HYPIC: A fast hybrid EM PIC-MCC code for ICRE in cylindrical coordinate system

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[M. Wu, A. Xu, C. Xiao, *HYPIC: A fast hybrid EM PIC-MCC code for ion cyclotron resonance energization in cylindrical coordinate system*, Computer Physics Communications **301**, 109207 (2024).]

Outline

- 1. HYPIC modelling
- 2. How to use HYPIC code
- 3. Optimization of HYPIC v1.1
- 4. Conclusions and discussions

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- **1. HYPIC modelling**
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HYPIC modelling

- **Motion of ions: PIC-MCC**

3D (x, y, z) Cartesian coordinate system

$$m\frac{d\boldsymbol{v}}{dt} = q\boldsymbol{E} + q\boldsymbol{v} \times \boldsymbol{B_0} + \boldsymbol{v}_{\mathrm{mcc}}$$

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}$$

$$\boldsymbol{E} = -\nabla\phi + \boldsymbol{E}_{mf}$$

Current carried by ions: Negligible (much less than electron current)

- **Motion of electrons: adiabatic fluid modeling**

The density and potential satisfy the Boltzmann distribution in 2D (r,z) column coordinate system

Suppressing the numerical instability caused by electrons and avoids the normalization of macroparticles

$$n_e m_e \frac{\partial \boldsymbol{u}_e}{\partial t} + m_e n_e (\boldsymbol{u}_e \cdot \nabla)\boldsymbol{u}_e = -\nabla p_e + e n_e (\nabla\phi - \boldsymbol{u}_e \times \boldsymbol{B}_0) - m_e n_e \nu_e \boldsymbol{u}_e \quad [m_e \to 0]$$

$$n_e = n_i$$

$$\nabla\phi = \frac{T_e \nabla n_e}{e n_e}$$

Current carried by electrons (EM response): cold plasma dielectric tensor

- **Adiabatic electron model: magnetic field term is negligible**

for example: $n_e = 2 \times 10^{13}\ \mathrm{cm}^{-3}, T_e = T_i = 10\ \mathrm{keV}, r_p = 0.1\ \mathrm{m}, v_e = 1.3 \times 10^3\ \mathrm{Hz}$

$$-\nabla p_e + en_e(\nabla\phi - \boldsymbol{u}_e \times \boldsymbol{B}_0) = 0$$

$$\nabla\phi - \boldsymbol{u}_e \times \boldsymbol{B}_0 = -\frac{\nabla p_e}{en_e}$$

Estimating magnitude perpendicular to the direction of the magnetic field:

$$\nabla_\perp\phi = -\frac{\nabla_\perp p_e}{en_e} \approx \frac{T_e}{er_p} = 10^5\ \mathrm{V/m}$$

$$B_0 \approx 1\ \mathrm{T}, u_{e\perp} \approx \frac{D_\perp}{r_p} \approx \frac{1}{0.1}\ \mathrm{m/s}:\ u_{e\perp}B_0 \approx 10\ \mathrm{V/m}$$

Conclusion: the magnetic field term in the adiabatic electron approximation is negligible.

HYPIC modelling

- **EM module: 3D RF antenna-plasma interaction**

Maxwell's equations in the frequency domain with a cold plasma response with collisions

$$\nabla(\nabla\cdot\boldsymbol{E}_{rf}) - \nabla^2\boldsymbol{E}_{rf} - \frac{\omega^2}{c^2}\overleftrightarrow{\varepsilon}\cdot\boldsymbol{E}_{rf} = i\omega\mu_0\boldsymbol{J}_a$$

where

$$\overleftrightarrow{\varepsilon} = \begin{bmatrix} \frac{B_{0z}^2}{B_0^2}K_\perp + \frac{B_{0r}^2}{B_0^2}K_\parallel & -\frac{B_{0z}}{B_0}iK_\phi & \frac{B_{0z}B_{0r}}{B_0^2}(K_\parallel - K_\perp) \\ iK_\phi\frac{B_{0z}}{B_0} & K_\perp & -iK_\phi\frac{B_{0r}}{B_0} \\ \frac{B_{0z}B_{0r}}{B_0^2}(K_\parallel - K_\perp) & i\frac{B_{0r}}{B_0}K_\phi & \frac{B_{0z}^2}{B_0^2}K_\parallel + \frac{B_{0r}^2}{B_0^2}K_\perp \end{bmatrix}$$

