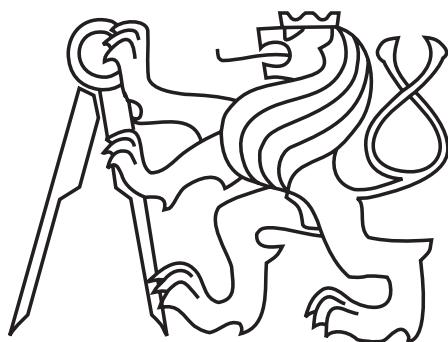


Czech Technical University in Prague  
Faculty of Nuclear Sciences and Physical Engineering  
Department of Physical Electronics



**Tight-focusing of short intense laser pulses in  
particle-in-cell simulations of  
laser-plasma interaction**

(Master thesis)

Author: Bc. Petr Valenta  
Supervisor: doc. Ing. Ondřej Klíma, Ph.D.  
Consultant: Dr. Stefan Andreas Weber  
Academic year: 2016/2017





**ČESKÉ VYSOKÉ UČENÍ TECHNICKÉ V PRAZE**  
**FAKULTA JADERNÁ A FYZIKÁLNĚ INŽENÝRSKÁ**  
*Katedra fyzikální elektroniky*

## **ZADÁNÍ DIPLOMOVÉ PRÁCE**

*Student:* **Bc. Petr Valent**

*Obor:* **Informatická fyzika**

*Školní rok:* **2016/2017**

*Název práce:* **Zaostření krátkého intenzivního laserového impulsu do velmi malého ohniska v PIC simulacích interakce s plazmatem**  
**Tight-focusing of short intense laser pulses in PIC simulations of laser-plasma interaction**

*Vedoucí práce:* **doc. Ing. Ondřej Klimo, PhD.**

*Konzultant:* **Dr. Stefan Weber**

*Cíl práce:*

Cílem práce je implementovat novou okrajovou podmíinku v PIC simulačním kódu EPOCH (případně vytvořit za tímto účelem zvláštní program), která umožní simulaci krátkého intenzivního laserového impulsu zaostřeného do ohniska menšího, než umožňuje paraxiální approximace. Tato okrajová podmínka bude otestována a použita v modelových simulacích, kde bude studován vliv zaostření laserového impulsu na průběh laserové interakce s plazmatem.

*Pokyny pro vypracování:*

- 1) Seznamte se s fyzikou šíření a fokusace krátkých ultra-intenzivních laserových impulsů. Popište paraxiální approximaci a její omezení a vypracujte přehled možností zaostření laserových impulsů do velmi malého ohniska.

- 2) Připravte metodu pro zadání okrajové podmínky v PIC simulacích s kódem EPOCH, která umožní zaostření laserového impulsu do ohniska menšího než je střední vlnová délka laserového záření. Metodu implementujte a otestujte.
- 3) Pro vybrané případy provádějte simulace interakce laserového záření s plazmatem a popište kvantitativní a kvalitativní rozdíly v závislosti na velikosti ohniska.

*Literatura:*

- 1) P. Gibbon, *Short Pulse Laser Interactions with Matter*, Imperial College Press, London, 2005.
- 2) T. D. Arber et al., Contemporary particle-in-cell approach to laser-plasma modelling, *Plasma Physics and Controlled Fusion* 57, 113001 (2015).
- 3) A. Macchi, A Superintense Laser-Plasma Interaction Theory Primer, SpringerBriefs in Physics, Springer, Dordrecht (2013).
- 4) C. K. Birdsall, A. B. Langdon, *Plasma Physics via Computer Simulation*, Hilger, Bristol (1991).
- 5) I. Thiele et al., Boundary conditions for arbitrarily shaped and tightly focused laser pulses in electromagnetic codes, *Journal of Computational Physics* 321, 1110 (2016).
- 6) R. L. Garay-Avendaño et al., Exact analytic solutions of Maxwell's equations describing propagating nonparaxial electromagnetic beams, *Applied Optics* 53, 4524 (2014).
- 7) JX. Li. et al., Fields of an ultrashort tightly focused laser pulse, *Journal of the Optical Society of America B* 33, 405 (2016).

Datum zadání: říjen 2016

Datum odevzdání: 5.květen 2017

.....  
Vedoucí katedry

.....  
Děkan

## **Prohlášení/Declaration**

Prohlašuji, že jsem předloženou práci vypracoval samostatně a že jsem uvedl veškerou použitou literaturu.

I declare that I carried out this work independently, and only with the cited sources, literature and other professional sources.

V Praze dne/In Prague on .....

.....  
Bc. Petr Valenta



Název práce: **Zaostření krátkého intenzivního laserového impulsu do velmi malého ohniska v částicových simulacích interakce s plazmatem**

Autor: Bc. Petr Valenta

Druh práce: Diplomová práce

Studijní program: (N3913) Aplikace přírodních věd

Vedoucí práce: Obor: (3901T065) Informatická fyzika

Vedoucí práce: doc. Ing. Ondřej Klimo, Ph.D.  
Katedra fyzikální elektroniky, Fakulta jaderná a fyzikálně inženýrská, České vysoké učení technické v Praze

Konzultant: Dr. Stefan Andreas Weber  
Projekt ELI-Beamlines, Fyzikální ústav Akademie věd České republiky, v. v. i.

### **Abstrakt**

Content...

Klíčová slova:

Title: **Tight-focusing of short intense laser pulses in particle-in-cell simulations of laser-plasma interaction**

Author: Bc. Petr Valenta

Type of work: Master thesis

Study programme: (N3913) Applications of Natural Sciences

Branch of study: (3901T065) Computational Physics

Supervisor: doc. Ing. Ondřej Klimo, Ph.D.  
Department of Physical Electronics, Faculty of Nuclear Sciences  
and Physical Engineering, Czech Technical University in Prague

Consultant: Dr. Stefan Andreas Weber  
Project ELI-Beamlines, Institute of Physics, The Czech Academy  
of Sciences, v. v. i.

## **Abstract**

Content...

Keywords: plasma-based amplification, PIC simulations, parametric instabilities

# Contents

<b>Introduction</b>	<b>11</b>
<b>1 Electromagnetic field</b>	<b>13</b>
1.1 Maxwell's equations . . . . .	13
1.2 Electrodynamic potentials . . . . .	15
1.3 Hertz vectors . . . . .	16
1.4 Energy and momentum . . . . .	17
1.5 Electromagnetic waves and Gaussian beam . . . . .	19
<b>2 Laser-plasma interaction</b>	<b>23</b>
2.1 Basic plasma parameters . . . . .	23
2.2 Plasma description . . . . .	25
2.3 Electromagnetic waves in plasmas . . . . .	27
2.4 Ponderomotive force . . . . .	29
2.4.1 Non-relativistic case . . . . .	30
2.4.2 Relativistic case . . . . .	32
2.5 Relativistic transparency . . . . .	33
2.6 Laser absorption and electron heating mechanisms . . . . .	33
2.6.1 Resonance absorption . . . . .	34
2.6.2 Brunel vacuum heating . . . . .	34
2.6.3 $\mathbf{J} \times \mathbf{B}$ heating . . . . .	34
2.7 Mechanisms of laser-driven ion acceleration . . . . .	34
2.7.1 Target normal sheath acceleration (TNSA) . . . . .	34
2.7.2 Radiation pressure acceleration (RPA) . . . . .	34
<b>3 Particle-in-cell (PIC)</b>	<b>35</b>
3.1 Mathematical derivation . . . . .	35
3.2 Particle pusher . . . . .	38
3.3 Field solver . . . . .	40
3.4 Particle and field weighting . . . . .	42
3.5 Stability and accuracy . . . . .	43

3.6	Code EPOCH . . . . .	43
<b>4</b>	<b>Tight-focusing of laser pulses</b>	<b>45</b>
4.1	Laser boundary conditions . . . . .	45
4.2	Implementation . . . . .	49
4.3	Evaluation . . . . .	50
<b>5</b>	<b>Results</b>	<b>59</b>
	<b>Conclusion</b>	<b>69</b>
	<b>Bibliography</b>	<b>71</b>
	<b>Appendices</b>	<b>75</b>
<b>A</b>	<b>Input files</b>	<b>75</b>
<b>B</b>	<b>Code listings</b>	<b>81</b>
<b>C</b>	<b>CD content</b>	<b>97</b>

# Introduction

Despite a wide variety of economic drives, the world energy consumption is continuously growing. Fossil fuels, crude oil and natural gas reserves are slowly shrinking and renewable resources alone will definitely not be able to meet the global energy demand. This energetic deficit might become a serious obstacle in the further sustainable development of human society. Therefore it is essential to find an alternative energy source; preferably one which could finally solve all of the aforementioned problems and, in addition, its utilization would be environmentally friendly.

During the 1950s, the demand for alternative and more feasible energy sources for the near future has led to the intensive research in the field of nuclear power engineering. Particularly, scientists became interested in a peaceful use of thermonuclear fusion. Firstly, they have tried to make required conditions for the fusion plasma using convenient geometry of magnetic fields. Early success, which has been expected by the scientific community, however, has not been achieved. Several years later, this fact also contributed to the idea of using lasers, at that time an entirely new source of intense radiation, to ignite thermonuclear fusion. It soon turned out, however, that by using lasers, a wide range of phenomena which might seriously complicate the ignition is inevitable as well.

One of the most negative effects in terms of inertial confinement fusion is the generation of hot electrons in a coronal plasma, in which the laser energy is transmitted to the kinetic energy of plasma. These electrons significantly preheat the core of the fuel target, which makes the required compression of plasma more difficult. Therefore, the laser-plasma interactions in this context have been intensively studied [13]. At the same time, new, more sophisticated methods, whereby laser energy is deposited into the target as efficiently as possible and with a minimal production of hot electrons, have been investigated as well [2].

The following work is focused on the interaction of laser radiation with plasma for the conditions according to current experiments in the Prague Asterix Laser System (PALS) facility, where the possibilities of fuel ignition are studied using a high-power iodine laser. More specifically, the interaction in terms of laser energy absorption efficiency, hot electron production and laser light scattering in a regime relevant to the shock ignition scheme, which has been proposed recently [3], have all been studied.

The work is structured as follows: the first chapter provides a brief description of the thermonuclear fusion, including the conditions of its ignition for both basic approaches.

## Introduction

---

The major part is devoted to inertial fusion. The second chapter summarizes the elementary knowledge of plasma physics and physics of laser-plasma interaction. The third chapter describes numerical simulation as an essential tool in modern science and engineering. Especially, one of the most popular methods in plasma physics, particle-in-cell (PIC), is thoroughly discussed. The characteristics of the code EPOCH[1], which has been used for the simulations within this work, can be found in the last section of this chapter. The last chapter demonstrates the results and benefits of this work. It contains the implementation of the boundary conditions in the code EPOCH and the results of performed two-dimensional simulations.

Although the most convenient unit system for most plasma applications is the Gaussian cgs system, throughout this work the SI (System Internationale) units are used, unless explicitly stated.

Symbols in bold represent vector quantities, and symbols in italics represent scalar quantities, unless otherwise indicated.

# Chapter 1

## Electromagnetic field

Since the laser beam is nothing but the electromagnetic wave, the opening chapter has to be logically devoted to the fundamental physical aspects of the classical electromagnetic field theory based on the elegant Maxwell's equations. The reader can find brief description of the microscopic as well as macroscopic variant of the Maxwell's equations and their general solutions exploiting electrodynamic potentials and Hertz vectors. A short part is devoted also to energy and momentum of the electromagnetic waves. In the last part, one finds the simplest mathematical description of the focused laser beam and conditions of its validity.

### 1.1 Maxwell's equations

The electromagnetic field is in general theory represented by two vectors, the intensity of the electric field  $\mathbf{E}(\mathbf{r}, t)$  and the magnetic induction  $\mathbf{B}(\mathbf{r}, t)$ . These vectors are considered to be finite and continuous functions of position  $\mathbf{r}$  and time  $t$ . The description of electromagnetic phenomena in classical electrodynamics is provided by the set of well-known Maxwell's equations. The microscopic variant for external sources in vacuum is formulated as follows,

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \quad (1.1)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (1.2)$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0, \quad (1.3)$$

$$\nabla \times \mathbf{B} - \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J}, \quad (1.4)$$

where  $\rho(\mathbf{r}, t)$  is total electric charge density and  $\mathbf{J}(\mathbf{r}, t)$  is total electric current density, which is constituted by the motion of a charge. These distributions may be continuous as well as discrete. As might be seen from Maxwell's equations (1.1 - 1.4), the charge density is the

source of the electric field, whilst the magnetic field is produced by the current density. The lack of symmetry in Maxwell's equations (1.2, 1.3 are homogeneous) is caused by the experimental absence of magnetic charges and currents. The universal constants appearing in the Maxwell's equations (1.1, 1.4) are the electric permittivity of vacuum  $\varepsilon_0$  and the magnetic permeability of vacuum  $\mu_0$ .

The first equation, 1.1, is Gauss's law for electric field in the differential form. It states that the flux of the electric field through any closed surface is proportional to the total charge inside. The second equation, 1.2, is Gauss's law for magnetic field. It expresses the fact that there are no magnetic monopoles, so the flux of magnetic field through any closed surface is always zero. The third equation, 1.3, is Faraday's law describing how the electric field is associated with a time varying magnetic field. And the last equation, 1.4, is Ampère's law with Maxwell's displacement current, which means that the time varying electric field causes the magnetic field. As a consequence, it predicts the existence of electromagnetic waves that can carry energy and momentum even in a free space.

To describe the effects of an electromagnetic field in the presence of macroscopic substances, the complicated distribution of charges and currents in matter over the atomic scale is not relevant. Thus one shall define a second set of auxiliary vectors that represent fields in which the material properties are already included in an average sense, the electric displacement  $\mathbf{D}(\mathbf{r}, t)$  and the magnetic vector  $\mathbf{H}(\mathbf{r}, t)$ ,

$$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} = \varepsilon \mathbf{E}, \quad (1.5)$$

$$\mathbf{H} = \frac{\mathbf{B}}{\mu_0} - \mathbf{M} = \frac{\mathbf{B}}{\mu}, \quad (1.6)$$

where  $\mathbf{P}(\mathbf{r}, t)$  and  $\mathbf{M}(\mathbf{r}, t)$  are the vectors of polarization and magnetization, respectively. Note that the vectors of polarization and magnetization can be interpreted as a density of electric or magnetic dipole moment of the medium, therefore they are definitely associated with the state of a matter and vanish in vacuum. Similarly as in the case of free space, the factors  $\varepsilon$  and  $\mu$  are called electric permittivity of medium and magnetic permeability of medium. In general case,  $\varepsilon$  and  $\mu$  are tensors. The constitutive relations above (1.5, 1.6) hold only if the medium is homogeneous and isotropic. For the sake of simplicity, only such materials will be considered in the following text.

The macroscopic variant of Maxwell's equations is formulated as follows,

$$\nabla \cdot \mathbf{D} = \rho, \quad (1.7)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (1.8)$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0, \quad (1.9)$$

$$\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J}, \quad (1.10)$$

where  $\rho(\mathbf{r}, t)$  and  $\mathbf{J}(\mathbf{r}, t)$  now stand for only external electric charge and current density, respectively.

By combining the time derivative of the equation 1.7 with the divergence of the equation 1.10, one obtains the following relation between the electromagnetic field sources,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0. \quad (1.11)$$

The important result 1.11, which is frequently referred to as the equation of continuity, expresses nothing but the conservation of total electric charge in an isolated system. In other words, the time rate of change of the electric charge in any closed surface is balanced by the electric current flowing through the surface.

## 1.2 Electrodynamic potentials

The first-order partial differential Maxwell's equations can be effectively converted to a smaller number of second-order equations by introducing electrodynamic potentials. Hence, one can express the electric and magnetic field as follows,

$$\mathbf{E} = -\nabla\Phi - \frac{\partial \mathbf{A}}{\partial t}, \quad (1.12)$$

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad (1.13)$$

where  $\Phi(\mathbf{r}, t)$  is the scalar potential and  $\mathbf{A}(\mathbf{r}, t)$  is the vector potential of the corresponding fields. One can clearly see that using the definitions 1.12, 1.13, six vector components are replaced by only four potential functions and two Maxwell's homogeneous equations (1.8, 1.9) are fulfilled identically.

However, by definitions 1.12, 1.13,  $\Phi(\mathbf{r}, t)$  and  $\mathbf{A}(\mathbf{r}, t)$  are not defined uniquely, thus an infinite number of potentials which lead to the same fields may be constructed. To avoid that, one has to impose a supplementary condition, for example

$$\nabla \cdot \mathbf{A} + \mu\epsilon \frac{\partial \Phi}{\partial t} = 0. \quad (1.14)$$

The condition 1.14 is called the Lorenz gauge. Lorenz gauge is commonly used in electromagnetism because its independence of the coordinate system. Furthermore, it leads to the following uncoupled equations,

$$\Delta\Phi - \mu\epsilon \frac{\partial^2 \Phi}{\partial t^2} = -\frac{\rho}{\epsilon}, \quad (1.15)$$

$$\Delta\mathbf{A} - \mu\epsilon \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu\mathbf{J}, \quad (1.16)$$

that are in all respects equivalent to the Maxwell's equations and in many situations much simpler to solve.

Equations 1.15, 1.16 correspond to the inhomogeneous wave equations for scalar potential  $\Phi(\mathbf{r}, t)$  and vector potential  $\mathbf{A}(\mathbf{r}, t)$ . Their general solutions are given by the following expressions,

$$\Phi(\mathbf{r}, t) = \frac{1}{4\pi\epsilon} \int \frac{\rho(\mathbf{r}', t')}{\|\mathbf{r} - \mathbf{r}'\|} dV, \quad (1.17)$$

$$\mathbf{A}(\mathbf{r}, t) = \frac{\mu}{4\pi} \int \frac{\mathbf{J}(\mathbf{r}', t')}{\|\mathbf{r} - \mathbf{r}'\|} dV, \quad (1.18)$$

where  $dV$  is a volume element and  $\|\cdot\|$  stands for the standard Euclidean norm. Note that the solutions 1.17, 1.18 are dependent only on charge and current densities at position  $\mathbf{r}'$  at so-called retarded time  $t' = t - \sqrt{\mu\epsilon}\|\mathbf{r} - \mathbf{r}'\|$  which takes into account the finite velocity of the wave. In other words, the fields at the observation point  $\mathbf{r}$  at the time  $t$  are proportional to the sum of all the electromagnetic waves that leave the source elements at point  $\mathbf{r}'$  at the retarded time  $t'$ .

### 1.3 Hertz vectors

There exists also other possibilities how to express the electromagnetic field. Under ordinary conditions, an arbitrary electromagnetic field may be defined in terms of a single vector function. This may be helpful for solving of many problems of classical electromagnetic theory, particularly the wave propagation.

First, let us introduce the electric Hertz vector  $\boldsymbol{\Pi}_e(\mathbf{r}, t)$  in terms of the scalar and vector potentials,

$$\Phi = -\nabla \cdot \boldsymbol{\Pi}_e, \quad (1.19)$$

$$\mathbf{A} = \mu\epsilon \frac{\partial \boldsymbol{\Pi}_e}{\partial t}. \quad (1.20)$$

Note that the definitions 1.19, 1.20 are consistent with the Lorenz gauge condition 1.14. In the absence of magnetization, it might be easily shown that  $\mathbf{J} = \partial \mathbf{P} / \partial t$  and the electric Hertz vector  $\boldsymbol{\Pi}_e(\mathbf{r}, t)$  is governed by an inhomogeneous wave equation

$$\Delta \boldsymbol{\Pi}_e - \mu\epsilon \frac{\partial^2 \boldsymbol{\Pi}_e}{\partial t^2} = -\frac{\mathbf{P}}{\epsilon}. \quad (1.21)$$

The equation 1.21 is of the same type as the equations 1.15, 1.16 and has therefore the familiar general solution

$$\boldsymbol{\Pi}_e(\mathbf{r}, t) = \frac{1}{4\pi\epsilon} \int \frac{\mathbf{P}(\mathbf{r}', t')}{\|\mathbf{r} - \mathbf{r}'\|} dV. \quad (1.22)$$

As might be seen from 1.22, the fields derived from the electric Hertz vector  $\boldsymbol{\Pi}_e(\mathbf{r}, t)$

can be interpreted as being due to a density distribution of electric dipoles. Every solution of 1.22 then uniquely determines the electromagnetic field through

$$\mathbf{E} = \nabla (\nabla \cdot \boldsymbol{\Pi}_e) - \mu\epsilon \frac{\partial^2 \boldsymbol{\Pi}_e}{\partial t^2}, \quad (1.23)$$

$$\mathbf{B} = \mu\epsilon \left( \nabla \times \frac{\partial \boldsymbol{\Pi}_e}{\partial t} \right). \quad (1.24)$$

Second, one may introduce the magnetic Hertz vector  $\boldsymbol{\Pi}_m(\mathbf{r}, t)$  in terms of the scalar and vector potentials by the following expressions,

$$\Phi = 0, \quad (1.25)$$

$$\mathbf{A} = \nabla \times \boldsymbol{\Pi}_m. \quad (1.26)$$

In the absence of polarization,  $\mathbf{J} = \nabla \times \mathbf{M}$  and the magnetic Hertz vector  $\boldsymbol{\Pi}_m(\mathbf{r}, t)$  defined by 1.25 and 1.26 fulfills an inhomogeneous wave equation

$$\Delta \boldsymbol{\Pi}_m - \mu\epsilon \frac{\partial^2 \boldsymbol{\Pi}_m}{\partial t^2} = -\mu\mathbf{M}. \quad (1.27)$$

As for the previous cases, one may easily find the solution of 1.27,

$$\boldsymbol{\Pi}_m(\mathbf{r}, t) = \frac{\mu}{4\pi} \int \frac{\mathbf{M}(\mathbf{r}', t')}{\|\mathbf{r} - \mathbf{r}'\|} dV, \quad (1.28)$$

thus the fields derived from the magnetic Hertz vector  $\boldsymbol{\Pi}_m(\mathbf{r}, t)$  may be imagined to be due to a density distribution of magnetic dipoles. Again, every solution of 1.28 uniquely determines the electromagnetic field via

$$\mathbf{E} = \nabla \times \frac{\partial \boldsymbol{\Pi}_m}{\partial t}, \quad (1.29)$$

$$\mathbf{B} = \nabla \times (\nabla \times \boldsymbol{\Pi}_m). \quad (1.30)$$

Note that the above derivations considered electric and magnetic Hertz vectors as a separate quantities. It is also possible, however, to introduce them together in the form of one six-vector [source].

