OPTIMIZATION OF SELF-CONSISTENT CODE FOR MODELLING OF RF PLASMA PRODUCTION

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The optimization to the radio frequency (RF) module of a self-consistent cylindrical model for plasma production is applied. Optimization includes avoiding repeated calculations and employing a parallelization. To suppress singularities in the lower hybrid resonance (LHR) zone a patching is in the code.

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INTRODUCTION

A self-consistent model of radio-frequency (RF) plasma production [1] contains transport equations for plasma density and electron energy, and includes ionization and excitation by electron impact, neoclassical transport, direct losses of plasma (convection to the plasma edge) and the neutral gas balance. The problem is solved in cylindrical geometry. The plasma is assumed to be azimuthally symmetrical and uniformly distributed along plasma column.

In the model the plasma is sustained by RF fields. The RF heating is calculated solving the Maxwell's equations. The part of the code with Maxwell's equations employs Fourier series in poloidal and toroidal angles and discretization in the radial direction. This part calculates the dielectric tensor, applies the regularity conditions for the electromagnetic fields at the magnetic axis and the boundary conditions at the metallic wall. The code uses finite differences for the balance part and finite elements method for the RF part.

The Maxwell's equations are written in the form:

$$\nabla\times\nabla\times\mathbf{E}-\frac{\omega^2}{c^2}\hat{\varepsilon}(r)\cdot\mathbf{E}=i\omega\mu_0\mathbf{j}_{\text{ext}}, \quad (1)$$

where $\mathbf{E}$ is the temporal Fourier harmonic of the electric field and $\mathbf{j}_{\text{ext}}$ is the density of the external RF (antenna) electric current.

The plasma dielectric tensor is a function of the radial coordinate and the plasma density and electron temperature,

$$\hat{\varepsilon}(r,t)=\sum_\alpha\hat{\varepsilon}_\alpha(r,t), \quad \hat{\varepsilon}_\alpha(r,t)=\begin{pmatrix}\varepsilon_{\perp\alpha} & ig_\alpha & 0\\ -ig_\alpha & \varepsilon_{\perp\alpha} & 0\\ 0 & 0 & \varepsilon_{\|\alpha}\end{pmatrix}.$$

Here α is the index enumerating types of particles.

The Maxwell's equations are solved at each time step for the running distributions of the plasma density and temperature. Discretization of the Maxwell's equations over the radial coordinate is performed by the method of weighted residuals with use of the third-order finite elements [2, 3].

Discretization is made by integration of the equations with weight (test) and basis (shape) functions.

Basis functions are: $\mathbf{B}_1=\Lambda^{(3)}(r)e^{im\varphi}e^{in\frac{z}{R}}\mathbf{e}_r$, $\mathbf{B}_2=\Lambda^{(3)}(r)e^{im\varphi}e^{in\frac{z}{R}}\mathbf{e}_\varphi$, $\mathbf{B}_3=\Lambda^{(3)}(r)e^{im\varphi}e^{in\frac{z}{R}}\mathbf{e}_z$, where $\Lambda^{(3)}(r)$ is the Hermitian finite element of the third order, R is the major radius of the torus.

Weight (test) functions are: $\mathbf{T}_1=\frac{d}{dr}\left[\Lambda^{(3)}(r)\right]e^{-im\varphi}e^{-in\frac{z}{R}}\mathbf{e}_r$, $\mathbf{T}_2=\frac{\Lambda^{(3)}}{r}(r)e^{-im\varphi}e^{-in\frac{z}{R}}\mathbf{e}_\varphi$, $\mathbf{T}_3=\Lambda^{(3)}(r)e^{-im\varphi}e^{-in\frac{z}{R}}\mathbf{e}_z$.

The generating function could be introduced $\mathbf{\Phi}=\Lambda^{(3)}(r)e^{-im\varphi}e^{-in\frac{z}{R}}$. Its gradient is the combination of the test functions $\nabla\Phi=\mathbf{T}_1-im\mathbf{T}_2-i\frac{n}{R}\mathbf{T}_3$.

