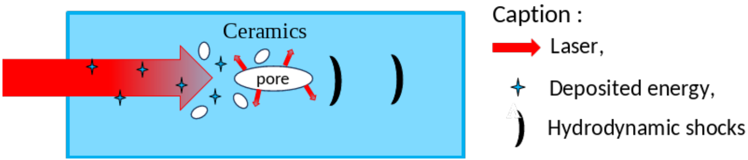
Modeling laser energy deposition in ceramics and induced hydrodynamic shock

Nicolas Bourdineaud [1,2], Guillaume Duchateau [1], Rodolphe Turpault [2]
[1] CEA CESTA, [2] IMB, Université de Bordeaux

Background and objectives



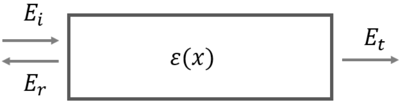
- Multiple irradiation, no aluminum layer
  $\Longrightarrow$ laser-dielectric material interaction
  $\Longrightarrow$ porosity must be considered
- Initially transparent medium, then laser induced excitation of electrons
  $\Longrightarrow$ Material becomes absorbing
- Coupling laser beam propagation and free electron dynamics in dielectric material
- Study of the influence of porosity on energy deposition
  $\Longrightarrow$ Implementation of a 2D code to efficiently evaluate laser energy deposition.

Contents

1. High-order finite-volume scheme for the Helmholtz equation

Laser propagation in dielectrics

Physical problem



Helmholtz equation [1]

$$\Delta E + k_0^2 \varepsilon(x) E = 0, \quad \text{with } E, \varepsilon \in \mathbb{C} \quad \text{and} \quad k_0 = \frac{2\pi}{\lambda}$$

[1] : M. Born, E. Wolf and al. *Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light* Cambridge University Press, 7 edition, 1999.

[2] X. Blanc, F. Hermeline, E. Labourasse, and J. Patela, *Arbitrary order positivity preserving finite-volume schemes for 2d elliptic problems*, Journal of Computational Physics 518, 113325 (2024)

[3] F. Ihlenburg and I. Babuska,*Finite element solution of the helmholtz equation with high wave number part i:The h-version of the fem*, Computers Mathematics with Applications 30, 9 (1995).

[4] A. Modave and T. Chaumont-Frelet, *A hybridizable discontinuous galerkin method with characteristic variables for helmholtz problems*, Journal of Computational Physics 493, 112459 (2023).

[5] A. Idesman and B. Dey, *A new numerical approach to thesolution of the 2d helmholtz equation with optimal accuracy on irregular domains and cartesian meshes*, Computational Mechanics 65(2020).

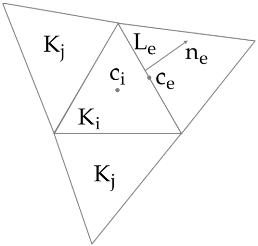
High-order finite volume scheme for 2D laser propagation

Polynomial reconstruction [6]

$$E(x, y, d, \nu, c) = \sum_{\alpha=0}^{d} \sum_{k=0}^{\alpha} \gamma_{\alpha k} \, (x - c_x)^{\alpha - k} \, (y - c_y)^{\alpha}$$

where γ minimizes the following functions :

$$G(\gamma) = \sum_{j \in \nu} w_j \left[E_j - \int_{K_j} E(x, y, d, \nu, c) dx \right]^2$$



- On each mesh edge L_e, we set the polynomial $\hat{E}_e(x, y, d, \nu_e, c_e)$.
- Similarly, on each cell K_i we set the polynomial $\tilde{E}_i(x, y, d, \nu_i, c_i)$ with the following constraint $E_i - \int_{K_i} \tilde{E}_i(x, y, d, \nu_i, c_i) dx = 0$.

