National Program of Controlled Thermonuclear Fusion
Association EURATOM - Hellenic Republic

EUROfusion
Horizon Europe

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


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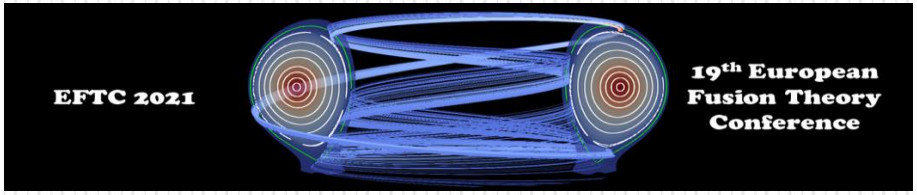


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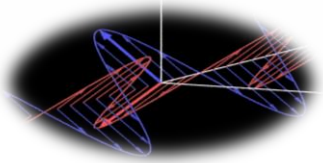
# The wave – plasma physical system

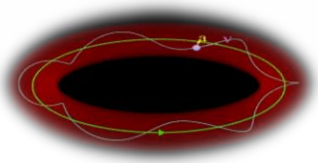
**Absorption & driven current**

**Wave** ⟶ **Plasma**

**Plasma** ⟶ **Wave**

**Instabilities & radiation**





***Model coupling***

## Wave modeling

*Solution of the wave equation*

Asymptotic methods
Ray tracing
QO/pWKB beam tracing

Full-wave methods
Spectral/Pseudospectral
Finite differences
Finite elements

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

## Plasma modeling

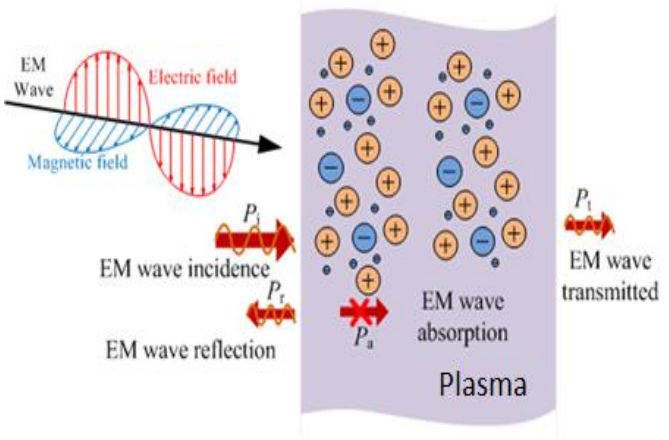
*Computation of the plasma response*

Macroscopic description
Effective dielectric tensor
EM fluid equations

Microscopic description
Fokker-Planck equation
Vlasov/Kinetic equation
Particle motion tracing

# 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



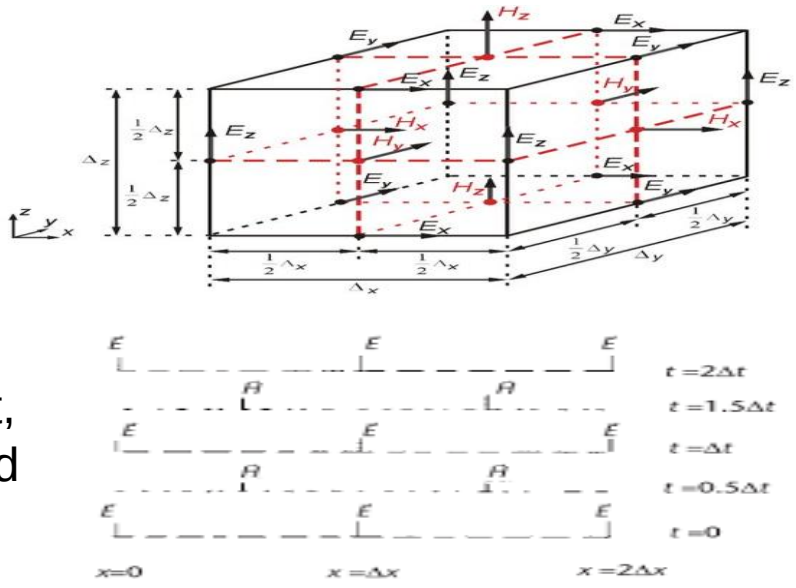

- **Approximate solution given by asymptotic methods**
  - *Ray tracing (geometrical optics):* Propagation described in analogy with particle dynamics (momentum → wave-vector, energy → frequency).
  - *Quasi-optical beam tracing:* Wave-vector generalized to include an imaginary part related to the transverse 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**
  - ***Approximations???*** Plasma stationarity, weakly-inhomogeneous plasma, cold plasma dispersion, linear & weakly-relativistic kinetics.

