

# Simulation of laser propagation in a plasma with a frequency wave equation

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## Abstract

The aim of this work is to perform numerical simulations of the propagation of a laser in a plasma. At each time step, one has to solve a Helmholtz equation in a domain which consists in some hundreds of millions of cells. To solve this huge linear system, we use an iterative Krylov method preconditioned by a separable matrix. The corresponding linear system is solved with a block cyclic reduction method. Some enlightenments on the parallel implementation are also given. Lastly, numerical results are presented including some features concerning the scalability of the numerical method on a parallel architecture.

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## 1. Introduction

The numerical simulation of propagation of high power intensity lasers in a plasma is important for the “NIF project” in USA and the “LMJ Facility project” in France. It is a very challenging area for scientific computing. Indeed the laser wave length  $2\pi/k_0$  is equal to a fraction of one micron and the simulation domain has to be much larger than 500  $\mu\text{m}$ . In a plasma the index of refraction is equal to  $\sqrt{1 - N(\mathbf{x})}$ , where  $N(\mathbf{x}) = N_e(\mathbf{x})/N_c$  and  $N_e$  is the electron plasma density at position  $\mathbf{x}$  and the critical density  $N_c$  is a constant depending only on the wave length. Of course, the laser propagates only in the region where  $N(\mathbf{x}) \leq 1$ . In macroscopic simulations (where the simulation lengths are of the order of some millimeters), geometrical optics models are used and numerical solutions are based on ray tracing methods. To take into account more specific phenomena such as diffraction, autofocusing and filamenta-

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tion, models based on a paraxial approximation of the full Maxwell equations are used. This kind of approximation is based on the assumption that the density  $N(\mathbf{x})$  is close to a mean value  $N_{av}$ ; it allows to make an expansion of W.K.B. type with a constant wave vector. At the end of Section 2, we recall the paraxial Eq. (7); see for example [5,1] in a classical framework and [6] for an analysis of this equation in a tilted frame and a numerical method. But, there are situations where the macroscopic variations of the plasma density  $N_e$  are not small, particularly in the zones which are just before the critical density. In this zone, the laser beam undergoes a strong change of direction near a surface called *caustic surface*. That is to say the wave vector is strongly varying near this surface, the paraxial approximation is no more valid and one has to deal with a model based on a frequency wave equation (obtained as a time envelope of the solution of the full Maxwell equations). The model is described in the Section 2. For a derivation of the models and a physical exposition of the phenomena under interest, see e.g. [23] or [12].

This paper is aiming at describing the numerical methods for solving the frequency wave equation and the coupling with the model for the plasma behavior. At each time step, one has to find the solution  $\psi = \psi(\mathbf{x})$  of the following Helmholtz problem

$$k_0^{-2} \Delta \psi + ((1 - N) + i\mu)\psi = f \quad (1)$$

where  $f$  is a given complex function and  $\mu$  a positive function related to the absorption of the laser by the plasma. Let us notice that  $\mu$  is usually very small and in some computation, we take  $\mu = 0$ .

In this paper, only 2D problems are considered but the method may be extended to 3D simulations, see Section 4.4. Let us set  $\mathbf{x} = (x, y)$  the two spatial coordinates. The key assumption is that the gradient of the density  $N(\mathbf{x}, y)$  is mainly parallel to the  $x$ -axis, then we set

$$N(x, y) = N_0(x) + \delta N(x, y) \quad (2)$$

where  $N_0$  depends on the  $x$  variable only and  $\delta N$  is small compared to 1. This allows to deal with real physical situations as it is shown in the numerical applications below.

The simulation domain is a rectangular box and a classical finite difference method is used for the spatial discretization. For an accurate solution it is necessary to have a spatial step equal to a fraction of the wave length. If  $n_x$  and  $n_y$  denote the number of discretization points in each direction, it leads to solve a linear system with  $n_x n_y$  degrees of freedom (which may be of the order of  $10^8$  for a typical 2D spatial domain).

One chooses an iterative method of Krylov type (cf. [9,22]) with a preconditioning by a matrix corresponding to the discretization of (1) with  $N$  replaced by  $N_0$ . This leads to solve a linear system corresponding to a separable tridiagonal block matrix (each block is a  $n_x \times n_x$  matrix), then a block cyclic reduction method may be used; see for instance [17,20] for this kind of method. The crucial point for this method is to decompose the unknown onto the basis of the  $n_x$  eigenvectors of the main-diagonal block matrix.

The paper is organized as follows. After the statement of the model in Section 2, we present the main difficulties for the numerical simulation of such problems in Section 3. In Section 4, the numerical scheme for the Helmholtz solver is presented, especially the method for solving the preconditioner with the block cyclic reduction method; some enlightenments on the parallel implementation and on the coupling with the hydrodynamics part are also given. Lastly, numerical results are presented including some features concerning the scalability of the numerical method.

## 2. Statement of the model

Our goal is to perform simulations taking into account diffraction, refraction and autofocusing phenomena. So it is necessary to perform a coupling between the fluid dynamics system for the plasma behavior and the frequency wave equation for the laser propagation (notice that the Brillouin parametric instabilities which create laser backscattering are not taken into account).

The laser beam is characterized by an electromagnetic wave with a fixed pulsation, so it may be modeled by the time envelope  $\Psi = \Psi(t, \mathbf{x})$  of this electric field. It is a slowly time varying complex function. On the other hand, for modeling the plasma behavior we introduce the non-dimensional electron density  $N = N(t, \mathbf{x})$  and the plasma velocity  $\mathbf{U} = \mathbf{U}(t, \mathbf{x})$ .

### 2.1. Modeling of the plasma

For the plasma, the simplest model is the following fluid model. Let us denote  $P = P(N, T_e)$  a smooth function of the density  $N$  and of the electron temperature  $T_e$  ( $T_e$  is a very smooth given function of the spatial variable  $\mathbf{x}$ ). Then one has to solve the following barotropic Euler system:

$$\frac{\partial}{\partial t} N + \nabla(N\mathbf{U}) = 0, \quad (3)$$

$$\frac{\partial}{\partial t} (N\mathbf{U}) + \nabla(N\mathbf{U}\mathbf{U}) + \nabla(P(N, T_e)) = -N\gamma_p \nabla|\Psi|^2. \quad (4)$$

The term  $\gamma_p \nabla|\Psi|^2$  corresponds to a ponderomotive force due to a laser pressure (the coefficient  $\gamma_p$  is a constant depending only on the ion species).

### 2.2. Modeling of the laser beam

Let us denote  $\epsilon = k_0^{-1}$ . The laser field  $\Psi = \Psi(t, \mathbf{x})$  is a solution to the following frequency wave equation (which is of Schrödinger type)

$$2i \frac{1}{c} \frac{\partial}{\partial t} \Psi + \epsilon \Delta \Psi + \frac{1}{\epsilon} (1 - N) \Psi + i\nu \Psi = 0, \quad (5)$$

where the absorption coefficient  $\nu$  is a real coefficient related to the absorption of the laser intensity by the plasma and  $c$  the light speed.