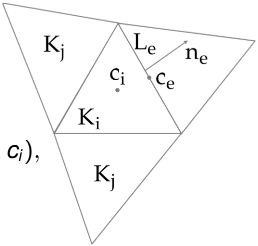
[6] : R. Costa, J. M. Nobrega, S. Clain, and G. J. Machado, *Very high-order accurate polygonal mesh finite volume scheme for conjugate heat transfer problems with curved interfaces and imperfect contacts*, Computer Methods in Applied Mechanics and Engineering 357, 112560 (2019).

High-order finite volume scheme for 2D laser propagation

Numerical Scheme [6]

$$\int_{K_i}\left(\Delta E + k_0^2\varepsilon(x)E\right)dx = \sum_{e\in\partial K_i}\int_{L_e}\nabla E.n_e dl + k_0^2\int_{K_i}\varepsilon(x)Edx,$$

$$\approx \sum_{e\in\partial K_i}|L_e|F_e + k_0^2|K_i|\sum_p w_p\varepsilon(x_p,y_p)\tilde{E}_i(x_p,y_p,d,\nu_i,c_i),$$



$$\text{BOR scheme}: \quad F_e(\hat{E}_e) = \sum_p w_p\nabla\hat{E}_e(x_p,y_p,d,\nu_e,c_e).n_e,$$

$$\text{CEN scheme}: \quad F_e(\tilde{E}_i,\tilde{E}_j) = \sum_p w_p\nabla\frac{\tilde{E}_i(x_p,y_p,d,\nu_i,c_i)+\tilde{E}_j(x_p,y_p,d,\nu_j,c_j)}{2}.n_e.$$

We obtain a linear system $AE = b$.

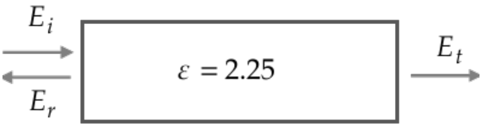
System is ill-conditioned and iterative solver hardly converge

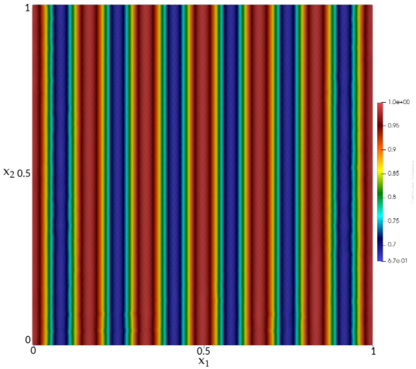
Direct solvers are used (Pastix [7])

[7] : P. Hénon, P. Ramet, J. Roman. *PaStiX: A High-Performance Parallel Direct Solver for Sparse Symmetric Definite Systems. Parallel Computing*, Elsevier, 2002, 28 (2).

Test case : homogeneous medium $\varepsilon = 2.25 + 0i$

Case 1



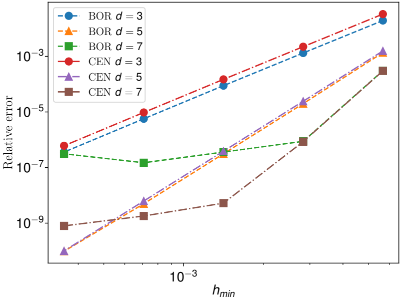


Exact solution for the electric field

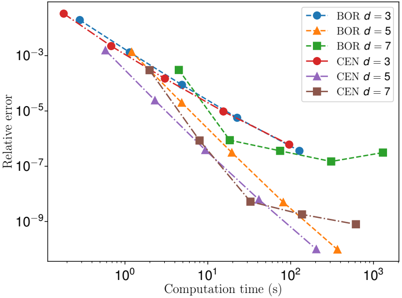
Parameters

- $\lambda = 0.5$
- $x_m = 1$
- Left : $(\frac{\partial}{\partial n} - ik_0)(E - S) = 0$
  with $S(x) = e^{ik_0 x_1}$
- Right : $(\frac{\partial}{\partial n} - ik_0)(E) = 0$
- Bottom/Top : $\frac{\partial E}{\partial n} = 0$
- Exact solution :
  $E^{exa}(x) = \frac{2\sqrt{\varepsilon}}{\sqrt{\varepsilon}+1} e^{ik_0 \varepsilon x_1} + \frac{\sqrt{\varepsilon}-1}{\sqrt{\varepsilon}+1} e^{-ik_0 \varepsilon x_1}$