## 1.4 Energy and momentum

To be able to describe the interaction of the electromagnetic field with matter, one has to know the energy distribution throughout the field as well as the momentum balance.

By scalar multiplications of 1.9 by  $\mathbf{H}(\mathbf{r}, t)$ , of 1.10 by  $\mathbf{E}(\mathbf{r}, t)$ , following subtraction of both obtained equations and using standard vector identities, one gets the expression

$$\mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} + \mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\mathbf{E} \cdot \mathbf{J}. \quad (1.31)$$

The equation 1.31 can be rewritten in the form of conservation law,

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{S} = -\mathbf{E} \cdot \mathbf{J}, \quad (1.32)$$

where

$$u = \frac{1}{2} (\mathbf{E} \cdot \mathbf{D} + \mathbf{H} \cdot \mathbf{B}), \quad \mathbf{S} = \mathbf{E} \times \mathbf{H}. \quad (1.33)$$

The quantity  $u(\mathbf{r}, t)$  in 1.33 describes the total energy density in the field and  $\mathbf{S}(\mathbf{r}, t)$  is so-called Poynting vector which represents, in the equation 1.32, the energy flow of the field per unit area. Note that the Poynting vector points in the same direction as the vector of the wave propagation.

The important statement 1.32, also referred to as the Poynting theorem, expresses the energy balance for the electromagnetic field. In other words, the time rate of change of the field energy within a certain region and the energy flowing out of that region is balanced by the conversion of the electromagnetic energy into mechanical or heat energy.

Besides energy, the electromagnetic wave can carry also momentum. To derive a balance of linear momentum, one has to know the way how charges and currents interact with the electromagnetic field. This is described by the Lorentz force which density  $\mathbf{f}_L(\mathbf{r}, t)$  is given by the following expression,

$$\mathbf{f}_L = \rho \mathbf{E} + \mathbf{J} \times \mathbf{B}. \quad (1.34)$$

Thus the electric and magnetic fields can be regarded as a forces produced by distribution of charge and currents.

By replacing sources in 1.34 using macroscopic Maxwell's equations 1.7, 1.10, one may express the density of Lorentz force  $\mathbf{f}_L(\mathbf{r}, t)$  entirely in terms of fields,

$$\mathbf{f}_L = (\nabla \cdot \mathbf{D}) \mathbf{E} + (\nabla \times \mathbf{H}) \times \mathbf{B} - \frac{\partial \mathbf{D}}{\partial t} \times \mathbf{B}. \quad (1.35)$$

Note that the last term on the right hand side of 1.35 can be rewritten using the Poynting vector  $\mathbf{S}(\mathbf{r}, t)$  derived above,

$$\frac{\partial \mathbf{D}}{\partial t} \times \mathbf{B} = \varepsilon \mu \frac{\partial \mathbf{S}}{\partial t} + \mathbf{D} \times (\nabla \times \mathbf{E}). \quad (1.36)$$

By plugging 1.36 into 1.35 and employing basic vector calculus identities, one eventually gets

the expression for the linear momentum balance in the form of conservation law,

$$\frac{\partial \mathbf{g}}{\partial t} + \nabla \cdot \mathbb{T} = -\mathbf{f}_L, \quad (1.37)$$

where

$$\mathbf{g} = \mathbf{D} \times \mathbf{B}, \quad T_{ij} = -E_i D_j - H_i B_j + \frac{1}{2} (\mathbf{E} \cdot \mathbf{D} + \mathbf{H} \cdot \mathbf{B}) \delta_{ij}. \quad (1.38)$$

The quantity  $\mathbf{g}(\mathbf{r}, t)$  in 1.37 may be interpreted as the density of linear electromagnetic momentum and  $\mathbb{T}(\mathbf{r}, t)$  is so-called Maxwell stress tensor which represents, in the equation 1.37, the momentum flow per unit area. The symbol  $\delta_{ij}$  in 1.38 stands for the Kronecker delta.

The important statement 1.37, which expresses the linear momentum balance for electromagnetic field, may be used to calculate the electromagnetic forces that act on objects or particles within that field. Notice that the contribution of the electromagnetic field to energy and momentum is completely characterized by the fluxes of  $\mathbf{S}(\mathbf{r}, t)$  and  $\mathbb{T}(\mathbf{r}, t)$ .

## 1.5 Electromagnetic waves and Gaussian beam

In this section, the simplest mathematical description of a focused laser beam based on approximations to the wave equation is deduced. Since in numerical codes it is a common practice to prescribe the laser beams by their propagation in free space, the set of the microscopic Maxwell's equations 1.1 - 1.4 will be exploited.

In the absence of external sources, it might be easily shown that the equations 1.1 - 1.4 may be alternatively formulated as an uncoupled homogeneous wave equations for electric field  $\mathbf{E}(\mathbf{r}, t)$  and magnetic field  $\mathbf{B}(\mathbf{r}, t)$ ,

$$\Delta \mathbf{E} - \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0, \quad (1.39)$$

$$\Delta \mathbf{B} - \frac{1}{c^2} \frac{\partial^2 \mathbf{B}}{\partial t^2} = 0, \quad (1.40)$$

where the universal constant  $c = 1/\sqrt{\mu_0 \epsilon_0}$  is the speed of light in vacuum, which leads to the essential fact, that the electromagnetic waves propagate in vacuum with the velocity of light  $c$ . However, the wave equations 1.39, 1.40 do not provide all the information about the electric and magnetic field of the wave. There are further constraints due to Maxwell's equations restricting the orientation and proportional magnitudes of the fields. From the set 1.1 - 1.4, it might be clearly seen that  $\mathbf{E}(\mathbf{r}, t)$  and  $\mathbf{B}(\mathbf{r}, t)$  must be mutually perpendicular to each other as well as to the direction of the wave propagation.

Without any loss of generality, consider the laser beam as a monochromatic electromagnetic wave propagating toward the positive direction of the z-axis. In many standard

references [source], the description of such a wave is given by the evolution of a single electric field component linearly polarized along the x-axis of the Cartesian coordinate system (although the more proper way would be to use the vector potential [source]), therefore one has to look for the solution of the equation 1.39.

According to the previous assumptions, the solution is expected to be in the form of the following plane wave,

$$\mathbf{E}(\mathbf{r}_\perp, z, t) = \Re E_0 \Psi(\mathbf{r}_\perp, z) e^{i(k_z z - \omega t)} \hat{\mathbf{e}}_x, \quad (1.41)$$

where  $\mathbf{r}_\perp = (x, y)^T$  is the vector of transverse Cartesian coordinates, symbol  $\Re$  stands for the real part of the complex quantity,  $E_0$  is a constant amplitude,  $\Psi(\mathbf{r}_\perp, z)$  is the part of the wave function which is dependent only on the spatial coordinates,  $\omega$  denotes the angular frequency,  $k_z$  is the z-component of the wave vector  $\mathbf{k}(\omega)$ ,  $i$  denotes the imaginary unit and  $\hat{\mathbf{e}}_x$  is the unit vector pointing in the direction of the x-axis.

Direct substitution of expression 1.41 into the equation 1.39 yields the time-independent form of the scalar wave equation

$$\Delta \Psi(\mathbf{r}_\perp, z) + 2ik_z \frac{\partial \Psi(\mathbf{r}_\perp, z)}{\partial z} = 0. \quad (1.42)$$

The equation 1.42 is called the Helmholtz equation. Note that it is sufficient to seek solutions to the equation 1.42 since the wave 1.41 is monochromatic.

It turned out, that the geometry of the focused laser beam can be expressed in terms of the laser wavelength  $\lambda$  and the following three parameters,

$$w_0, \quad z_R = \frac{k_z w_0^2}{2} = \frac{\pi w_0^2}{\lambda}, \quad \Theta = \frac{w_0}{z_R} = \frac{\lambda}{\pi w_0}. \quad (1.43)$$

The parameter  $w_0$  in 1.43 is the beam waist, defined as a radius at which the laser intensity fall to  $1/e^2$  of its axial value at the focal spot. The second parameter,  $z_R$ , is so-called Rayleigh range which is a distance in the longitudinal direction from the focal spot to the point where the beam radius is  $\sqrt{2}$  larger than the beam waist  $w_0$ . And the last parameter,  $\Theta$ , is the divergence angle of the beam that represents the ratio of transverse and longitudinal extent.

Because of the symmetry about the longitudinal axis of the equation 1.42, the following calculations may be made simpler by introducing a dimensionless cylindrical coordinates that use the parameters 1.43,

$$\rho = \frac{\|\mathbf{r}_\perp\|}{w_0}, \quad \zeta = \frac{z}{z_R}. \quad (1.44)$$

After performing a transformation of coordinates, the Helmholtz equation 1.42 becomes

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \Psi(\rho, \zeta)}{\partial \rho} \right) + 4i \frac{\partial \Psi(\rho, \zeta)}{\partial \zeta} = -\Theta^2 \frac{\partial^2 \Psi(\rho, \zeta)}{\partial \zeta^2}. \quad (1.45)$$

In the following calculations, the beam divergence angle  $\Theta$  is assumed to be small ( $\Theta \ll 1$ ),

thus it can be used as an expansion parameter for  $\Psi$  and the solution of 1.45 will always be consistent,

$$\Psi = \sum_{n=0}^{+\infty} \Theta^{2n} \Psi_{2n}. \quad (1.46)$$

Next, one shall insert 1.46 into 1.45 and collect the terms with the same power of  $\Theta$ . Then the zeroth-order function  $\Psi_0$  obeys the following equation,

$$\frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \Psi_0(\rho, \zeta)}{\partial \rho} \right) + 4i \frac{\partial \Psi_0(\rho, \zeta)}{\partial \zeta} = 0. \quad (1.47)$$

The equation 1.47, which is called the paraxial Helmholtz equation, is the starting point of traditional Gaussian beam theory. One can expect the solution of 1.47 in the form of a Gaussian function with a width varying along the longitudinal direction, thus

$$\Psi_0(\rho, \zeta) = h(\zeta) e^{-f(\zeta)\rho^2}, \quad (1.48)$$

where  $f(\zeta)$  and  $h(\zeta)$  are unknown complex functions that have to satisfy a condition  $f(0) = h(0) = 1$ . After plugging 1.48 into 1.47, one gets the following equation,

$$-f(\zeta)h(\zeta) + i \frac{dh(\zeta)}{d\zeta} + \rho^2 h(\zeta) \left( f(\zeta)^2 - i \frac{df(\zeta)}{d\zeta} \right) = 0. \quad (1.49)$$

Since the equation 1.49 has to hold for arbitrary value of  $\rho$ , one may find two independent equations that are equivalent to 1.49

$$\frac{1}{f(\zeta)^2} \frac{df(\zeta)}{d\zeta} + i = 0, \quad \frac{1}{f(\zeta)h(\zeta)} \frac{dh(\zeta)}{d\zeta} + i = 0. \quad (1.50)$$

It might be easily shown, that under specified conditions the solutions of equations 1.50 have to be

$$h(\zeta) = f(\zeta), \quad f(\zeta) = \frac{1}{\sqrt{1+\zeta^2}} e^{-i \arctan \zeta}, \quad (1.51)$$

and therefore the complete expression for the zeroth-order wave function  $\Psi_0(\rho, \zeta)$  is

$$\Psi_0(\rho, \zeta) = \frac{1}{\sqrt{1+\zeta^2}} \exp \left[ -\frac{\rho^2}{1+\zeta^2} + i \left( \frac{\rho^2 \zeta}{1+\zeta^2} - \arctan \zeta \right) \right]. \quad (1.52)$$

In many situations, it is also useful to evaluate the expression 1.52 in terms of Cartesian coordinates, in which the zeroth-order wave function  $\Psi_0(\mathbf{r}_\perp, z)$  is

$$\Psi_0(\mathbf{r}_\perp, z) = \frac{w_0}{w(z)} \exp \left[ -\frac{\mathbf{r}_\perp^2}{w(z)^2} + i \left( k_z \frac{\mathbf{r}_\perp^2}{2R(z)} - \varphi_G(z) \right) \right], \quad (1.53)$$

where the parameters used to simplify the expression 1.53 are defined as

$$w(z) = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2}, \quad R(z) = z \left[1 + \left(\frac{z_R}{z}\right)^2\right], \quad \varphi_G(z) = \arctan\left(\frac{z}{z_R}\right). \quad (1.54)$$

One shall discuss the physical meaning of the three parameters 1.54. The function  $w(z)$  represents the spot size parameter of the beam, that is the radius at which the laser intensity fall to  $1/e^2$  of its axial value at any position  $z$  along the beam propagation. Note that the minimum of the spot size  $w(0) = w_0$ , consequently the focal spot is stationary and located at the origin of a Cartesian coordinate system. The second parameter,  $R(z)$  is known to be the radius of curvature of the beam's wavefront at any position  $z$  along the beam propagation. Note that  $\lim_{z \rightarrow 0^\pm} R(z) = \pm\infty$ , therefore the beam behaves like a plane wave at focus as required. The last parameter,  $\varphi_G(z)$ , is the so-called Guoy phase of the beam at any position  $z$  along the beam propagation, which describes a phase shift in the wave as it passes through the focal spot.

Finally, by substituting 1.53 for  $\Psi(\mathbf{r}_\perp, z)$  in 1.41 and taking the real part of that complex quantity, one obtains the electric field of the so-called paraxial Gaussian beam,

$$\mathbf{E}(\mathbf{r}_\perp, z, t) = E_0 \frac{w_0}{w(z)} \exp\left(-\frac{\mathbf{r}_\perp^2}{w(z)^2}\right) \cos\left(\omega t - k_z \left(z + \frac{\mathbf{r}_\perp^2}{2R(z)}\right) + \varphi_G(z)\right) \hat{\mathbf{e}}_x. \quad (1.55)$$

Although given electric field 1.55 describes the main features of the focused laser beam, it might be clearly seen that it does not satisfy Gauss's law (1.1). The correct electric field cannot vary with the direction of its polarization or has to have at least two non-zero vector components. To fix that, one would have to solve the wave equation for the vector potential 1.16 and afterwards exploit the solution to deduce all components of the electric and magnetic fields.

In addition, since one assumed  $\Theta \ll 1$ , the solution 1.55 is not accurate for strongly diverging beams. Since the divergence angle is inversely proportional to the beam waist, the previous condition yields  $w_0 \gg \lambda$ . In other words, it means that 1.55 is not valid for tightly focused laser beams and the need may arise for higher-order corrections.

# Chapter 2

## Laser-plasma interaction

When a high-power laser pulse is focused onto the surface of a solid target, a high density plasma layer is produced almost immediately due to the presence of strong electromagnetic fields. The whole plasma region, which expands at sonic velocities, is dominated by laser-plasma interactions. The laser-plasma interactions offer an environment full of non-linear processes that take place during the propagation of the laser light through the plasma. In this chapter, a brief introduction to this field of research, which is rich both in physics and in applications, is provided.

### 2.1 Basic plasma parameters

A plasma, one of the four fundamental states of matter, is a quasi-neutral gas of charged and neutral particles which exhibits collective behavior [source]. It is necessary to closer explain some terms used in this definition.

By collective behavior one means motions that depend not only on local conditions but on the state of the plasma in remote regions as well. As charged particles move around, they can generate local concentrations of positive or negative charge, which give rise to electric fields. Motion of charges also generates currents, and hence magnetic fields. These fields affect the motion of other charged particles far away. Thus, the plasma gets a wide range of possible motions.

Quasi-neutrality describes the apparent charge neutrality of a plasma over large volumes, while at smaller scales, there can be charge imbalance, which may give rise to local electric fields. This fact can be expressed mathematically as

$$\sum_s q_s n_s \approx 0, \quad (2.1)$$

where  $q_s$  and  $n_s$  is, respectively, the charge and density of particles of species  $s$ . The index of summation is taken over all the particle species of given system.

One of the most important parameters, which allows to predict the behavior of plasmas more accurately, is the degree of its ionization. For a gas containing only single atomic species in thermodynamic equilibrium, the ionization can be clearly recognized from the Saha-Langmuir equation, which is most commonly written in the following form,

$$\frac{n_{k+1}}{n_k} = \frac{2}{n_e h^3} (2\pi m_e k_B T)^{\frac{3}{2}} \frac{g_{k+1}}{g_k} \exp\left(-\frac{\varepsilon_{k+1} - \varepsilon_k}{k_B T}\right). \quad (2.2)$$

Here  $n_k$  is the density of atoms in the  $k$ -th state of ionization,  $n_e$  is the electron density,  $m_e$  stands for the mass of electron,  $k_B$  is Boltzmann's constant,  $T$  is the gas temperature,  $h$  is Planck's constant,  $g_k$  is the degeneracy of the energy level for ions in the  $k$ -th state and  $\varepsilon_k$  is the ionization energy of the  $k$ -th level. From the equation (2.2), it may be clearly seen that the fully ionized plasmas exist only at high temperatures. That is the main reason why plasmas do not occur naturally on Earth (with a few exceptions).

A fundamental characteristics of the plasma behavior is its ability to shield out the electric potentials that are applied to it. Therefore, another important quantity  $\lambda_{Ds}$  which is called the Debye length of species  $s$  is established,

$$\lambda_{Ds} = \sqrt{\frac{\varepsilon_0 k_B T_s}{q_s^2 n_s}}. \quad (2.3)$$

The physical constant  $T_s$  denotes the temperature of the particles of species  $s$ . It often happens that a different species of particles in plasma have separate distributions with different temperatures, although each species can be in its own thermal equilibrium. The Debye length is a measure of the shielding distance or thickness of the sheath.

In plasma, each particle tries to gather its own shielding cloud. The previously mentioned concept of Debye shielding is valid only if there are enough particles in that cloud. Therefore, another important dimensionless number  $N_{Ds}$ , which is called plasma parameter of species  $s$ , is established. Definition of this parameter is given by the average number of particles of species  $s$  in a plasma contained within a sphere of radius of the Debye length, thus

$$N_{Ds} = \frac{4}{3} \pi n_s \lambda_{Ds}^3. \quad (2.4)$$

Consider an electrically neutral plasma in equilibrium. Suppose an amount of electrons is displaced with respect to the ions, for example by intense laser pulse, and then allowed to move freely. An electric field will be set up, causing the electrons to be pulled back toward ions. Thus, the net result is a harmonic oscillation. The frequency of the oscillation is called the electron plasma frequency  $\omega_{pe}$ ,

$$\omega_{pe} = \sqrt{\frac{e^2 n_e}{\varepsilon_0 m_e}}. \quad (2.5)$$

By analogy with the electron plasma frequency (2.5) one could define the ion plasma frequency  $\omega_{pi}$  for a general ion species. However, the ions are much heavier than electrons, so they do not respond to the high frequency oscillation of the electromagnetic field. It is often possible to treat the massive ions as an immobile, uniform, neutralizing background. However, if the frequency of external radiation source or the waves induced in plasmas is close to this frequency, the ion motion must also be included, an example may be stimulated Brillouin scattering.

A typical charged particle in a plasma simultaneously undergo Coulomb collisions with all of the other particles in the plasma. The importance of collisions is contained in an expression called the collision frequency  $\nu_c$ , which is defined as the inverse of the mean time that it takes for a particle to suffer a collision. Relatively accurate calculation of electron-ion collision frequency  $\nu_{ei}$  can be obtained from the following relation,

$$\nu_{ei} = \frac{Ze^4 n_e}{4\pi\varepsilon_0^2 m_e^2 v^3} \ln \Lambda, \quad \Lambda = \frac{\lambda_D}{b_0}. \quad (2.6)$$

The coefficient  $Z$  denotes the charge number,  $v$  is relative velocity of colliding particles and  $\ln \Lambda$  is the so-called Coulomb logarithm. It is ratio of the Debye to Landau length. Landau length  $b_0$  is the impact parameter at which the scattering angle in the center of mass frame is  $90^\circ$ . For many plasmas of interest Coulomb logarithm takes on values between  $5 - 15$ . In a plasma a Coulomb collision rarely results in a large deflection. The cumulative effect of the many random small angle collisions that it suffers, however, is often larger than the effect of the few large angle collisions. Notice that the collision frequency  $\nu_{ei}$  is proportional to  $v^{-3}$ , therefore the effect of collisions in hot plasmas is usually weak.

In a constant and uniform magnetic field, one can find that a charged particle spirals in a helix about the line of force. This helix, however, defines a fundamental time unit and distance scale,

$$\omega_{cs} = \frac{|q_s| \|\mathbf{B}\|}{m_s}, \quad r_{Ls} = \frac{v_\perp}{\omega_{cs}}. \quad (2.7)$$

These are called the cyclotron frequency  $\omega_{cs}$  and the Larmor radius  $r_{Ls}$  of species  $s$ . Here  $v_\perp$  is a positive constant denoting the speed in the plane perpendicular to  $\mathbf{B}$ .

## 2.2 Plasma description

Currently, there exist three different approaches to plasma physics. The particle theory, the kinetic theory and the hydrodynamic theory. Each approach has some advantages and limitations that stem from the simplified assumptions appropriate only for certain phenomena and time scales.

The time evolution of the system containing charged particles in plasma is influenced by the electromagnetic fields formed due to the movement of particles as well as the external

fields (e.g. laser). The particle approach is based on solving the equations of motion for all the particles in the system. In this case, the motion of particles is governed by the Newton's equations with the Lorentz force,

$$m_s \frac{d\mathbf{r}}{dt} = q_s (\mathbf{E} + \mathbf{v} \times \mathbf{B}). \quad (2.8)$$

The particle theory is useful for tracking a single particle motion in prescribed electromagnetic field. Obviously, the general solution for the system of charged particles using this approach can be complicated since the plasma typically consist of a large number of such particles interacting in a self-consistent fields. However, the full analysis for certain cases may be applied with the help of computing infrastructures and particle simulation codes.