PROBLEM OF TREATMENT OF LHR

The point of the lower hybrid resonance (LHR) $|\varepsilon_\perp|=0$ appears in single-ion species plasma at frequencies higher than ion cyclotron. In ion cyclotron range of frequencies (ICRF) the characteristic plasma densities are $n_e\sim10^{11}$ cm^{-3}. In cold plasma, in the LHR point the RF field has a singularity. The singularity cannot be described in finite elements approach and, after discretization, its existence may result in ill conditioned problem.

The dispersion of the slow wave is

$$k_\perp^2=k_{sw}^2\equiv-\frac{\varepsilon_\|}{\varepsilon_\perp}\left(k_z^2-k_0{}^2\varepsilon_\perp\right). \quad (2)$$

Here $k_0=\omega/c$. This equation determines the propagating waves $E_x=A_\pm(x)\exp(\pm i\int k_{sw}dx)$ in the WKB limit. The amplitude of the wave $A(x)$ remains unknown. The corresponding differential equation for the wave which one can construct from common sense does not contribute to determining the amplitude since the general form of such an equation

$$\frac{d}{dx}\left[B(x)\frac{d}{dx}D(x)E_x\right]+B(x)D(x)k_{sw}^2E_x=0 \quad (3)$$

contains two unknown slowly varying functions $B(x)$ and $D(x)$ that influence on the amplitude of the solution. To find them, the analysis of Maxwell's equations is necessary.

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To separate the slow wave from the fast wave, two small parameters are used $\alpha = \sqrt{k_x^2, k_y^2, k_0^2|\varepsilon_\perp|, k_0^2|g|} << 1$ and $\beta = \sqrt{|\varepsilon_\perp|/|\varepsilon_\|\||} << 1$. In the analysis, the last component of Maxwell's equations is substituted by the equation $\nabla \cdot \varepsilon \cdot \mathrm{E} = 0$

The Maxwell's equations are:

$$\left(k_z^2 + k_y^2 - k_0^2\varepsilon_\perp\right)E_x + ik_y \frac{d}{dx}E_y - ik_0^2 gE_y + ik_z \frac{d}{dx}E_z = 0,$$

$$ik_0^2 gE_x + ik_y \frac{d}{dx}E_x - \frac{d^2}{dx^2}E_y - k_0^2\varepsilon_\perp E_y - k_y k_z E_z = 0,$$

$$\frac{d}{dx}\left(\varepsilon_\perp E_x + igE_y\right) + ik_y\left(-igE_x + \varepsilon_\perp E_y\right) + ik_z\varepsilon_\| E_z = 0. \quad (4)$$

If zero- and first-order terms in α and β are retained, then the system becomes

$$\left(k_z^2 + k_y^2 - k_0^2\varepsilon_\perp\right)E_x + ik_y \frac{d}{dx}E_y + ik_z \frac{d}{dx}E_z = 0,$$

$$ik_y \frac{d}{dx}E_x - \frac{d^2}{dx^2}E_y = 0,$$

$$\frac{d}{dx}\left(\varepsilon_\perp E_x\right) + ik_z\varepsilon_\| E_z = 0. \quad (5)$$

Finally, we have the following equations

$$\frac{d}{dx}\left[\frac{1}{\varepsilon_\|}\frac{d}{dx}\left(\varepsilon_\perp E_x\right)\right] + \frac{k_{sw}^2}{\varepsilon_\|}\left(\varepsilon_\perp E_x\right) = 0\,. \quad (6)$$

For the propagating wave the WKB solution of this equation is

$$E_x = \frac{C_\pm\sqrt{|\varepsilon_\||}}{\varepsilon_\perp\sqrt{|k_{sw}|}}\exp(\pm i\int k_{sw}dx)\,,$$

$$E_z = \mp\frac{C_\pm\sqrt{|k_{sw}|}}{k_z\sqrt{|\varepsilon_\||}}\exp(\pm i\int k_{sw}dx). \quad (7)$$

Note here that $|E_x| \propto |\varepsilon_\perp|^{-3/4}$ and $|E_z| \propto |\varepsilon_\perp|^{-1/4}$. Thus, on approach to LHR point both components of the field increase. This is natural since the group velocity of the wave decreases but the energy flux should be unchanged.

The check is to calculate the energy flux $\Pi_x = \frac{c}{8\pi}\left(\mathbf{E}^* \times \mathbf{B}\right)_x = -\frac{c}{8\pi}\left(E_z^* B_y\right)$ to make sure that it does not change when the wave propagates. For negligible damping the flux is

$$\Pi_x = \pm\frac{c}{8\pi}\frac{k_0}{k_z^2}|C_\pm|^2\,. \quad (8)$$

It does not depend on the plasma parameters.