2D test case : homogeneous medium $\varepsilon = 2.25 + 0i$



Convergence curves in space

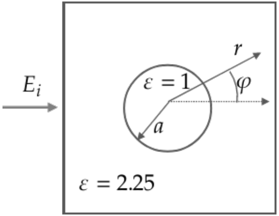


Relative error as a function of computation time

h	BOR $d = 3$		BOR $d = 5$		BOR $d = 7$	
	Error	Order	Error	Order	Error	Order
5.66E-03	1.77E-02	NA	1.17E-03	NA	2.60E-04	NA
2.83E-03	1.21E-03	3.88	1.72E-05	6.09	7.33E-07	8.47
1.41E-03	8.09E-05	3.90	2.76E-07	5.96	3.22E-07	1.19
7.07E-04	5.22E-06	3.95	4.49E-09	5.94	1.33E-07	1.28
3.54E-04	3.31E-07	3.98	8.71E-11	5.69	2.77E-07	-1.06

- Expected order obtained, odd degrees superconverge
- Degree $d = 5$ is the most efficient

2D test case : scattering of a plane wave by a cylinder

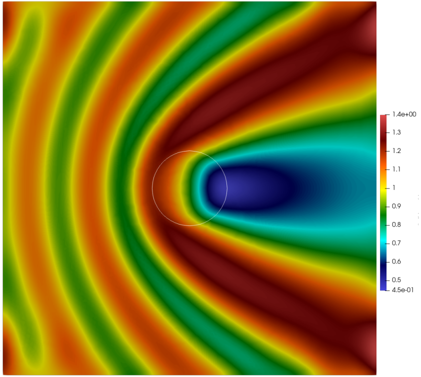


Parameters

- $\lambda = 0.5$
- $a = 0.1$
- Neumann BC
- Exact solution :

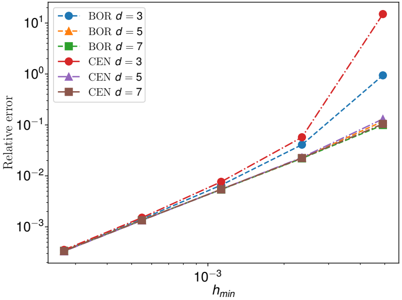
$$E^{exa}(x) = \sum_{n=-\infty}^{+\infty} (-1)^n \left(J_n(k_0\sqrt{\varepsilon}r) - b_n H_n(k_0\sqrt{\varepsilon}r)\right) e^{in\varphi}$$

with $b_n = \dfrac{J_n(a)J_n'(k_0\sqrt{\varepsilon}a) - \frac{1}{\sqrt{\varepsilon}}J_n'n(a)J_n(k_0\sqrt{\varepsilon}a)}{J_n(a)H_n'(k_0\sqrt{\varepsilon}a) - \frac{1}{\sqrt{\varepsilon}}J_n'n(a)H_n(k_0\sqrt{\varepsilon}a)}$



Exact solution for the electric field

2D test case : scattering of a plane wave by a cylinder



Convergence curves in space

- Permittivity discontinuity $\longrightarrow$ E is of class C^1
- Maxwell's interface equations : $[\![E]\!] = 0$ and $\left[\!\left[\frac{\partial E}{\partial n}\right]\!\right] = 0$
- The numerical solution of the electric field is of class C^∞
- Limited order due to the permittivity discontinuity