$$K_\perp = 1 - \sum_{l=i,e}\frac{\widetilde{\omega}_{pl}^2}{\omega^2 - \omega_{cl}^2}, K_\phi = \sum_{l=i,e}\frac{\widetilde{\omega}_{pl}^2\widetilde{\omega}_{cl}}{\omega(\omega^2 - \widetilde{\omega}_{cl}^2)}, K_\parallel = 1 - \sum_{l=i,e}\frac{\widetilde{\omega}_{pl}^2}{\omega^2},$$

$$\widetilde{\omega}_{pl} = \sqrt{q_l^2 n_l/(\varepsilon_0 m_l^\nu)}, \widetilde{\omega}_{cl} = q_l B_0/m_l^\nu, m_l^\nu = m_l\left(1 + i\frac{\nu_l}{\omega}\right), \boldsymbol{J}_a = \sum_{-\infty}^{\infty}\boldsymbol{J}_{am}(r,z,t)\exp(-im\theta)$$

2D (r,z) column coordinate system with Fourier transform on azimuthal component

[This module was developed by Andong Xu]

HYPIC modelling

- **Summary of governing equations**

$$m\frac{d\boldsymbol{v}}{dt} = q\boldsymbol{E} + q\boldsymbol{v}\times\boldsymbol{B_0} + \boldsymbol{v}_{\mathrm{mcc}}$$

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}$$

$$n_e = n_i$$

$$\boldsymbol{E} = -\nabla\phi + \boldsymbol{E}_{mf}$$

$$\frac{3}{2}\frac{\partial}{\partial t}(nT_e) + \nabla\cdot\boldsymbol{q}_e = p_p + nQ_{ie}$$

$$\nabla(\nabla\cdot\boldsymbol{E}_{rf}) - \nabla^2\boldsymbol{E}_{rf} - \frac{\omega^2}{c^2}\overleftrightarrow{\varepsilon}\cdot\boldsymbol{E}_{rf} = i\omega\mu_0\boldsymbol{J}_a$$

$$\frac{\partial}{\partial t}(nT_e) = -\frac{2}{3k}\nabla\cdot\boldsymbol{q}_e + \frac{2}{3k}p_p + \frac{2}{3k}nQ_{ie}$$

Suitable for axisymmetric background magnetic field ($B_\theta = 0$) , and 3D RF antennas

HYPIC v1.0 : without purple terms

HYPIC v1.1 : with purple terms

HYPIC modelling: numerical method

- **PIC module**

Ions moving in 3D Cartesian coordinate system (3D3V), time step pushing in RK4 format

The background magnetic field is obtained by numerically solving $\nabla \times \boldsymbol{B_0} = \mu \boldsymbol{J}$ using iterative method

Interpolation between particles and fields: linear interpolation

Typical number of particles: 100 000

- **MCC module**

Using Nanbu's method, with the idea of grouping small-angle binary collisions in plasmas into a unique binary collision with a large scattering angle

- **code verification**

Details in ref. [M. Wu, A. Xu, C. Xiao, Computer Physics Communications 301, 109207 (2024)]

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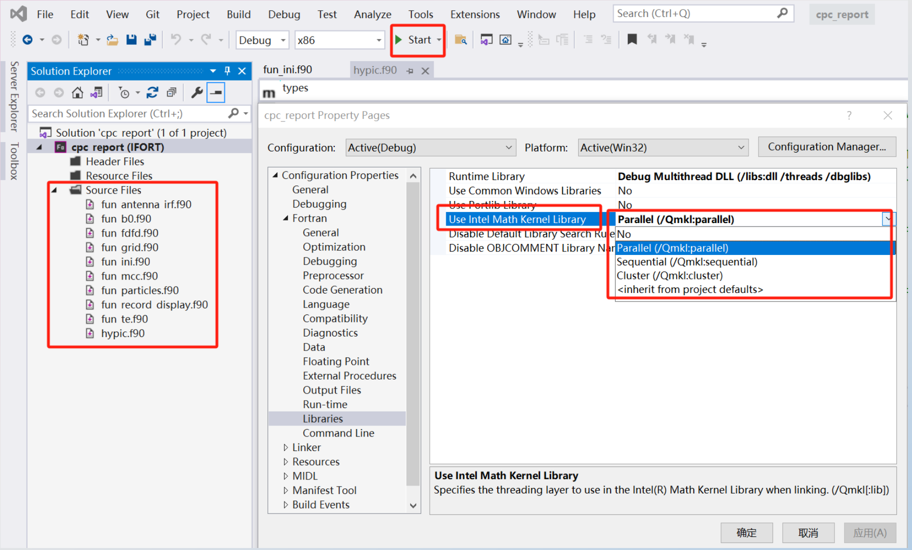
How to use HYPIC code