To avoid singularities, the patch proportional to $\delta\varepsilon$ is added to the Maxwell's equations

$$\nabla\times\nabla\times\mathbf{E} - k^2\varepsilon(r)\cdot\mathbf{E} - i\delta\varepsilon\left(\mathbf{E} - \mathbf{e}_z\mathbf{e}_z\cdot\mathbf{E}\right) = i\omega\mu_0\mathbf{j}_{\mathrm{ext}}. (9)$$

It is applied at the narrow zone where $|\varepsilon_\perp| < \varepsilon_{\min}$ ($\varepsilon_{\min}$ is a calculation parameter).

If the solution of Eq. (9) is an analytical function, the patching changes the solution only in the patching area and does not influence on the solution outside it. The solution would not also depend on the patch magnitude.

In first series of calculations the following formula for the patch is used $\delta\varepsilon = i\left[\sqrt{\varepsilon_{\min}^2 - \mathrm{Re}^2\,\varepsilon_\perp} - \mathrm{Im}\,\varepsilon_\perp\right]$ (linear patching). Its application results in constancy of the $|\varepsilon_\perp|$ (see curve 2 in Fig. 1) in the patching area.

Parabolic patching (see curve 3 in Fig. 1)

$$\delta\varepsilon = i\left[\sqrt{\left(\frac{\mathrm{Re}^2\,\varepsilon_\perp/2}{\varepsilon_{\min}} + \frac{\varepsilon_{\min}}{2}\right)^2 - \mathrm{Re}^2\,\varepsilon_\perp} - \mathrm{Im}\,\varepsilon_\perp\right]$$

is more robust following the results of the numerical experiments.

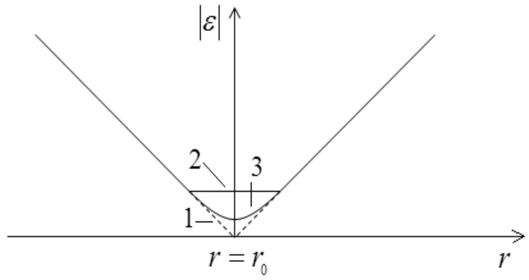

Fig. 1 Radial dependence of $|\varepsilon_\perp|$ in vicinity of LHR point: 1 – without patching; 2 – with linear patching; 3 – with parabolic patching

The structure of the fields and the convergence illustrated in Fig. 2.

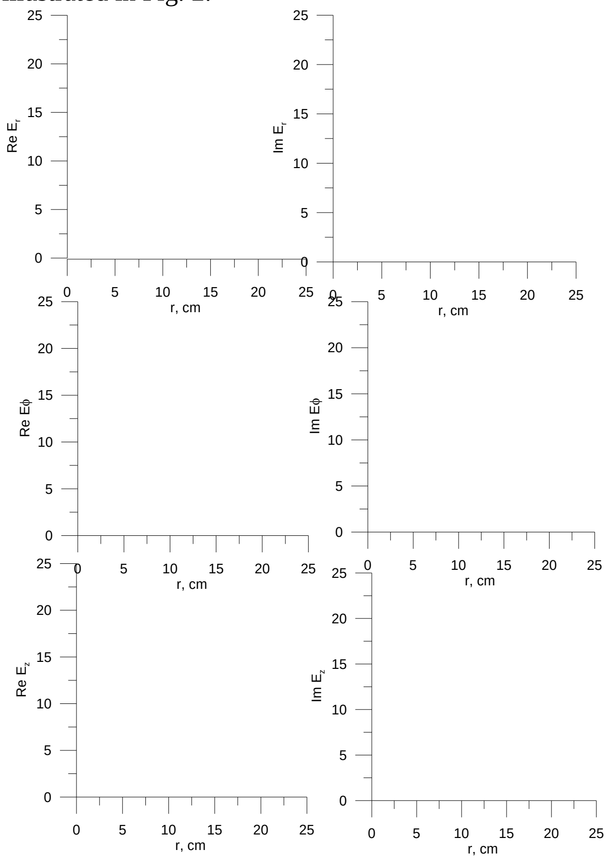

Fig. 2. Example of three calculations with different mesh node numbers: green is for 101, red is for 201, blue is for 1001

The three curves correspond to different mesh node numbers. We see that when the patch is applied the solution converges with increasing number of mesh points. The convergence is slower than in regular case.

