Question description

The equation system consists of the following equations coupled with the application mode of Electromagnetic Waves. $w(\mathbf{r})$ and $\rho(\mathbf{r})$ are the dependent variables of the PDEs. $\mathbf{E}(\mathbf{r})$ is electric field. Other variable coefficients are known and defined in the attached model file.

$$w(\chi) = \frac{\psi}{4}\frac{\omega_P(\mathbf{r})}{\beta^2}\frac{\mathring{a}^2 E_h}{m_e}\nabla^2\frac{\rho(\mathbf{r})}{\omega_P(\mathbf{r})}$$

$$\nabla\cdot\left(\chi(\mathbf{r})\nabla\frac{\beta^2(\mathbf{r})\rho(\mathbf{r})-\beta_0 w(\mathbf{r})}{\omega_P^2(\mathbf{r})}\right)-\rho(\mathbf{r})$$

$$=\varepsilon_0\nabla\cdot\left(\chi(\mathbf{r})\mathbf{E}(\mathbf{r})\right)$$

The variables and constants in the equation and those defined in the model file are corresponded as in the following table.

Table

Equation	**Model**
w	wInt
ρ	RouInd
ω_P	OmegaP
χ	Chi
β^2	BetaSq
β_0^2	BetaSq0
ψ	Psi
$\mathring{a}$	rBohr
E_h	EHartree
m_e	eMass

These two PDEs are coupled with Maxwell's equations through $\mathbf{J}_P$,

$$\mathbf{J}_P(\mathbf{r}) = i\omega\chi(\mathbf{r})\nabla\frac{\beta_0^2 w(\mathbf{r})-\beta^2(\mathbf{r})\rho(\mathbf{r})}{\omega_P^2(\mathbf{r})}$$

and $\mathbf{J}_P$ is inserted into Maxwell's equation as

$$\nabla\times\mathbf{H} = i\omega(\varepsilon_\infty+\chi)\varepsilon_0\mathbf{E}+\mathbf{J}_P$$

The two dependent variables $w(\mathbf{r})$ and $\rho(\mathbf{r})$ approach sufficiently zero at the exterior boundary of the cylindrical structure. These BCs are utilized when deriving weak forms. As for the enforcement of boundary conditions, I'm not quite sure which ones are proper to ensure a unique solution.

My major problem is how to solve the model. I tried many solvers in COMSOL 4.3a and all failed (see below).

MUMPS: Convergence cannot be achieved. The estimated error is large and the solution doesn't look reasonable.
Pardiso: Since singular matrix occurs, the model can't be solved with Pardiso solver.
Spooles: Internal error. Returned solution not converged.

Since MUMPS seems a choice to solve the model, is it possible to improve the results from MUMPS solver?

According to the error message from Pardiso solver, the model has a singular stiffness matrix. This may be the cause of the problem. I searched around and found singular matrix can be due to improper boundary conditions or initial values. I'm curious about how initial values are used when solving a linear model with a direct solver. Some people told me initial values are only used for nonlinear, time dependent and iterative solvers, not for direct solvers. Then boundary condition is the reason for singular matrix. But how should I choose proper boundary conditions?

Thanks a lot!