Parallelization of a 3D FDTD code and physics studies of EC heating and current drive in fusion plasmas

C. Tsironis
A. Papadopoulos
M. Martone

School of Electrical and Computer Engineering
National Technical University of Athens
Athens, Greece
The wave – plasma physical system

**Wave**

- Solution of the wave equation
  - Asymptotic methods
  - Ray tracing
  - QO/pWKB beam tracing
  - Full-wave methods
  - Spectral/Pseudospectral
  - Finite differences
  - Finite elements

**Plasma**

- Computation of the plasma response
  - Macroscopic description
  - Effective dielectric tensor
  - EM fluid equations
  - Microscopic description
  - Fokker-Planck equation
  - Vlasov/Kinetic equation
  - Particle motion tracing

**Model coupling**

- Uncoupled
  - Solve separately each model equations

- Quasi-self-consistent
  - Solve separately each model equations & couple the results

- Self-consistent
  - Solve coupled system of model equations

- Absorption & driven current
- Instabilities & radiation
EC wave (beam) propagation in plasma

- The wave equation describes EM propagation in plasmas
  - Full problem solution: Extremely hard!
    - Wave equation → Inhomogeneous PDE
    - Dynamic equation for plasma current?
  - Numerical solution of PDEs?
    - Resource-demanding code execution!!!
    - Spatial grid progressing onto temporal grid

- Approximate solution given by asymptotic methods
  - Ray tracing (geometrical optics): Propagation described in analogy with particle dynamics (momentum → wave-vector, energy → frequency).
  - Quasi-optical beam tracing: Wave-vector generalized to include an imaginary part related to the transverse beam electric field profile.
  - Paraxial WKB beam tracing: Beam trajectory identified as a GO ray & described by scalar functions for the amplitude, width and curvature.

- Advanced EC codes are based on asymptotic methods
Need for full-wave methods???

- The approximations present in asymptotic methods break down in several cases of practical interest:
  - ① $\lambda \ll \max(\text{inhomogeneity scale})$ • ② $T \ll \max(\text{transients scale})$
  - Hot plasma dispersion, mode conversion, steep plasma gradients etc.
  - *Alternative* → Full-wave methods (albeit computationally expensive…)

- **Option:** Finite Difference Time Domain (FDTD) method
  - Maxwell’s curl equations transformed to *central finite-differences*.
  - **Spatial grid:** Placement of the electric & magnetic field vectors on *interlinked contours* in order to have Maxwell’s divergence equations as *valid by identity*.
  - **Temporal grid:** The electric field is computed at a given time instant, then the magnetic field is computed at the next time instant and so on (*leapfrog integration scheme*).
The code **RFFW** (Radio Frequency Full Wave)

- **Numerical FDTD solver for the propagation of EM waves with generic electric field profile in arbitrary plasmas:**
  - 1D/2D/3D propagation grid (optimal choice ↔ based on the problem)
  - Scattered field formalism (separation of incident & response EM field)
  - Cold/Warm/Hot plasma dielectric response (time-domain current density equation vs frequency-domain “effective” dielectric tensor)
  - Arbitrary plasma geometry (fusion device equilibria, space plasmas, …)
  - Generic wave/beam geometry (plane wave, Gaussian beam, …)
  - Various boundary condition schemes (conducting, absorbing,…)

- **Example: Plane wave @ 1D hot plasma (AUG parameters)**
  - $R_{\text{tor}} = 1.65 \text{ m}$ ● $r_{\text{pol}} = 0.6 \text{ m}$
  - $B_{\text{tor}} (x = 0) = 2.5 \text{ T}$
  - $n_e = [1.4, 1.6] \cdot 10^{13} \text{ cm}^{-3}$
  - $T_e = [0.2, 2] \text{ KeV}$
  - $f = 140 \text{ GHz}$ (mode X2)
  - $P_0 = 1 \text{ MW}$

\[
\omega_{de}(x) = \frac{\omega_{de}|_{z=0}}{1 + \frac{x}{r_{\text{tor}}}}
\]

\[
\omega_{pe}^2(x) = \omega_{pe}^2|_{z=0} + \left( \omega_{pe}^2|_{z=r_{\text{pol}}^2} - \omega_{pe}^2|_{z=0} \right) \left( \frac{x}{r_{\text{pol}}} \right)^2
\]

\[
v_{\text{ce}}(x) = v_{\text{ce}}|_{z=0} + \left( v_{\text{ce}}|_{z=r_{\text{pol}}}^2 - v_{\text{ce}}|_{z=0} \right) \left( \frac{x}{r_{\text{pol}}} \right)^2
\]