RF MODULE

The calculations related to the Maxwell's equations are comprised into the RF module. It is designed on the base of 1D RF code [1].

In the numerical code, the RF module is made as a separate subroutine. The RF module input parameters are the ion component composition (the ion charges in units of proton charge, the ion mass number, number of sorts of ions, ion density radial distributions), the radial mesh node coordinates and the number of the mesh points, the magnetic field radial profile, the collision frequencies and the total input power. The RF power deposition profile to each ion sort, electrons and to the LHR zone and the full RF power are the output quantities.

Operation of the RF module is organized as follows. On first call it makes reading and storing calculation parameters (heating frequency, mesh size etc.) written in the input file and, after this, makes memory management. The subroutine creates its own adaptive mesh with mesh node accumulation in the vicinity of the LHR point. The right-hand side of the Maxwell's equations is calculated.

At further calls for each Fourier harmonic the Maxwell's equations are projected to the mesh. Using given plasma density and temperature profiles, the RF module calculates the dielectric tensor. Further the finite element algorithm is applied and the matrix of the system of linear equations is filled. The boundary conditions are imposed. The proprietary subroutine makes LU decomposition of the matrix and solves the algebraic equations. For each Fourier harmonic the power density is calculated and summed up. After termination of the loops over Fourier harmonics the power densities are remapped from the internal mesh to the external one, the mesh of the balance equations.

OPTIMIZATION

The optimization is applied to the RF module. It includes avoiding repeated calculations and employing a parallelization.

Main computational load in the code is due to the calculation of the electromagnetic fields and absorbed RF power. In the aspect of avoiding repetition of the same computations, useful properties of the problem are as follows:

- The dielectric tensor of cold plasma which is used in the code is independent on the axial and azimuthal wave numbers *m* and *n*. The dielectric tensor of the plasma is used both in the boundary problem and in the calculation of the absorbed power.
- The $\nabla\times\nabla\times$ operator can be represented as a second-order polynomial by *m* and *n*. After discretization the polynomial coefficients (matrices) are calculated once and then used to calculate the matrices for different Fourier harmonics.
- Parallelization of computations can be used in the calculation of electromagnetic fields for different Fourier harmonics and in the calculation of the absorbed RF power since harmonics with different *m* and *n* are uncoupled.

Inside the RF module parallelization directives implemented using open standard for parallelizing of programs, OpenMP. The dielectric tensor of the plasma is calculated only once and stored in memory. Also in the numerical code, a single calculation of the right-hand sides is implemented. Parallelization of calculations of different azimuthal harmonics is used with OpenMP directives.

DISCUSSION

Patching allows to make a correct calculation of the RF fields and to determine the specific absorption in the LHR zone. Application of the patch results in disappearing fine field structure in the LHR zone and allows one to avoid spurious solutions.

Test calculations demonstrated that the optimizations made in the numerical code result in the acceleration of the code more than 10 times as compared with the initial non-optimized version.

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ОПТИМИЗАЦИЯ САМОСОГЛАСОВАННОГО КОДА ДЛЯ МОДЕЛИРОВАНИЯ ВЧ-СОЗДАНИЯ ПЛАЗМЫ

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Проведена оптимизация высокочастотного (ВЧ) модуля самосогласованной цилиндрической модели для создания плазмы. Оптимизация заключалась в отказе от повторных вычислений и использовании распараллеливания. Для подавления сингулярности в области нижнего гибридного резонанса (НГР) в коде использован патчинг.

ОПТИМІЗАЦІЯ САМОУЗГОДЖЕНОГО КОДУ ДЛЯ МОДЕЛЮВАННЯ ВЧ-СТВОРЕННЯ ПЛАЗМИ

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Проведена оптимізація високочастотного (ВЧ) модуля самоузгодженої циліндричної моделі для створення плазми. Оптимізація полягала у відмові від повторних обчислень і використанні розпаралелювання. Для придушення сингулярності в області нижнього гібридного резонансу (НГР) у коді використаний патчінг.