### 2.3. Boundary conditions

The laser beam is assumed to enter into the domain at  $x = 0$ . Denote by  $\mathbf{e}_b$  the unit vector in the direction of the incoming beam. Since the density  $N$  depends mainly on the  $x$ -variable, we may denote by  $N^{\text{in}}$  the mean value of the incoming density on the boundary and by  $N^{\text{out}}$  the mean value of the density on the outgoing boundary. The boundary condition at  $x = 0$  reads (with  $\mathbf{n}$  the outwards normal to the boundary)

$$(\epsilon \mathbf{n} \cdot \nabla + i\mathbf{K} \cdot \mathbf{n})(\Psi - \alpha^{\text{in}} e^{ik_0 \mathbf{K} \cdot \mathbf{x}}) = 0. \quad (6)$$

where  $\mathbf{K} = \mathbf{e}_b \sqrt{1 - N^{\text{in}}}$ ,  $\alpha^{\text{in}} = \alpha^{\text{in}}(y)$  is a smooth function which is, roughly speaking, independent of the time. On the part of the boundary  $x = x_{\text{max}}$ , there are two cases according to the value  $N^{\text{out}}$ :

- (i) If  $N^{\text{out}} > 1$ , the wave does not propagate up to the boundary and the boundary condition may read as  $\partial \Psi / \partial x = 0$ .
- (ii) If  $N^{\text{out}} \leq 1$ , one has to consider an absorbing boundary condition. Here we take the simplest one, that is to say  $(\epsilon \mathbf{n} \cdot \nabla + i\sqrt{1 - N^{\text{out}}}) \Psi = 0$ .

In addition, on the part of the boundary corresponding to  $y = 0$  and  $y = y_{\text{max}}$ , it is crucial to have a good transparent boundary condition, so we introduce perfectly matched layers (PML), see [3]. For the simple equation  $-\Delta \psi - \omega^2 \psi = f$ , this technique amounts to replace in the neighborhood of the boundary, the operator  $\frac{\partial}{\partial y}$  by  $(1 + \frac{\sigma}{i\omega})^{-1} \frac{\partial}{\partial y}$ , where  $\sigma$  is a damping function which is not zero only on two or three wave lengths and which increases very fast up to the boundary. Notice that the feature of this method is that it is necessary to modify the discretization of the Laplace operator on a small zone near the boundaries.

**Remark 1** (On the system (3)–(5)). Even if the non-linearities are withdrawn in the barotropic Euler equations, it is difficult to prove the well-posedness of the considered system which is of the Zakharov type (to check this point, it is enough to check that  $w = 1 - N$  satisfies a wave equation with a right hand side term containing  $\Delta(|\Psi|^2)$ ). Another mathematical difficulty comes from the incoming boundary condition (6). Nevertheless, if the laser intensity  $|\Psi|^2$  is not very large, it is generally assumed that there exists a solution of this system. See [8,15] for some mathematical considerations on the Zakharov system.

**Remark 2 (The paraxial equation).** For the sake of completeness, we recall now the paraxial approximation equation which is valid only if the plasma density is a very smooth function, in such a way that we can take  $N_0 = N_{av}$  where  $N_{av}$  is a constant. So we can define a mean wave vector  $\mathbf{K} = \mathbf{e}_b \sqrt{1 - N_{av}}$  and the laser beam is now characterized by the space and time envelope of the electric field  $E = E(t, \mathbf{x})$ , that is to say

$$\Psi(t, \mathbf{x}) = E(t, \mathbf{x})e^{i\mathbf{K}\cdot\mathbf{x}/\epsilon}.$$

The envelope  $E$  is assumed to be slowly varying with the space variable and thus satisfies

$$i\left(\frac{2}{c}\frac{\partial E}{\partial t} + 2\mathbf{K} \cdot \nabla E + vE\right) + \epsilon(\Delta_{\perp}^K E) - \frac{1}{\epsilon}(N - N_{av})E = 0. \tag{7}$$

where  $\Delta_{\perp}^K$  denotes the Laplace operator in the hyperplane transverse to  $K$ . It is necessary to supplement Eq. (7) with a boundary condition on the incoming boundary which is  $E(0, \cdot) = \alpha^{in}$  with an initial condition, see [5,1,6].

### 3. Difficulties

The discretization and the solving of the above system of partial differential equations is very challenging since different space scales are to be considered. Moreover, it leads to very large linear systems.

#### 3.1. Multiscale in space

For solving (5), the spatial mesh has to be very fine,  $h_{\text{Helmholtz}} \simeq \lambda_0/10$  or less in each direction (recall that  $\lambda_0 = 2\pi/k_0$ ); this mesh is called in the sequel the Helmholtz grid. But the modulus  $|\psi|$  of the electric field is slowly varying with respect to the spatial variable, thus one can use a coarse mesh for the simulation of the Euler system, typically one can set  $h_{\text{fluid}} \simeq \lambda_0/2$ .

For the numerical solution of the fluid system, we refer to the method described in [14] or [1] which has been implemented in a parallel platform called HERA. The ponderomotive force is taken into account by adding a force proportional to  $\nabla|\psi|^2$  to the pressure force. The plasma density  $N$ , the velocity  $\mathbf{U}$  and the laser intensity  $|\psi|^2$  are evaluated at the center of each cell.

So we handle a two-level mesh of finite difference type: in a 2D simulation, each cell of the fluid system is divided into  $p_0 \times p_0$  cells for the Helmholtz level, with  $p_0 = 5$  or more. At each time step  $\delta t$  determined by the CFL criterion for the Euler system, one has to solve the frequency wave Eq. (5). For the time discretization of this equation, an implicit scheme is used. The length  $c\delta t$  is very large compared to the spatial step therefore the time derivative term may be considered as a perturbation. So, at each time step, if  $\psi^{ini}$  denotes the value of the solution of the previous time step, one has to find  $\psi$  solution of the following equation of Helmholtz type

$$\epsilon^2 \Delta \psi + ((1 - N) + i\mu_1)\psi = i\mu_0 \psi^{ini}, \tag{8}$$

where  $\mu_0 = \epsilon 2/(c\delta t)$ ,  $\mu_1 = \epsilon(2/(c\delta t) + v)$ . This equation is supplemented by a boundary condition at  $x = 0$

$$\left(\epsilon \frac{\partial}{\partial x} + i\mathbf{K}_x\right)\psi = \left(\epsilon \frac{\partial}{\partial x} + i\mathbf{K}_x\right)(\alpha^{in} e^{i\mathbf{K}_y \cdot y/\epsilon}). \tag{9}$$

and another one in  $x = x_{\text{max}}$  as above.