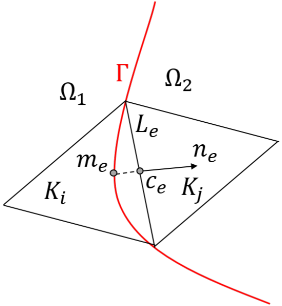
h	BOR $d = 3$		BOR $d = 5$		BOR $d = 7$	
	Error	Order	Error	Order	Error	Order
4.91E-03	7.64E-01	NA	9.70E-02	NA	8.23E-02	NA
2.35E-03	3.37E-02	4.24	1.85E-02	2.25	1.83E-02	2.04
1.12E-03	5.44E-03	2.48	4.52E-03	1.92	4.48E-03	1.91
5.48E-04	1.18E-03	2.12	1.13E-03	1.93	1.12E-03	1.92
2.70E-04	2.83E-04	2.01	2.82E-04	1.96	2.81E-04	1.95

High-order scheme : consideration of discontinuity and curvature

Let Γ be a curve describing the boundary between two materials Ω_1 and Ω_2 of different ε, then the solution of E is of class $C^1(\Omega_1 \bigcup \Omega_2)$.

On edge L_e, two polynomials $\hat{E}_e^{\Omega_1}(x, y, d, \nu_e^{\Omega_1}, c_e)$ and $\hat{E}_e^{\Omega_2}(x, y, d, \nu_e^{\Omega_2}, c_e)$ are defined with the following constraints :

$$\begin{aligned} \hat{E}_e^{\Omega_1}(x_{m_e}, y_{m_e}, d, \nu_e^{\Omega_1}, c_e) &= \tilde{E}_j(x_{m_e}, y_{m_e}, d, \nu_j, c_j), \\ \nabla \hat{E}_e^{\Omega_2}(x_{m_e}, y_{m_e}, d, \nu_e^{\Omega_2}, c_e).n_e &= \nabla \hat{E}_e^{\Omega_1}(x_{m_e}, y_{m_e}, d, \nu_e^{\Omega_1}, c_e).n_e. \end{aligned}$$

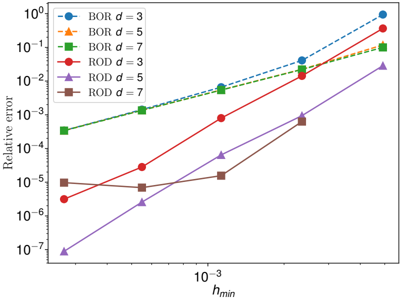


Thus, the numerical flux at interface L_e are expressed as [6]:

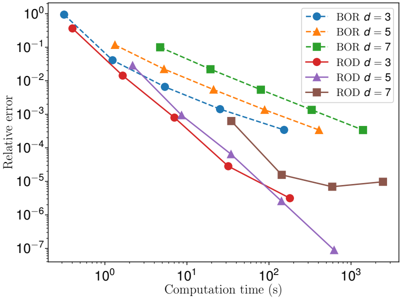
$$\begin{aligned} F_{e,j\to i}(\hat{E}_e^{\Omega_1}) &= \sum_p w_p \nabla \hat{E}_e^{\Omega_1}(x_p, y_p, d, \nu_e^{\Omega_1}, c_e).n_e, \\ F_{e,i\to j}(\hat{E}_e^{\Omega_2}) &= \sum_p w_p \nabla \hat{E}_e^{\Omega_2}(x_p, y_p, d, \nu_e^{\Omega_2}, c_e).n_e. \end{aligned}$$

[6] : R. Costa, J. M. Nobrega, S. Clain, and G. J. Machado, *Very high-order accurate polygonal mesh finite volume scheme for conjugate heat transfer problems with curved interfaces and imperfect contacts*, Computer Methods in Applied Mechanics and Engineering 357, 112560 (2019).

