sections.

The challenging features of Elmfire with respect to the conservation of energy and toroidal angular momentum are both that it is a particle-in-cell code and that it resolves the full 5D distribution of drift-kinetic electrons, in addition to gyrokinetic ions, under 3D electrostatic potential [5]. Under the circumstances, first, the simulated plasma is non-neutral in the space between the grid points although the charge neutrality at the grid points is enforced. This inhomogeneity results in asymmetric electric force interpolation between ions and electrons and therefore in toroidal angular momentum drive unless the so-called momentum conserving interpolation scheme is employed. In the standard version of the scheme, the electric force is interpolated from the grid to the particle location by the same interpolation function as the charge is sampled to the grid. Ideally, the quasi-neutrality at the grid points guarantees then zero toroidal

angular momentum drive. Second, in the simulations of the full electron distribution, the numerical electron heating (or cooling) determines the time-evolution of total energy for the most part. The numerical heating is associated with inaccuracies in the time integration of the electron parallel acceleration by $\vec{E} \cdot \hat{b}$, and as such, there is no ready-made numerical scheme to remove the heating at once.

In Elmfire, the gyrocenter motion of ions and the guiding center motion of electrons are followed by an implicit-explicit integration scheme. The implicit time integration, i.e., of the ion polarization drift and the electron parallel acceleration by $\vec{E} \cdot \hat{b}$, is utilized for solving the electric potential from the quasi-neutrality condition. The exact formulas for the gyrocenter equations of motion including the polarization drift are given in Ref. [2]; the missing effect of the inhomogeneous magnetic field can be included by a separate guiding center expansion. Now, in Elmfire, the momentum conserving interpolation scheme is used only for the electric field in the $\vec{E} \times \vec{B}$ drift velocity, and even in this case the radial component of the electric field has to be redefined from the standard version to ensure stable simulations [3]. The so-called energy conserving interpolation scheme is applied to the electric field in the implicit ion polarization drift and electron parallel acceleration, instead, since the use of the momentum conserving scheme would result in severe numerical problems. For symmetry reasons, the ion parallel acceleration is treated similarly to electrons. Concerning the numerical electron heating and its reduction in Elmfire simulations, a second-order implicit time integration scheme is introduced for the electron parallel acceleration by $\vec{E} \cdot \hat{b}$ [6]. The parallel electric field is evaluated by a continuous (energy conserving) interpolation method, while the former first-order implicit time integration scheme is found stable only with a piecewise continuous parallel electric field.

To measure the accuracy of the conservation of total toroidal angular momentum and energy in Elmfire simulations, a turbulent, collisional deuterium plasma is simulated with the parameters similar to FT-2 tokamak discharges: minor radius 8 cm, major radius 55 cm, on-axis magnetic field 2.2 T, total plasma current 55 kA, initial electron and ion temperatures on axis 120 eV and at separatrix 10 eV, and initial electron density on axis $5.0 \cdot 10^{19}$ m^{-3} and at separatrix $0.1 \cdot 10^{19}$ m^{-3}. The initial radial temperature and density profiles are set parabolic, while the fixed radial current density profile is linear. The main numerical parameters are chosen as follows: inner simulation boundary at 2 cm, outer simulation boundary at 8 cm, grid of $50 \times 200 \times 8$ in radial, poloidal and toroidal direction, time step 30 ns (near the limit of the electron parallel accuracy condition), and average number of electrons (and ions) per grid cell 1100. During the simulations, total energy and toroidal angular momentum are diagnosed in the simulation domain excluding five innermost and outermost radial grid shells. Therefore, from the physical

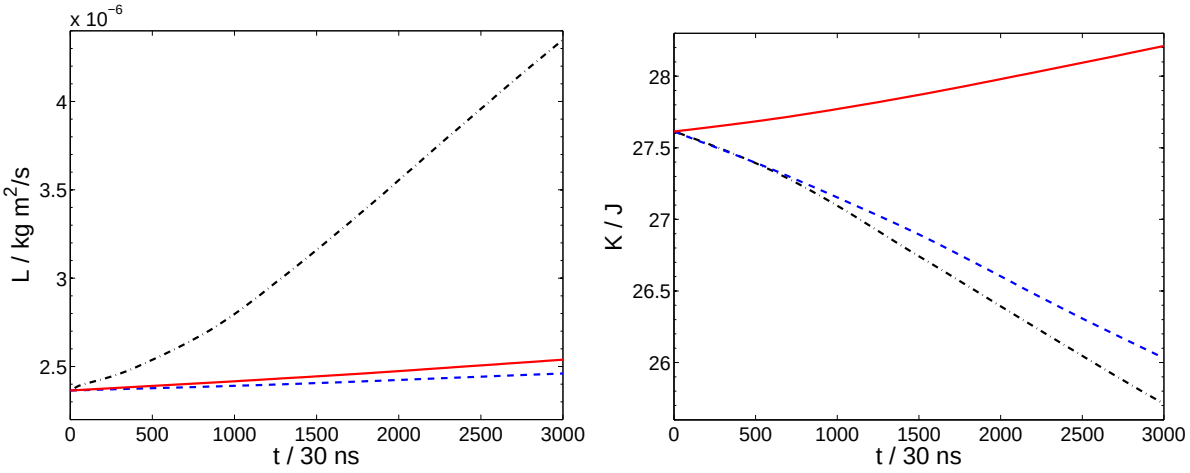

Figure 1: Accuracy of the conservation of toroidal angular momentum (left) and energy (right) in a turbulent Elmfire simulation. The black dash-dot line refers to schemes E2 and A2, the blue dashed line to E1 and A2, and the red solid line to E1 and A1.

point of view, the only energy and momentum sources/sinks to be considered are energy and toroidal angular momentum transport through the boundaries of the diagnostic domain. From the numerical point of view, one should note that total toroidal angular momentum and energy cannot be measured exactly inside a toroidal annulus because particles inside the annulus interact with the electric field outside the annulus, and vice versa, due to the finite ion Larmor radius and finite particle size.