#### 3.2. Large scale problem

As we shall see, the main difficulty comes from the Helmholtz equation: the number of unknowns is quite large and the properties of the resulting linear system make it hard to solve. The linear system is symmetric but not Hermitian; these properties are inherited by the discretized equations. The resulting linear systems are thus difficult to precondition. Concerning the preconditioning, the assumption (2) leads to replace the original system by another one which is simpler since it does not take into account the perturbation  $\delta N(x, y)$ . The corresponding linear system to be solved leads to a five-diagonal symmetric non-hermitian matrix  $A_G$

$$A_G = \begin{pmatrix} \beta + A & -T & & & & \\ -T & A & -T & & & \\ & \ddots & \ddots & \ddots & & \\ & & & -T & A & -T \\ & & & & -T & \beta + A \end{pmatrix} \tag{10}$$

where  $T$  is equal to a constant times the identity matrix of dimension  $n_x$ , the matrix  $A$  of dimension  $n_x$  and  $\beta$  is a complex constant. The matrix  $A_G$  is separable and therefore a block cyclic reduction method may be used for its numerical solution.

Note that a realistic simulation with a domain of size  $500 \mu\text{m} \times 700 \mu\text{m}$  and with a wave length of  $0.35 \mu\text{m}$ , results in 12 millions fluid unknowns and 300 millions unknowns on the Helmholtz grid.

### 4. Numerical strategies

#### 4.1. Helmholtz solver

Even though we consider a 2D problem, the very large size of the problem prevents us from using a direct solver, even a parallel one. We have to use an iterative method, in our case a preconditioned Krylov solver, see for instance [9,22]. As for the preconditioner, it seems difficult to propose one which would be valid both in the central zone where a pure Helmholtz equation is considered and in the Perfectly Matched Layers (PML). Therefore, we first perform a decomposition of the domain into three subdomains: two thin PML layers and a large central domain with appropriate interface conditions, see Section 4.1.1. The preconditioning of the central problem is presented in Section 4.1.2, it corresponds to the solution to an approximate equation.

Let us mention right away that a multigrid method for the Helmholtz Eq. (11) would not work. Indeed, multigrid methods are efficient only if a large enough damping parameter is present in the equation. Here, the coefficient  $c\delta t$  is larger than 100 wave lengths and the term  $v$  is typically given by the formula:

$$v = v_C N_0(x)^2$$

with  $1/v_C$  in the order of  $15 \mu\text{m}$  (typical values of the density are around 0.4). So the damping term  $k_0\mu_1 = k_0(\mu_0 + v)$  is quite small when compared to the wave length  $2\pi k_0^{-1}$  and it is too weak for a multigrid method.

To solve the linear system arising from the discretization of the Helmholtz equation

$$\epsilon^2 \Delta \psi + i\mu_1 \psi + (1 - N_0(x))\psi - \delta_N(x, y)\psi = i\mu_0 \psi^{\text{ini}}, \tag{11}$$

we use the fact that the function  $N_0$  depends only of a one-dimension variable and we deal with a Krylov method with a preconditioner which corresponds to a separable matrix. This preconditioner may be interpreted as the discretization of the operator

$$\psi \mapsto \epsilon^2 \Delta \psi + i\mu_1 \psi + (1 - N_0(x))\psi. \tag{12}$$

(recall  $\mu_1 = \mu_0 + v$ ) with the same boundary conditions. A block cyclic reduction method is then used for solving the corresponding linear system.

Let us mention that the idea of preconditioning a variable coefficient Helmholtz equation by a problem amenable to the separation of variables technique was investigated in [19] in the context of seismic modeling. Although in this context the method was not satisfactory, we shall see that in our context (laser–plasma interaction), results are indeed very good. We mention as well another method [7] based on the preconditioning of (11) by a shifted Helmholtz equation with  $\beta_0 \simeq 0.3 - 0.5$

$$\epsilon^2 \Delta \psi + i\mu_1 \psi + (1 + i\beta_0)[(1 - N)\psi]$$

that would be amenable to a multigrid solver.

Let us also mention that it is not possible to use a simple FFT in the  $y$ -direction. Indeed, that would amount to assume periodicity in this direction. It is not the case since the laser goes out through a side of the domain (say  $\Omega_t$ ) and not through the other.

4.1.1. Domain decomposition

The computational domain is divided into three overlapping subdomains: a purely Helmholtz zone  $\Omega_c$  and two zones bordering it above  $\Omega_t$  and below  $\Omega_b$ , see Fig. 1. In  $\Omega_t$  and  $\Omega_b$ , we have both a PML and a Helmholtz region.

The coupling between the subdomains is made via Robin interface conditions, see [16,2]. So solving (8) leads to the following coupled system of equations, where the unknown functions are  $\psi_t, \psi_c, \psi_b$

$$\begin{cases} \epsilon^2 \left[ \eta(y) \frac{\partial}{\partial y} \left( \eta(y) \frac{\partial}{\partial y} \right) + \frac{\partial^2}{\partial x^2} \right] \psi_t + i\mu_1 \psi_t + (1 - N_0) \psi_t = 0 & \text{in } \Omega_t \\ \frac{\partial \psi_t}{\partial y} + i\alpha \psi_t = \frac{\partial \psi_c}{\partial y} + i\alpha \psi_c & \text{on } \Gamma_t^2 \\ \epsilon^2 \Delta \psi_c + i\mu_1 \psi_c + (1 - N_0) \psi_c - \delta_N \psi_c = i\mu_0 \psi^{\text{ini}} & \text{in } \Omega_c \\ \frac{\partial \psi_c}{\partial y} + i\alpha \psi_c = \frac{\partial \psi_t}{\partial y} + i\alpha \psi_t & \text{on } \Gamma_t^1 \\ -\frac{\partial \psi_c}{\partial y} + i\alpha \psi_c = -\frac{\partial \psi_b}{\partial y} + i\alpha \psi_b & \text{on } \Gamma_b^1 \\ \epsilon^2 \left[ \eta(y) \frac{\partial}{\partial y} \left( \eta(y) \frac{\partial}{\partial y} \right) + \frac{\partial^2}{\partial x^2} \right] \psi_b + i\mu_1 \psi_b + (1 - N_0) \psi_b = 0 & \text{in } \Omega_b \\ -\frac{\partial \psi_b}{\partial y} + i\alpha \psi_b = -\frac{\partial \psi_c}{\partial y} + i\alpha \psi_c & \text{on } \Gamma_b^2 \end{cases}$$

The coupling interface condition are of Robin type with  $\alpha = 0.5/\epsilon$ . The boundary condition at  $x = 0$  is given by (9) for  $\psi_c$  and by  $(\epsilon \frac{\partial}{\partial x} + i\mathbf{K}_x) \psi = 0$ , for  $\psi_t$  and  $\psi_b$ . These equations are discretized by a finite difference scheme. Let us denote by  $\Psi_t, \Psi_c$  and  $\Psi_b$  the corresponding unknown vector in domains  $\Omega_t, \Omega_c$  and  $\Omega_b$ . The linear system to be solved reads:

$$M \begin{pmatrix} \Psi_t \\ \Psi_c \\ \Psi_b \end{pmatrix} = \begin{pmatrix} b_t \\ b_c \\ b_b \end{pmatrix} \quad \text{where } M = \begin{bmatrix} A_{P1} & C_1 & 0 \\ C_2 & A_H & C_3 \\ 0 & C_4 & A_{P2} \end{bmatrix}. \tag{13}$$

The blocks  $(C_i)_{1 \leq i \leq 4}$  are related to the discrete Robin interface conditions.