2D test case : scattering of a plane wave by a cylinder



Convergence curves in space

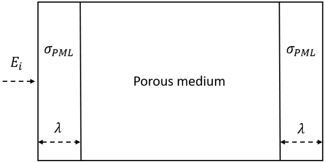


Relative error as a function of computation time

h	ROD $d=3$		ROD $d=5$		ROD $d=7$	
	Error	Order	Error	Order	Error	Order
4.91E-03	2.98E-01	NA	2.36E-02	NA	NA	NA
2.35E-03	1.18E-02	4.39	7.98E-04	4.60	5.23E-04	NA
1.12E-03	6.64E-04	3.91	5.43E-05	3.66	1.29E-05	5.04
5.48E-04	2.53E-05	4.54	2.16E-06	4.47	5.73E-06	1.13
5.48E-04	2.88E-06	3.07	7.44E-08	4.75	8.17E-06	-0.50

- Expected order obtained
- Odd degrees superconverge for straight discontinuities

Towards a representative test case



The boundary conditions are :

- Top/Bottom : Periodic
- Left : $(\frac{\partial}{\partial n} - ik_0)(E - S) = 0$
- Right : $(\frac{\partial}{\partial n} - ik_0)E = 0$

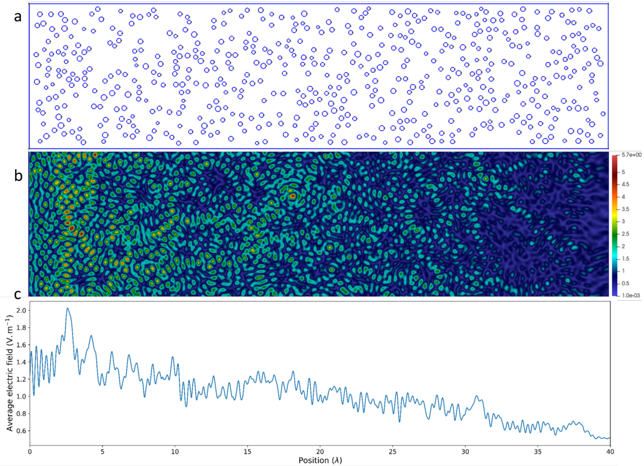
A conductivity profile σ_{PML} is defined at the edges to minimise the reflection and transmission of the electric field [8]:

$$\frac{\partial}{\partial x}\left(f(x)\frac{\partial}{\partial x}E\right) + \frac{\partial}{\partial y}\left(\frac{1}{f(x)}\frac{\partial}{\partial y}E\right) + k_0^2\frac{\varepsilon}{f(x)} = 0$$

$$\text{with} \quad f(x) = \frac{1}{1 + i\sigma_{PML}(x)} \quad \text{and} \quad \sigma_{PML}(x) = \sigma_m s\left(\frac{x}{\lambda}\right)$$

[8] : J.-P. Berenger, *A perfectly matched layer for the absorption of electromagnetic waves*, Journal of Computational Physics 114, 185 (1994).

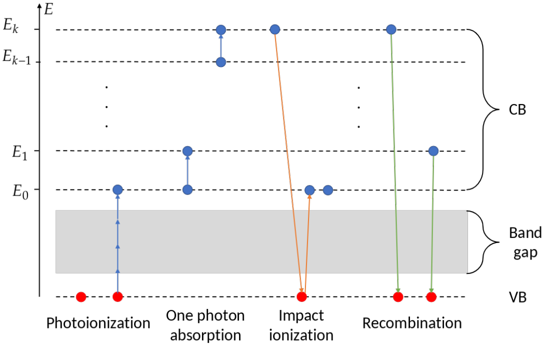
Towards a representative test case



Porous medium (10% of porosity) : a) topology of the case, b) electric field and c) mean value of the electric field along y axis. Calculation domain $40\lambda \times 10\lambda$ with 444842 cells. Computation time : 80s (64CPU).