The plasma kinetic theory takes into account the motion of all charged particles in the system as well. However, the evolution of such system is not described by the exact motion of the particles, but only via certain average properties. The kinetic theory is based on a set of equations for the distribution function  $f_s(\mathbf{x}, \mathbf{v}, t)$  of each particle of species  $s$  in plasma. The distribution function may be interpreted as a statistical description of a large number of interacting particles in the system. If collisions can be neglected (for example in hot plasmas), the distribution function is governed by the collisionless Vlasov equation,

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla f_s + \frac{q_s}{m_s} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_s}{\partial \mathbf{v}} = 0. \quad (2.9)$$

The Vlasov equation 2.9 is obtained only by making the assumption that the particle density is conserved, such that the time rate of change in a phase-space volume is equal to the flux of particles in or out of that volume. Due to its simplicity, the equation 2.9 is probably the most commonly used equation in the kinetic theory. However, the assumption to neglect collisions in a plasma is not valid generally. If it is necessary to take them into account, the collision term can be approximated using several methods [source].

In spite of the fact that the hydrodynamic theory is the roughest approximation for the description of plasma, it is sufficiently accurate to describe the majority of observed phenomena. The velocity distribution of each species is assumed to be Maxwellian everywhere, so the dependent variables are functions of only space and time coordinates. In other words, the fluid equations are the first three moments of the Vlasov equation (2.9). These yield the following hydrodynamic equations for the density, momentum and the energy,

$$\frac{\partial n_s}{\partial t} + \nabla \cdot (n_s \mathbf{u}_s) = 0, \quad (2.10)$$

$$m_s n_s \left[ \frac{\partial \mathbf{u}_s}{\partial t} + (\mathbf{u}_s \cdot \nabla) \mathbf{u}_s \right] + \nabla \cdot \mathbb{P}_s = q_s n_s (\mathbf{E} + \mathbf{u}_s \times \mathbf{B}), \quad (2.11)$$

$$\frac{\partial}{\partial t} \left( \frac{1}{2} n_s m_s u_s^2 + e_s \right) + \nabla \cdot \left( \frac{1}{2} n_s m_s u_s^2 \mathbf{u}_s + e_s \mathbf{u}_s + \mathbb{P}_s \mathbf{u}_s + \mathbf{Q}_s \right) = q_s n_s \mathbf{u}_s \cdot \mathbf{E}. \quad (2.12)$$

The zeroth-order moment (2.10) yields the continuity equation, where  $\mathbf{u}_s(\mathbf{x}, t)$  is the velocity of the fluid of species  $s$ . This equation essentially states that the total number of particles is conserved. The first-order moment (2.11) leads to a momentum equation. Here  $\mathbb{P}_s(\mathbf{x}, t)$  is the pressure tensor. This comes about by separating the particle velocity into the fluid and a thermal component of velocity. The thermal velocity then leads to the pressure term. Finally, the second-order moment (2.12) corresponds to the energy equation, where  $e_s$  is the density of the internal energy and  $\mathbf{Q}_s$  describes the heat flux density.

Note that the moment equations form an infinite set. Thus, in order to solve these equations, a truncation is required. For the system of equations 2.10 - 2.12 to be complete, it has to be supplemented by the equation of state, which describes the relation between pressure and density in the plasma. However, the equations of state are well defined only in local thermodynamic equilibrium. Otherwise, the system cannot provide sufficiently exact description and thus the fluid equations 2.10 - 2.12 are not appropriate.

## 2.3 Electromagnetic waves in plasmas

In this section, general properties of the electromagnetic wave propagation in magnetized plasmas are described. Particularly, consider in some detail the waves traveling parallel to and perpendicular to magnetic field.

First, the dispersion relation is derived from the hydrodynamic plasma equations. Since one assume plasma response to a high frequency field, the ions are treated as a stationary, neutralizing background. Thermal motion of particles is also ignored, thus the pressure term in 2.11 can be neglected. According to previous assumptions, one shall solve the following set of equations,

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{u}_e) = 0, \quad (2.13)$$

$$m_e n_e \left[ \frac{\partial \mathbf{u}_e}{\partial t} + (\mathbf{u}_e \cdot \nabla) \mathbf{u}_e \right] = -en_e (\mathbf{E} + \mathbf{u}_e \times \mathbf{B}). \quad (2.14)$$

The symbol  $e$  denotes the elementary charge.

To obtain the wave equations for the oscillating electric and magnetic field, Faraday's law (1.3) and Ampere's law (1.4) are also needed. Next, the system of equations will be linearized by using the methods of perturbation theory. Consider a small perturbations from the stationary state,

$$n_e = n_{e0} + \delta n_e, \quad \mathbf{u}_e = \mathbf{u}_{e0} + \delta \mathbf{u}_e, \quad \mathbf{B} = \mathbf{B}_0 + \delta \mathbf{B}, \quad \mathbf{E} = \mathbf{E}_0 + \delta \mathbf{E}, \quad (2.15)$$

where  $\mathbf{u}_{e0}$  and  $\mathbf{E}_0$  are obviously identically equal to zero vector. After substituting per-

turbed quantities (2.15) into initial system of equations and performing Fourier transform one obtains

$$\delta n_e = i \frac{n_{e0}}{\omega} \mathbf{k} \cdot \delta \mathbf{u}_e, \quad (2.16)$$

$$\delta \mathbf{u}_e = -i \frac{e}{m_e \omega} \delta \mathbf{E} - i \frac{e}{m_e \omega} \delta \mathbf{u}_e \times \mathbf{B}_0, \quad (2.17)$$

$$\delta \mathbf{B} = \frac{1}{\omega} \mathbf{k} \times \delta \mathbf{E}, \quad (2.18)$$

$$\delta \mathbf{E} = -\frac{1}{\varepsilon_0 \mu_0 \omega} \mathbf{k} \times \delta \mathbf{B} + i \frac{en_0}{\varepsilon_0 \omega} \delta \mathbf{u}_e. \quad (2.19)$$

Note that the equation for density perturbation 2.16 may be ignored. Eliminating  $\delta \mathbf{B}$  and  $\delta \mathbf{u}_e$  from the equation 2.19 one gets the equation for perturbation of the electric field,

$$\begin{aligned} & (\omega^2 - \omega_{pe}^2 - c^2 k^2) \delta \mathbf{E} + i \frac{\omega_{ce}}{\omega} (\omega^2 - c^2 k^2) \delta \mathbf{E} \times \mathbf{e}_B + \\ & + c^2 (\mathbf{k} \cdot \delta \mathbf{E}) \mathbf{k} + i \frac{\omega_{ce}}{\omega} c^2 (\mathbf{k} \cdot \delta \mathbf{E}) \mathbf{k} \times \mathbf{e}_B = 0. \end{aligned} \quad (2.20)$$

Here  $\mathbf{e}_B$  is a unit vector in the direction of the magnetic field,

$$\mathbf{e}_B = \frac{\mathbf{B}_0}{B_0}. \quad (2.21)$$

If one choose, without the loss of generality, the coordinate system where  $\mathbf{B}_0 = (0, 0, B_0)$  and  $\mathbf{k} = (k \sin \alpha, 0, k \cos \alpha)$ , one obtains the equation  $\mathbb{M} \cdot \delta \mathbf{E} = 0$  with the matrix

$$\mathbb{M} = \begin{pmatrix} \omega^2 - \omega_{pe}^2 - c^2 k^2 \cos^2 \alpha & i \frac{\omega_{ce}}{\omega} (\omega^2 - c^2 k^2) & c^2 k^2 \cos \alpha \sin \alpha \\ -i \frac{\omega_{ce}}{\omega} (\omega^2 - c^2 k^2 \cos^2 \alpha) & \omega^2 - \omega_{pe}^2 - c^2 k^2 & -i \frac{\omega_{ce}}{\omega} c^2 k^2 \cos \alpha \sin \alpha \\ c^2 k^2 \cos \alpha \sin \alpha & 0 & \omega^2 - \omega_{pe}^2 - c^2 k^2 \sin^2 \alpha \end{pmatrix}. \quad (2.22)$$

The system of equations has non-trivial solution if and only if  $\det(\mathbb{M}) = 0$ . This condition leads to the desired dispersion relation for an arbitrary angle  $\alpha$ ,

$$\begin{aligned} & \left[ (\omega^2 - \omega_{pe}^2 - c^2 k^2 \cos^2 \alpha) (\omega^2 - \omega_{pe}^2 - c^2 k^2 \alpha) - \left( \frac{\omega_{ce}}{\omega} \right)^2 (\omega^2 - c^2 k^2) (\omega^2 - c^2 k^2 \cos^2 \alpha) \right] \\ & (\omega^2 - \omega_{pe}^2 - c^2 k^2 \sin^2 \alpha) - c^4 k^4 \cos^2 \alpha \sin^2 \alpha \left[ (\omega^2 - \omega_{pe}^2 - c^2 k^2) - \left( \frac{\omega_{ce}}{\omega} \right)^2 (\omega^2 - c^2 k^2) \right] = 0. \end{aligned} \quad (2.23)$$

Now, it is necessary to find dispersion relations for the two simplest cases, propagation along and perpendicular to the magnetic field. For the waves propagating along  $\mathbf{B}_0$  is  $\alpha = 0$  and the dispersion relation 2.23 gets relatively simple form,

$$(\omega^2 - \omega_{pe}^2) \left[ (\omega^2 - \omega_{pe}^2 - c^2 k^2)^2 - \left( \frac{\omega_{ce}}{\omega} \right)^2 (\omega^2 - c^2 k^2)^2 \right] = 0. \quad (2.24)$$

The equation 2.24 has three solutions. The first describes plasma oscillations at frequency  $\omega = \omega_{pe}$ . The second and third solutions give right-handed (R) and left-handed (L) circularly polarized waves,

$$N_R^2 = 1 - \frac{(\omega_{pe}/\omega)^2}{1 - \omega_{ce}/\omega}, \quad N_L^2 = 1 - \frac{(\omega_{pe}/\omega)^2}{1 + \omega_{ce}/\omega}. \quad (2.25)$$

The symbol  $N$  stands for the index of refraction, which is more useful for describing how the waves propagate through medium.

In a similar manner, for the waves propagating perpendicular to  $\mathbf{B}_0$  is  $\alpha = \pi/2$  and the dispersion relation 2.23 has the following form,

$$(\omega^2 - \omega_{pe}^2 - c^2 k^2) [(\omega^2 - \omega_{pe}^2) (\omega^2 - \omega_{pe}^2 - c^2 k^2) - \omega_{ce}^2 (\omega^2 - c^2 k^2)] = 0. \quad (2.26)$$

The equation 2.26 has two solutions, which give ordinary (O) and extraordinary (X) waves,

$$N_O^2 = 1 - \left( \frac{\omega_{pe}}{\omega} \right)^2, \quad N_X^2 = 1 - \left( \frac{\omega_{pe}}{\omega} \right)^2 \frac{1 - (\omega_{pe}/\omega)^2}{1 - (\omega_{pe}/\omega)^2 - (\omega_{ce}/\omega)^2}. \quad (2.27)$$

The ordinary wave corresponds to a linearly polarized wave with electric field lying along the magnetic field direction, so that the motion remains unaffected. The extraordinary wave has the electric fields that are perpendicular to magnetic field, but with components both perpendicular and parallel to the wave vector.

The important properties of these waves are distinguished by their cut-offs ( $N \rightarrow 0$ ) and resonances ( $N \rightarrow \infty$ ). In the vicinity of the resonance there is a total absorption, at a cut-off frequency there is a total reflection of incident waves. All of the cut-offs and resonances of waves (including ions) are listed in the table 1.

## 2.4 Ponderomotive force

The ponderomotive force is probably the most important quantity that describes the interaction of high intensity laser pulses with plasma. It represents the gradient of the laser electric field that pushes charged particles in plasma into the regions of a lower field amplitude and it consequently leads to a wide range of non-linear phenomena that make the plasma inherently unstable. The ponderomotive force is involved e. g. in filamentation and self-focusing of laser beam, in the formation of cavities and solitons in the plasma profile or

Wave	Cut-offs	Resonances
R	$\omega_R = \frac{1}{2}\omega_{ce} + \frac{1}{2}\sqrt{\omega_{ce}^2 + 4\omega_{pe}^2}$	$\omega_{ce} = \frac{eB_0}{m_e}$
L	$\omega_L = -\frac{1}{2}\omega_{ce} + \frac{1}{2}\sqrt{\omega_{ce}^2 + 4\omega_{pe}^2}$	$\omega_{ci} = \frac{ZeB_0}{m_i}$
O	$\omega = \sqrt{\omega_{pe}^2 + \omega_{pi}^2}$	-
X	$\omega = \omega_R, \quad \omega = \omega_L$	$\omega_{lh} = \sqrt{\omega_{ce} \omega_{ci}}, \quad \omega_{uh} = \sqrt{\omega_{pe}^2 + \omega_{ce}^2}$

**Table 1:** Summary of cut-offs and resonances for all the principal waves. Note that  $\omega_{lh}$  and  $\omega_{uh}$  are so-called lower hybrid frequency and upper hybrid frequency, respectively.

various parametric instabilities.

Note that since the mass of the ions is much higher than the electron mass, the ponderomotive force acting on ions is in most cases negligible. However, the ponderomotive force exerted on the electrons may be consequently transmitted to the ions by the electric field which is created due to the charge separation in plasma.

In the following two subsections, one can find the derivation of the ponderomotive force for the non-relativistic as well as the relativistic case. The derivation of the non-relativistic formula for ponderomotive force is easy to understand and clearly depicts its main characteristics that are valid even for the relativistic case. However, one has to be aware that the non-relativistic approximation breaks down if the laser intensity exceeds the values of  $10^{16}$  W/cm<sup>2</sup>. This may be the case of short or tightly focused laser beams. For this reason, the relativistic case is briefly discussed as well in the second subsection.

### 2.4.1 Non-relativistic case

The ponderomotive force can be derived from the motion of single particle in prescribed electromagnetic field. Thus one may exploit the Newton's equation of motion with the Lorentz force (2.8). As the laser propagates through plasma, one may expect the oscillation of charged particles in a high-frequency electromagnetic field. For the mathematical description, one may exploit the so-called oscillation-center approximation in this case. It consists of splitting the radius vector  $\mathbf{r}$  and velocity  $\mathbf{v}$  of an arbitrary charged particle into two parts,

$$\mathbf{r} = \mathbf{r}_0 + \delta\mathbf{r}, \quad \mathbf{v} = \mathbf{v}_0 + \delta\mathbf{v}, \quad (2.28)$$

where the index 0 denotes the quantities at the center of oscillation and  $\delta\mathbf{x} = \mathbf{x} - \mathbf{x}_0$  stands for the oscillating vector.

Next, one may exploit the Taylor series to expand both, the electric field  $\mathbf{E}(\mathbf{r}, t)$  and magnetic field  $\mathbf{B}(\mathbf{r}, t)$  around the oscillation center  $\mathbf{r}_0$ ,

$$\mathbf{E}(\mathbf{r}_0 + \delta\mathbf{r}, t) \cong \mathbf{E}(\mathbf{r}_0, t) + (\delta\mathbf{r} \cdot \nabla) \mathbf{E}(\mathbf{r}_0, t), \quad (2.29)$$

$$\mathbf{B}(\mathbf{r}_0 + \delta\mathbf{r}, t) \cong \mathbf{B}(\mathbf{r}_0, t) + (\delta\mathbf{r} \cdot \nabla) \mathbf{B}(\mathbf{r}_0, t). \quad (2.30)$$

Note that taking only the zeroth and first-order terms of the fields is sufficiently accurate approximation for the description of ponderomotive force.

By substituting 2.28, 2.29 and 2.30 into ?? and collecting the terms of the same order, one obtains following two equations,

$$m_s \frac{d^2 \delta\mathbf{r}}{dt^2} = q_s [\mathbf{E}(\mathbf{r}_0, t) + \mathbf{v}_0 \times \mathbf{B}(\mathbf{r}_0, t)], \quad (2.31)$$

$$m_s \frac{d^2 \mathbf{r}_0}{dt^2} = q_s [(\delta\mathbf{r} \cdot \nabla) \mathbf{E}(\mathbf{r}_0, t) + \delta\mathbf{v} \times \mathbf{B}(\mathbf{r}_0, t)]. \quad (2.32)$$

To solve equations 2.31 and 2.32, assume further the laser fields in the form of standing monochromatic wave,

$$\mathbf{E}(\mathbf{r}_0, t) = \mathbf{E}_0(\mathbf{r}_0) \cos \omega t, \quad \mathbf{B}(\mathbf{r}_0, t) = -\frac{1}{\omega} \nabla \times \mathbf{E}_0(\mathbf{r}_0) \sin \omega t. \quad (2.33)$$

Note that the magnetic field in 2.33 has been obtained by the integration of Faraday's law (1.3). For the non-relativistic case, the term  $\mathbf{v}_0 \times \mathbf{B}(\mathbf{r}_0, t)$  is small in comparison with the term  $\mathbf{E}(\mathbf{r}_0, t)$  in the equation 2.31, thus it can be neglected. Taking into account the previous considerations, the solution of 2.31 yields the oscillating quantities,

$$\delta\mathbf{r} = -\frac{q_s}{m_s \omega^2} \mathbf{E}_0(\mathbf{r}_0) \cos \omega t, \quad \delta\mathbf{v} = \frac{q_s}{m_s \omega} \mathbf{E}_0(\mathbf{r}_0) \sin \omega t. \quad (2.34)$$

Since the integration constants can be considered as a slowly varying time functions, they have been included in  $\mathbf{r}_0$ .

By inserting 2.34 into 2.32 one gets immediately the following formula,

$$m_s \frac{d^2 \mathbf{r}_0}{dt^2} = -\frac{q_s^2}{m_s \omega^2} [(\mathbf{E}_0(\mathbf{r}_0) \cdot \nabla) \mathbf{E}_0(\mathbf{r}_0) \cos^2 \omega t + \mathbf{E}_0(\mathbf{r}_0) \times (\nabla \times \mathbf{E}_0(\mathbf{r}_0)) \sin^2 \omega t]. \quad (2.35)$$

To get the quasi-stationary ponderomotive force, one shall compute the time average values over the laser period  $T = 2\pi/\omega$ . Thus by performing the time average of 2.35 (note

that  $\langle \sin^2 \omega t \rangle_T = \langle \cos^2 \omega t \rangle_T = 1/2$  ) one gets

$$m_s \left\langle \frac{d^2 \mathbf{r}_0}{dt^2} \right\rangle_T = -\frac{q_s^2}{2m_s \omega^2} [(\mathbf{E}_0(\mathbf{r}_0) \cdot \nabla) \mathbf{E}_0(\mathbf{r}_0) + \mathbf{E}_0(\mathbf{r}_0) \times (\nabla \times \mathbf{E}_0(\mathbf{r}_0))]. \quad (2.36)$$

The first term on the right-hand side of 2.36 contributes to the transverse component of the ponderomotive force, whilst its longitudinal component originates from the second term. Utilizing standard identities of vector calculus, one finally gets the resulting quasi-stationary ponderomotive force  $\mathbf{F}_p(\mathbf{r})$  in the non-relativistic case,

$$\mathbf{F}_p = -\nabla \Phi_p, \quad \Phi_p = \frac{q_s^2}{4m_s \omega^2} \mathbf{E}_0^2, \quad (2.37)$$

where  $\Phi_p(\mathbf{r})$  is the corresponding ponderomotive potential, which may be interpreted as a cycle-averaged oscillation energy.

Sometimes, it may be yet useful to have the expression for the ponderomotive force per unit volume  $\mathbf{f}_p(\mathbf{r})$ . To obtain it, one has to multiply the formula 2.36 by the particle density. In the case of the electron fluid and normal laser light incidence on plasma, one gets the following easy-to-remember form,

$$\mathbf{f}_p = -\frac{\varepsilon_0 \omega_{pe}^2}{4 \omega^2} \nabla \mathbf{E}_0^2. \quad (2.38)$$

#### 2.4.2 Relativistic case

The non-relativistic case is based on neglecting the term  $\mathbf{v} \times \mathbf{B}$  in the Newton's equation of motion (2.8). However, this approximation is not valid for particles moving with velocities close to the velocity of light  $c$ . The following derivation of relativistic ponderomotive force follows [source].

A system containing a charged particle in an arbitrary electromagnetic field can be rigorously described using Lagrangian mechanics. The relativistic Lagrangian  $L(\mathbf{r}, \mathbf{v}, t)$  for this case is given by the following expression,

$$L = -\frac{m_s c^2}{\gamma} - q_s (\Phi - \mathbf{v} \cdot \mathbf{A}), \quad \gamma = \left(1 - \frac{\mathbf{v}^2}{c^2}\right)^{-\frac{1}{2}}. \quad (2.39)$$

For the traveling monochromatic wave, the Lagrangian  $L(\mathbf{r}, \mathbf{v}, t)$  in 2.39 can be transformed to  $L(\varphi)$  using the wave phase  $\varphi = \mathbf{k} \cdot \mathbf{r} - \omega t$ . The reason of doing this is that the transformed

Lagrangian can be used to obtain the average over the wave period of motion,

$$\mathcal{L}_0(\varphi) = \frac{1}{2\pi} \int_{\varphi}^{\varphi+2\pi} \mathcal{L}(\varphi') d\varphi', \quad \mathcal{L}(\varphi) = L(\varphi) \left( \frac{d\varphi}{dt} \right)^{-1}. \quad (2.40)$$

Note that the Langrangian 2.40 depends only on the quantities at the center of oscillation  $\mathbf{r}_0$  and  $\mathbf{v}_0$  defined through  $\varphi$ . Then the motion of the oscillation center is governed by the Lagrange equations,

$$\frac{d}{dt} \left( \frac{\partial L_0}{\partial \mathbf{v}_0} \right) - \frac{\partial L_0}{\partial \mathbf{r}_0} = 0, \quad L_0(\varphi) = \mathcal{L}_0(\varphi) \left( \frac{d\varphi}{dt} \right). \quad (2.41)$$

The complete proof of assertions above can be found in [source].