# *Need for full-wave methods???*

- **The approximations present in asymptotic methods break down in several cases of practical interest:**
  - ① $\lambda$ << *max(inhomogeneity scale)* ● ② $T$ << *max(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,…)
- **<u>Example:</u> Plane wave @ 1D hot plasma (AUG parameters)**

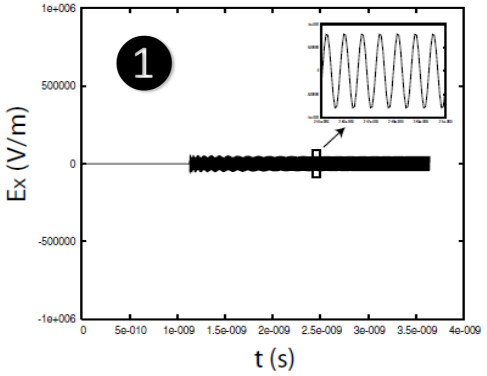
ASDEX Upgrade

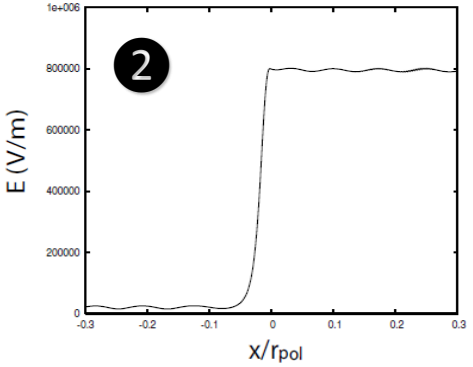
**$R_{tor}$** = 1.65 m ● **$r_{pol}$** = 0.6 m
**$B_{tor}$ (x = 0)** = 2.5 T
**$n_e$** = [1.4, 1.6] · $10^{13}$ $cm^{-3}$
**$T_e$** = [0.2, 2] KeV
**f** = 140 GHz (mode X2)
**$P_0$** = 1 MW

$$\omega_{ce}(x) = \frac{\omega_{ce}|_{x=0}}{1+\frac{x}{r_{tor}}}$$

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

$$v_{te}^2(x) = v_{te}^2|_{x=0} + \left(v_{te}^2|_{x=r_{pol}} - v_{te}^2|_{x=0}\right)\left(\frac{x}{r_{pol}}\right)^2$$




❶ Dynamic evolution of the x-component of the electric field ● ❷ Spatial profile of the electric field amplitude

# Inside RFFW: FDTD formalism

- **Scattered field formalism:** ***Separation of EM wave field***
  - $E_t = E_i + E_s$ ***[Total field] = [Incident field] + [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

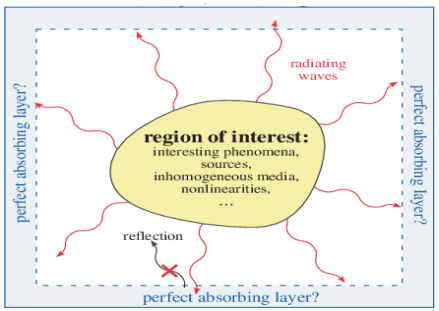
- ***Discretized FDTD equations:***

$$\nabla \times \mathbf{E_s} = -\mu_0 \frac{\partial \mathbf{H_s}}{\partial t} \Rightarrow H_{qs}\big|_{i,j,k}^{n+1/2} = H_{qs}\big|_{i,j,k}^{n-1/2} - \frac{\Delta t}{\mu_0 \Delta l}\psi_q\left[\mathbf{E_s}\big|_{i,j,k}^{n}\right]$$