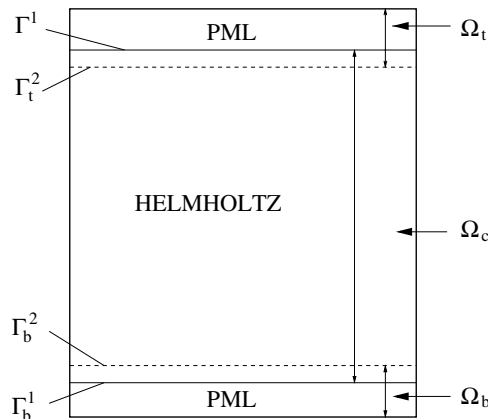


Fig. 1. Domain decomposition into three overlapping subdomains.

4.1.2. The matrix system

Denote by  $A_{\delta N}$  the diagonal matrix corresponding to the discretization of the operator of multiplication by  $-\delta_N + i(\mu_1 - \mu_0)$  and by  $A_G$  the one corresponding to the discretization of Eq. (12), that is to say  $A_H = A_G + A_{\delta N}$ , then the matrix  $M$  may be decomposed as

$$M = M_D + M_E,$$

with

$$M_D = \begin{bmatrix} A_{P1} & 0 & 0 \\ 0 & A_G & 0 \\ 0 & 0 & A_{P2} \end{bmatrix} \quad \text{and} \quad M_E = \begin{bmatrix} 0 & C_1 & 0 \\ C_2 & A_{\delta N} & C_3 \\ 0 & C_4 & 0 \end{bmatrix}$$

The principle for solving the linear system (13) is to use a Krylov method preconditioned by  $M_D$  which is a block diagonal matrix; here we choose a GMRES algorithm (without restart since the number of iterations is quite low, see below Section 5.2). To apply the preconditioner, since matrices  $A_{P1}, A_{P2}$  are small ones, they can be factorized by a direct method and from the computational point of view, the key step is to use a fast solver for the matrix  $A_G$ .

Let us describe the structure of the matrix  $A_G$  coming from the discretization of Eq. (12). Denote by  $\delta y$  the mesh size in  $y$ , by  $\mathbf{I}$  the identity matrix of dimension  $n_x$ . Let  $A_0$  be the symmetric tridiagonal matrix which corresponds to the discretization of the following 1D problem

$$\epsilon^2 \frac{\partial^2}{\partial x^2} \psi + (1 - N_0(x))\psi,$$

with the boundary condition (9). Their coefficients are real except the one in the first row and the first column (due to the boundary condition). Then we set

$$\begin{aligned} A &= A_0 + i\mu_0 \mathbf{I} - \frac{2\epsilon^2}{\delta y^2} \mathbf{I} \\ T &= -\frac{\epsilon^2}{\delta y^2} \mathbf{I}, \\ B &= A_0 + i\left(\mu_0 - \frac{\alpha\epsilon^2}{\delta y}\right) \mathbf{I} - \frac{\epsilon^2}{\delta y^2} \mathbf{I} = A + \beta \mathbf{I} \end{aligned}$$

where  $\beta = -i\alpha\epsilon^2/\delta y + \epsilon^2/\delta y^2$ . Now, if we denote  $\Psi_c = (u_1, u_2, \dots, u_{n_y})$  and  $f = (f_1, f_2, \dots, f_{n_y})$  where the elements  $u_m$  and  $f_m$  are  $n_x$ -vectors, the system  $A_G \Psi_c = f$  reads as follows:

$$\begin{pmatrix} B & -T & & & & \\ -T & A & -T & & & \\ & & \ddots & \ddots & \ddots & \\ & & & -T & A & -T \\ & & & & -T & B \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n_y-1} \\ u_{n_y} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{n_y-1} \\ f_{n_y} \end{pmatrix} \tag{14}$$

4.1.3. Cyclic reduction

In order to solve system (14), we use the block cyclic reduction method, see for instance [10]. Let us recall the principle of this method. Assuming that  $n_y = 2^k - 1$  for the sake of simplicity. We know that  $A$  and  $T$  commute. Consider three successive lines of (14) for  $i = 2, 4, \dots, n_y - 1$ :

$$\begin{cases} -Tu_{i-2} + Au_{i-1} - Tu_i = f_{i-1} \\ -Tu_{i-1} + Au_i - Tu_{i+1} = f_i \\ -Tu_i + Au_{i+1} - Tu_{i+2} = f_{i+1}. \end{cases} \tag{15}$$



After a linear combination of these lines, we get:

$$-T^2 A^{-1} u_{i-2} + (A - 2T^2 A^{-1}) u_i - T^2 A^{-1} u_{i+2} = f_i + T A^{-1} (f_{i-1} + f_{i+1}) \tag{16}$$

After this first step, the elimination procedure may be performed again by induction. That is to say, denote  $A^{(0)} = A$ ,  $B^{(0)} = B$ ,  $T^{(0)} = T$  et  $f^{(0)} = f$ ; after  $r$  elimination steps, the reduced system for  $0 \leq r \leq k - 1$  owns  $2^{k-r} - 1$  blocs and reads as:

$$\begin{pmatrix} B^{(r)} & -T^{(r)} & & & & & \\ -T^{(r)} & A^{(r)} & -T^{(r)} & & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -T^{(r)} & A^{(r)} & -T^{(r)} & \\ & & & & -T^{(r)} & B^{(r)} & \end{pmatrix} \begin{pmatrix} u_{2^r} \\ u_{2 \cdot 2^r} \\ \vdots \\ u_{(n_y-1)-2^r+1} \\ u_{n_y-2^r+1} \end{pmatrix} = \begin{pmatrix} f_{2^r}^{(r)} \\ f_{2 \cdot 2^r}^{(r)} \\ \vdots \\ f_{(n_y-1)-2^r+1}^{(r)} \\ f_{n_y-2^r+1}^{(r)} \end{pmatrix}$$

where for  $r = 1, \dots, k - 2$ :

$$\begin{aligned} A^{(r)} &= A^{(r-1)} - 2(T^{(r-1)})^2 (A^{(r-1)})^{-1} \\ B^{(r)} &= A^{(r-1)} - (T^{(r-1)})^2 ((A^{(r-1)})^{-1} + (B^{(r-1)})^{-1}) \\ T^{(r)} &= (T^{(r-1)})^2 (A^{(r-1)})^{-1} \end{aligned} \tag{17}$$

For the right hand side, we get the induction formula:

$$f_{i \cdot 2^r}^{(r)} = f_{i \cdot 2^r}^{(r-1)} + T^{(r-1)} (A^{(r-1)})^{-1} (f_{i \cdot 2^r - 2^{r-1}}^{(r-1)} + f_{i \cdot 2^r + 2^{r-1}}^{(r-1)}) \tag{18}$$

After all the elimination steps, it remains only one equation for finding  $u_{2^{k-1}}$ . Once this value is obtained, one deduces all the other values step by step recursively.