The relativistic ponderomotive force in the oscillation center system can be easily found from the Lagrange equations 2.41,

$$\mathbf{F}_p \equiv \frac{d}{dt} \left( \frac{\partial L_0}{\partial \mathbf{v}_0} \right) = -c^2 \nabla m_{\text{eff}}, \quad (2.42)$$

where the so-called effective mass  $m_{\text{eff}}$  is the space and time dependent quantity that has been introduced as follows,

$$m_{\text{eff}} = -\mathcal{L}_0 \frac{\gamma_0}{c^2} \left( \frac{d\varphi}{dt} \right), \quad \gamma_0 = \left( 1 - \frac{\mathbf{v}_0^2}{c^2} \right)^{-\frac{1}{2}}. \quad (2.43)$$

Note that the assertion 2.43 holds for any electromagnetic field in vacuum in which it is possible to define the oscillation center. In an ordinary conditions, the effective mass  $m_{\text{eff}}$  can be rewritten as

$$m_{\text{eff}} = m_s \sqrt{1 + \frac{q_s \mathbf{A}^2}{\alpha m_s^2 c^2}} \quad (2.44)$$

with  $\alpha = 1$  for circular and  $\alpha = 2$  for linear polarization of the electromagnetic wave.

## 2.5 Relativistic transparency

## 2.6 Laser absorption and electron heating mechanisms

Absorption of laser energy in laser-plasma interactions is an important issue, which has been closely related to the applications including the inertial fusion research ever since the invention of laser. Intense laser pulse can be absorbed in plasma by different non-linear mechanisms. In the following, the three main mechanisms of absorption of laser radiation

are briefly described.

### 2.6.1 Resonance absorption

The energy of laser beam may be, among others, absorbed by resonance absorption in the plasma. It is a linear process in which an incident laser wave is partially absorbed by conversion into an electron wave at the critical density of plasma  $n_c(\omega)$ .

Resonance absorption takes place when a linearly p-polarized laser pulse is obliquely incident on a plasma with an inhomogeneous density profile. A component of the electric laser field perpendicular to the target surface then resonantly excites an electron plasma wave also along the plasma density gradient, thus a part of the laser wave energy is transferred into the electrostatic energy of the electron plasma wave. This wave propagates into the underdense plasma and is damped either by collision or collisionless absorption mechanisms. Consequently, energy is further converted into the thermal energy which heats the plasma and may possibly produce hot electrons.

Particularly, resonance absorption is the main absorption process for the higher laser intensities and longer wavelengths. The efficiency of the resonance absorption may also be higher for hot plasmas, low critical density, or short scale length of the plasma density profile.

### 2.6.2 Brunel vacuum heating

### 2.6.3 $\mathbf{J} \times \mathbf{B}$ heating

## 2.7 Mechanisms of laser-driven ion acceleration

### 2.7.1 Target normal sheath acceleration (TNSA)

### 2.7.2 Radiation pressure acceleration (RPA)

# Chapter 3

## Particle-in-cell (PIC)

This chapter is devoted to numerical simulations, particularly to the particle-in-cell (PIC) method, which represents one of the most popular numerical algorithms in plasma physics. There can be found the mathematical background of this method, description of the individual steps of the computational cycle as well as the stability conditions. The last section provides a brief overview of the particle-in-cell code EPOCH, which has been used for simulations within this work.

### 3.1 Mathematical derivation

Laser-plasma interaction involves a collective behavior of particles and electromagnetic fields which is in general case complex and strongly non-linear problem to solve. The investigation of such systems cannot be usually carried out only through the theoretical and experimental work. Since a large amount of simultaneous interactions with many degrees of freedom may be present there, analytical modeling seems to be impractical. On the other hand, many of the significant details of laser-plasma interaction may be extremely difficult or even impossible to obtain experimentally. Hence, for the further progress in this field of research, other tools and techniques are required [10].

Numerical simulations help researchers to develop models covering a wide range of physical scenarios as well as to investigate their properties. With the advent of powerful computational systems, numerical simulations now play an important role as an essential tool in developing theoretical models and understanding experimental results in various fields of modern science [12]. These so-called computer experiments are often faster and much cheaper than a single real experiment in laboratory [8]. In addition, one numerical code can solve a broad range of tasks only by modification of its initial and boundary conditions.

Nowadays, it is clear that detailed understanding of the physical mechanisms in the laser-plasma interaction can be achieved only through the combination of theory, experiment and simulation. Development of parallel algorithms that are able to provide sufficiently exact

solutions in reasonable time, however, belongs to the most challenging fields of modern science.

The PIC method refers to a technique that has been used to solve a certain class of partial differential equations. The method has been proposed in the mid-fifties and it has early gained a great popularity in the field of plasma physics. It is based on the kinetic description approach, thus the evolution of the system is conducted in principle via the motion of the charged particles.

However, real systems are often extremely large in terms of the number of particles they contain. In order to make simulations computationally tractable, so-called macro-particles are used. The macro-particle is a finite-size computational particle representing a group of physical particles that are near each other in the phase space. Notice that it is allowed to rescale the number of particles, because the Lorentz force depends only on the charge to mass ratio, which is invariant to this transformation. Thus, the macro-particle will follow the same trajectory as the corresponding real particles would [9].

Although this approach significantly reduces the number of computational particles in simulation, the binary interactions for every pair of a system cannot be taken into account. The cost would scale quadratically as the number of particles increases and that makes the computational effort unmanageable in the case of larger systems. Fortunately, many of the phenomena occur in high-temperature plasmas where the collective behavior dominates and the collisional effects are very weak (see 2.6), thus one can neglect them. Otherwise, one has to exploit other techniques to estimate the collisional effects [11].

In the collisionless plasma, the phase space particle distribution function  $f_s(\mathbf{r}, \mathbf{v}, t)$  for a given species  $s$  is governed by the Vlasov equation (2.9). The mathematical formulation of the PIC method is obtained by assuming that the distribution function  $f_s(\mathbf{r}, \mathbf{v}, t)$  is given by the sum of distribution functions for macro-particles  $f_{p,s}(\mathbf{r}, \mathbf{v}, t)$ ,

$$f_s = \sum_p f_{p,s}. \quad (3.1)$$

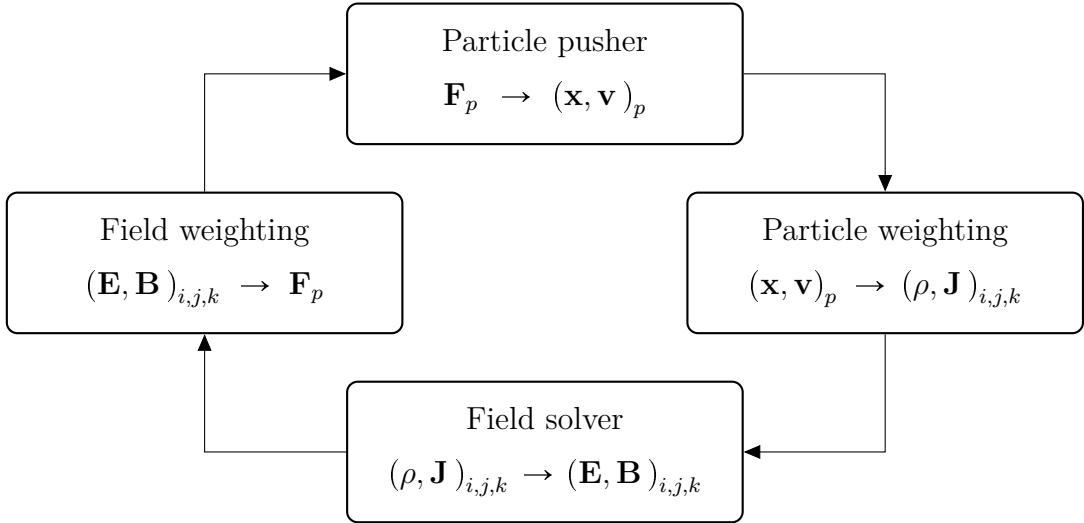
Index  $p$  denotes hereafter the quantities attributable to macro-particles. The distribution function for each macro-particle is further assumed to be

$$f_{p,s}(\mathbf{r}, \mathbf{v}, t) = w_p S_r(\mathbf{r} - \mathbf{r}_p(t)) S_v(\mathbf{v} - \mathbf{v}_p(t)), \quad (3.2)$$

where  $w_p$  is a weight depending on the number of physical particles represented by each macro-particle, and  $S_r(\mathbf{r} - \mathbf{r}_p(t))$ ,  $S_v(\mathbf{v} - \mathbf{v}_p(t))$  are the so-called shape functions for the spatial and velocity coordinate, respectively.

The shape functions cannot be chosen arbitrarily. They have to fulfill several special properties. Let  $S_\xi$  be the shape function of the phase space coordinate  $\xi$ . Then:

1. The support of the shape function is compact,  $\exists R > 0$ ,  $\text{supp } S_\xi \subset (-R, R)$ .



**Figure 1:** Computational cycle of the particle-in-cell method

2. Integral of the shape function is unitary,  $\int_{-\infty}^{+\infty} S_\xi(\xi) d\xi = 1$ .
3. The shape function is symmetrical,  $S_\xi(\xi) = S_\xi(-\xi)$ .

While these restrictive conditions still offer a wide range of options, the standard PIC method is essentially determined by the choice of the shape function in the velocity coordinate as a Dirac  $\delta$ -function and in the spatial coordinate as a m-th order b-spline basis function  $b_m$ . Note that the choice of the shape functions has strong impact on the stability and accuracy of the simulation. Higher-order basis functions results in less numerical noise and reduces non-physical phenomena in simulations, obviously at the cost of increased computational time.

Substituting the discretization 3.1 into the Vlasov equation 2.9 and taking into account the properties of shape functions mentioned above, one obtains the set of equations of motion for macro-particle  $p$ ,

$$\frac{d\mathbf{r}_p}{dt} = \mathbf{v}_p, \quad \frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{F}_p}{m_s}, \quad (3.3)$$

where  $\mathbf{F}_p(t)$  represents a spatial average of the force acting on the macro-particle,

$$\mathbf{F}_p = q_s (\mathbf{E}_p + \mathbf{v}_p \times \mathbf{B}_p). \quad (3.4)$$

The fields at the macro-particle position  $\mathbf{E}_p(t)$  and  $\mathbf{B}_p(t)$  in 3.4 are given by the spatial shape function, which implies some form of interpolation. This will be closer discussed in the fourth section of this chapter.

The PIC method combines Lagrangian and Eulerian frame of reference. It means that the macro-particles are tracked in continuous phase space, whereas the electromagnetic fields

are calculated only on stationary grid points. Therefore, it is necessary to perform the discretization of the spatial coordinates  $\mathbf{r} \rightarrow \mathbf{r}_{ijk}$  where  $(i, j, k) \in \mathbb{Z}^3$  are grid indices. It is also necessary to perform discretization of the temporal coordinate  $t \rightarrow t^n$ , where  $n \in \mathbb{N}$  is the time level index. The algorithm will be outlined for a three-dimensional equidistant rectangular grid, thus  $\mathbf{r}_{ijk} = (i\Delta x, j\Delta y, k\Delta z)$ , where  $\Delta x, \Delta y, \Delta z$  are the spatial steps in each direction and  $t^n = n\Delta t$ , where  $\Delta t$  is the time step. Each quantity  $A(\mathbf{r}_{ijk}, t^n)$  will be hereafter denoted as  $A_{ijk}^n$ .

The computational cycle of the PIC method is shown in Figure 1. Individual steps are closer described in several following sections. The influence of the choice of the time and spatial step on the stability and accuracy of the PIC method will be demonstrated as well.

## 3.2 Particle pusher

As one could already see from 3.3, the motion of macro-particles in simulation is governed by the Newton equations with spatially averaged Lorentz force. Since the particles can reach velocities near the velocity of light, it is necessary to perform relativistic generalization,

$$\mathbf{u}_p = \gamma \mathbf{v}_p, \quad \gamma = \sqrt{1 + \left(\frac{\mathbf{u}_p}{c}\right)^2}. \quad (3.5)$$

Assume that the electric and magnetic fields are interpolated from the grid points to the particles at the time level  $t^n$ . Then the equations of motion to be integrated are

$$\frac{d\mathbf{r}_p}{dt} = \frac{\mathbf{u}_p}{\gamma}, \quad \frac{d\mathbf{u}_p}{dt} = \frac{q_s}{m_s} \left( \mathbf{E}_p + \frac{\mathbf{u}_p}{\gamma} \times \mathbf{B}_p \right). \quad (3.6)$$

To discretize the equations of motion 3.6, a time-centered leap-frog scheme is used. One obtains

$$\frac{\mathbf{r}_p^{n+1} - \mathbf{r}_p^n}{\Delta t} = \frac{\mathbf{u}_p^{n+1/2}}{\gamma^{n+1/2}}, \quad (3.7)$$

$$\frac{\mathbf{u}_p^{n+1/2} - \mathbf{u}_p^{n-1/2}}{\Delta t} = \frac{q_s}{m_s} \left( \mathbf{E}_p^n + \frac{\mathbf{u}_p^{n+1/2} + \mathbf{u}_p^{n-1/2}}{2\gamma^n} \times \mathbf{B}_p^n \right). \quad (3.8)$$

Although these equations appear to be very simple, the solution is the most time-consuming part of the simulation, because they must be solved for every single macro-particle at each time step. Standard approach for particle pushing in plasma simulation PIC codes involves elegant Boris method, which completely separates the effect of electric and magnetic fields [4]. Substitute

$$\mathbf{u}_p^{n-1/2} = \mathbf{u}_p^- - \frac{q_s \mathbf{E}_p^n \Delta t}{m_s} \frac{\Delta t}{2}, \quad \mathbf{u}_p^{n+1/2} = \mathbf{u}_p^+ + \frac{q_s \mathbf{E}_p^n \Delta t}{m_s} \frac{\Delta t}{2} \quad (3.9)$$

into the equation 3.8, then the electric field cancels entirely,

$$\frac{\mathbf{u}_p^+ - \mathbf{u}_p^-}{\Delta t} = \frac{q_s}{2\gamma^n m_s} (\mathbf{u}_p^+ + \mathbf{u}_p^-) \times \mathbf{B}_p^n. \quad (3.10)$$

The equation 3.10 describes a rotation of the vector  $\mathbf{u}_p^-$  to  $\mathbf{u}_p^+$  in one simulation time step  $\Delta t$ . The angle  $\theta$  between the vector  $\mathbf{u}_p^-$  and  $\mathbf{u}_p^+$  is expected to be  $\theta = \omega_c \Delta t$ .

To implement the Boris method, first add half the electric impulse  $\mathbf{E}_p^n$  to  $\mathbf{u}_p^{n-1/2}$ , then perform the full rotation by the angle  $\theta$ , and finally, add another half the electric impulse  $\mathbf{E}_p^n$ . From the basic geometry Boris derived following steps to obtain  $\mathbf{u}_p^{n+1/2}$ . From the first of the equations 3.9, express the vector  $\mathbf{u}_p^-$ ,

$$\mathbf{u}_p^- = \mathbf{u}_p^{n-1/2} + \frac{q_s \mathbf{E}_p^n \Delta t}{m_s} \frac{\Delta t}{2} \quad (3.11)$$

and construct an auxiliary vector  $\mathbf{u}'_p$ , which is simultaneously perpendicular to  $(\mathbf{u}_p^+ - \mathbf{u}_p^-)$  and to  $\mathbf{B}_p^n$ ,

$$\mathbf{u}'_p = \mathbf{u}_p^- + \mathbf{u}_p^- \times \mathbf{t}, \quad \mathbf{t} = \frac{q_s \mathbf{B}_p^n \Delta t}{\gamma^n m_s} \frac{\Delta t}{2}. \quad (3.12)$$

The vector  $\mathbf{t}$  has to be logically parallel to  $\mathbf{B}_p^n$  with the length of  $\tan(\theta/2) \approx \theta/2$  for small angles. Next, exploit the fact that the vector  $(\mathbf{u}'_p \times \mathbf{B}_p^n)$  is parallel to  $(\mathbf{u}_p^+ - \mathbf{u}_p^-)$  and express the vector  $\mathbf{u}_p^+$ ,

$$\mathbf{u}_p^+ = \mathbf{u}_p^- + \mathbf{u}'_p \times \mathbf{s}, \quad \mathbf{s} = \frac{2\mathbf{t}}{1+t^2}. \quad (3.13)$$

Here the vector  $\mathbf{s}$  is parallel to  $\mathbf{B}_p^n$  and its length has to fulfill the condition  $\|\mathbf{u}_p^+\| = \|\mathbf{u}_p^-\|$ . The transition from  $\mathbf{u}_p^-$  to  $\mathbf{u}_p^+$  can be written more clearly using the matrix,

$$\mathbf{u}_p^+ = \mathbb{M} \mathbf{u}_p^-, \quad (3.14)$$

where

$$\mathbb{M} = \begin{pmatrix} 1 - s_2 t_2 - s_3 t_3 & s_2 t_1 + s_3 & s_3 t_1 - s_2 \\ s_1 t_2 - s_3 & 1 - s_1 t_1 - s_3 t_3 & s_3 t_2 + s_1 \\ s_1 t_3 + s_2 & s_2 t_3 - s_1 & 1 - s_1 t_1 - s_2 t_2 \end{pmatrix}. \quad (3.15)$$

Finally, substitute the vector  $\mathbf{u}_p^+$  into the second from the equations 3.9,

$$\mathbf{u}_p^{n+1/2} = \mathbf{u}_p^+ + \frac{q_s \mathbf{E}_p^n \Delta t}{m_s} \frac{\Delta t}{2}. \quad (3.16)$$

The position of macro-particle particle is then advanced according to

$$\mathbf{r}_p^{n+1} = \mathbf{r}_p^n + \frac{\mathbf{u}_p^{n+1/2}}{\gamma^{n+1/2}} \Delta t, \quad \gamma^{n+1/2} = \sqrt{1 + \left( \frac{\mathbf{u}_p^{n+1/2}}{c} \right)^2}. \quad (3.17)$$

### 3.3 Field solver

As already mentioned, the behavior of the time varying electromagnetic field in free space is governed by the microscopic variant of Maxwell equations (1.1 - 1.4). A typical numerical technique to resolve the Maxwell's equations with respect to time is finite-difference time-domain method (FDTD), because it is probably the simplest technique in terms of the implementation.

The vector components of the fields  $\mathbf{E}_{ijk}^n$  and  $\mathbf{B}_{ijk}^n$  are spatially staggered about rectangular cells of the computational grid,

$$\mathbf{E}_{ijk}^n \rightarrow \left[ (E_x)_{i,j+1/2,k+1/2}^n, (E_y)_{i+1/2,j,k+1/2}^n, (E_z)_{i+1/2,j+1/2,k}^n \right], \quad (3.18)$$

$$\mathbf{B}_{ijk}^n \rightarrow \left[ (B_x)_{i+1/2,j,k}^n, (B_y)_{i,j+1/2,k}^n, (B_z)_{i,j,k+1/2}^n \right]. \quad (3.19)$$

This scheme, which has proven to be very robust, is now known as a Yee lattice [15]. The illustration of a standard Cartesian Yee cell used for FDTD is shown in Figure 2. Components of the current density  $\mathbf{J}_{ijk}^n$  are defined in the same way as the components of  $\mathbf{E}_{ijk}^n$ , charge density  $\rho_{ijk}^n$  is defined in the middle of the cell,

$$\mathbf{J}_{ijk}^n \rightarrow \left[ (J_x)_{i,j+1/2,k+1/2}^n, (J_y)_{i+1/2,j,k+1/2}^n, (J_z)_{i+1/2,j+1/2,k}^n \right], \quad (3.20)$$

$$\rho_{ijk}^n \rightarrow \rho_{i+1/2,j+1/2,k+1/2}^n. \quad (3.21)$$

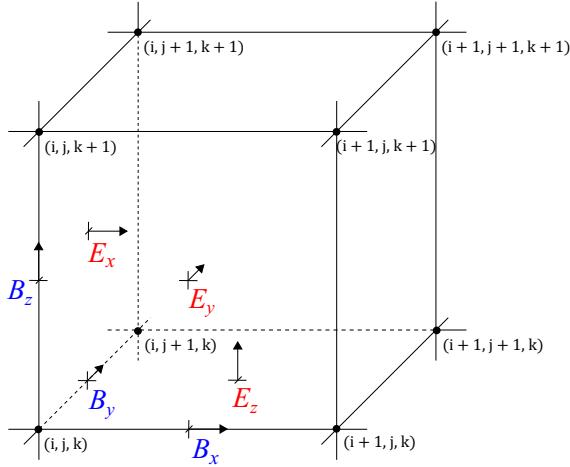
For marching in time a leap-frog scheme is used, thus discretized Maxwell's equations 1.1 - 1.4 have the following form,

$$\nabla^+ \cdot \mathbf{E}_{ijk}^n = \frac{\rho_{ijk}^n}{\epsilon_0}, \quad (3.22)$$

$$\nabla^- \cdot \mathbf{B}_{ijk}^{n+1/2} = 0, \quad (3.23)$$

$$\frac{1}{c^2} \frac{\mathbf{E}_{ijk}^{n+1} - \mathbf{E}_{ijk}^n}{\Delta t} = \nabla^+ \times \mathbf{B}_{ijk}^{n+1/2} - \mu_0 \mathbf{J}_{ijk}^{n+1/2}, \quad (3.24)$$

$$\frac{\mathbf{B}_{ijk}^{n+1/2} - \mathbf{B}_{ijk}^{n-1/2}}{\Delta t} = -\nabla^- \times \mathbf{E}_{ijk}^n. \quad (3.25)$$



**Figure 2:** Standard Cartesian Yee cell used for FDTD method

Notice that this scheme achieves second-order accuracy in both, space and time. Discrete operators ( $\nabla^+$ ) and ( $\nabla^-$ ) used in 3.22 - 3.25 act on a scalar field  $f_{ijk}$  as follows,

$$\nabla^+ f_{ijk} = \left( \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta x}, \frac{f_{i,j+1,k} - f_{i,j,k}}{\Delta y}, \frac{f_{i,j,k+1} - f_{i,j,k}}{\Delta z} \right), \quad (3.26)$$

$$\nabla^- f_{ijk} = \left( \frac{f_{i,j,k} - f_{i-1,j,k}}{\Delta x}, \frac{f_{i,j,k} - f_{i,j-1,k}}{\Delta y}, \frac{f_{i,j,k} - f_{i,j,k-1}}{\Delta z} \right). \quad (3.27)$$

These operators have the following properties,

$$\nabla^- \cdot \nabla^- \times = \nabla^+ \cdot \nabla^+ \times = 0, \quad \nabla^- \cdot \nabla^+ = \nabla^+ \cdot \nabla^- = \Delta^\pm. \quad (3.28)$$

Symbol  $\Delta^\pm$  stands for the discrete Laplace operator in central differences,

$$\Delta^\pm f_{i,j,k} = \frac{f_{i-1,j,k} + 2f_{i,j,k} + f_{i+1,j,k}}{\Delta x^2} + \frac{f_{i,j-1,k} + 2f_{i,j,k} + f_{i,j+1,k}}{\Delta y^2} + \frac{f_{i,j,k-1} + 2f_{i,j,k} + f_{i,j,k+1}}{\Delta z^2}. \quad (3.29)$$

Before trying to find the solution of discretized Maxwell equations 3.22 - 3.25, one must realize that this system of equations is not independent. In the three-dimensional case, there are eight first-order differential equations, but only six unknown vector components. Acting on the equations 3.24 and 3.25 by operators ( $\nabla^- \cdot$ ) and ( $\nabla^+ \cdot$ ), respectively, one obtains

$$\frac{\nabla^- \cdot \mathbf{B}_{ijk}^{n+1/2} - \nabla^- \cdot \mathbf{B}_{ijk}^{n-1/2}}{\Delta t} = 0, \quad (3.30)$$

$$\frac{\rho_{ijk}^{n+1} - \rho_{ijk}^n}{\Delta t} + \nabla^+ \cdot \mathbf{J}_{ijk}^{n+1/2} = 0. \quad (3.31)$$

It means that it is possible to solve only the equations 3.24 and 3.25, while the divergence equations 3.22, 3.23 can be considered as the initial conditions. Note that in this case, the continuity equation in the finite differences (3.31) has to be fulfilled.