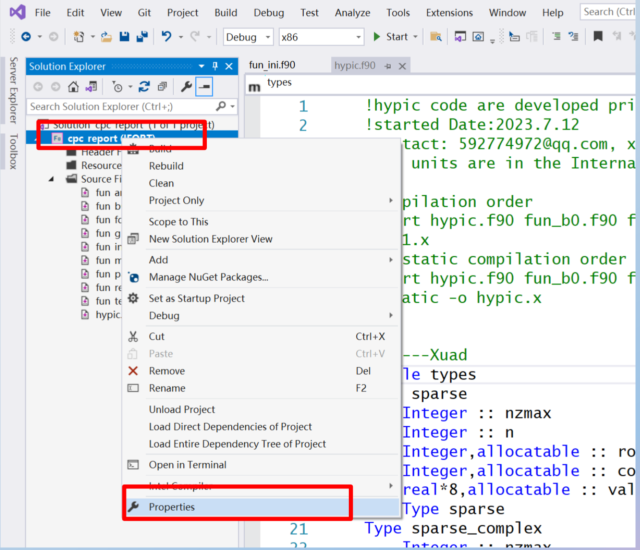
- **Visual studio in Windows (Fortran compiling with MKL library)**

(1) Create a new empty f90 project and include all the f90 files to 'Source Files' (see left figure)

(2) set 'Project'->'Properties'->'Fortran'->'Libraries'->'Use Intel Math Kernel Library'->'Parallel(/Qmkl:parallel)' (see right figure)

(3) run 'start'





How to use HYPIC code

- **ifort compiler in linux**

(1) Go to the folder where the codes are located and input the compiling command

>>ifort hypic.f90 fun_b0.f90 fun_record_display.f90 fun_grid.f90 fun_ini.f90

fun_antenna_irf.f90 fun_particles.f90 fun_mcc.f90 fun_fdfd.f90 fun_te.f90 -mkl -o hypic.x

(2) Run HYPIC

#insure iswitch_display= 1, display the running state on screen

./3-1.x

or

#insure iswitch_display= 0, display nothing when running, suitable for backstage running

./3-1.x &

```
wumy@cjxiao-Precision-Tower-7910:~$ cd hypic/
wumy@cjxiao-Precision-Tower-7910:~/hypic$ ifort hypic.f90 fun_b0.f90 fun_record_display.f90  fun_grid.f90 fun_ini.f90 fun_antenna_irf.f90 fun_particles.f90
fun_mcc.f90 fun_fdfd.f90 fun_te.f90 -mkl -o hypic.x
wumy@cjxiao-Precision-Tower-7910:~/hypic$ ./hypic.x
 the background_B0 subroutine is running ......
 mr,mz=         151          601
 iteration number is         52737
 the background_B0 subroutine is finished.
 Fun_ini finished. Fun_fdfd is running.
 Main loop is running.
```

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Optimization of HYPIC v1.1

- **Compared to HYPIC v1.0, this release (v1.1) has the following upgrades**

(1) The electron temperature evolution equation is introduced to describe the electron temperature more reasonably.

(2) Added the power-mode antenna. User can set the total power of the antenna.

(3) Multiple types of ions can be used at the same case.

(4) 0-2 RF frequencies can be used at the same case.

(5) The axial origin (z=0) was moved from the left end of the magnetic mirror to the center of the magnetic mirror.

(6) Optimized the antenna current mode.