From a practical point of view, one has to perform these computations in the spectral basis of the eigenvectors of the matrix  $A$ , which are of course also eigenvectors of  $T$ ,  $B$ ,  $A^{(r)}$ ,  $T^{(r)}$ ,  $B^{(r)}$  for all  $r$ .

#### 4.2. Parallel implementation

The implementation of the method has been made in the HERA platform, see [1,14]. For the Helmholtz solver, one first has to find a orthonormal basis of eigenvectors of  $A_0$ . As a matter of fact, the matrix  $A_0$  is symmetric non-hermitian, all their coefficients are real but the one at the top corner which is complex due to the boundary condition. Since the matrix  $A_0$  is symmetric complex but not hermitian, we search a set of eigenvectors which are orthogonal for the pseudo inner product  $\langle u, v \rangle = u^T \cdot v$ . To compute this set, we use the “new QD” algorithm of Parlett (cf. [18]) although it was designed for real matrix. We conjecture that it is always possible to find such a basis of eigenvectors for our class of matrices, where one diagonal coefficient is complex. The only difficulty would be to find a non zero eigenvector  $v$  such that  $v^T \cdot v = 0$ . Let us mention that this problem is addressed in [11] and that it is equivalent to suppose that matrix  $A_0$  is diagonalizable. In practice, we never encountered any problem by using the method. In the method proposed in [18], which follows an idea of [21], the computation of the eigenvalues is based on a series of LU factorization of tridiagonal matrices. This step is sequential but very cheap in terms of memory and CPU time requirements especially when compared to the QR algorithm which would manipulate full matrices. Once the eigenvalues have been computed, the computation of the eigenvectors consists in finding the kernel of tridiagonal matrices. One uses the algorithm proposed by Dhillon [4] based on the “new QD” algorithm which produces directly an orthogonal basis of eigenvectors. This task is distributed among the processors and is thus parallel. The great contribution of [18,4] is to explain how to perform the above mentioned tasks in a stable and robust way. In the real case, the stability analysis was performed in [18]. Here, we use the “new QD” algorithm in the symmetric complex framework. In our tests, this method is very stable, accurate and 40 times faster than the QR method.



Let  $Q$  denote the matrix whose columns are the eigenvectors of  $A^0$ . The matrix  $Q$  is orthonormal for the pseudo scalar product, that is to say

$$QQ^T = Q^TQ = \mathbf{I}$$

Since  $T$  is the identity matrix up to a multiplicative constant, one can introduce the diagonal matrices  $A^{(0)}$  and  $\Gamma^{(0)}$

$$A = QA^{(0)}Q^T, \quad T = Q\Gamma^{(0)}Q^T. \tag{19}$$

So we get

$$A^{(r)} = QA^{(r)}Q^T, \quad T^{(r)} = Q\Gamma^{(r)}Q^T \tag{20}$$

with the following induction formulas

$$A^{(r)} = A^{(r-1)} - 2(\Gamma^{(r-1)})^2(A^{(r-1)})^{-1}, \quad \Gamma^{(r)} = (\Gamma^{(r-1)})^2(A^{(r-1)})^{-1} \tag{21}$$

Let us summarize the algorithm

- Introduce the vectors  $\tilde{f}_i$  transformed of  $f_i$  in the eigenvector basis

$$\tilde{f}_i = Q^T f_i \quad \text{for } i = 1, \dots, n_y.$$

- At each step  $r$ , the vector  $\tilde{f}_i^r$  transformed of  $f_i^r$  of the right hand side, reads

$$\tilde{f}_{i,2^r}^{(r)} = \tilde{f}_{i,2^r}^{(r-1)} + \Gamma^{(r-1)}(A^{(r-1)})^{-1} \left( \tilde{f}_{i,2^{r-2}2^r}^{(r-1)} + \tilde{f}_{i,2^r+2^{r-1}}^{(r-1)} \right)$$

- One computes the vectors  $\tilde{u}_{2^{k-1}}$  by solving

$$A^{(k-1)}\tilde{u}_{2^{k-1}} = \tilde{f}_{2^{k-1}}^{(k-1)}$$

- One recursively distributes the solutions by solving sub-systems of the following type

$$A^{(r)}\tilde{u}_{j,2^{r+1}-2^r} = \tilde{g}_{j,2^{r+1}-2^r}^{(r)}$$

where

$$\tilde{g}_{j,2^{r+1}-2^r}^{(r)} = \tilde{f}_{j,2^{r+1}-2^r}^{(r)} + \Gamma^{(r)}(\tilde{u}_{(j-1),2^{r+1}} + \tilde{u}_{(j),2^{r+1}})$$

- Lastly, the solution  $u$  is given by

$$u_i = Q\tilde{u}_i \quad \text{for } i = 1, \dots, n_y.$$

For the parallel implementation, the processors are shared out according to horizontal slabs in a balanced way. Let us note that the first and last processors contain PML layers and some lines of the central grid. The crucial point of the algorithm is the multiplication of a full matrix  $Q$  (and its transpose) of dimension  $n_x \times n_x$  by the set of  $n_y$  vectors, i.e. a matrix–matrix multiplication. Within a realistic framework for Symmetric MultiProcessors (SMP) architecture, the matrix  $Q$  of a size of several giga octets can be stored only in the memory of the nodes of processors. This led us to use a technique of hybrid parallelization of MPI-multithreading type. One wishes to profit from the locality of the data between processors of the same node and to use MPI for the others communications between nodes. Cutting is carried out in order to avoid conflict of writing of the threads. For example, shearing in  $N_q \times N_b$  threads leads to

$$\begin{bmatrix} Q_1 \\ \vdots \\ Q_{N_q} \end{bmatrix} \times [B_1 \quad \dots \quad B_{N_b}] = \begin{bmatrix} Q_1 B_1 & \dots & Q_1 B_{N_b} \\ \vdots & \ddots & \vdots \\ Q_{N_q} B_1 & \dots & Q_{N_q} B_{N_b} \end{bmatrix}.$$

Each product  $Q_i B_j$  is carried out by a call to the BLAS library. Let us specify that the steps of computation in the spectral basis (i.e.  $A^{(r)}, \Gamma^{(r)}, \tilde{f}_{i,2^r}^{(r)}, \dots$ ) are of a very negligible cost in comparison to matrix–matrix products. Our tests show a good scalability of the cyclic reduction and a great speed of execution.