## 3.4 Particle and field weighting

In order to solve the Maxwell's equations, as shown in the previous section of this chapter, one has to know the source terms produced by the motion of the charged particles. In other words, it is necessary to assign charge and current densities from the continuous macro-particle positions to the discrete grid points. This simulation step is usually referred to as particle weighting and it involves some form of interpolation.

According to the kinetic theory, charge density  $\rho(\mathbf{x}, t)$  and current density  $\mathbf{J}(\mathbf{x}, t)$  are given by the following integrals over the velocity space,

$$\rho(\mathbf{x}, t) = \sum_s q_s \int f_s(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}, \quad \mathbf{J}(\mathbf{x}, t) = \sum_s q_s \int f_s(\mathbf{x}, \mathbf{v}, t) \mathbf{v} d\mathbf{v}. \quad (3.32)$$

After discretization of 3.32 using macro-particles and exploiting the properties of the shape functions, one gets immediately

$$\rho_{ijk}^n = \sum_p q_p S_r(\mathbf{r}_{ijk} - \mathbf{r}_p^n), \quad \mathbf{J}_{ijk}^n = \sum_p q_p \mathbf{v}_p^n S_r(\mathbf{r}_{ijk} - \mathbf{r}_p^n), \quad (3.33)$$

where  $q_p = q_s w_p$ . However, using the formulas 3.33 for charge and current deposition in PIC codes may violate the discrete continuity equation (3.31) and in turn cause errors in Gauss's law (3.22). In this case, one would have to solve the Poisson's equation for the correction of the electric field at every simulation time step or use a numerical scheme that satisfies the continuity equation exactly. These schemes are referred to as a charge conservation methods ([14], [5], [source]).

Similarly, to advance macro-particle positions, as shown in the second section of this chapter, one has to know the force acting on them. Hence, it is necessary to assign electric and magnetic fields that are calculated at the discrete grid points to the continuous macro-particle positions. This simulation step is usually referred to as field weighting.

By analogy to the particle weighting, one may exploit the shape functions to calculate the spatial averages of the all electric and magnetic field components,

$$\mathbf{E}_p^n = \sum_{ijk} \mathbf{E}_{ijk}^n S_r(\mathbf{r}_{ijk} - \mathbf{r}_p^n), \quad \mathbf{B}_p^n = \sum_{ijk} \mathbf{B}_{ijk}^n S_r(\mathbf{r}_{ijk} - \mathbf{r}_p^n). \quad (3.34)$$

Note that it is recommended to use the same weighting for both, particles and fields, in order to eliminate a self-force and ensure the conservation of momentum [6].

## 3.5 Stability and accuracy

The stability and accuracy of the standard PIC method is directly dependent on the size of the spatial and temporal simulation steps. In order to find correct parameters, one has to know the absolute accuracy and corresponding stability conditions.

The effect of the spatial grid is to smooth the interaction forces and to couple plasma perturbations to perturbations at other wavelengths, called aliases. It may lead to non-physical instabilities and numerical heating. To avoid these effects, the spatial step needs to resolve the Debye length (see 2.3). Thus, it is desirable to fulfill the following condition,

$$\Delta x, \Delta y, \Delta z \leq \lambda_D. \quad (3.35)$$

In the general electromagnetic case, the time step has to satisfy the Courant–Fridrichs–Levy (CFL) condition [10],

$$C = c^2 \Delta t^2 \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right), \quad (3.36)$$

where the dimensionless number  $C \leq 1$  is called the CFL number. This condition limits the range of motion of all objects in the simulation during one time step. It ensures, that these particles would not cross more than one cell in one simulation time step. When this condition is violated, the growth of non-physical effects can be very rapid.

The leap-frog scheme, used to solve the field equations and equations of motion, is second-order accurate in both, time and space. In addition, this scheme is explicit and time-reversible. An extensive study of PIC method can be found in [source].

## 3.6 Code EPOCH

The abbreviation EPOCH refers to an Extendable PIC Open Collaboration project [1]. EPOCH is a multi-dimensional, relativistic, electromagnetic code designed for plasma physics simulations based on the PIC method. The code, which has been developed at University of Warwick, is written in FORTRAN and parallelized using MPI library. EPOCH is able to cover physical processes that may take place at ultra-high laser intensities, such as barrier suppression ionization, quantum electrodynamics emission and pair production.

The main features include dynamic load balancing option for making optimal use of all processors when run in parallel, allowing restart on an arbitrary number of processors. The setup of EPOCH is controlled through a customizable input deck. An input deck is a text file which can be used to set simulation parameters for EPOCH without necessity to edit or recompile the source code. Most aspects of a simulation can be controlled, such as the number of grid points in the simulation domain, the initial distribution of particles and the initial electromagnetic field configuration. In addition, EPOCH has been written to add more modern features and to structure the code in such a way that the future expansion of

the code may be made as easily as possible. The entire core of the code uses SI units.

By default, EPOCH uses triangular particle shape functions with the peak located at the position of computational particle and a width of two cells, which provides relatively clean and fast solution. However, user can select higher order particle shape functions based on a spline interpolation by enabling compile-time option in the makefile.

The electromagnetic field solver uses a FDTD scheme with second order of accuracy. The field components are spatially staggered on a standard Cartesian Yee cell. The solver is directly based on the scheme derived by Hartmut Ruhl [7]. The particle pusher is relativistic, Birdsall and Landon type [4] and uses Villasenor and Buneman current weighting [14].

EPOCH offers several types of boundary conditions for fields and particles, such as periodic, transmissive, reflecting and also Convolutional Perfectly Matched Layer (CPML) boundary conditions. Laser beams can be attached to arbitrary boundary via special boundary condition as well.

As a side project within this work, the code EPOCH has been instrumented to enable in situ diagnostics and visualization of the electromagnetic fields using ParaView Catalyst [source]. The increasing demands of the simulations need more data to be stored on a disk and analysed. However, the capabilities of computing environment which is responsible for transferring the data and communication have not grown up as rapid as the computational power. Dumping and processing of all the data calculated during the simulation would take too much time, so in practice this usually means that they are stored only at several time steps or at much coarser resolution than the original data. The rest is just discarded and the significant part of information may be potentially lost.

In situ visualization describes techniques where data can be visualized in real-time as it is generated during a simulation and without it being stored on a storage resource. By coupling the visualization and simulation, the data transfer bottleneck can be overcome. Furthermore, this approach allows scientists to monitor and interact with a running simulation, allowing for its parameters to be modified and allowing to immediately view the effects of these changes.

While a simulation is running, a user can see the size of the datasets that a simulation produces. But none of this data is physically stored on a storage system. The computationally expensive operations are carried out using ParaView's graphical interface. So, the user can select data structures and analyze them in the same way as in post-processing. But there is one difference, the simulation is in progress so a user can observe the data as it is being generated. With Catalyst, it is also possible to pause the simulation or specify a break-point at a selected time step. This can be helpful if a user expects some interesting behavior of investigated phenomena or for identifying regions where numerical instability arises. For the implementation details, see appendix B.

The main goal of this work has been to implement a solution that would enable to simulate tightly focused laser beams using simulation code EPOCH. This will be closer described in the following chapter.

# Chapter 4

## Tight-focusing of laser pulses

The investigation of laser-matter interaction also involves exploring of specific themes of the ultra-relativistic regime, which requires extremely high intensities of the external field. These intensities, that are experimentally inaccessible at present, could be potentially achieved by tight-focusing and that would allow a broad spectrum of many multidisciplinary applications.

As mentioned in the previous chapter, various aspects of electromagnetic interaction are usually studied using sophisticated numerical simulation codes. Vast majority of these codes, however, use a paraxial approximation (closer described in chapter 1) to prescribe the laser fields at the boundaries, and afterwards, a field solver guides the beam across the simulation domain. As already mentioned, the paraxial approximation is valid only if the angular spectrum of laser pulse is sufficiently narrow, therefore it is not possible to simulate tightly focused laser beams using this approach. As might be seen later, paraxial approximation in this case leads to a distorted field profiles which have strong impact on the results of laser-matter interaction.

Several interesting solutions, how to simulate strongly focused beams, have been already proposed [source]. Within this work, a simple and efficient algorithm for a Maxwell consistent calculation of the electromagnetic fields at the boundaries of the computational domain [source] (also called laser boundary conditions) has been used and implemented into the PIC code EPOCH [source]. Note, that this algorithm is able to describe laser beams with arbitrary shape.

### 4.1 Laser boundary conditions

In this section, another mathematical description of a focused laser beam based on a rigorous solution of the wave equation 1.39 is presented. All the following calculations are reproduced from the excellent work of Illia Thiele et al. [source].

Assume that the laser beam propagates in vacuum without external sources along the z-axis of the Cartesian coordinate system. The wave equation 1.39 in temporal Fourier space

has the following form,

$$\Delta \hat{\mathbf{E}}(\mathbf{r}, \omega) + \frac{\omega^2}{c^2} \hat{\mathbf{E}}(\mathbf{r}, \omega) = 0, \quad (4.1)$$

where the hat symbol placed on the top of a variable denotes the Fourier transform with respect to time. Next, one shall perform a spatial Fourier transform of 4.1 with respect to transverse coordinates  $\mathbf{r}_\perp$  only,

$$\left( -k_x^2 - k_y^2 + \frac{\partial^2}{\partial z^2} \right) \bar{\mathbf{E}}(k_x, k_y, z, \omega) + \frac{\omega^2}{c^2} \bar{\mathbf{E}}(k_x, k_y, z, \omega) = 0, \quad (4.2)$$

where the bar symbol placed on the top of a variable denotes the Fourier transform with respect to time and spatial transverse coordinates. The equation 4.2 can be simplified as follows,

$$k_z^2(\mathbf{k}_\perp, \omega) \bar{\mathbf{E}}(\mathbf{k}_\perp, z, \omega) + \frac{\partial^2}{\partial z^2} \bar{\mathbf{E}}(\mathbf{k}_\perp, z, \omega) = 0. \quad (4.3)$$

where  $k_z(\mathbf{k}_\perp, \omega) = \sqrt{-\mathbf{k}_\perp^2 + \omega^2/c^2}$  and  $\mathbf{k}_\perp = (k_x, k_y)^T$ . The fundamental solution of the equation 4.3 consists of the forward (+) and backward (-) propagating waves,

$$\bar{\mathbf{E}}^\pm(\mathbf{k}_\perp, z, \omega) = \bar{\mathbf{E}}_0^\pm(\mathbf{k}_\perp, \omega) e^{\pm i k_z(\mathbf{k}_\perp, \omega)(z - z_0)}. \quad (4.4)$$

Where  $\bar{\mathbf{E}}_0^\pm(\mathbf{k}_\perp, \omega)$  is the electric laser field at some plane  $z = z_0$ . It might be clearly seen, that only two out of six vector components of the electric and magnetic fields are independent, therefore one may prescribe for example the transverse components  $\bar{\mathbf{E}}_{0,\perp}^\pm(\mathbf{k}_\perp, \omega)$  at the plane  $z = z_0$  and all other components can be derived from the Maxwell's equations 1.1, 1.3,

$$\bar{\mathbf{E}}_\perp^\pm(\mathbf{k}_\perp, z, \omega) = \bar{\mathbf{E}}_{0,\perp}^\pm(\mathbf{k}_\perp, \omega) e^{\pm i k_z(\mathbf{k}_\perp, \omega)(z - z_0)}, \quad (4.5)$$

$$\bar{E}_z^\pm(\mathbf{k}_\perp, z, \omega) = \mp \frac{\mathbf{k}_\perp \cdot \bar{\mathbf{E}}_\perp^\pm(\mathbf{k}_\perp, z, \omega)}{k_z(\mathbf{k}_\perp, \omega)}, \quad (4.6)$$

$$\bar{\mathbf{B}}_\perp^\pm(\mathbf{k}_\perp, z, \omega) = \frac{1}{\omega k_z(\mathbf{k}_\perp, \omega)} \mathbb{R}^\pm(\mathbf{k}_\perp, \omega) \bar{\mathbf{E}}^\pm(\mathbf{k}_\perp, z, \omega), \quad (4.7)$$

where

$$\mathbb{R}^\pm(\mathbf{k}_\perp, \omega) = \begin{pmatrix} \mp k_x k_y & \mp [k_z^2(\mathbf{k}_\perp, \omega) + k_y^2] & 0 \\ \pm [k_z^2(\mathbf{k}_\perp, \omega) + k_x^2] & \pm k_x k_y & 0 \\ -k_y k_z(\mathbf{k}_\perp, \omega) & -k_x k_z(\mathbf{k}_\perp, \omega) & 0 \end{pmatrix}. \quad (4.8)$$

Analogically, one could solve the wave equation for the magnetic field 1.40, prescribe two transverse components of  $\bar{\mathbf{B}}_{0,\perp}^\pm(\mathbf{k}_\perp, \omega)$  at the plane  $z = z_0$  and afterwards calculate all other fields using Maxwell's equations 1.2, 1.4. The complete proof, that the fields 4.5 - 4.7

are consistent with the Maxwell's equations in vacuum 1.1 - 1.4 can be found in the original paper [source].

Note that for  $\mathbf{k}_\perp^2 > \omega^2/c^2$ ,  $k_z(\mathbf{k}_\perp, \omega)$  becomes imaginary and equation 4.4 describes evanescent waves that are unphysical in free space. Thus the Fourier spectrum of laser waves has to be filtered in the transverse Fourier space. On the other hand, if the spatial Fourier spectrum contains only components with  $\mathbf{k}_\perp^2 \ll \omega^2/c^2$ , then  $k_z(\mathbf{k}_\perp, \omega)$  can be approximated using the first few terms of a Taylor series,

$$k_z(\mathbf{k}_\perp, \omega) \approx \frac{|\omega|}{c} - \frac{c}{2|\omega|} \mathbf{k}_\perp^2. \quad (4.9)$$

Note that by plugging 4.9 into equations 4.5 - 4.7 one gets the paraxial approximation.

In the last part of this section, the practical algorithm for implementation of the boundary conditions based on the previously derived solution of Maxwell's equations is presented. Assume that the laser beam propagates in a forward direction along the z-axis. In the beginning, it is necessary to prescribe the electric laser field  $\mathbf{E}_{0,\perp}(\mathbf{r}_\perp, t)$  in the plane  $\mathcal{P}$  at  $z = z_0$ . Note, that it can be defined by arbitrary function of space and time. The goal is then to find the fields  $\mathbf{E}_B(\mathbf{r}_\perp, t)$  and  $\mathbf{B}_B(\mathbf{r}_\perp, t)$  at the corresponding boundary  $z = z_B$ .

Consider that the transverse part of simulation domain is made of equidistant rectangular grid described by  $x^i, y^j$ , where  $i, j \in \{1, \dots, N_{x,y}\}$ , and the grid steps  $\delta x, \delta y$ . The simulation time  $t^n$ , where  $n \in \{1, \dots, N_t\}$ , is also divided into equidistant time steps of size  $\delta t$ .

The algorithm allows to calculate fields  $\mathbf{E}_B^{ij}(t)$  and  $\mathbf{B}_B^{ij}(t)$  for any given time  $t$  from the interval  $[t^1 - \frac{z_B - z_0}{c}, t^{N_t} - \frac{z_B - z_0}{c}]$ . In order to preserve clarity, the algorithm below is given in the exact form as in the original paper [source].

1. Calculate  $\hat{\mathbf{E}}_{0,\perp}^{ijn}$  via discrete Fourier transforms in time:

$$\omega^n = \frac{2\pi}{N_t \delta t} \left( -\frac{N_t}{2} + n \right), \quad (4.10)$$

$$\hat{\mathbf{E}}_{0,\perp}^{ijn} = \frac{\delta t}{2\pi} \sum_{l=1}^{N_t} \mathbf{E}_{0,\perp}^{ijl} e^{i\omega^n t^l}, \quad n \in \{1, \dots, N_t\}. \quad (4.11)$$

2. Calculate  $\bar{\mathbf{E}}_{0,\perp}^{ijn}$  via two-dimensional discrete Fourier transforms in transverse space:

$$k_x^i = \frac{2\pi}{N_x \delta x} \left( -\frac{N_x}{2} + i \right), \quad k_y^j = \frac{2\pi}{N_y \delta y} \left( -\frac{N_y}{2} + j \right), \quad (4.12)$$

$$\bar{\mathbf{E}}_{0,\perp}^{ijn} = \frac{\delta x \delta y}{(2\pi)^2} \sum_{l,m=1}^{N_x, N_y} \hat{\mathbf{E}}_{0,\perp}^{lmn} e^{-i(k_x^i x^l + k_y^j y^m)}, \quad i, j \in \{1, \dots, N_{x,y}\}. \quad (4.13)$$

3. Calculate transverse electric field components at the boundary  $z = z_B$ :

$$k_z^{ijn} = \Re \sqrt{\frac{(\omega^n)^2}{c^2} - (k_x^i)^2 - (k_y^j)^2}, \quad (4.14)$$

$$\bar{\mathbf{E}}_{B,\perp}^{ijn} = \begin{cases} \bar{\mathbf{E}}_{0,\perp}^{ijn} e^{ik_z^{ijn}(z_B - z_0)} & \text{for } k_z^{ijn} > 0 \\ 0 & \text{for } k_z^{ijn} = 0 \end{cases}. \quad (4.15)$$

4. Calculate longitudinal electric field components at the boundary  $z = z_B$ :

$$\bar{E}_{B,z}^{ijn} = \begin{cases} -\frac{k_x^i \bar{E}_{B,x}^{ijn} + k_y^j \bar{E}_{B,y}^{ijn}}{k_z^{ijn}} & \text{for } k_z^{ijn} > 0 \\ 0 & \text{for } k_z^{ijn} = 0 \end{cases}. \quad (4.16)$$

5. Calculate the magnetic field at the boundary  $z = z_B$ :

$$\mathbb{R}^{ijn} = \begin{pmatrix} -k_x^i k_y^j & (k_x^i)^2 - (\omega^n)^2/c^2 \\ (\omega^n)^2/c^2 - (k_y^j)^2 & k_x^i k_y^j \\ -k_y^j k_z^{ijn} & k_x^i k_z^{ijn} \end{pmatrix}, \quad (4.17)$$

$$\hat{\mathbf{B}}_B^{ijn} = \begin{cases} (\omega^n k_z^{ijn})^{-1} \mathbb{R}^{ijn} \bar{\mathbf{E}}_{B,\perp}^{ijn} & \text{for } k_z^{ijn} > 0 \\ 0 & \text{for } k_z^{ijn} = 0 \end{cases}. \quad (4.18)$$

6. Calculate  $\hat{\mathbf{E}}_B^{ijn}$ ,  $\hat{\mathbf{B}}_B^{ijn}$  via two-dimensional inverse discrete Fourier transforms:

$$\hat{\mathbf{E}}_B^{ijn} = \frac{(2\pi)^2}{N_x N_y \delta x \delta y} \sum_{l,m=1}^{Nx,Ny} \bar{\mathbf{E}}_B^{lmn} e^{i(k_x^l x^i + k_y^m y^j)}, \quad (4.19)$$

$$\hat{\mathbf{B}}_B^{ijn} = \frac{(2\pi)^2}{N_x N_y \delta x \delta y} \sum_{l,m=1}^{Nx,Ny} \bar{\mathbf{B}}_B^{lmn} e^{i(k_x^l x^i + k_y^m y^j)}. \quad (4.20)$$

7. Calculate  $\mathbf{E}_B^{ij}(t)$ ,  $\mathbf{B}_B^{ij}(t)$  for any given time  $t \in [t^1 - \frac{z_B - z_0}{c}, t^{N_t} - \frac{z_B - z_0}{c}]$ .

$$\mathbf{E}_B^{ij}(t) = \frac{2\pi}{N_t \delta t} \sum_{n=1}^{N_t} \hat{\mathbf{E}}_B^{ijn} e^{-i\omega^n t}, \quad (4.21)$$

$$\mathbf{B}_B^{ij}(t) = \frac{2\pi}{N_t \delta t} \sum_{n=1}^{N_t} \hat{\mathbf{B}}_B^{ijn} e^{-i\omega^n t}. \quad (4.22)$$

## 4.2 Implementation

One of the main goals of this work has been to implement the algorithm mentioned in the previous section, to evaluate its correctness in several test simulations and finally, to exploit resulting implementation for simulations of tightly focused Gaussian beams in laser-matter interaction. The main requirement on implementation has been easy to use with 2D version of particle-in-cell simulation code EPOCH [source]. For this reason, several possible solutions has been taken into account.

The final decision has been to create a static library, which will be able to compute desired quantities and will provide functions for communication with the main simulation code. The essential advantage is that it could be basically linked with any laser-plasma simulation code. Also, since it is necessary to call only two additional functions, the instrumentation will be fast, easy and the main simulation code will not be excessively disturbed. Furthermore, the implementation itself come with the CMake [source] support, which simplify the compilation process using platform and compiler independent configuration files.

