Speed-up of SOLPS-ITER code for tokamak edge modeling

E. Kaveeva[1], V. Rozhansky[1], I. Senichenkov[1], I. Veselova[1], S. Voskoboynikov[1],

X. Bonnin[2], D. Coster[3]

[1]*Peter the Great St.Petersburg Polytechnic University, St.Petersburg, Russia*

[2]*ITER Organization, St Paul Lez Durance Cedex, France*

[3]*Max-Planck Institut für Plasmaphysik, EURATOM Association, Garching, Germany*

Account of drifts and currents dramatically decreases the accessible time step for the integration of time dependent equations of the code SOLPS-ITER [1]. In the present paper the mechanisms leading to the numerical instability and time step limitations associated with drifts in SOLPS-ITER are analyzed as well as the ways to relax these limitations.

Scheme of numerical instability

The main feature of the instability, when the "limiting" time step is exceeded, is oscillation of the electrostatic potential inside the separatrix. The potential oscillations have no poloidal structure, and they lead to the rise of a big radial electric field changing its sign at each time step. Such behavior resembles geodesic acoustic mode (GAM) formation with a characteristic frequency $\omega_{GAM} \approx \sqrt{(T_e + T_i)/m_i} / R$ [2]. The simplest description of GAM includes the radial balance of the polarization and a diamagnetic current, and the particle balance in which the $\vec{E} \times \vec{B}$ drift leads to the density perturbation. In a simple toroidal co-ordinates (r, θ, φ) of flux surfaces with circular cross section and no Shafranov shift the GAM electric field is $E_r = E_0 + E_1 \exp(-i\omega t)$ and the density distribution is $n = n_0 + n_1 \sin\theta \exp(-i\omega t)$. The linearization of the continuity equation gives

$$-i\omega n_1 + 2\frac{E_1}{RB}n_0 = 0. \tag{1}$$

The pressure perturbation leads to the average diamagnetic current through the flux surface $\left\langle j_r^{(dia)} \right\rangle = -\frac{T_e + T_i}{BR}n_1$, which is compensated by the polarization current $\left\langle j_r^{(P)} \right\rangle = -\frac{m_i n_0}{B^2}i\omega E_1$,

$$\left\langle j_r^{(dia)} \right\rangle = -\left\langle j_r^{(P)} \right\rangle \tag{2}$$

Combining Eqs.(1), (2) the GAM frequency ω_{GAM} and the limiting time step of iterations $\delta t_{max} < \omega_{GAM}^{-1}$ in the code describing the GAM physics can be obtained.

The polarization current in the SOLPS-ITER set of equations is replaced by the anomalous current $j_r^{(AN)} = \sigma_{AN} E_r$ which was initially introduced for numerical reasons and should not influence the steady-state solution. Then, instead of Eq. (2) the current balance is

$$\left\langle j_r^{(dia)} \right\rangle = -\left\langle j_r^{(AN)} \right\rangle. \tag{3}$$

Combining Eqs.(1), (3) the imaginary oscillation frequency can be obtained leading to the exponential decrease for the pressure perturbation and perturbation of $\vec{E} \times \vec{B}$ drift: $n_1, E_1 \sqcup \exp(-\gamma t)$ where

$$\gamma = \frac{2n(T_e + T_i)}{\sigma_{AN}(BR)^2}.$$ To produce the solution of an equation for each quantity $(V_{||}, n, \varphi, T_e, T_i)$ the numerical scheme of SOLPS-ITER uses the four other quantities calculated previously. The characteristic time step for this partially explicit iteration scheme is then limited by the decrement:

$$\delta t < \gamma^{-1}, \quad \delta t_{max} \approx \sigma_{AN}(BR)^2 / n(T_e + T_i).$$ According to our experience this estimate remains correct for limiting time steps of the iterations both for ITER and ASDEX-Upgrade (AUG) modeling. An accurate analysis shows that the temperature perturbations are also involved in the oscillations, giving the time step limitation of the same order as density perturbations. The maximal time step is proportional to the anomalous conductivity value. Still, the simple solution to increase σ_{AN} can't be applied directly. The neoclassical radial conductivity [3] $\sigma_\perp^{NEO} \approx \mu_{i1} / (BR)^2$ where μ_{i1} is the classic parallel viscosity coefficient, should be bigger than σ_{AN}, otherwise the code would not reproduce the radial electric field.