### 4.3. Coupling with the hydrodynamics part

Notice first that, since the absorption coefficient is very small, the modulus of the solution of the Helmholtz equation is slowly varying with the space variable and therefore also the laser intensity  $|\psi|^2$ . Therefore, one can deal with the ponderomotive force  $\nabla|\psi|^2$  and the hydrodynamics equations on the coarse grid (whose size is equal to one half of the wave length). The general numerical scheme is the following at each time step.

- First step : Solve the Helmholtz Eq. (11) on the fine grid according to the above described method.
- Second step : Evaluation the laser intensity  $|\psi|^2$  on this coarse grid: one simply takes the mean value of the quantities  $|\psi|^2$  defined on the fine grid.
- Third step : Solving the hydrodynamics system (3) and (4) on the coarse grid. One uses a standard explicit scheme for dealing with the classical part of this system. For the ponderomotive force, we use a centered discretization of the gradient of the laser intensity. Let us sketch in 1D the resulting scheme; the extension in 2D is straightforward. For a cell  $j$  whose adjacent cells in the direction  $x$  are denoted by  $j + 1$  and  $j - 1$ , we denote by  $N_j$ ,  $p_j$ , and  $u_j$  the density, the pressure and the velocity in the cell  $j$  evaluated at the beginning of the time step (without superscript) and at the end of of the time step (with the superscript  $\bullet^{\delta t}$ ). If one uses a numerical solver à la Roe, the resulting values at the end of the time step take the following form

$$N_j^{\delta t} = N_j - \frac{\delta t}{\delta x} (f_{j+1/2} - f_{j-1/2}), \tag{22}$$

$$(Nu)_j^{\delta t} = (Nu)_j - \frac{\delta t}{\delta x} (g_{j+1/2} - g_{j-1/2}), \tag{23}$$

where the numerical fluxes  $f_\bullet$  and  $g_\bullet$  on cell edge  $j - 1/2$  depend only on the quantities  $N_j$ ,  $p_j$ , and  $u_j$  on the two neighbor cells (for first order schemes) or on the four neighbor cells (for second order schemes); see for instance [1] or [14] for details. Moreover, for taking into account the ponderomotive force  $\gamma_p \nabla|\psi|^2$ , we use a standard centered discretization: one has to add to the right hand side of (23) the following term evaluated with the last known values of  $\psi$

$$\delta t N_j \gamma_p \frac{|\psi_{j+1}|^2 - |\psi_{j-1}|^2}{2\delta x}$$

- Fourth step : We have to perform a linear interpolation between the coarse grid and the fine grid for getting a suitable electron density  $N_0$  and  $\delta_N$  on the fine grid for solving the Helmholtz equation at the future time step.

Of course in the PML zones, the ponderomotive force terms have not to be taken into account.

### 4.4. Remarks about 3D computations

For 3D computations, one may assume that the third direction  $z$  is orthogonal to the propagation plane, therefore the laser beam does not go out of the domain through the  $z$ -boundary. So one could use a periodic structure in the  $z$ -direction with a large artificial absorption coefficient near the  $z$ -boundary. Then, one can apply the same block cyclic reduction method with  $A$  a square matrix whose dimensions are equal to  $n_x \times n_z$ . That corresponds to the discrete 2D operator following:

$$\epsilon^2 \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) + (1 - N_0) + \mu_1.$$

So, the eigenfunctions read as  $\psi_j(x) e^{ikz2\pi/L_z}$  where  $L_z$  is the size of the domain. From the discrete point of view, the matrix  $A$  (see (14)) is penta-diagonal and has the form

$$\begin{pmatrix} M & -I & & -I \\ -I & M & -I & \\ & \ddots & \ddots & \ddots \\ & & -I & M & -I \\ -I & & & -I & M \end{pmatrix}$$

One can check that if the eigenvalues of  $M$  are  $(\lambda_j)_{1 \leq j \leq n_x}$ , the eigenvalues of  $A$  may read as  $(\lambda_j - bk^2)_{1 \leq j \leq n_x, 0 \leq k \leq n_z - 1}$  with  $b$  positive. The eigenvectors may be factorized as in the continuous case.

But the key problem is the data storage. Indeed, for a realistic case with a domain of about  $10^{11}$  cells, the main unknown would be a complex vector of size about  $10^{11}$ . Thus, by extrapolating our simulation needs in 2D, it leads to about more than one thousand nodes with at least 16 processors per node. This will be a real high performance computing challenge for the future supercomputer architectures.

## 5. Numerical results

### 5.1. Test cases

The boundary value  $\alpha^{\text{in}}$  has to mimic laser beam; to be realistic the profile of  $\alpha^{\text{in}}$  corresponds to a juxtaposition of a lot of small hot spots, called *speckles* whose intensity is very high compared to the mean intensity of the beam. The shape of a speckle is generally a Gaussian function whose width is about a few micrometers.

One considers here a simulation domain of  $100 \times 300$  wave lengths; the initial density profile is a linear function increasing from 0.1 at  $x = 0$  to 1.1 at  $x = x_{\text{max}}$ . The profile of  $\alpha^{\text{in}}$  contains only three speckles. At the Helmholtz level, one handles only 3 millions of cells. With 32 PEs (of the type EV67 HP-Compaq), the CPU time is only a few minutes per time step with approximately 10 Krylov iterations at each time step.

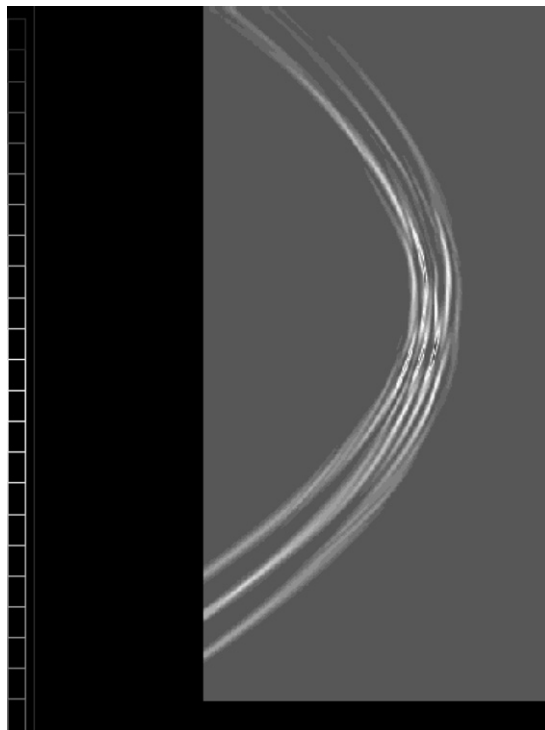


Fig. 2. Laser intensity of a schematic beamlet.