$$\nabla \times \mathbf{H_s} = \bar{\bar{\sigma}}\mathbf{E_s} + \bar{\bar{\varepsilon}}\frac{\partial \mathbf{E_s}}{\partial t} + \bar{\bar{\sigma}}\mathbf{E_i} + \left(\bar{\bar{\varepsilon}} - \varepsilon_0 \bar{\bar{I}}\right)\frac{\partial \mathbf{E_i}}{\partial t} \Rightarrow$$

$$E_{qs}\big|_{i,j,k}^{n+1} = \sum_{l=1}^{3}\sum_{m=1}^{3}\alpha_{ql}\big|_{i,j,k}\left\{\tau_{lm}\big|_{i,j,k}E_{ms}\big|_{i,j,k}^{n} + \psi_q\left[\mathbf{H_s}\big|_{i,j,k}^{n+1/2}\right] - \sigma_{lm}\big|_{i,j,k}E_{mi}\big|_{i,j,k}^{n+1/2} - \left(\varepsilon_{lm}\big|_{i,j,k} - \varepsilon_0\delta_{lm}\right)\frac{\partial E_{mi}}{\partial t}\Big|_{i,j,k}^{n+1/2}\right\}$$

- **Boundary conditions:**
  - Provision of the “missing” nearest-neighbour grid components for the boundary EM field evaluation.
  - Several options of FDTD BC schemes:
    - Outer radiating ⇒ $E_z\big|_0^{n+1} = -E_z\big|_1^{n-1} + \frac{c\Delta t - \Delta x}{c\Delta t + \Delta x}\left(E_z\big|_1^{n+1} + E_z\big|_0^{n-1}\right) + \frac{2\Delta x}{c\Delta t + \Delta x}\left(E_z\big|_0^{n} + E_z\big|_1^{n}\right)$
    - Absorbing boundary ⇒ $\frac{1}{\kappa_y}\frac{\partial E_z^{sc.}}{\partial y} - \frac{1}{\kappa_z}\frac{\partial E_y^{sc.}}{\partial z} + \psi_{H_{x,y}}^{sc.} - \psi_{H_{x,z}}^{sc.} = -\mu\frac{\partial H_x^{sc.}}{\partial t} - (\mu - \mu_0)\frac{\partial H_x^{in.}}{\partial t}$ + $\psi_{E_{x,y}}^{sc.}\big|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} = b_{y_j}\psi_{E_{x,y}}^{sc.}\big|_{i+\frac{1}{2},j,k}^{n-\frac{1}{2}} + c_{y_j}\frac{\partial H_z^{sc.}}{\partial y}\Big|_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}}$



# 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*

$$\frac{\partial \mathbf{J}}{\partial t} = \boldsymbol{\varepsilon}_0 \boldsymbol{\omega}_\mathbf{p}^2(\mathbf{r},t)\mathbf{E} + \boldsymbol{\omega}_\mathbf{c} \times \mathbf{J}$$

**Hot plasma**

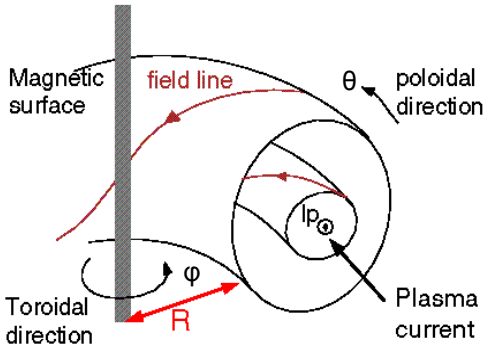
*Weakly-relativistic, inhomogeneous, anisotropic & linear plasma dielectric tensor in frequency domain*

$$\tilde{\epsilon} = \tilde{\mathrm{I}} + \frac{\omega_{pe}^2}{\omega} \sum_{l=-\infty}^{\infty} \int \frac{\frac{1}{\gamma p}\frac{df_0}{dp}}{\omega - k_{||}\mathrm{v}_{||} - \frac{l\omega_{ce}}{\gamma}} \begin{bmatrix} \frac{l^2}{\beta_j^2} J_l^2 p_\perp^2 & i\frac{l}{\beta_j} J_l J_l' p_\perp^2 & \frac{l}{\beta_j} J_l^2 p_{||} p_\perp \\ -i\frac{l}{\beta_j} J_l J_l' p_\perp^2 & J_l'^2 p_\perp^2 & -i J_l J_l' p_{||} p_\perp \\ \frac{l}{\beta_j} J_l^2 p_{||} p_\perp & i J_l J_l' p_{||} p_\perp & J_l^2 p_{||}^2 \end{bmatrix} d^3p$$