The library has been written in C++ language and is object oriented so the algorithm can be easily extended to three dimensional geometry. In order to speedup the whole underlying computation, the algorithm has been parallelized using hybrid techniques. The time domain has been decomposed into the stripes corresponding to individual computational processes, the communication between these processes is ensured by MPI library. Furthermore, the computationally most expensive cycles are parallelized using OpenMP implementation of multi-threading. Later on, the speedup and parallel scaling performance will be briefly discussed.

Fourier transforms form the core of the computational process and their performance is crucial for the overall performance of the code. For this reason, many currently available libraries have been considered. Eventually, the Fourier transforms in the algorithm can be computed using FFTW [source] library, Intel® MKL [source] library or it is also possible to directly evaluate the formulas without using any additional library. The user specifies his option before the compilation. Regarding both libraries, a threaded versions of 1D in-place complex fast Fourier transforms have been used throughout the code. According to several measures, there is no significant difference between the speed of both implementations.

One potential bottleneck could happen during the computation of spatial Fourier transforms since the arrays with spatial data are decomposed into different processes. The cluster versions of functions performing the Fourier transforms have been tested, however they did not bring any significant speedup. The reason is as follows. They require to have the global array in memory and use its own distribution which involves overlapping. Since the size of global arrays is usually not so large and since it is necessary to perform a lot of different Fourier transforms, the majority of computational time is spent rather for communication, mainly if many of computational cores are used.

This issue has been solved by gathering the data on master process, performing the Fourier transforms in space by only one processor and scattering the data back to corre-

sponding processes. This is the reason why the code does not scale well, however, the time to compute all desired quantities is in most cases negligible in comparison with the time required by main simulation cycle. Nevertheless, this issue could be improved in future.

Since it is necessary to compute the whole time evolution of the laser field at boundary for each grid point before the simulation starts, the resulting amount of data can be significantly large and does not have to fit in a computer memory. Thus, it is inevitable to dump the data into a file, which will be then accessed by the main simulation code. Due to the performance purposes, each computational process stores its data into a shared file with corresponding offset and in binary coding. Therefore, the output operations are as fast as possible and save the storage resources. Library then provide a function which allows to seek an arbitrary position in a file. This function is then called each time step of the main simulation loop to fill the laser source arrays with all the relevant data. This way of accessing data does not cause any significant slowdown or memory overhead.

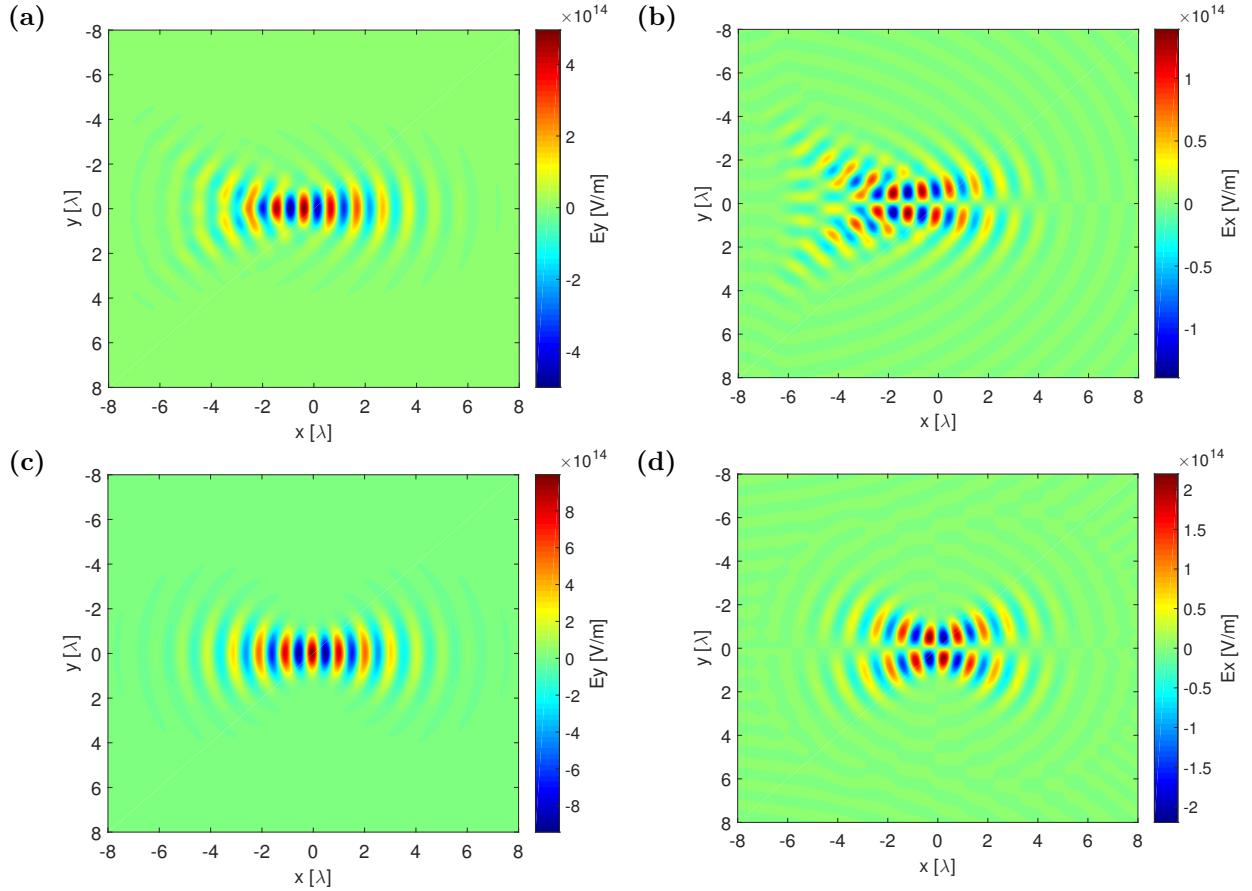
The EPOCH [source] code require only transverse components of laser electric field, all other quantities are computed by the FDTD solver. The implementation of the library allows fully connection with EPOCH [source]. In practice, if the user wants to simulate tight-focusing, is is necessary to enable the corresponding flag as a compile-time option and then to specify all required parameters in the input file. The code then automatically computes all necessary data. It works generally regardless the number of lasers in the simulation or boundaries that they are attached to.

The current version of library does not work for obliquely incident laser pulses, because in this case one cannot exploit the advantage of an efficient computation with fast Fourier transforms. However, the code allows to compute the laser fields at boundary by evaluating Fourier integrals directly, so it could be easily extended. Second, it is at the moment possible to simulate only Gaussian laser pulses. However, the user can easily prescribe its own shape and position of the beam in focal plane by modifying corresponding part of the code.

Several most important data structures, functions and methods that form the core of the library for tight-focusing can be seen in appendix B.

### 4.3 Evaluation

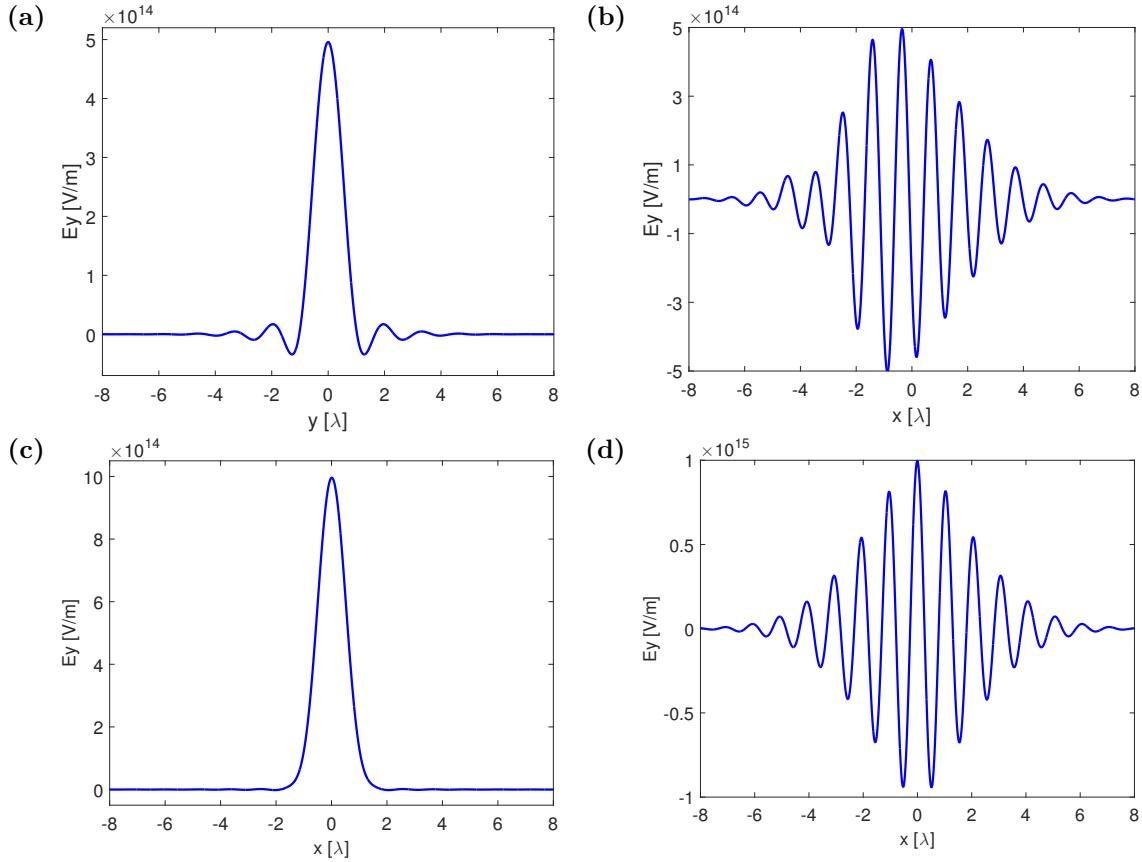
To evaluate the correctness of the algorithm presented in the previous section of this chapter as well as to demonstrate the drawbacks of the paraxial approximation, several test simulations in 2D geometry have been performed. In the following text, a two limit cases are presented. The first pair of simulations employs tightly focused Gaussian laser beam with the size at focus comparable with the center laser wavelength, whilst the second one shows the case of the Gaussian beam with the size at focus one order of magnitude larger than the center laser wavelength, where both approaches should return identical results. Note, that all the simulations have been computed using 2D version of PIC code EPOCH [source] instrumented with library for tight-focusing.



**Figure 3:** Transverse ( $E_y$ ) and longitudinal ( $E_x$ ) electric laser field components captured at the time step of their maximal intensity at the focal spot. The cases (a), (b) correspond to the laser pulse propagating under the paraxial approximation, whilst (c), (d) come from the simulation where the beam propagation has been resolved within the Maxwell consistent approach. In the case of paraxial approximation, both components reveal strong distortions and asymmetry, their focal spot is located about  $1\lambda$  closer to the left boundary than specified and the corresponding amplitude is significantly lower. The laser has been attached to the left hand side boundary.

First, have a look at the simulation of a tightly focused Gaussian beam. The p-polarized laser pulse with center wavelength  $\lambda = 1\text{ }\mu\text{m}$  propagates from left hand side boundary to the right. Its duration has been chosen to  $\tau = 20\text{ fs}$  in FWHM and amplitude  $E_0 = 1 \cdot 10^{15}\text{ V/m}$ . The beam waist  $w_0 = 0.7\text{ }\mu\text{m}$  is shorter than the laser wavelength, which implies that non-negligible parts of  $\bar{\mathbf{E}}_{0,\perp}(k_x, \omega)$  are evanescent. The focus is located at a distance  $x = 8\text{ }\mu\text{m}$  from the boundary that the laser is attached to.

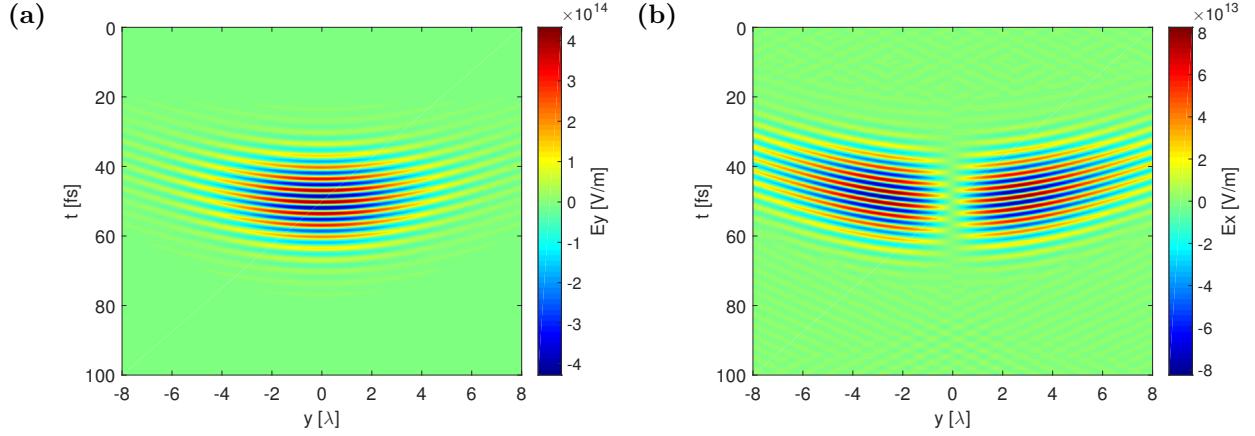
The size of the simulation domain is  $16\lambda \times 48\lambda$ , with 100 cells per laser wavelength in both directions, thus  $\Delta x = \Delta y = \lambda/100 = 10\text{ nm}$ . The one simulation time step is according to CFL condition  $\Delta t = 0.95\sqrt{2}\lambda/100c \approx 0.05\text{ fs}$ , the whole simulation time is then  $t = 150\text{ fs}$ .



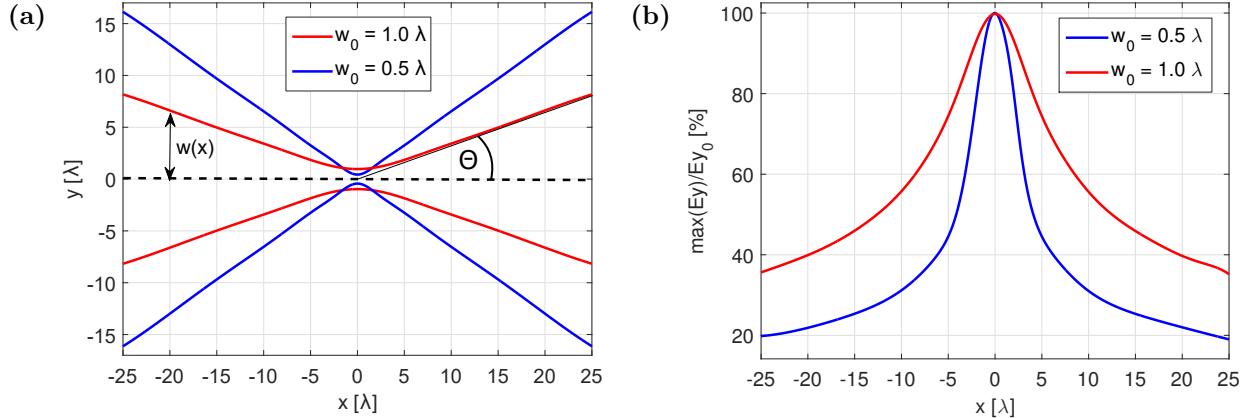
**Figure 4:** Transverse (a), (c) and longitudinal (b), (d) slices of the transverse electric laser field ( $E_y$ ) at the time step when it reaches maximal intensity at the focal spot. The cases (a), (b) correspond to the laser pulse propagating under the paraxial approximation, whilst (c), (d) come from the simulation where the beam propagation has been resolved within the Maxwell consistent approach. In the case of paraxial approximation, one can clearly see strong side-wings in the spatial beam profile (a) as well as the asymmetry of the field in the longitudinal line-out (b).

The pulse propagates in vacuum in order to get rid of all effects that could be potentially caused by plasma. All the simulation parameters can be found in the attached input files in the appendix A.

In the following paragraph, the results of the first simulation are discussed in a more detail. Fig. 3 shows transverse and longitudinal electric field components at their maximal intensity at focus for both cases, laser beam propagating under the paraxial approximation (Fig. 3 - a, b) and according to the approach consistent with Maxwell equations (Fig. 3 - c, d). In the case of paraxial approximation, one can clearly see strong distortions and asymmetry in the shape of both electric field components. In addition, the focus location is shifted about  $1\mu\text{m}$  closer to the left boundary and the corresponding amplitude at focus is less than half the required value. In contrast, the fields produced by the simulation using



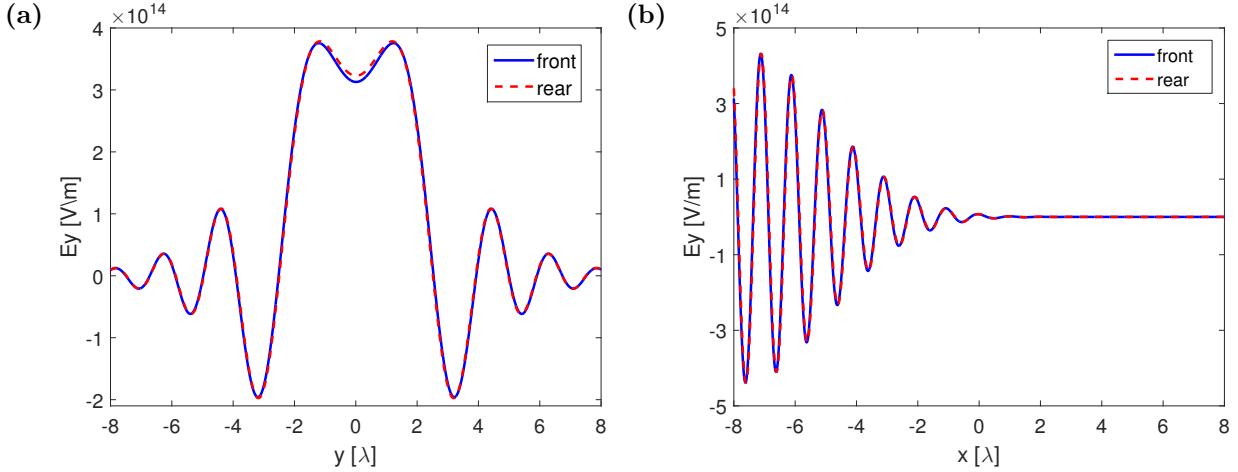
**Figure 5:** The time evolution of transverse ( $E_y$ ) (a) and longitudinal ( $E_x$ ) (b) electric laser field components at the boundary that the laser is attached to. Both components have been calculated according to the Maxwell consistent approach.



**Figure 6:** (a) Graph of the spot size parameter  $w(x)$  of the beams with  $w_0 = 1\lambda$  and  $0.5\lambda$  calculated using Maxwell consistent approach. From the plotted lines, one can roughly estimate the beam divergence angle  $\Theta$ . The divergence angles for both beams are surprisingly in a good accordance with the divergence angles of corresponding Gaussian beams. (b) Graph of the transverse ( $E_y$ ) electric laser field amplitude with respect to the distance from focal spot according to the Maxwell consistent approach. The values on vertical axis are given in a percentage of the amplitude at focus  $E_{0,y}$ .

Maxwell consistent calculation of laser fields at boundary are symmetric with respect to the focal spot and without any distortions. Furthermore, the focus location as well as the amplitude fulfills the initial requirements precisely.

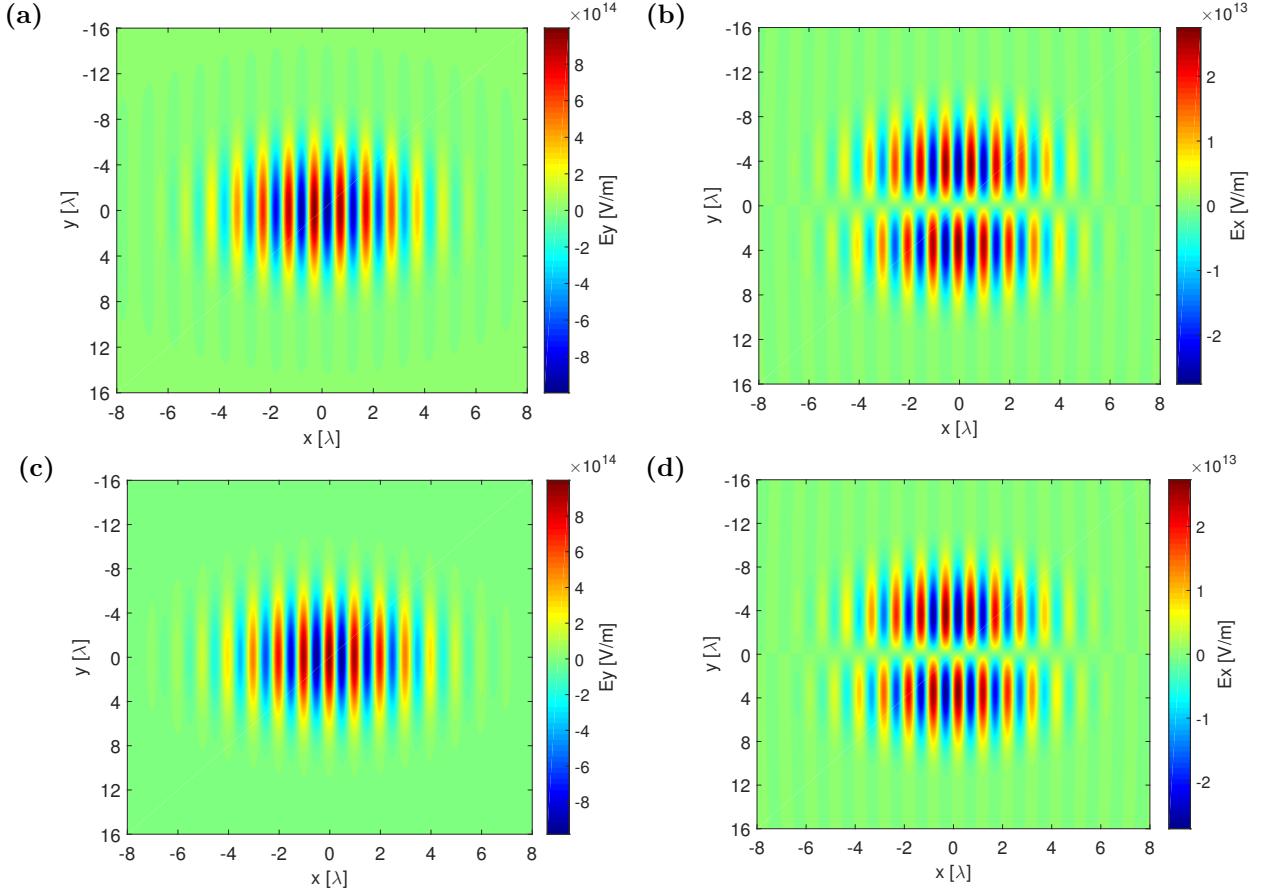
Fig. 4 shows transverse and longitudinal slices of transverse electric field component at focus for the case of laser beam propagating under the paraxial approximation (Fig. 4 - a,



**Figure 7:** Transverse (a) and longitudinal (b) slice of the transverse electric laser field ( $E_y$ ) when it reaches its maximal intensity at the front (blue) and rear (red) boundary. The results come from the simulation where the Maxwell consistent approach for laser propagation has been used. For better comparison, the field at the rear boundary in (b) has been horizontally flipped. The exact match between the field shapes at a different time steps of simulation proves the correctness of the laser beam propagation.

b) as well as for the case where the beam propagation has been resolved within the Maxwell consistent approach (Fig. 4 - c, d). For the case of paraxial approximation, one can clearly see the asymmetry of the field shape in the longitudinal slice (Fig. 4 - b), which consequently leads to a decrease of the amplitude at focus and to the strong side-wings in the spatial beam profile, as might be better seen from the transverse slice (Fig. 4 - a). On the other hand, Maxwell consistent approach calculates fields of perfect symmetry with respect to the focal spot (Fig. 4 - c) and no side-wings or distortions are present (Fig. 4 - d).