Without the coupling with the plasma, it is well known that the solution is very close to the one given by Geometrical Optics approximation and corresponds to parallel speckles or beamlets which are curved and tangent to a caustic line; this line corresponds to  $x = x_\star$  such that  $N_0(x_\star) = \cos^2(\theta)$ , with  $\theta$  denoting the incidence angle of the beamlets where they enter into the simulation box (see for example [13] for this approximation and for examples of beamlet travel in a plasma with a linear density profile). With our model, if the laser intensity is small (which corresponds to a weak coupling with the plasma), one notices that a small digging of the plasma density occurs. This digging is more significant when the laser intensity is larger, then an autofocusing phenomenon takes place. On Fig. 2, one sees the map of the laser intensity that is to say the quantity  $|\psi|^2$ , which corresponds to this situation after some time steps. We see here that the three beamlets behave as in Geometrical Optics approximation in the first part of their path; but since they undergo autofocusing, something like a filamentation may be observed in the region where the beamlets are curved.

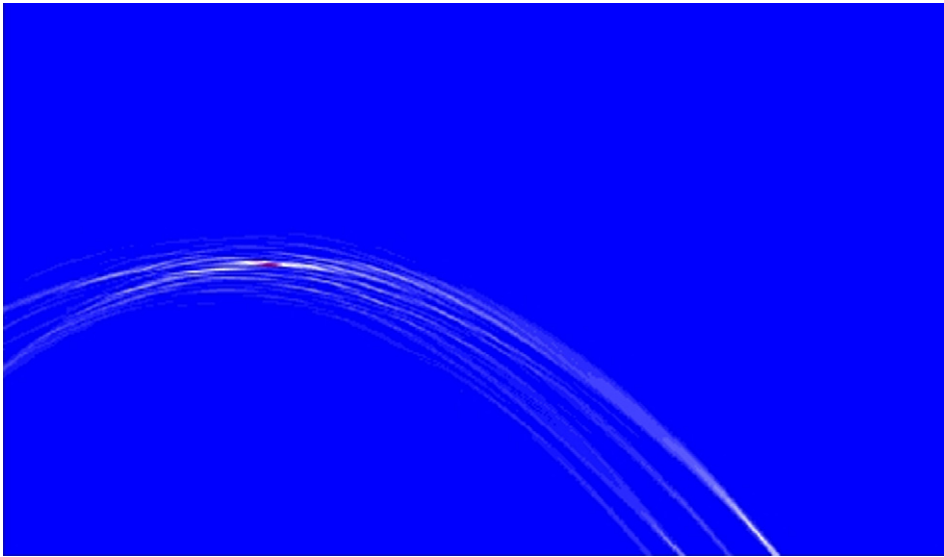


Fig. 3. Laser intensity of a beamlet in a plasma after 6 ps without absorption. Notice the autofocusing of the beamlet near the caustic. The  $x$  axis is here vertical.

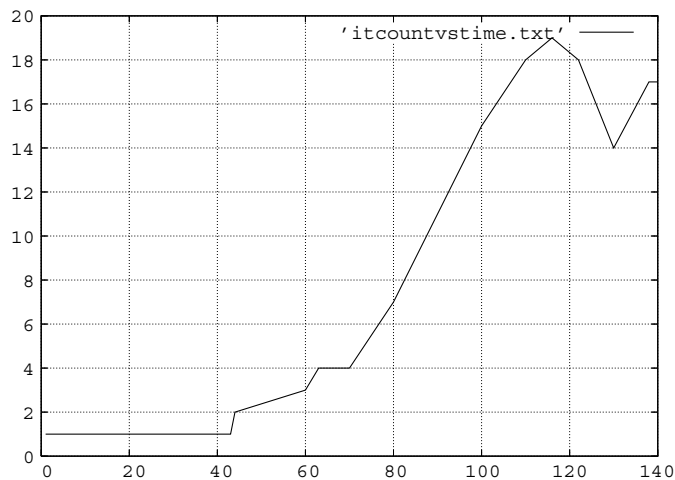


Fig. 4. Number of GMRES iterations versus time.

Table 1  
Scalability for a fixed size problem

Number of processes	16	32	64	128
Elapsed time per GMRES iteration (s)	492	249	126	64
Efficiency GMRES algorithm	1	0.987	0.976	0.96

Table 2  
Scalability for problems of increasing sizes

Number of Processes	1	4	16	64	256
No. of d.o.f. $\times 10^6$	0.4	1.6	6.3	25.4	101.6
Elapsed time for QD algorithm (s)	1	3	12	48	189
Elapsed time per GMRES iteration	4.8	11.6	24	47	93

Another case will be presented, corresponding to simulation domain of  $700 \times 1200$  wave lengths. At the Helmholtz level, one handles 84 millions of cells and the simulation have run on 128 PEs. The map of the laser intensity is shown on Fig. 3 after 6 ps (corresponding to about 15 time steps). We have set to zero the absorption coefficient in order to have a sharp problem. The caustic lines corresponds to about  $N_0(x_\star) = 0.5$ . Here the digging of the plasma is locally very important since the variation of density  $\delta N$  reaches 0.07 in a region where  $N_0(x) = 0.45$ .

## 5.2. Numerical performance

We focus on the solution of the very large system (13) arising from the discretization of the Helmholtz equation by the preconditioned GMRES method presented above. At each time step, the computation is ini-

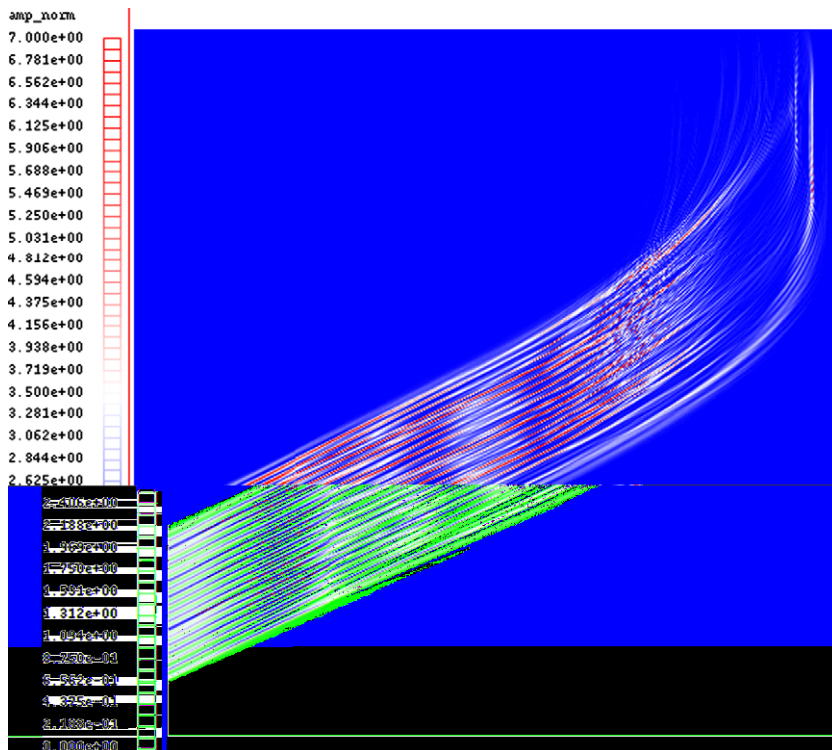


Fig. 5. Laser intensity for a multiple beams laser for a plasma density ranging up to 1.