- **1.** Dynamic evolution of the x-component of the electric field ● **2.** Spatial profile of the electric field amplitude
Inside RFFW: FDTD formalism

- **Scattered field formalism:** *Separation of EM wave field*
  - \( \mathbf{E}_t = \mathbf{E}_i + \mathbf{E}_s \)  
    
    \[ [\text{Total field}] = [\text{Incident field}] + [\text{Scattered field}] \]
  - **Incident field:** EM field as in absence of the medium (i.e. in vacuum)
  - **Scattered field:** Generated by the medium in response to incident field

- **Discretized FDTD equations:**
  \[
  \nabla \times \mathbf{E}_s = -\mu_0 \frac{\partial \mathbf{H}_s}{\partial t} \quad \Rightarrow \quad H_{qs}^{n+1/2}_{i,j,k} = H_{qs}^{n-1/2}_{i,j,k} - \frac{\Delta t}{\mu_0 \Delta l} \psi_q [\mathbf{E}_s]^n_{i,j,k} \\
  \nabla \times \mathbf{H}_s = \delta \mathbf{E}_s + \frac{\varepsilon}{\varepsilon_0} \frac{\partial \mathbf{E}_s}{\partial t} + \bar{\delta} \mathbf{E}_i + \left( \bar{\varepsilon} - \varepsilon_0 \bar{l} \right) \frac{\partial \mathbf{E}_i}{\partial t} \quad \Rightarrow \quad E_{qs}^{n+1}_{i,j,k} = \sum_{l=1}^3 \sum_{m=1}^3 \alpha_{ql} E_{ms}^{n}_{i,j,k} + \psi_q [\mathbf{H}_s]^{n+1/2}_{i,j,k} \\
  - \sigma_{lm} E_{mi}^{n+1/2}_{i,j,k} - (\varepsilon_{lm} E_{mi}^{n+1/2}_{i,j,k} - \varepsilon_0 \delta_{lm}) \frac{\partial E_{mi}}{\partial t}^{n+1/2}_{i,j,k} \}
  \\

- **Boundary conditions:**
  - Provision of the “missing” nearest-neighbour grid components for the boundary EM field evaluation.
  - Several options of FDTD BC schemes:
    - Outer radiating \( E_{z0}^{n+1} = -E_{z0}^{n-1} + \frac{c \Delta t - \Delta x}{c \Delta t + \Delta x} (E_{z0}^{n+1} + E_{z0}^{n-1}) + \frac{2 \Delta x}{c \Delta t + \Delta x} (E_{z0}^{n} + E_{z0}^{n}) \)
    - Absorbing boundary
      \[
      \frac{\partial E_{zc}}{\partial y} + \frac{\partial E_{zc}}{\partial z} + \psi_{zc} - \psi_{zc} = -\frac{\partial H_{zc}}{\partial t} - (\mu - \mu_0) \frac{\partial H_{zc}}{\partial t} + \psi_{zc}^{n+1/2}_{i+1/2,j,k} = b_{xj} \psi_{zc}^{n+1/2}_{i+1/2,j,k} + \mu_{xj} \frac{\partial E_{zc}}{\partial y}^{n+1/2}_{i+1/2,j,k} 
      \]
Inside RFFW: Medium formalism

- Availability of different response models to EM waves depending on the plasma kinetic state:

  **Cold plasma**  
  Non-relativistic, inhomogeneous, anisotropic & linear plasma  
  Current equation in time domain

  \[
  \frac{\partial \mathbf{J}}{\partial t} = \varepsilon_0 \omega_p^2 (r, t) \mathbf{E} + \omega_c \times \mathbf{J}
  \]