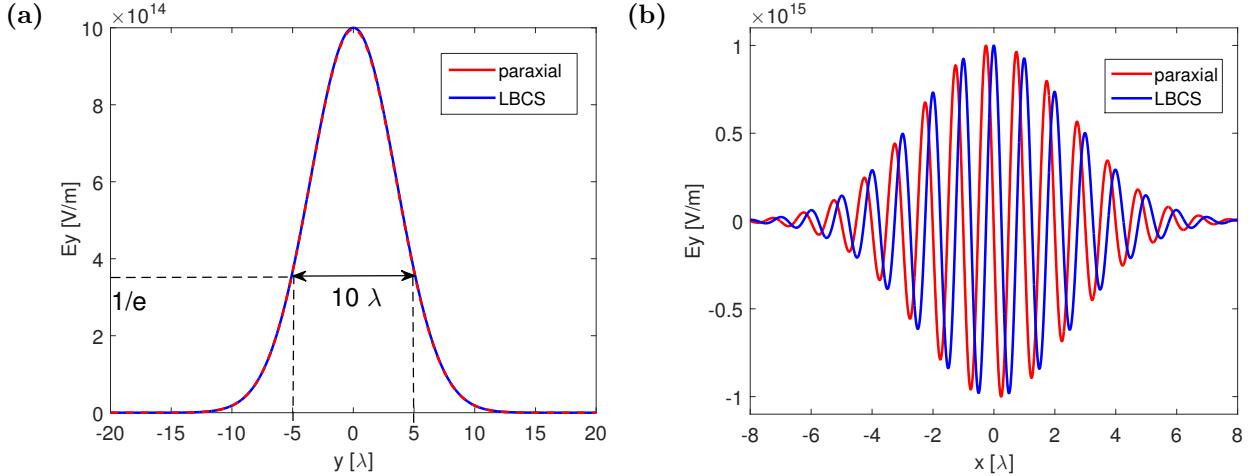
In Fig. 5 one can examine the time evolution of transverse (Fig. 5 - a) and longitudinal (Fig. 5 - b) electric field components at boundary as computed using Maxwell consistent approach. Note, that one have to chose carefully the transverse size of the domain, since the beam width at boundary may be much larger than at focus because of a diffraction. To estimate the beam width at boundary, one has to know the beam divergence angle  $\Theta$ . In Fig. 6 - a, one can find a graph of the spot size parameter  $w$  as calculated using the Maxwell consistent approach for the beams focused to  $w_0 = 1 \lambda$  and  $0.5 \lambda$ . From the plotted lines, one can roughly estimate the beam divergence angle  $\Theta$ . For the beam focused to  $w_0 = 1 \lambda$ , the beam divergence angle has been around  $\Theta = 18.2^\circ$  which is almost identical value as for the Gaussian beam of the same parameters. For the beam with  $w_0 = 0.5 \lambda$  the divergence has been estimated to  $\Theta = 32.9^\circ$ , while the Gaussian beam with the same size at focus has divergence  $\Theta = 36.5^\circ$ . Consequently, in spite of the fact that the divergence of the tightly focused beams calculated using the Maxwell consistent approach is a little bit lower, both approaches are in quite a good accordance regarding this parameter.



**Figure 8:** Transverse ( $E_y$ ) and longitudinal ( $E_x$ ) electric laser field components captured at the time step of their maximal intensity at the focal spot. The cases (a), (b) correspond to the laser pulse propagating under the paraxial approximation, whilst (c), (d) come from the simulation where the beam propagation has been resolved within the Maxwell consistent approach. The size of the focus has been chosen to be one order of the magnitude larger than the center laser wavelength. One can clearly see, that there is no significant difference between the shapes of the electric field components.

In Fig. 6 - b, one can see the amplitude of the transverse electric laser field with respect to the distance from the focal spot calculated using Maxwell consistent approach. This could be particularly useful for experimenters since it is not always easy to focus the beam onto the target surface perfectly.

To evaluate a correctness of the beam propagation using Maxwell consistent approach, several criteria has been defined. The correctness of the amplitude and beam waist as well as the right focus location has already been verified. Additional criteria has been set on a beam symmetry. In Fig. 7, one can find a comparison of the transverse electric laser field component when it achieves its maximal intensity at front and rear boundary. One can clearly see the



**Figure 9:** Transverse (a) and longitudinal (b) slices of the transverse electric laser field ( $E_y$ ) at the time step when it reaches maximal intensity at focus. Red lines correspond to the laser pulse propagating under the paraxial approximation, whilst blue lines come from the simulation where the beam propagation has been resolved within the Maxwell consistent approach. The size of the focus has been chosen to be one order of magnitude larger than the center laser wavelength. In the case of paraxial approximation, the focus is slightly shifted closer to the left boundary (b), otherwise the size of the focus as well as the amplitude is correct for both cases (a).

exact match between the field shapes at different time steps of the simulation in transverse (Fig. 7 - a) and longitudinal (Fig. 7 - b) slices. Moreover, all the aforementioned criteria has been fulfilled also in other simulations with different input parameters that are not presented here. Consequently, these observations prove the correctness of the propagation at least for the tightly focused Gaussian laser beams.

For the second simulation, all the input parameters remained the same except the beam waist. Now, the parameter  $w_0 = 5\mu\text{m}$ , which is about the limit case for the beam propagating under the paraxial approximation. Thus, one would expect that the simulation results will be almost identical.

Similarly as in Fig. 3, Fig. 8 shows again transverse and longitudinal electric field components at their maximal intensity at focus for both cases, laser beam propagating under the paraxial approximation (Fig. 8 - a, b) and according to the approach consistent with Maxwell equations (Fig. 8 - c, d). Here, one cannot register any difference between the results corresponding to both approaches.

Also, the transverse slice of the transverse electric laser field component at focus (Fig. 9 - a) shows the correct shape and amplitude for both cases. The longitudinal slice (Fig. 9 - b), however, points out the fact that the location of the focal spot is still a little bit shifted closer to the left hand side boundary. Nevertheless, this difference could be in practice neglected. At the end of the day, for the Gaussian beams propagating under the paraxial approximation, the beam diameter at focus should be at least one order of magnitude larger than the center

laser wavelength.

In conclusion, one should be aware that the propagation of tightly focused laser pulses cannot be described by paraxial approximation. Above, it has been shown that for the beams focused to a spot with the size comparable to a center laser wavelength, paraxial approximation leads to a shifted location of the focus, asymmetric laser field profiles with distortions and lower amplitude. These deviations are far from negligible and have without any doubt strong impact on the laser-matter or laser-plasma interaction results. On the other hand, the propagation of tightly focused Gaussian laser beams prescribed at boundaries according to the Maxwell consistent approach has been proven to be correct.



# Chapter 5

## Results

First set (8 simulations const. int or const. e, target 2 micron, 2000 ppc): Laser:

- wavelength:  $\lambda = 0.8 \mu m$
- const intensity:  $I = 1e20 \text{ W/cm}^2$  or const. energy:  $E = 2.8306e4 \text{ J}$  (corresponds to  $I = 1e20 \text{ W/cm}^2$  for  $w_0 = 1.0 \mu m$ )
- duration:  $t = 30 \text{ fs}$  (in FWHM)
- beam waist in focus:  $w_0 = 0.5, 1.0, 2.0, 4.0 \mu m$
- focus distance from boundary:  $x_B - x_0 = 8 \mu m$
- polarization: P
- boundary: left

Domain:

- x min:  $0 \mu m$
- x max:  $15 \mu m$
- y min:  $-20 \mu m$
- y max:  $20 \mu m$
- $N_x$ : 1875 cells ( $\delta x = \lambda/100 = 8 \text{ nm}$ )
- $N_y$ : 5000 cells ( $\delta y = \lambda/100 = 8 \text{ nm}$ )
- time step:  $\delta t = 1/(\sqrt{2}c)\lambda/100 \approx 0.05 \text{ fs}$

- simulation time:  $\tau = 200 \text{ fs}$

Target:

- x min:  $8 \mu\text{m}$
- x max:  $10 \mu\text{m}$
- y min:  $-15 \mu\text{m}$
- y max:  $15 \mu\text{m}$
- electrons: 2000 ppc
- protons: 100 ppc
- density: 100 critical
- temperature: 100 eV

Seconds set (2 simulations with higher intensity, 1000 ppc): Laser:

- wavelength:  $\lambda = 0.8 \mu\text{m}$
- const intensity:  $I = 1\text{e}21 \text{ W/cm}^2$
- duration:  $t = 30 \text{ fs}$  (in FWHM)
- beam waist in focus:  $w_0 = 0.5, 2.0 \mu\text{m}$
- focus distance from boundary:  $x_B - x_0 = 8 \mu\text{m}$
- polarization: P
- boundary: left

Domain:

- x min:  $0 \mu\text{m}$
- x max:  $15 \mu\text{m}$
- y min:  $-20 \mu\text{m}$
- y max:  $20 \mu\text{m}$
- $N_x$ : 1875 cells ( $\delta x = \lambda/100 = 8 \text{ nm}$ )
- $N_y$ : 5000 cells ( $\delta y = \lambda/100 = 8 \text{ nm}$ )

- 
- time step:  $\delta t = 1/(\sqrt{2}c)\lambda/100 \approx 0.05$  fs
  - simulation time:  $\tau = 200$  fs

Target:

- x min:  $8 \mu m$
- x max:  $10 \mu m$
- y min:  $-15 \mu m$
- y max:  $15 \mu m$
- electrons: 1000 ppc
- protons: 100 ppc
- density: 100 critical
- temperature: 100 eV

Third set (2 simulations with higher intensity, thiner target (0.25 micron), 2000 ppc): Laser:

- wavelength:  $\lambda = 0.8 \mu m$
- const intensity:  $I = 1e21 \text{ W/cm}^2$
- duration:  $t = 30$  fs (in FWHM)
- beam waist in focus:  $w_0 = 0.5, 2.0 \mu m$
- focus distance from boundary:  $x_B - x_0 = 8 \mu m$
- polarization: P
- boundary: left

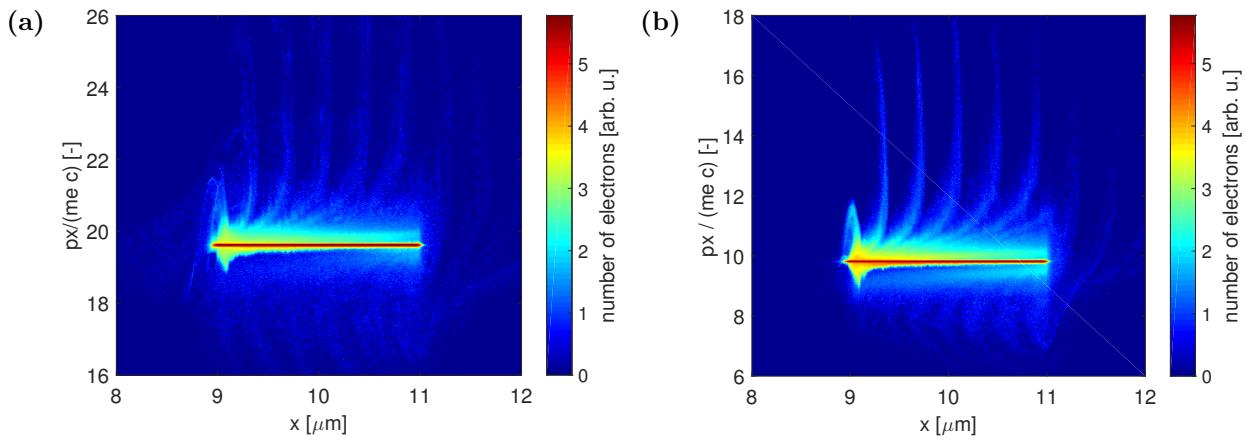
Domain:

- x min:  $0 \mu m$
- x max:  $15 \mu m$
- y min:  $-20 \mu m$
- y max:  $20 \mu m$
- $N_x$ : 1875 cells ( $\delta x = \lambda/100 = 8 \text{ nm}$ )

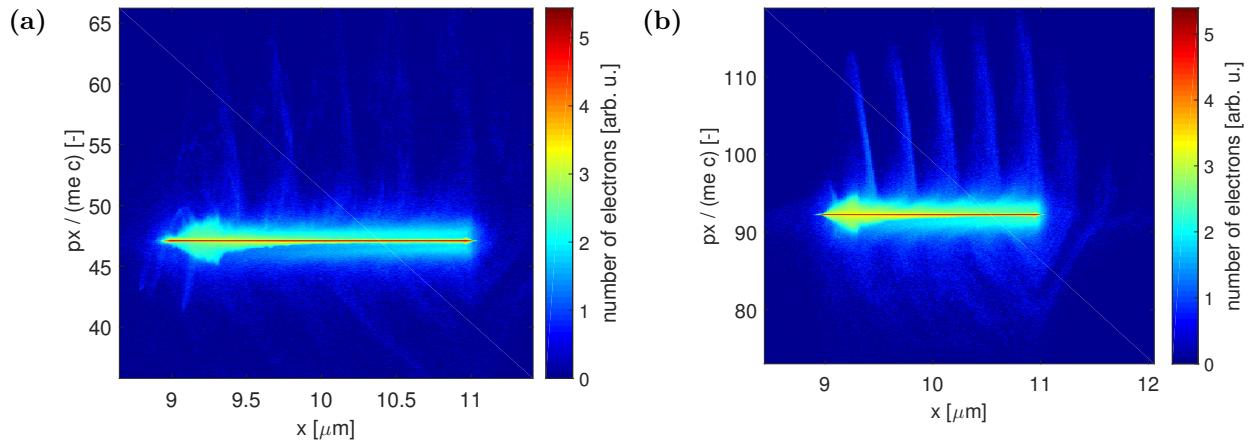
- $N_y$ : 5000 cells ( $\delta y = \lambda/100 = 8 \text{ nm}$ )
- time step:  $\delta t = 1/(\sqrt{2}c)\lambda/100 \approx 0.05 \text{ fs}$
- simulation time:  $\tau = 200 \text{ fs}$

Target:

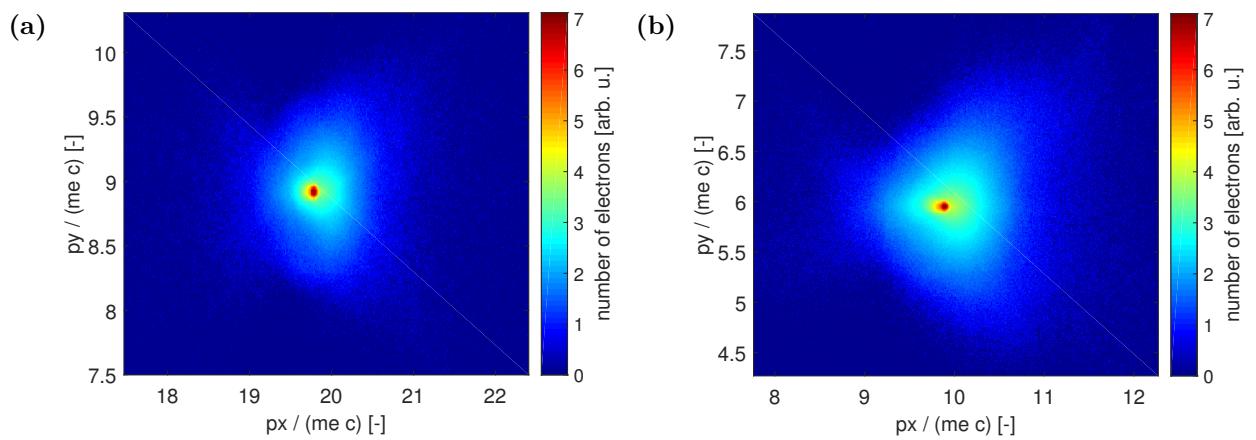
- x min:  $8 \mu\text{m}$
- x max:  $8.25 \mu\text{m}$
- y min:  $-15 \mu\text{m}$
- y max:  $15 \mu\text{m}$
- electrons: 2000 ppc
- protons: 100 ppc
- density: 100 critical
- temperature: 100 eV



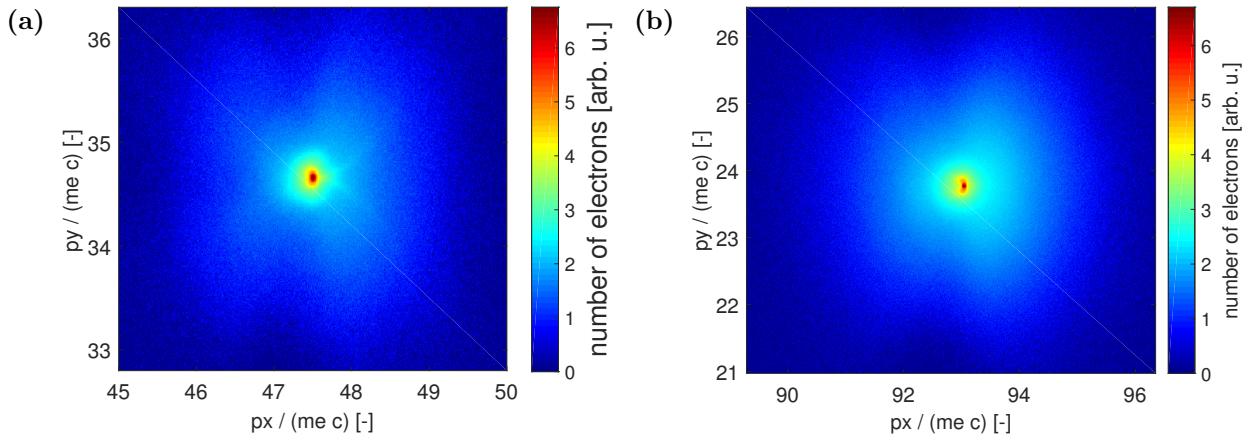
**Figure 10:** (a)  $w_0 = 0.5 \text{ micron}$ ,  $I = 1e20 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$  (b)  $w_0 = 2 \text{ micron}$ ,  $I = 1e20 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$



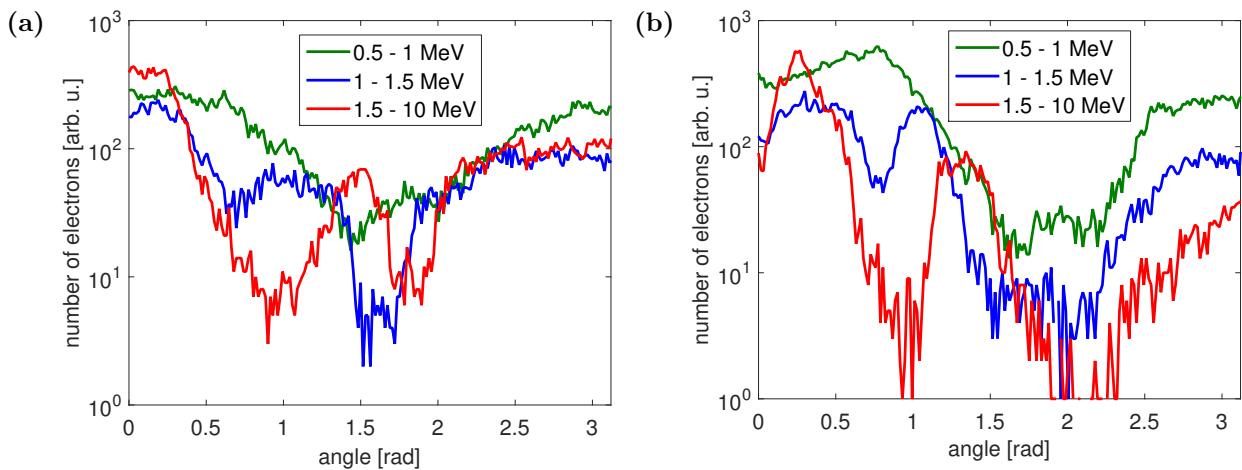
**Figure 11:** (a)  $w_0 = 0.5 \text{ micrometer}$ ,  $I = 1\text{e}21 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$  (b)  $w_0 = 2 \text{ micrometer}$ ,  $I = 1\text{e}21 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$