2. Coupling the Helmholtz solver with the time-dependent electron dynamics

Free electron dynamics



Free electron dynamics equations [9]

$$\frac{\partial n_{cb}}{\partial t} = \alpha W_{pi}(E) + \alpha W_{1pt}(E) n_{cb} - \nu_{rec} n_{cb}.$$

$$\text{Depopulation}: \alpha = 1 - \frac{n_{cb}}{n_{max}}$$

$$\text{Photoionization rate}: W_{pi}$$

$$\text{One photon absorption rate}: W_{1pt}$$

Permittivity of the material (Drude's model [10])

$$\varepsilon(n_{cb}) = 1 + (\varepsilon_\infty - 1)\left(1 - \frac{n_{cb}}{n_{init}}\right) - \frac{e^2 n_{cb}}{m_e \varepsilon_0 \omega(\omega - i\nu_{imp})}.$$

[9] : B. Rethfeld. *Unified model for the free-electron avalanche in laser-irradiated dielectrics.* Phys. Rev. Lett., 92:187401, May 2004.

[10] : E. G. Gamaly and A. V. Rode. *Transient optical properties of dielectrics and semiconductors excited by an ultrashort laser pulse* J. Opt. Soc. Am. B, 31(11):C36–C43, Nov 2014.

Laser energy deposition model

Free electron dynamics [10]

$$\frac{\partial n_{cb}}{\partial t} = \alpha(n_{cb})W_{pi}(E)+\alpha(n_{cb})W_{1pt}(E)n_{cb}-\nu_{rec}n_{cb}.$$

$W_{pi} \propto E^8$ and $W_{1pt} \propto E^2 \longrightarrow$ strongly non-linear

Laser beam propagation [1]

$$\Delta E + k_0^2\varepsilon(n_{cb})E = 0,$$

Optical properties of the material under laser irradiation (Drude's model [11])

$$\text{Permittivity} : \varepsilon = 1 + (\varepsilon_\infty - 1)\left(1 - \frac{n_{cb}}{n_{init}}\right) - \frac{e^2 n_{cb}}{m_e \varepsilon_0 \omega(\omega - i\nu_{imp})}.$$

[1] : M. Born, E. Wolf and al. *Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light* Cambridge University Press, 7 edition, 1999.

[10] : E. G. Gamaly and A. V. Rode, *Transient optical properties of dielectrics and semiconductors excited by an ultrashort laser pulse*, J. Opt. Soc. Am. B31, C36 (2014).

[11] : B. C. Stuart, M. D. Feit, S. Herman, A. M.Rubenchik, B. W. Shore, and M. D. Perry, *Nanosecond to femtosecond laser induced breakdown in dielectrics*,Phys. Rev. B53, 1749 (1996).

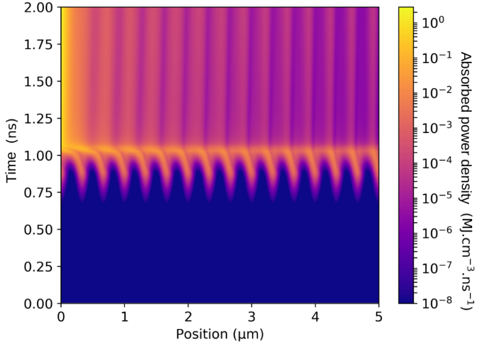
Numerical solution of coupled equations

Splitting method

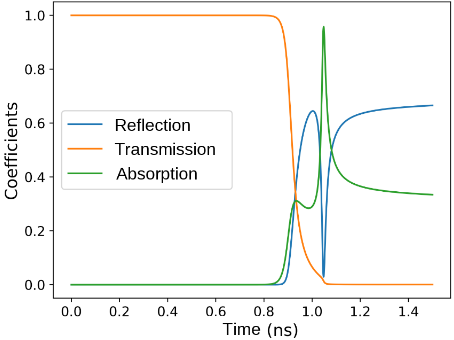
At each time step :