  **Hot plasma**  
  Weakly-relativistic, inhomogeneous, anisotropic & linear plasma dielectric tensor in frequency domain

  \[
  \varepsilon = \mathbb{1} + \frac{\omega_p^2}{\omega} \sum_{l=-\infty}^{\infty} \int \frac{1}{\omega - k_{||} v_{||} - \text{Im} \omega} \left[ \begin{array}{ccc}
  \frac{\beta_p}{\beta_\perp} & \frac{J_{\perp}^2 p_{\perp}}{J_{\perp}^2} & \frac{J_{\perp}^2 p_{\perp}}{J_{\perp}^2 p_{||}} \\
  \frac{\beta_\perp}{\beta_p} & \frac{J_{\perp}^2 p_{||}}{J_{\perp}^2} & \frac{J_{\perp}^2 p_{||}}{J_{\perp}^2} \\
  \frac{J_{\perp}^2 p_{||}}{J_{\perp}^2} & \frac{J_{\perp}^2 p_{||}}{J_{\perp}^2} & \frac{J_{\perp}^2 p_{||}}{J_{\perp}^2}
  \end{array} \right] d^3 \mathbf{p}
  \]

- Axisymmetric model for the magnetic field:

  \[
  \mathbf{B} = B_t \mathbf{e}_\phi + B_p \mathbf{e}_\theta
  \]

  \[
  B_t (r, \theta) = \frac{B_0}{1 + \epsilon_A (r) \cos \theta} \quad B_p (r, \theta) = \frac{\epsilon_A (r)}{q (r)} B_t (r)
  \]

  **Profile parameters:** Aspect ratio & safety factor

  - **Inverse aspect ratio:** \( \epsilon_A (r) = r/R_0 \)
  - **q-profile:** \( q(r) = q_{\text{min}} + (q_{\text{max}} - q_{\text{min}}) \cdot r^2/\alpha^2 \)

- Inclusion of non-axisymmetric perturbations (e.g. magnetic islands):

  - \( \mathbf{B} \) defined by flux functions *(Clebsch formalism)*

  \[
  \mathbf{B} = \nabla \psi_t \times \nabla \theta - \nabla \psi_p \times \nabla \phi
  \]
Need for code parallelization!!

- The serial version of RFFW comes with very important computational limitations!
  - Non-fusion plasma: Realistic simulation times & memory requirements.
    - Plasma density << Average densities of medium-sized tokamaks.
    - Plasma dimensions << Average medium-size tokamaks poloidal radius.
  - Without multi-core exploitation & distributed memory parallelism, the code cannot handle problems that involve ITER-sized plasmas.
    - *Cases relevant to fusion:* CPU time ~ 20-180 days, RAM ~ 32-96 GB.

- Apply hybrid parallelization scheme (coordinated by EUROfusion HLST)
  - Analysis of grids type & code variables
    - Staggered vs collocated grids?
    - Annotate to-be-affected code variables.
  - *OpenMP workload partitioning*
    - Introduction of shared memory constructs.
  - *MPI data & workload partitioning*
    - Based on ghost & boundary cell exchange communication primitives.
    - Implemented in separate code module.
Step #1: Identify grids type & the impacted variables

- RFFW uses *staggered* grids → Advantage!!!
  - Scalar and vector variable computations may be “coupled”.
  - Avoidance of singularities & convergence problems is easier.
- Some variables & indices have to be pertained to the local domain only.

Step #2: OpenMP primitives

- Different portions of the grid space get updated *in parallel*.
  - Many threads per array copy.
- Introduce *thread local* (private) variables where required.
  - Declared bounds remain *global*
**Hybrid parallelization: MPI**

- **Step #3a: MPI data management**
  - **Transition from global to local structures:**
    - Introduction of process local subdomains (subsets of the global one).
    - Replace local loop indices with global ones (in order to optimize loop iterations).
  - **Optimize boundary condition routines:**
    - Retain code via preprocessor conditionals.

  ```plaintext
  Example:
  orbcexsz1: do ix=lx,lx+1,1
  kx1T0R.Typ.1 ct1=ct1+xszl(1x,1)+...
  kx1T0R.Typ.2 ct1=ct1+xszl(1x,3)+...
  end do orbcexsz1
  ```

- **Step #3b: MPI communication**
  - **Ghost/boundary cell exchanges.**
    - Required in finite difference schemes at the vicinity of the grid boundaries.
    - Direction: From owner task to neighbors.
    - Realization with command MPI Sendrecv().
Tests for parallel code strong scaling