tialized using the solution of the previous time step. In Fig. 4, we plot the iteration counts as a function of the physical time. As time increases, the density fluctuation  $\delta_N$  gets larger and it is necessary to perform more iterations of the GMRES method. Nevertheless, we do not have more than 20 iterations.

Let us address now the scalability of our computational method. So we consider a fixed size problem of 40 million unknowns and we increase the number of processors. Table 1 gives the elapsed time of one GMRES iteration. Due to the good parallel properties of the cyclic reduction, we see that the speed up is almost perfect. Now when the number of unknowns increases, one can easily check that the computational effort grows proportionally to  $n_x^2 n_y$ . In Table 2, from one column to the next, the number of points is doubled in each direction so the CPU time is 8 times larger. Since the number of processors is multiplied by four, we check that the elapsed time is about two times larger. These two tables show that the parallelization of the cyclic reduction method work very well.

### 5.3. A more realistic case

In the realistic configurations, it may be useful to solve the paraxial equations on a part of the simulation domain in which this approximation is valid and the Helmholtz equations on the remainder where the validity of this approximation is no more true. The mesh size for to numerical solution of the paraxial equation is the same as for the fluid system (see [14,5]). The coupling between the paraxial and Helmholtz parts is performed according to the classical boundary condition for the Helmholtz Eq. (9) with  $\alpha^{\text{in}}$  replaced by  $E^{\text{out}}$ , which is the value of the solution to the paraxial equation at the interface boundary. The advantage of the paraxial equation is that it can be solved by a marching method in space where only 1D systems have to be solved at each vertical line of unknowns; see [5,6].

Here we have performed a simulation with an initial density which is equal to 0.15 up the third of the simulation domain and which ranges linearly up to 1 at  $x = x_{\text{max}}$ , the boundary value  $\alpha^{\text{in}}$  mimics a multispeckle

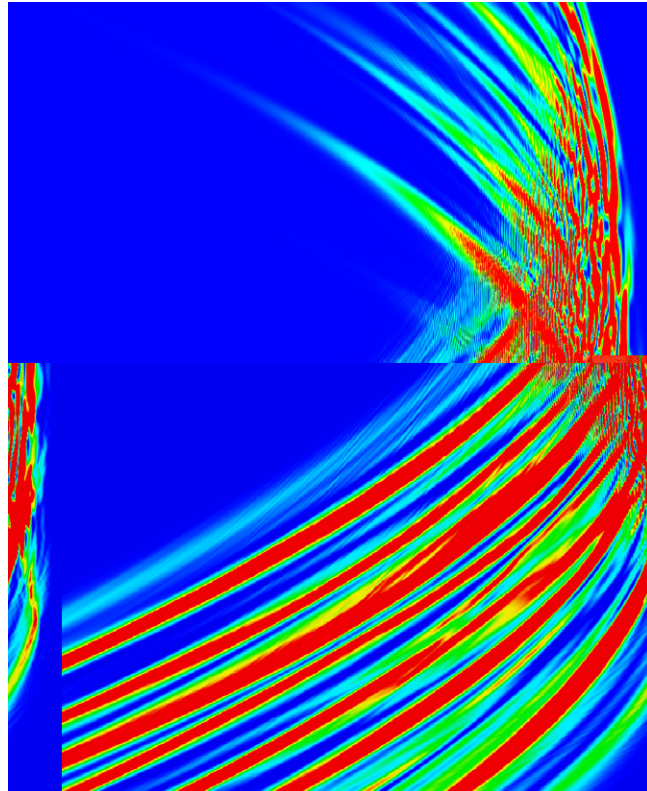


Fig. 6. Zoom near the caustic line of the laser intensity for a multi-speckle beam.

laser beam. We use the paraxial model in the third of the simulation domain and the frequency wave equation in the complementary part, then we have much less unknowns to deal with for the Helmholtz problem. In this simulation, the computational domain size was  $2000 \times 2000$  wave lengths. There were 200 million cells in the Helmholtz zone and 4 millions unknowns for the paraxial zone. The hydrodynamics equations are solved on a domain which consists of 16 million cells. The computation was performed using 256 processors. The physical time of the simulation is equal to 11 ps. The elapsed time for the full simulation was 8 h. On Fig. 5, the map of the laser intensity is represented at the end of simulation.

Lastly, we show on Fig. 6, a zoom of the laser intensity near the caustic line in a numerical simulation of the same type than the previous one, except that the absorption coefficient is small but not zero. One can notice the great accuracy of simulation which shows interference patterns of the speckles.

## 6. Conclusion and prospects

In the framework of the hydrodynamics parallel platform HERA, we have developed a solver for the laser propagation based on the Helmholtz equation that can handle realistic computations on very large computational domains. The Helmholtz zone is coupled with a paraxial zone and a fluid plasma model. The assumption that the initial density  $N$  depends mainly on the  $x$ -variable only allows us to precondition by a domain decomposition method (two PMLs and a large Helmholtz zone) where the linear system corresponding to the Helmholtz zone with a matrix  $A_G$  may be solved efficiently by the block cyclic reduction method. Most of the computer time is spent by applying a dense  $n_x \times n_x$  matrix  $Q$  to a set of  $n_y$  vectors. We can thus achieve a very good scalability w.r.t to the number of unknowns in the  $y$ -direction.

As the physical time evolves the fluctuation of the density increases. We notice then an increase in the number of GMRES iterations per time step, but this number remains small enough to have an acceptable CPU time. In the future some CPU time may be saved by using a domain decomposition in the large central Helmholtz zone. For instance, simply dividing the Helmholtz zone in two vertical subdomains would decrease the size of the matrices  $Q$  by a factor 4. Moreover the use of local (and thus more accurate) averages for the density in the preconditioner could break the increase in the number of iterations as the time increases. Another interesting strategy could be to not consider inside the inner iteration loop of the Krylov method all the spatial domain that is to say all the  $n_y$  vectors but only the vectors which do not belong to some subinterval  $[n_y^1, n_y^2]$  for instance the ones where the solution varies very few from an iteration to the other.

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