- Compute n_{cb} from E : $\frac{\partial n_{cb}}{\partial t} = \alpha \frac{\rho}{\rho_0} W_{pi} + \alpha W_{1pt} n_{cb} - \nu_{rec} n_{cb}$.
  $\longrightarrow$ Embedded adaptive time step
- Compute ε from n_{cb} : $\varepsilon = 1 + (\varepsilon_\infty - 1)\left(1 - \frac{n_{cb}}{n_{init}}\right) - \frac{e^2 n_{cb}}{m_e \varepsilon_0 \omega(\omega - i\nu_{imp})}$.
- Compute $E(x)$ from updated ε : $\Delta E + k_0^2 \varepsilon E = 0$.
  $\longrightarrow$ High-order finite volume scheme
- Evaluation of deposited power density e from new E et n_{cb}: $e = |\sigma E.E|$, with $\sigma = \frac{e^2 \nu_c n_{cb}}{m_e \omega(\omega - i\nu_c)}$

1D physical results



Power density deposited as a function of time



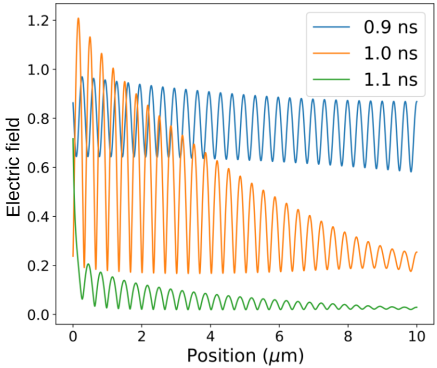
Transmission, reflection and absorption coefficients as a function of time.

Short times: volume energy deposition

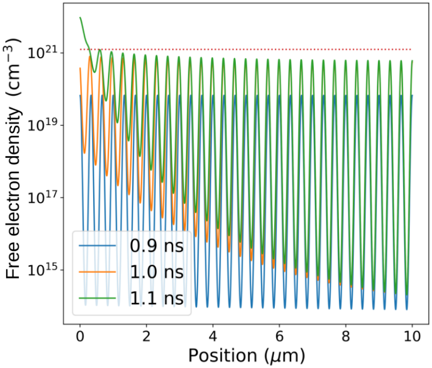
Long times: surface energy deposition

$\Longrightarrow$ Transition from transparent to absorbing medium

1D physical results



Laser electric field at different times.



Free electron density field at different times

Sharp variation near critical plasma density n_{cr} : $\Re(\varepsilon(n_{cr})) = 0$

$\Longrightarrow$ Transision from a propagating to an evanescent wave

$\Longrightarrow$ Adaptive time step scheme

Adaptive time step scheme for free electron dynamics

Embedded adaptive step scheme:

$$n_{cb}^{n+1} \leftarrow n_{cb}^{n} + \Delta t_n \sum_i b_i k_i$$
$$\tilde{n}_{cb}^{n+1} \leftarrow n_{cb}^{n} + \Delta t_n \sum_i \tilde{b}_i k_i$$
$$e_{n+1} \leftarrow n_{cb}^{n+1} - \tilde{n}_{cb}^{n+1}$$

if $e_{n+1} \leq tol_e$ **then**

Save n_{cb}^{n+1}

$$\Delta t_{n+1} = 0.9 \Delta t_n \left(\frac{tol_e}{e_{n+1}}\right)^{\frac{1}{d}}$$

end if

Second criterion on permittivity variation to adapt the time step during the transparent/absorbing transition:

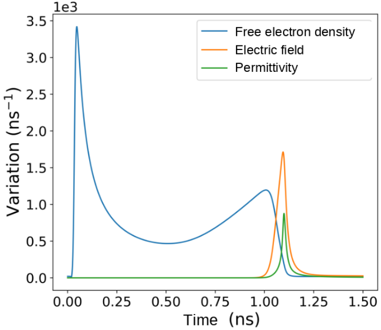
if $\Delta\epsilon_{n+1} \leq tol_\epsilon$ **then**