- **Axisymmetric model for the magnetic field:**

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

$$B_t(r,\theta) = \frac{B_0}{1 + \epsilon_A(r)\cos\theta} \qquad B_p(r,\theta) = \frac{\epsilon_A(r)}{q\,(r)} B_t(r)$$

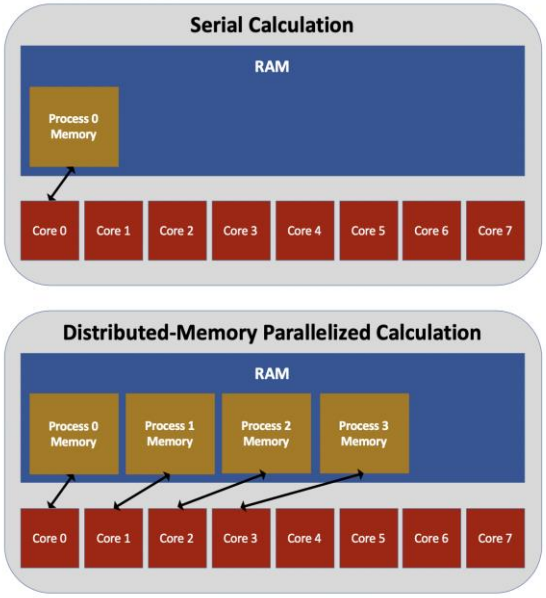



- *Profile parameters:* Aspect ratio & safety factor
  - *Inverse aspect ratio:* $\epsilon_A(r) = r/R_0$
  - q-profile: $q(r)=q_{min}+(q_{max}-q_{min})\cdot r^2/\alpha^2$
- Inclusion of non-axisymmetric perturbations (e.g. magnetic islands):
  - **B** defined by flux functions *(Clebsch formalism)* → $\mathbf{B} = \nabla\psi_t \times \nabla\theta - \nabla\psi_p \times \nabla\phi$

# *Need for code parallelization!!!*

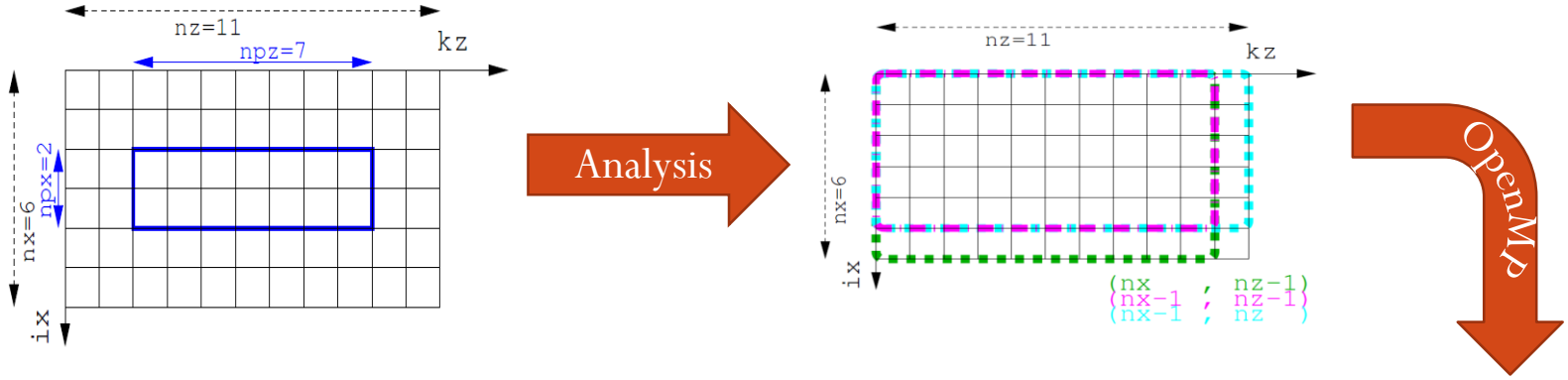
- **The serial version of RFFW comes with <u>very important computational limitations!</u>**
  - <u>Non-fusion plasma:</u> Realistic simulation times & memory requirements.
    - Plasma density << Average densities of medium-sized tokamaks.
    - Plasma dimensions << Average medium-size tokamaks poloidal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