(7) Automatic selection of the appropriate time step, according to the nature of energy conservation (loss <1%) in the RK4 format.

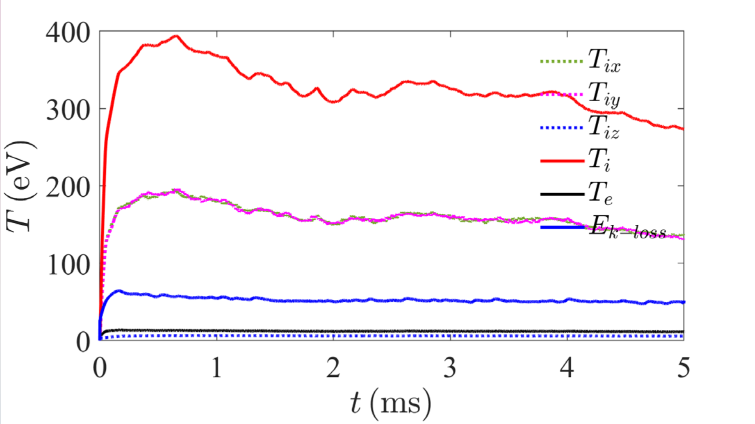
(8) Optimized the plotting code (in matlab language).

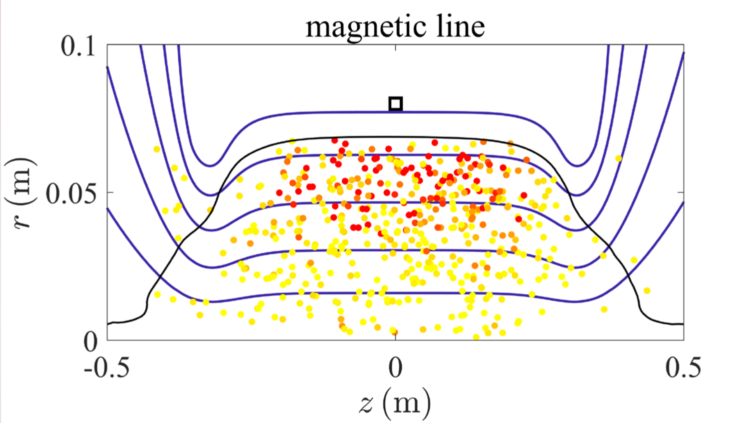
Please note: these improvements increase the computational effort. The latest version of HYPIC can be seen in https://github.com/DrMYWu

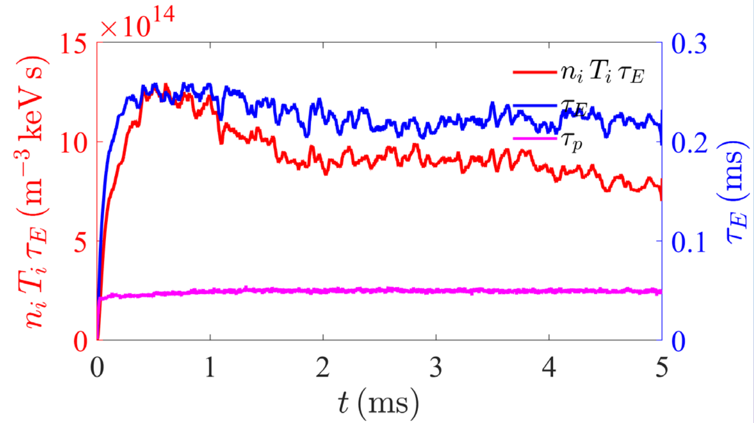
Numerical results of HYPIC v1.1

- **The ICRE process in a magnetic mirror**

parameters	value
ion	H^+
RF frequency f	13.56 MHz
resonant magnetic fieldB_0	0.89 T
plasma density n_e	10^{19} m^{-3}
power	~10 kW
Equivalent antenna resistance R_a	0.1 Ω