Now, Fig. 1 illustrates the effect of the above-mentioned numerical methods on the accuracy of the conservation of toroidal angular momentum and energy. The conservation of toroidal angular momentum, first, improves significantly by applying the momentum conserving interpolation scheme (E1) to the electric field in the $\vec{E} \times \vec{B}$ drift velocity instead of the former energy conserving interpolation scheme (E2). The difference between the schemes is effectively that the momentum conserving scheme makes the radial $\vec{E} \times \vec{B}$ flux of ions and electrons ambipolar. Second, the second-order implicit time integration scheme (A1) for the electron parallel acceleration together with a continuous electric field interpolation shows to improve the conservation of energy over the former first-order implicit time integration scheme (A2) with a piecewise continuous electric field interpolation. The simultaneous deterioration of the conservation of toroidal angular momentum underlines that the time integration of the parallel acceleration by $\vec{E} \cdot \hat{b}$ is asymmetric between ions and electrons and that the asymmetry is larger when the integration scheme A1 is employed.

The results in Fig. 1 are produced rather low number of particles per grid cell, and thus the accuracy of the conservation of toroidal angular momentum and energy is represented in

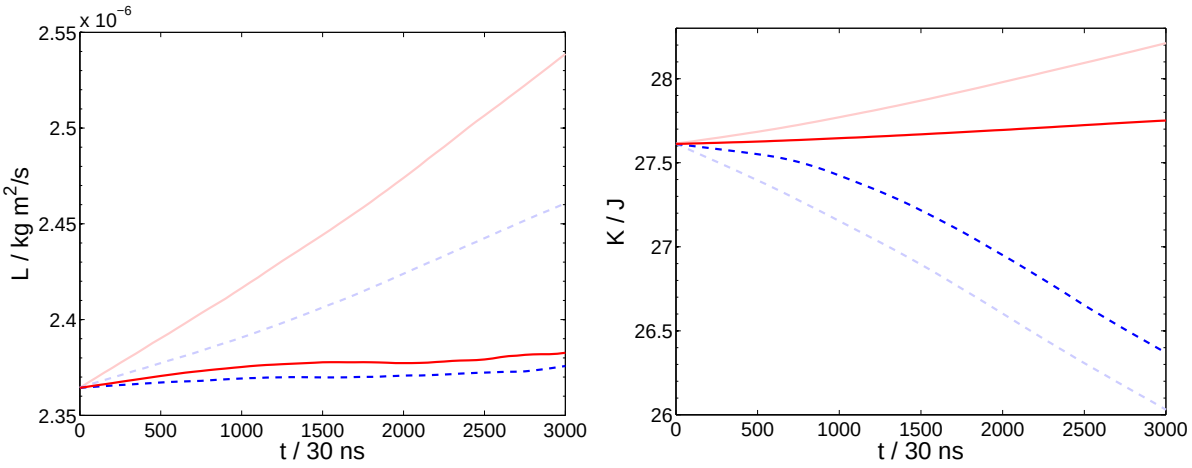

Figure 2: Accuracy of the conservation of toroidal angular momentum (left) and energy (right) with respect to particle number. The bright lines correspond to 4400 particles per grid cell and the faint lines to 1100 particles per grid cell. The line coding corresponds to Fig. 1.

Fig. 2 using four times more particles. The conservation of toroidal angular momentum shows now a big improvement regardless of whether the integration scheme A1 or A2 is applied to the electron parallel acceleration. The conservation of energy, on the other hand, improves by a factor of four with the integration scheme A1 while the integration scheme A2 shows practically no improvement. In the simulations, the growth of turbulent modes starts around the 500th time step.

As a conclusion, the momentum conserving interpolation scheme for the electric field in the $\vec{E} \times \vec{B}$ drift velocity [3] and the second-order implicit time integration scheme for the electron parallel acceleration by $\vec{E} \cdot \hat{b}$ [6] provide numerically stable methods to obtain good toroidal angular momentum and energy conservation in Elmfire simulations.

Acknowledgements: This work was supported by the Academy of Finland (Grant No 122435 and No 134977), EFDA Topical Group Activities, High Level Support Team, and the supercomputing facilities of CSC, HPC-FF and PRACE.

References

[1] S. Leerink et al., submitted to Phys. Rev. Lett. (2012)

[2] J.A. Heikkinen et al., Phys. Plasmas **18**, 022310 (2011)

[3] J.A. Heikkinen et al., Comp. Phys. Commun. **183**, 1719 (2012)

[4] F.I. Parra et al., Plasma Phys. Control. Fusion **50**, 065014 (2008)

[5] J.A. Heikkinen et al., J. Comput. Phys. **227**, 5582 (2008)

[6] T. Korpilo et al., submitted to J. Comput. Phys. (2012)