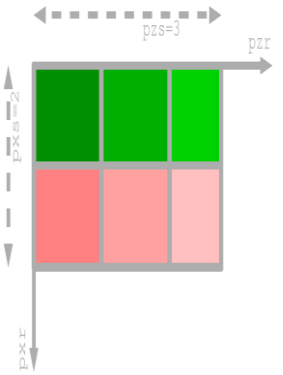
# Hybrid parallelization: Design & OpenMP

- **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

```
!$OMP PARALLEL DEFAULT(SHARED) PRIVATE
(ix,kz,...,exs_interp,...)
...
!$OMP DO SCHEDULE (STATIC)
eysloopz:  do kz=2,nz-1
!kz set by OpenMP on each thread
eysloopx:  do ix=2,nx-1
!ix ranging 2 to nx-1
...
eys(ix,kz)=exs_interp...+eys(ix,kz)*...
...
end do eysloopx
end do eysloopz
!$OMP END DO
...
!$OMP END PARALLEL
```



# 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).

EXAMPLE

```
do kz=npz_1,npz_2                do kz=lpz_1,lpz_2
do ix=npx_1,npx_2                do ix=lpx_1,lpx_2
 ...                              ...
end do                           end do
end do                           end do
```

  - *Optimize boundary condition routines:*
    - Retain code via preprocessor conditionals.

EXAMPLE

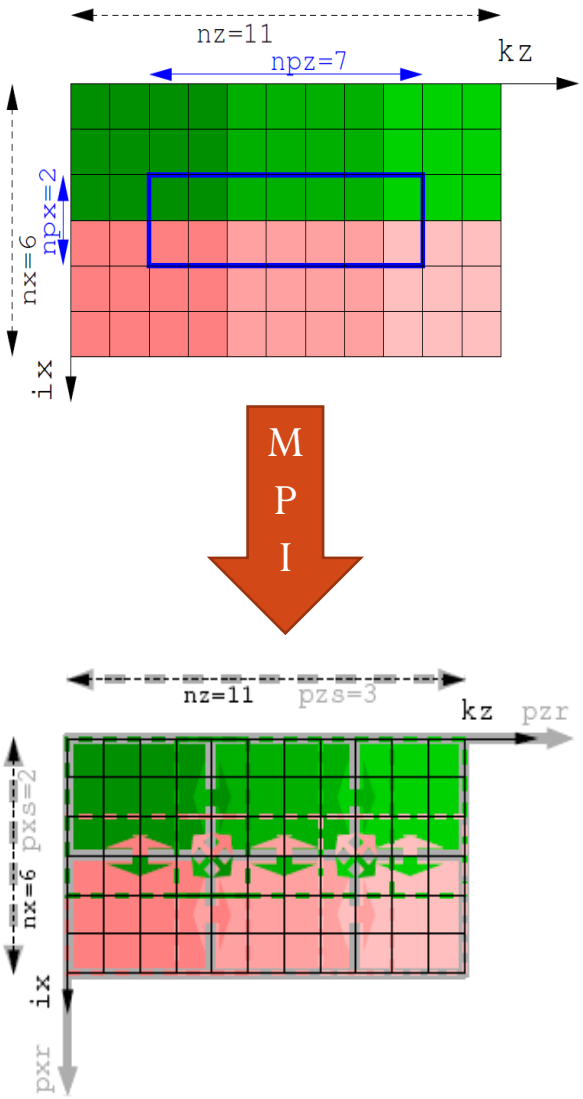
```
orbcexsz1:   do ix=lx_1,lxm_2,1
FWTOR_IF_Z_1 exs(ix,1)=exsz_1(ix,2)+...
FWTOR_IF_Z_2 exs(ix,nz)=exsz_1(ix,3)+...
end do orbcexsz1
```

- **Step #3b: MPI communication**
  - Ghost/boundary cell exchanges.
    - Required in finite difference schemes at the vicinity of the grid boundaries.