Numerical results of HYPIC v1.1

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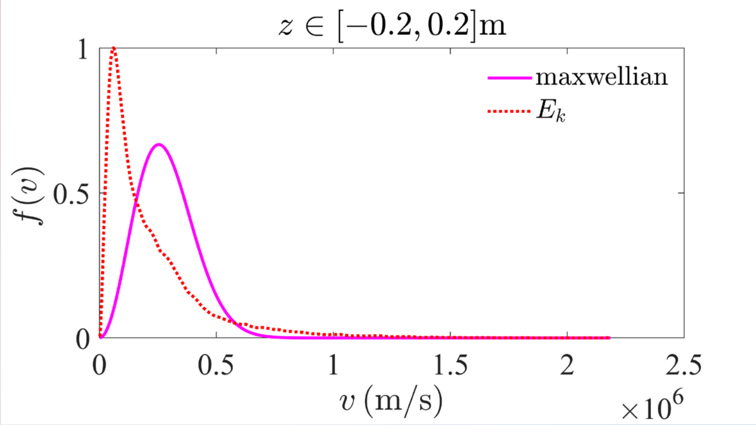

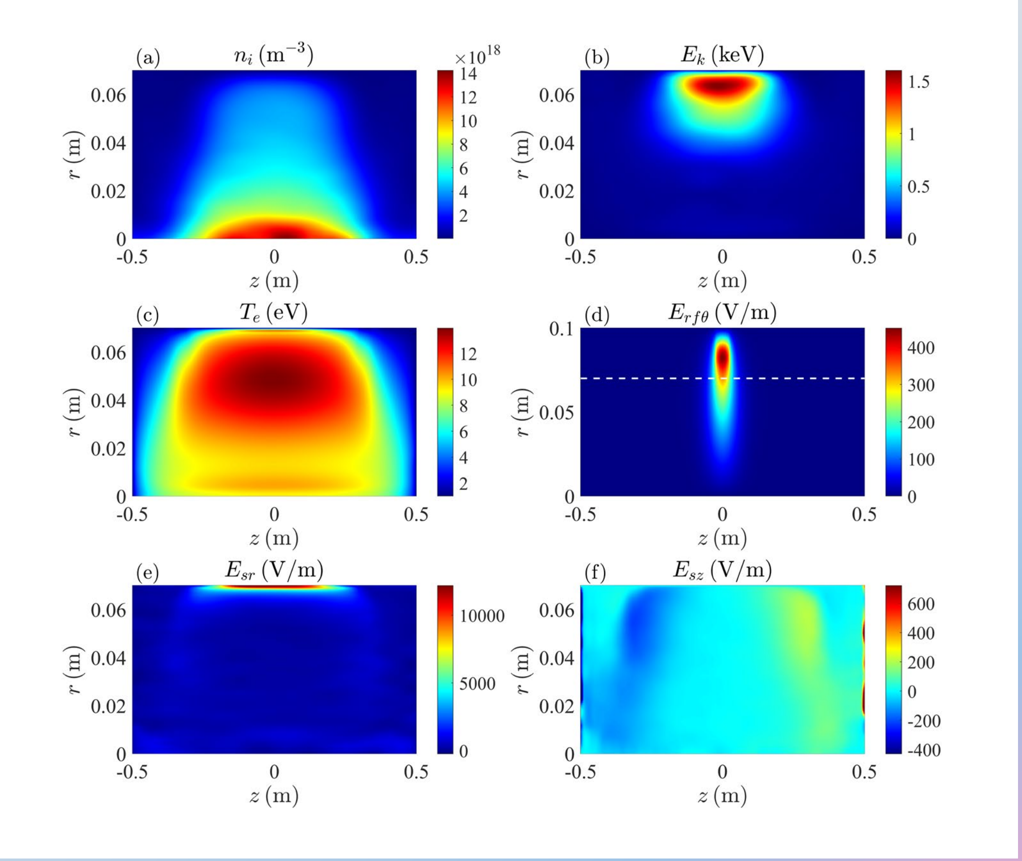

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Conclusions and discussions

- **HYPIC code are able to fast simulate the antenna-plasma interactions and the ICRE processes in linear devices, such as high-power electric propulsion, magnetic mirror, and FRC, etc.**
- **inclusion of the kinetic effects of ions, the ES and EM effects, the collisions between ions and electrons, and with a small computation.**
- **In HYPIC v1.1, we have made several optimizations, in particular the introduction of the electron temperature evolution equation.**

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The latest version of HYPIC can be seen in https://github.com/DrMYWu

Thanks！