Possible solutions for convergence speed-up: Method of partial flux surface averaging

To get the converged solution one should numerically follow the evolution of flux-averaged density and temperatures for several slow characteristic time scales determined by anomalous transport, $\tau_D \sim L^2 / D$. Taking the transport barrier width and the diffusion coefficient for estimate, we get $\tau_D \sim 100 \, ms$ for ITER $(L \sim 5cm, D \sim 0.03 m^2 / s)$ and $1 \, ms$ for AUG $(L \sim 1.5cm, D \sim 0.2 m^2 / s)$. The instability is driven by the density and temperature perturbations at faster time scales, of the order of $10^{-8} \, s$ for ITER and $10^{-7} \, s$ for AUG. So it is possible to decrease numerically the time derivative of the density perturbation retaining the evolution of flux-averaged quantities unchanged.

The implementation of this scheme in the code is described below. First, the corrections for plasma component densities $\delta n_{al,m}^{(k)}$ ($a -$ ion species, $k -$ time step index, l - radial and m - poloidal indexes of numerical grid cells), and for electron and ion temperatures $\delta T_{el,m}^{(k)}$, $\delta T_{il,m}^{(k)}$ are calculated routinely at the time step. Next, inside the separatrix the average corrections are calculated for each flux surface and are applied to each cell. Then, the corrections for densities and temperatures perturbations are calculated and applied with scaling coefficients $\alpha_a < 1$, $\alpha_T < 1$, $\alpha_T \sim \alpha_a$, so that at the beginning of the next time step:

$$n_{al,m}^{(k+1)} = n_{al,m}^{(k)} + \left\langle \delta n_a^{(k)} \right\rangle_l + \alpha_a (\delta n_{al,m}^{(k)} - \left\langle \delta n_a^{(k)} \right\rangle_l), \quad T_{l,m}^{(k+1)} = T_{l,m}^{(k)} + \left\langle \delta T^{(k)} \right\rangle_l + \alpha_T (\delta T_{l,m}^{(k)} - \left\langle \delta T^{(k)} \right\rangle_l)$$

The correction modification is applied only inside the separatrix and should not be applied to the partially ionized impurity states that have very strong poloidal density variation and almost no influence on the plasma pressure. It permits the increase of time step roughly by a factor $\alpha_T^{-1} \sim \alpha_{a\,main}^{-1}$ (here "*main*" is the label for the ion species contributing most to the plasma pressure) and does not affect the converged solution. The scheme should not be used for the modeling of deep detachment, where the density perturbation at the flux surfaces next to X-point is of the order of unity.

The scheme was tested for ITER and AUG calculations. For AUG conditions the possible increase in the time step was from $2 \cdot 10^{-7} \, s$ for no speed-up to $10^{-5} \, s$, for ITER from $2 \cdot 10^{-8} \, s$ to $10^{-6} \, s$.

As an example the AUG shot evolution traced after the drifts turning on is shown in Fig.1(a). Tracings for speed-up coefficients $\alpha_T = \alpha_a = 0.04$ and time step $2.5 \cdot 10^{-6}$ s (solid lines) are compared to tracings for $\alpha_T = \alpha_a = 0.01$ and time step 10^{-5} s (dashed lines). The two sets of speed-up parameters give the same evolution of the calculation with the only difference that the steady state solution for time step 10^{-5} s can be obtained 4 times faster in terms of CPU. The convergence without the speed-up scheme would take about 10^2 times longer, for our calculation capacities it would be several years. Therefore, to make the test of converged solution it was obtained in a month of calculation with speed-up and then the calculation was continued without speed-up scheme and with small time step $2 \cdot 10^{-7} s$. The points in time where the calculations were continued are shown in Fig. 1(a) with arrows. The time tracings before and after the change of the time step are shown in Fig.1(b). The calculation without the speed-up scheme shows that the stationary solution does not change if the scheme is turned off.
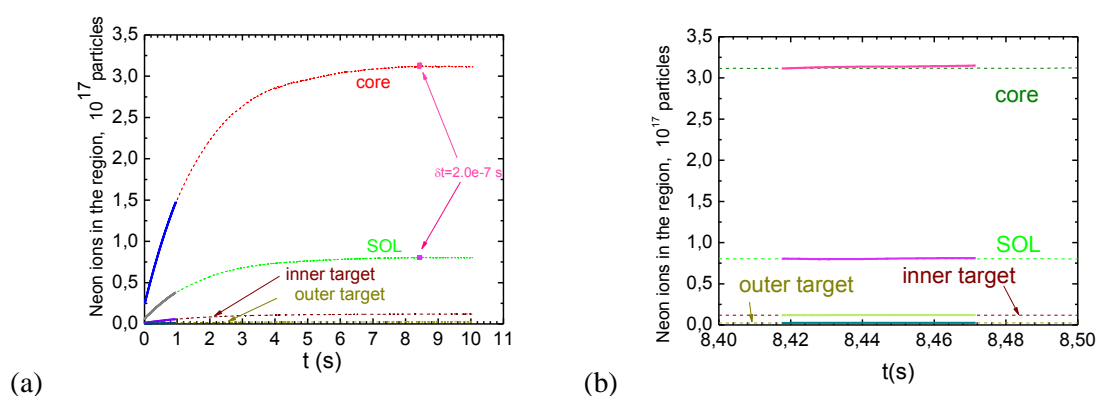

Fig.1. Time evolution for AUG modeling (a) with two sets of speed-up parameters (b) speed-up turning off.