EXAMPLE

```
Problem: When e.g. pxr=1.AND.ix=lxp_1
eysloopz:   do kz=lzp_1,lzm_2
eysloopx:   do ix=lxp_1,lxm_2
 ...
exs_interp=0.5*(exs(ix-1,kz)+exs(ix,kz))
 ...
end do eysloopx
end do eysloopz
```

    - Direction: From owner task to neighbors.
    - Realization with command MPI Sendrecv().



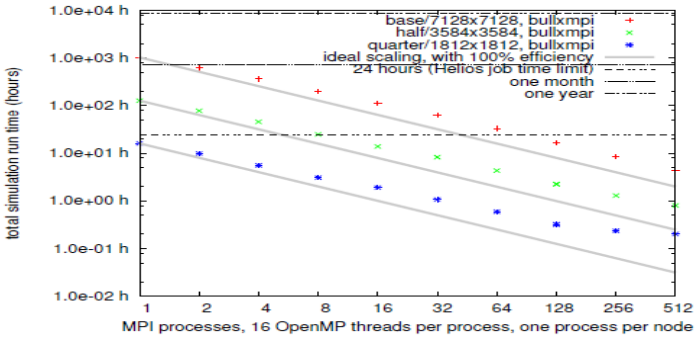
# Tests for parallel code strong scaling

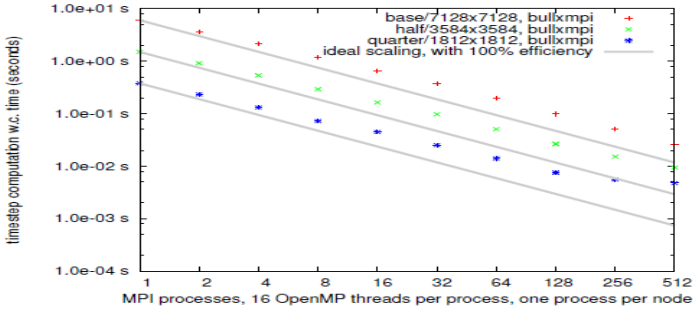
- **Tests performed @ HELIOS supercomputer:**
  - Fortran module → *intel/15.0.2.164*
  - Cluster module → *oscar-modules/1.0.3 srun/1.0*
  - MPI Modules → *bullxmpi/1.2.8.4 vs intelmpi/5.0.3.048*
  - Studied 3 different cases (wrt grid size and number of steps to termination) by scaling MPI parallelism:
    - 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).

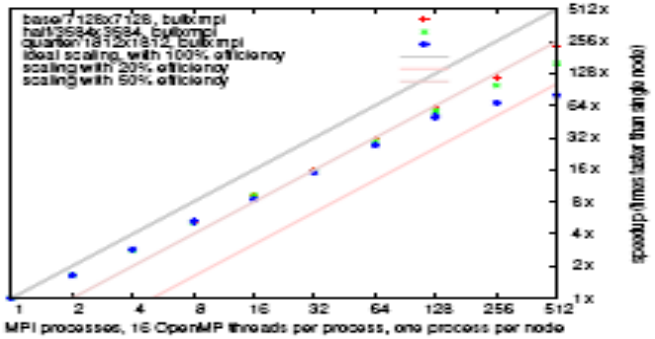
# Strong scaling results

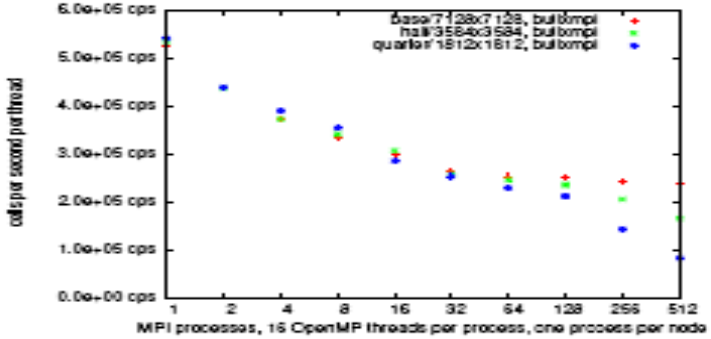
- **Total projected runtime & timestep computation time:**
  - *max_helios_node case:* ~380d serial; ~35d OpenMP; ~5h hybrid!!!
  - Smallest case saturates @ 256nodes ($113^2$ cells/node, $28^2$ cells/thread).