- **Tests performed @ HELIOS supercomputer:**
  - Fortran module → *intel/15.0.2.164*
  - Cluster module → *oscar-modules/1.0.3 srn/1.0*
  - MPI Modules → *bullxmpi/1.2.8.4 vs intelmpi/5.0.3.048*
  - Studied 3 different cases (wrt grid size and number of steps to termination) by scaling MPI parallelism:
    - Case 1 → max_helios_node (7128 x 7128 cells)
    - Case 2 → 3564 x 3564 cells (Case 1/4)
    - Case 3 → 1782 x 1782 cells (Case 1/16)

- **General assessment & comments of the results:**
  - Max 2500x code acceleration in the largest parallel run.
  - Intel's MPI occurred to be consistently slightly faster (< 5%) than Bull's.
  - OpenMP scaling of ≈ 12x on one node, ≈ 8x (of max 16x) for the largest case on many nodes.
  - With message passing off, super-linear scaling is achieved.
    - Likely due to the case fitting in the last level cache.
    - In these cases, OpenMP scaling is reduced (e.g. < 8x).
Strong scaling results

- **Total projected runtime & timestep computation time:**
  - *max helios node case:* ~380d serial; ~35d OpenMP; ~5h hybrid!!
  - Smallest case saturates @ 256nodes (113^2 cells/node, 28^2 cells/thread).

- **Speedup & scalability:**
  - Speedup increases wrt the grid size (in the range 80x to 200x).
  - Scalability reduces as a function of the grid size.
**Numerical results: Cold plasma**

- **2D propagation of Gaussian beam in cold plasma @ AUG**
  - *Device parameters:* \(r_{\text{tor}} = 1.65 \text{ m}, r_{\text{pol}} = 0.6 \text{ m}, B_0 = 2.5 \text{ T}.\)
  - *Plasma parameters:* \(n_e = [1.4, 1.6] \cdot 10^{13} \text{ cm}^{-3}, T_e = 0 \text{ KeV}, q = [1, 4].\)
  - *Beam parameters:* \(f = 140 \text{ GHz (mode X2)}, w_0 = 4 \text{ cm}, P_0 = 1 \text{ MW}.\)

- **Visualization of the EC beam electric field amplitude:**

- **Result:** Focused beam propagation with no power losses
  - Beam reaches its minimum width (*waist*) \(\approx 0.5w_0\) near \(0.5 \cdot r_{\text{pol}}.\)
  - Cold plasma → No EC absorption mechanism → No power damping.
Numerical results: Hot plasma

- **3D propagation of plane wave in hot plasma @ TCV**
  - *Device parameters*: \( r_{\text{tor}} = 0.88 \text{ m}, \quad r_{\text{pol}} = 0.25 \text{ m}, \quad B_0 = 1.44 \text{ T}. \)
  - *Plasma parameters*: \( n_e = [0.5, 1] \cdot 10^{13} \text{ cm}^{-3}, \quad T_e = [0.2, 2] \text{ KeV}, \quad q = [1, 4]. \)
  - *Wave parameters*: \( f = 118 \text{ GHz (mode X3)}, \quad w_0 = \infty, \quad P_0 = 0.5 \text{ MW}. \)

- **Plots of the EC wave power damping & generated current:**
  1. Wave power variation along propagation
  2. Spatial profile of generated electric current

- **Result:** Wave damping occurs at the EC resonance layer
  - Absorption begins near \( 0.5 \cdot r_{\text{pol}} \) and is relatively broad (width \( \approx 0.2 \cdot r_{\text{pol}} \)).
  - Electric current is generated as a consequence of wave damping.
Employ frequency-domain tensor in FDTD scheme

- Unavailability of the hot-plasma dielectric tensor in time-domain
- When is it inconsistent to use the frequency-domain tensor?
  - **Answer:** When both wave spectrum & plasma response depend on $k$
  - **OK:** Beam @ cold plasma, plane wave @ hot plasma
  - **Not OK (but case with practical interest...):** Beam @ warm/hot plasma

**Physically-consistent solution:** Convolution scheme for plasma response calculation

\[
\sigma(k, \omega; r, t) = \int d^3r' \int_0^\infty dt' \sigma(r', t'; r, t) e^{-ik\cdot r + i\omega t'}
\]

Implement a fully-inhomogeneous plasma tensor

- Based on inhomogeneous kinetic equation (Brunner & Vaclavic 1993)
  - Tensor operator contains the spatial derivatives of the distribution function
  - Plasma response → Convolution integral of tensor with the electric field
  - Small Larmor radius over wave field & plasma inhomogeneity