Possible solutions for convergence speed-up: Method of intermediate solution

The idea of the speed-up scheme is to seek first an intermediate solution, using a large value of anomalous conductivity σ_{AN} thus permitting big time step. At this stage, neoclassical radial conductivity is increased artificially by introducing artificial large parallel viscosity coefficient μ_{i1} inside the separatrix, to have intermediate profile of radial electric field close to the final one. Other modifications of the equations are introduced in order to avoid unphysical acceleration in the toroidal directon and unphysical change of the electron density profiles [4]. At the second stage all modifications are switched off, σ_{AN} is reduced and the true solution is obtained.

The main predictable discrepancy between the true and the intermediate solution is a radial scale $\delta \sim \left(B^2 r^2 \eta / B_x^2 \mu_{i1} \right)^{1/2}$ for transition from SOL to neoclassic electric field [5] (η - anomalous perpendicular viscosity coefficient) depending on parallel viscosity coefficient. When the anomalous conductivity, classical viscosity and time step are decreased at the second stage, the radial electric field in the separatrix vicinity should change correspondingly. The physical time of the change of electric field can be estimated as time of redistribution of the parallel velocity due to perpendicular viscosity on the scale δ, of the order of several mm. This time scale is orders of magnitude smaller than the scales of the diffusive processes, which are required to reach stationary solution at first stage. So, the speed-up scheme can give considerable decrease of the computation time. The calculations

focused on the physical processes in the SOL can be stopped at first stage since the solution inside the separatrix, which serves as a boundary condition to the problem in SOL, differs at first and second stages only by small details of the poloidal distribution of parallel velocity.

The proposed scheme was tested in ITER simulations. The preliminary calculations were continued for about two CPU months with the time step 10^{-6} s, $\sigma_{AN} = 4 \cdot 10^{-6} en_e$ and with the viscosity coefficient increased by a factor 20. Then for a CPU month the calculations were performed from the solution converged at first step, with the time step $2 \cdot 10^{-8} s$, $\sigma_{AN} = 10^{-7} en_e$ and with physically correct viscosity. The preliminary and final calculations results are shown in Fig. 2.

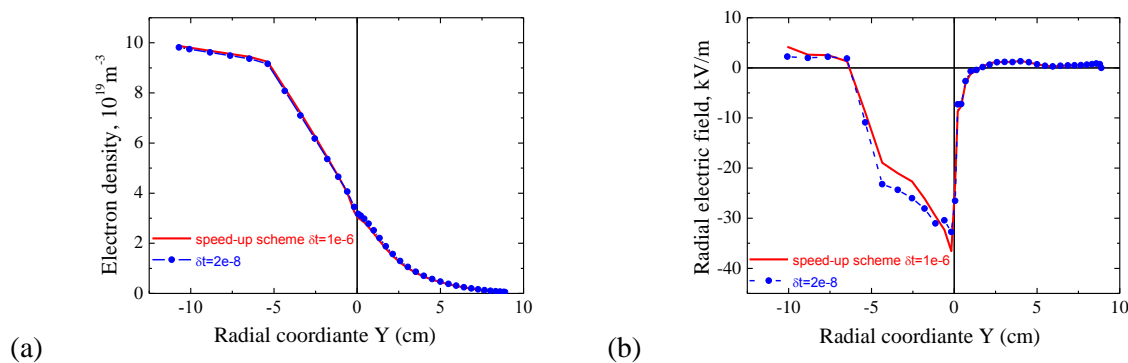(a)   (b)

Fig.2. Parameters after initial and final stage of calculations for ITER geometry and typical input parameters.
(a) Electron density at the outer midplane; (b) radial electric field at the outer midplane

Conclusions

Simulations of edge tokamak plasmas with the full SOLPS-ITER model including EIRENE neutrals and charged particle drifts are possible with acceptable convergence time scales only with implementation of improved numerical schemes. The most challenging limitation of convergence time step is associated with the poloidal redistribution of particles inside the separatrix by drifts of the GAM nature. It can be overcome with one of two methods. The first one uses artificial slowing down of poloidal density and temperatures redistribution on the closed flux surfaces. In the second one the equations are modified so that they can be solved faster, with the fast solution very close to one we are seeking, as an initial approximation for convergence to the true solution. Implementation of these methods can speed up the modeling time by more than an order of magnitude.

Acknowledgement

Reference

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