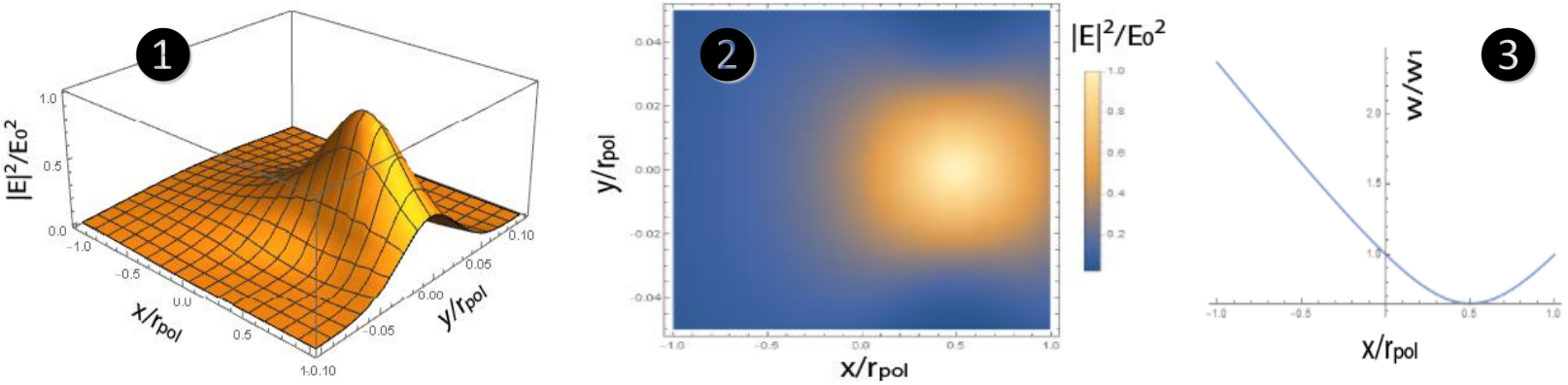

- ***Speedup & scalability:***
  - Speedup increases wrt the grid size (in the range 80x to 200x).
  - Scalability reduces as a function of the grid size.



# Numerical results: Cold plasma

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

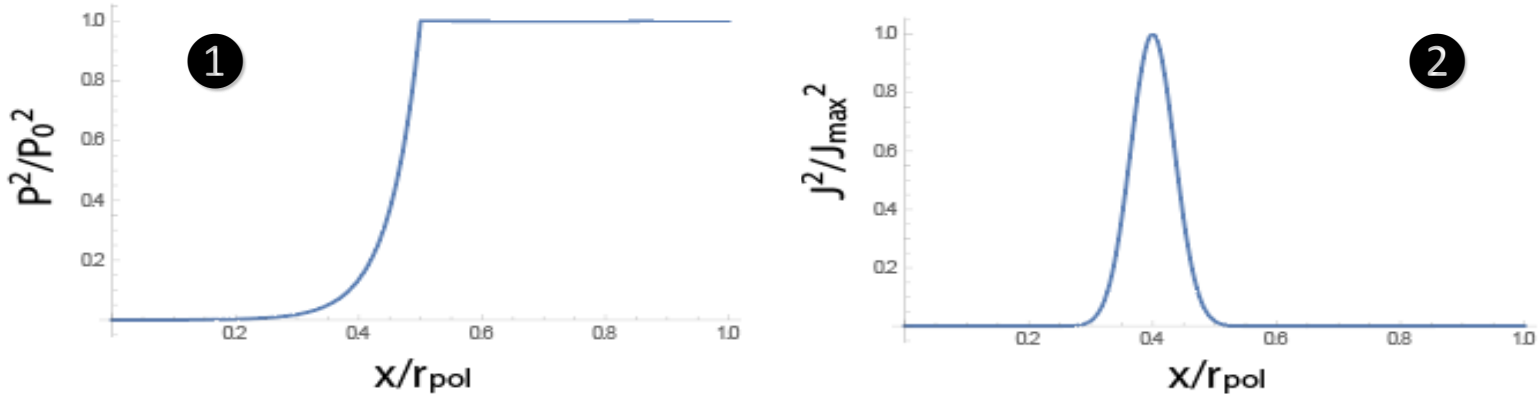



❶ Surface plot of electric field amplitude • ❷ Electric field amplitude contours • ❸ Width variation along propagation