Save n_{cb}^{n+1}

$$\Delta t_{n+1} = 0.9 \Delta t_n \frac{tol_\epsilon}{\Delta\epsilon_{n+1}}$$

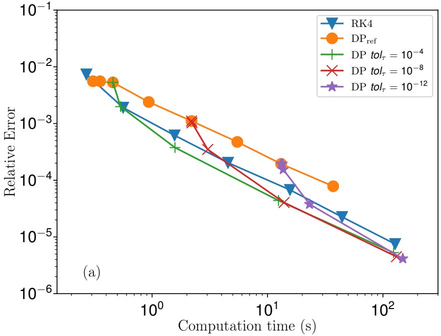
end if

Schemes used : Euler Richardson, RK3/8 et Dormand Prince (4/5)

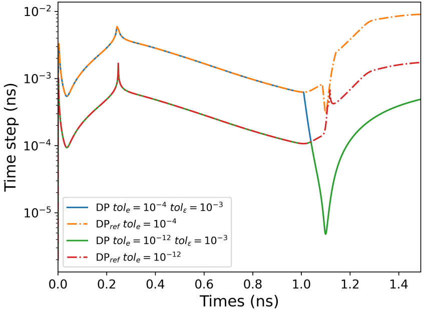


Time derivative of free electron density,electric field and permittivity.

1D time convergence



Relative error in deposited energy for modified Dormand and for RK4 and classic Dormand Prince.



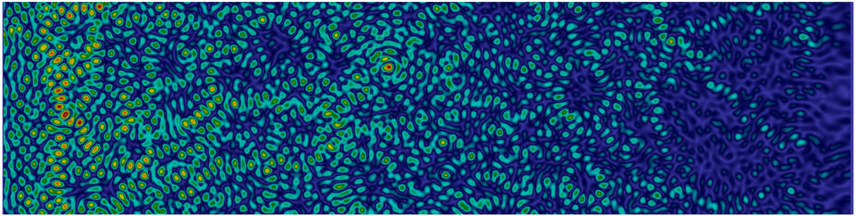
Modified Dormand Prince time step in function of time.

Adding a second tolerance reduces the number of iterations for a given error.

[12] :N. Bourdineaud, G. Duchateau, and R. Turpault, *Efficient numerical approach for modeling coupled electronand nanosecond laser pulse propagation dynamics in dielectric materials*, Phys. Rev. E111, 035309 (2025).

Conclusion and future work

- High-order finite volume scheme works well to solve Helmholtz in 1D and 2D,
  $\Longrightarrow$ Very effective scheme
  $\Longrightarrow$ Efficient interface conditions
- Embedded adaptive time step scheme works well to electron dynamics equation,
  $\Longrightarrow$ Capture the usual optical and interaction behaviors
  $\Longrightarrow$ Reduces calculation time
- Perform laser energy deposition calculations on representative cases to study the influence of porosity :



Thank you for your attention.

Bibliography

Max Born, Emil Wolf, A. B. Bhatia, P. C. Clemmow, D. Gabor, A. R. Stokes, A. M. Taylor, P. A. Wayman, and W. L. Wilcock.
Principles of Optics: Electromagnetic Theory of Propagation, Interference and Diffraction of Light.
Cambridge University Press, 7 edition, 1999.

Xavier Blanc, Francois Hermeline, Emmanuel Labourasse, and Julie Patela.
Arbitrary order positivity preserving finite-volume schemes for 2d elliptic problems.
Journal of Computational Physics, 518:113325, 2024.

F. Ihlenburg and I. Babuška.
Finite element solution of the helmholtz equation with high wave number part i: The h-version of the fem.
Computers Mathematics with Applications, 30(9):9–37, 1995.

Axel Modave and Théophile Chaumont-Frelet.
A hybridizable discontinuous galerkin method with characteristic variables for helmholtz problems.
Journal of Computational Physics, 493:112459, 2023.

Alexander Idesman and Bikash Dey.
A new numerical approach to the solution of the 2-d helmholtz equation with optimal accuracy on irregular domains and cartesian meshes.
Computational Mechanics, 65, 04 2020.

Ricardo Costa, João M. Nóbrega, Stéphane Clain, and Gaspar J. Machado.
Very high-order accurate polygonal mesh finite volume scheme for conjugate heat transfer problems with curved interfaces and imperfect contacts.