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

# Numerical results: Hot plasma

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




❶ Wave power variation along propagation • ❷ Spatial profile of generated electric current

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

# *Improvements & future work*

- **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 $\tilde{\epsilon}(\mathrm{r},t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\tilde{\epsilon}(\mathrm{r},\omega_0)e^{-i\omega' t}d\omega'=\tilde{\epsilon}(\mathrm{r},\omega_0)\delta(t)$
    - *Not OK (but case with practical interest…):* Beam @ warm/hot plasma
  - *Physically-consistent solution:* Convolution scheme for plasma response calculation $\boldsymbol{\sigma}(\mathbf{k},\omega;\mathbf{r},t)\equiv\int d^3\mathbf{r}'\int_0^{\infty}dt'\;\boldsymbol{\sigma}(\mathbf{r}',t';\mathbf{r},t)e^{-i\mathbf{k}\cdot\mathbf{r}'+i\omega t'}$
- **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

$$\begin{aligned}
\epsilon^{(1)}_{nn} &= \epsilon^{(1)}_{bb}=\frac{k_\varphi}{2\omega\Omega b_p}\left\{\nabla'_n\left[\frac{\partial}{\partial\Omega}(Z_1-Z_{-1})-\frac{1}{\omega}(Z_1+Z_{-1})\right]\right\}\\
&\quad+\frac{K}{2}\left[X_1+X_{-1}+4+\lambda\frac{\Omega}{\omega}(W_1-W_{-1})\right],\\
\epsilon^{(1)}_{nb} &= -\epsilon^{(1)}_{bn}=\frac{i}{b_p}\left\{\nabla'_n\left[B_{n\|}+\frac{k_\varphi}{2\omega^2\Omega}(Z_{-1}-Z_1)\right]\right\}\\
&\quad+i\frac{K}{2}\left[X_1-X_{-1}+\lambda\frac{\Omega}{\omega}(W_1+W_{-1}-\frac{2}{\lambda})\right],\\
\epsilon^{(1)}_{\|\|} &= \frac{1}{\Omega b_p}\left(\nabla'_n\frac{\partial\tilde{Z}_0}{\partial k_\varphi}\right)+2K\left(\frac{\omega}{k_\varphi v_{th}}\right)^2\left[\lambda(Y_0-Y_0^\lambda)-\left(\frac{\omega}{k_\varphi v_{th}}\right)^2 Y_0+1\right]
\end{aligned}$$

$$\begin{aligned}
\epsilon^{(1)}_{n\|} &= B_{b\|}\left(\nabla_p+\beta_{\|n}\right)+iB_{n\|}\left(\nabla_n-\beta_{\|b}\right)\\
&\quad+\frac{2}{\Omega}\left[\omega\left(\beta_{\|n}B_{n\|}-i\beta_{\|b}B_{b\|}\right)+\frac{1}{k_\varphi}\left(\nabla_p\,\tilde{Z}_0\right)\right]\\
\epsilon^{(1)}_{\|n} &= \left(-\nabla_p+\beta_{n\|}\right)B_{b\|}+i\left(\nabla_n+\beta_{b\|}\right)B_{n\|}\\
&\quad+\frac{2}{\Omega}\left[\omega\left(\beta_{\|n}B_{n\|}+i\beta_{\|b}B_{b\|}\right)+\frac{1}{k_\varphi}\left(\nabla_p\,\tilde{Z}_0\right)\right]
\end{aligned}$$

$$\begin{aligned}
\epsilon^{(1)}_{b\|} &= B_{b\|}\left(-\nabla_n+\beta_{\|b}\right)+iB_{n\|}\left(\nabla_p+\beta_{\|n}\right)\\
&\quad+\frac{2\omega}{\Omega}\left(\beta_{\|b}B_{n\|}+i\beta_{\|n}B_{b\|}\right)+G_{b\|},\\
\epsilon^{(1)}_{\|b} &= \left(\nabla_n+\beta_{b\|}\right)B_{b\|}+i\left(\nabla_p-\beta_{n\|}\right)B_{n\|}\\
&\quad+\frac{2\omega}{\Omega}\left(\beta_{\|b}B_{n\|}-i\beta_{\|n}B_{b\|}\right)+G_{b\|}.
\end{aligned}$$