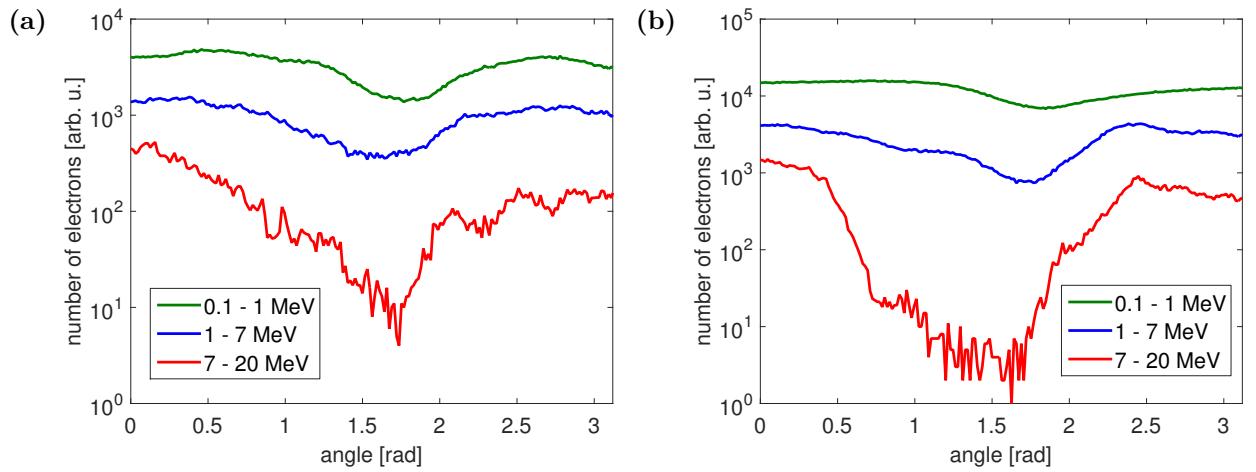
**Figure 12:** (a)  $w_0 = 0.5 \text{ micrometer}$ ,  $I = 1\text{e}20 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$  (b)  $w_0 = 2 \text{ micrometer}$ ,  $I = 1\text{e}20 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$



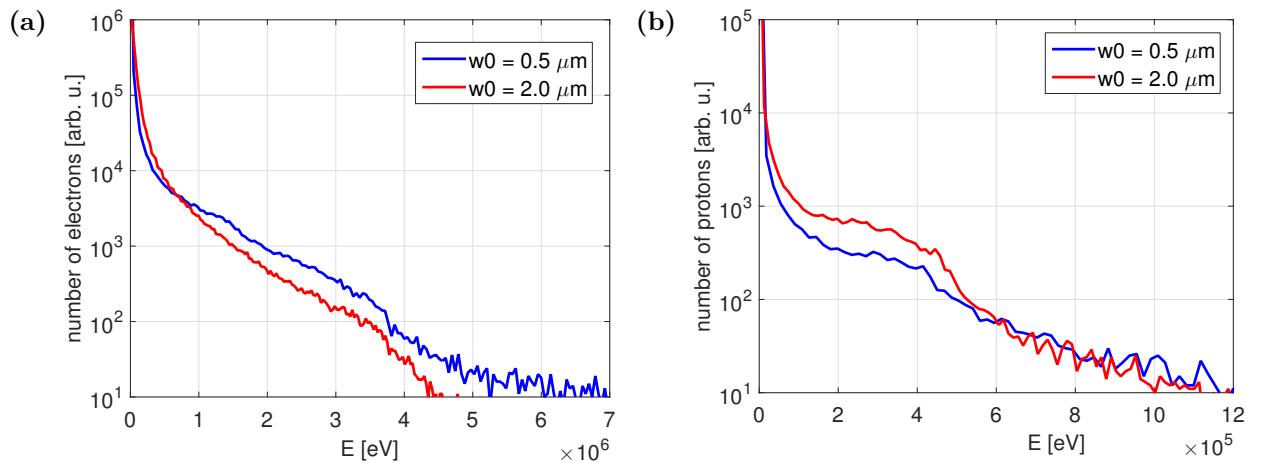
**Figure 13:** (a)  $w_0 = 0.5 \text{ micron}$ ,  $I = 1\text{e}21 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$  (b)  $w_0 = 2 \text{ micron}$ ,  $I = 1\text{e}21 \text{ W/cm}^2$ ,  $t = 100 \text{ fs}$



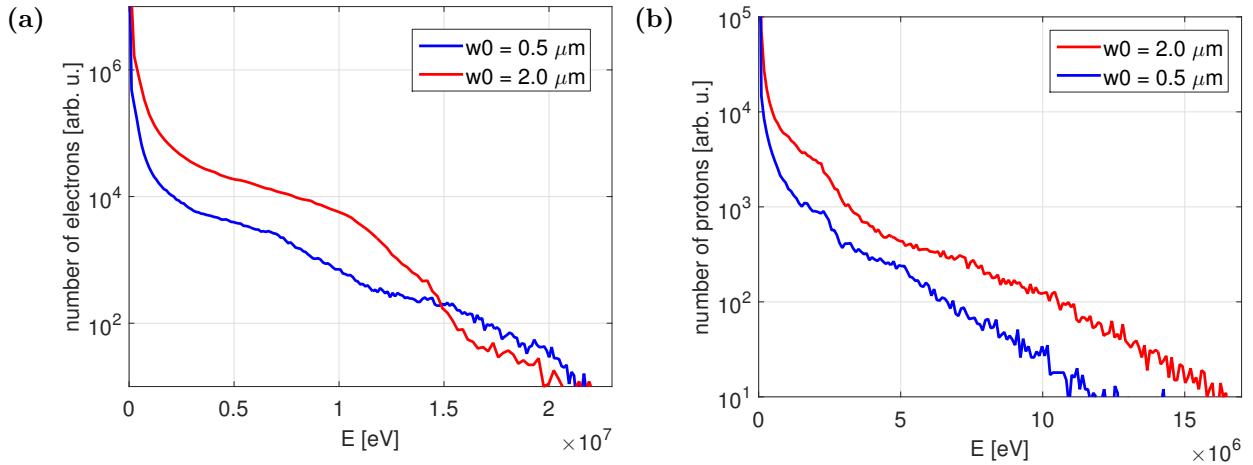
**Figure 14:** (a)  $w_0 = 0.5 \text{ micron}$ , electrons,  $t = 100 \text{ fs}$ ,  $I = 1\text{e}20 \text{ W/cm}^2$  (b)  $w_0 = 2 \text{ micron}$ , electrons,  $t = 100 \text{ fs}$ ,  $I = 1\text{e}20 \text{ W/cm}^2$



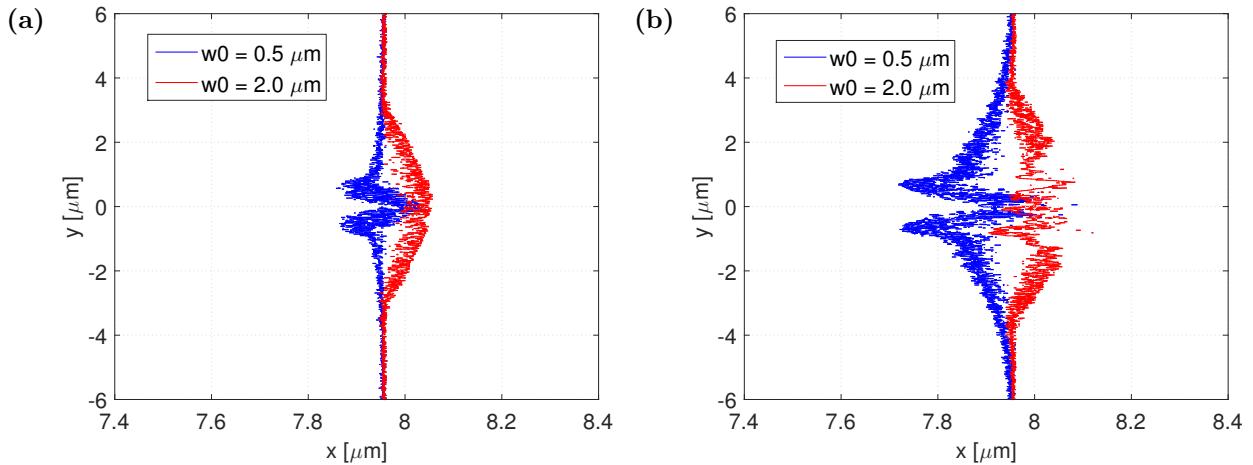
**Figure 15:** (a)  $w_0 = 0.5 \mu\text{m}$ , electrons,  $t = 100 \text{ fs}$ ,  $I = 1 \text{ e21 W/cm}^2$  (b)  $w_0 = 2 \mu\text{m}$ , electrons,  $t = 100 \text{ fs}$ ,  $I = 1 \text{ e21 W/cm}^2$



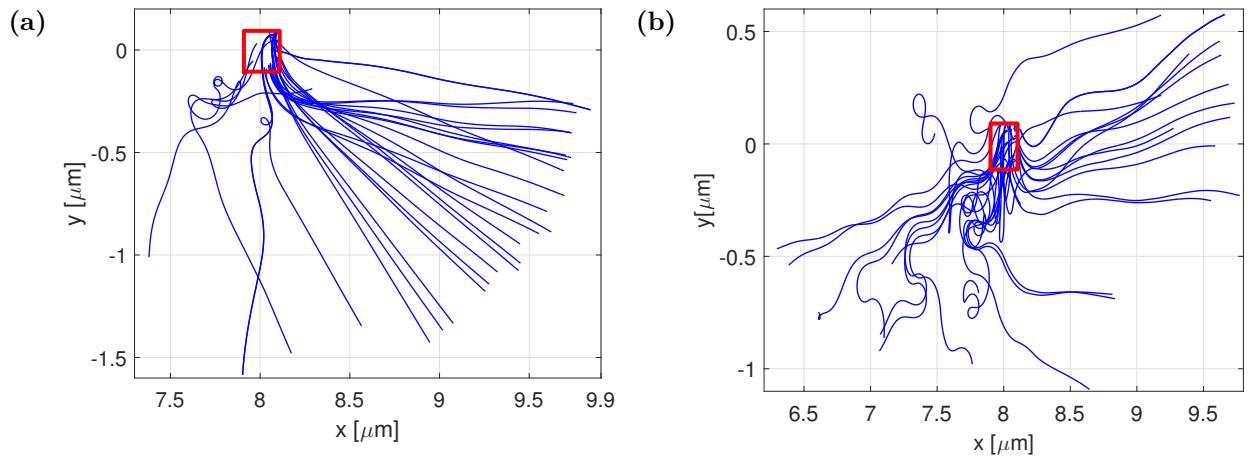
**Figure 16:** (a) electrons,  $t = 100 \text{ fs}$ ,  $I = 1 \text{ e20 W/cm}^2$  (b) protons,  $t = 200 \text{ fs}$ ,  $I = 1 \text{ e20 W/cm}^2$



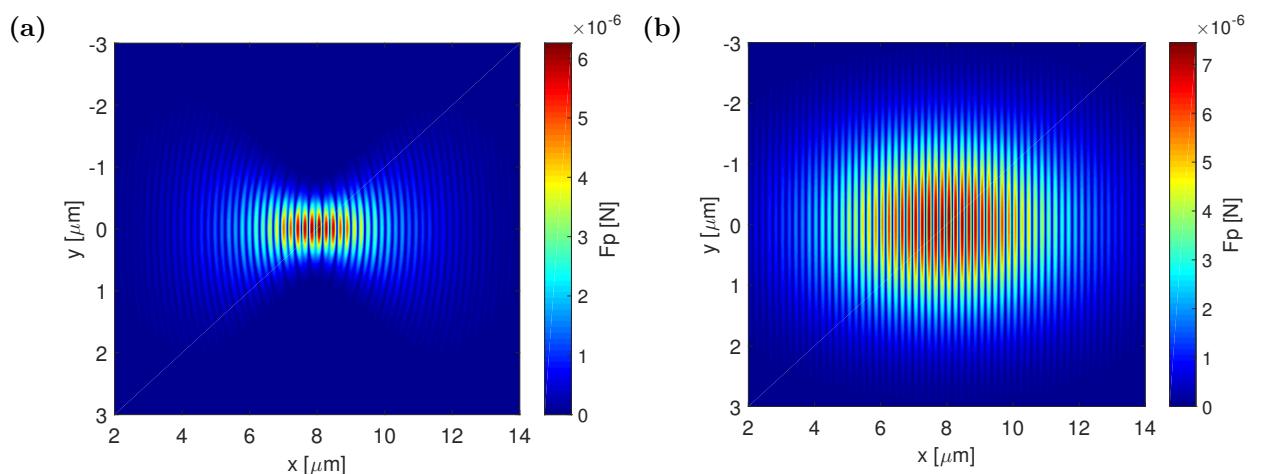
**Figure 17:** (a) electrons,  $t = 100$  fs,  $I = 1\text{e}21$  W/cm $^2$  (b) protons,  $t = 200$  fs,  $I = 1\text{e}21$  W/cm $^2$



**Figure 18:** (a) nc protons,  $t = 100$  fs,  $I = 1\text{e}20$  W/cm $^2$  (b) nc protons,  $t = 100$  fs,  $I = 1\text{e}21$  W/cm $^2$



**Figure 19:** (a) electrons,  $w_0 = 0.5$  micron,  $t = 100$  fs,  $I = 1e21$  W/cm $^2$  (b) electrons,  $w_0 = 2$  micron,  $t = 100$  fs,  $I = 1e21$  W/cm $^2$



**Figure 20:** (a)  $w_0 = 0.5$  micron,  $I = 1e20$  W/cm $^2$  (b)  $w_0 = 2$  micron,  $I = 1e20$  W/cm $^2$



# Conclusion

The work briefly presents the introduction to the inertial fusion research as well as basic physical processes which take place during the interaction of intense laser pulse with plasma. Particularly, for better interpretation and understanding of ongoing experiments that study the possibilities of nuclear fusion ignition by shock wave, the conditions of interaction have been set accordingly to them.

The main benefits of this work are successful implementation of boundary conditions for the effective absorption of hot electrons in the two-dimensional version of the computational code EPOCH. Its correct functionality has been later verified by plenty of numerical tests. Afterwards, two large scale simulations of laser system PALS in two-dimensional geometry on its fundamental wavelength  $1,315 \mu\text{m}$  with intensity  $1 \cdot 10^{20} \text{W/m}^2$  and with initial electron temperatures  $T_e = 0.5 \text{keV}$  and  $T_e = 2.5 \text{keV}$  have been performed. Both simulations capture the time period of 20 ps. Simulations have been performed using the particle-in-cell code EPOCH [1]. Initial profiles of plasma density and temperature have been approximated from hydrodynamic simulations, which have been performed previously.

The total absorption of incident laser energy in plasma for the case of the simulation with  $T_e = 0.5 \text{ keV}$  was estimated to 42.4 %, for the case of the simulation with  $T_e = 2.5 \text{ keV}$ , the total absorption was significantly lower, about 33.1 %. The temperature of the hot electrons in the case of the simulation with  $T_e = 0.5 \text{ keV}$  was estimated to 36 keV, in the case of the simulation with  $T_e = 2.5 \text{ keV}$  the temperature was about 25 keV. In both cases, the number of hot electrons is relatively low and their temperatures are not too high to prevent the fuel target compression in the later phase. However, it is necessary to further investigate their effect performing more accurate simulations.

## Acknowledgments

I wish express my gratitude to both, my supervisor doc. Ing. Ondřej Klímo, Ph.D. and consultant Dr. Stefan Andreas Weber for constant support and guidance, as well as for providing invaluable advice and direction.

Access to computing and storage facilities owned by parties and projects contributing to the National Grid Infrastructure MetaCentrum, provided under the programme "Projects of Large Infrastructure for Research, Development, and Innovations" (LM2010005), is greatly appreciated.

Access to the CERIT-SC computing and storage facilities provided under the programme Center CERIT Scientific Cloud, part of the Operational Program Research and Development for Innovations, reg. no. CZ. 1.05/3.2.00/08.0144, is greatly appreciated.

The development of the EPOCH code was funded in part by the UK EPSRC grants EP/G054950/1, EP/G056803/1, EP/G055165/1 and EP/ M022463/1.

Bc. Petr Valenta

# Bibliography

- [1] T D Arber, K Bennett, C S Brady, A Lawrence-Douglas, M G Ramsay, N J Sircombe, P Gillies, R G Evans, H Schmitz, A R Bell, and C P Ridgers. Contemporary particle-in-cell approach to laser-plasma modelling. *Plasma Physics and Controlled Fusion*, 57(11):113001, 2015.
- [2] D. Batani, S. Baton, A. Casner, S. Depierreux, M. Hohenberger, O. Klimo, M. Koenig, C. Labaune, X. Ribeyre, C. Rousseaux, G. Schurtz, W. Theobald, and V.T. Tikhonchuk. Physics issues for shock ignition. *Nuclear Fusion*, 54(5):054009, 2014.
- [3] R. Betti et al. Shock ignition: A new approach to high gain inertial confinement fusion on the national ignition facility. *Phys. Rev. Lett.*, 103(4), 2009.
- [4] C. K. Birdsall and A. B. Langdon. *Plasma Physics via Computer Simulation*. Series in Plasma Physics. CRC Press, 2004.
- [5] T. Zh. Esirkepov. Exact charge conservation scheme for particle-in-cell simulation with an arbitrary form-factor. *Computer Physics Communications*, 135(2), 2001.
- [6] H. Fehske, R. Schneider, and A. Weiße. *Computational Many-Particle Physics*. Springer, 2008.
- [7] Kai Germaschewski, William Fox, Narges Ahmadi, Liang Wang, Stephen Abbott, Hartmut Ruhl, and Amitava Bhattacharjee. The plasma simulation code: A modern particle-in-cell code with load-balancing and gpu support. *arXiv preprint arXiv:1310.7866*, 2013.
- [8] H. Gould, J. Tobochnik, and W. Christian. *An introduction to computer simulation methods: applications to physical systems*. Addison–Wesley series in physics. Addison–Wesley, 3 edition, 2007.
- [9] R. W. Hockney and J. W. Eastwood. *Computer Simulation Using Particles*. CRC Press, 2010.
- [10] D. A. Jaroszynski, R. Bingham, and R. A. Cairns. *Laser-Plasma Interactions*. Scottish Graduate Series. CRC Press, 2009.

- [11] G. Lapenta. Particle in cell methods with application to simulations in space weather. Lecture notes.
- [12] T. Pang. *An introduction to computational physics*. Cambridge University Press, 2 edition, 2006.
- [13] V T Tikhonchuk, A Colaïtis, A Vallet, E Llor Aisa, G Duchateau, Ph Nicolaï, and X Ribeyre. Physics of laser-plasma interaction for shock ignition of fusion reactions. *Plasma Physics and Controlled Fusion*, 58(1):014018, 2016.
- [14] J. Villasenor and O. Buneman. Rigorous charge conservation for local electromagnetic field solvers. *Computer Physics Communications*, 69(2-3), 1992.
- [15] K. Yee. Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media. *IEEE Transactions on Antennas and Propagation*, 14(3), 1966.

# **Appendices**



# Appendix A

## Input files

This part contains input files of several most important simulations that have been performed within this work.

**Listing A.1:** test\_lbcs

```
1 begin:control
2   nx = 1600
3   ny = 4800
4   x_min = -8 * micron
5   x_max = 8 * micron
6   y_min = -24 * micron
7   y_max = 24 * micron
8   t_end = 150 * femto
9   field_order = 2
10  stdout_frequency = 1
11  smooth_currents = T
12  dt_multiplier = 0.95
13 end:control
14
15 begin:boundaries
16   cpml_thickness = 16
17   cpml_kappa_max = 20
18   cpml_a_max = 0.2
19   cpml_sigma_max = 0.7
20   bc_x_min_field = cpml_laser
21   bc_x_max_field = cpml_outflow
22   bc_x_min_particle = thermal
23   bc_x_max_particle = thermal
24   bc_y_min_field = cpml_outflow
25   bc_y_max_field = cpml_outflow
26   bc_y_min_particle = thermal
27   bc_y_max_particle = thermal
28 end:boundaries
29
30 begin:laser
31   boundary = x_min
32   id = 1
33   fwhm_time = 20 * femto
34   t_0 = 50 * femto
35   w_0 = 0.7 * micron # 5.0 * micron
36   pos = 0.0 * micron
37   focus = 0.0 * micron
```

```

38 amp = 1.0e15
39 lambda = 1.0 * micron
40 pol_angle = 0.0 * pi
41 t_start = 0.0 * femto
42 t_end = 300 * femto
43 end:laser
44
45 begin:output
46   name = fields
47   file_prefix = field
48   dump_at_times = 50.00 * femto, 76.685127616 * femto, 103.370255232 * femto
49   grid = always + single
50   ex = always + single
51   ey = always + single
52   bz = always + single
53   dump_first = F
54   dump_last = F
55   restartable = F
56 end:output

```

**Listing A.2:** test paraxial

```

1 begin:control
2   nx = 1600
3   ny = 4800
4   x_min = -8 * micron
5   x_max = 8 * micron
6   y_min = -24 * micron
7   y_max = 24 * micron
8   t_end = 150 * femto
9   field_order = 2
10  stdout_frequency = 1
11  smooth_currents = T
12  dt_multiplier = 0.95
13 end:control
14
15 begin:boundaries
16   cpml_thickness = 16
17   cpml_kappa_max = 20
18   cpml_a_max = 0.2
19   cpml_sigma_max = 0.7
20   bc_x_min_field = cpml_laser
21   bc_x_max_field = cpml_outflow
22   bc_x_min_particle = thermal
23   bc_x_max_particle = thermal
24   bc_y_min_field = cpml_outflow
25   bc_y_max_field = cpml_outflow
26   bc_y_min_particle = thermal
27   bc_y_max_particle = thermal
28 end:boundaries
29
30 begin:constant
31   cell_xsize = (x_max - x_min) / nx
32   cell_ysize = (y_max - y_min) / ny
33   las_lambda0 = 1.0 * micron
34   las_omega = 2.0 * pi * c / las_lambda0
35   las_time = 2.0 * pi / las_omega
36   theta = 0
37   w0 = 0.7 * micron # 5.0 * micron
38   fwhm_time = 20 * femto
39   w_time = fwhm_time / (2.0 * (sqrt(log(e(2.0)))))


```

```

40 xfocus = 8 * micron
41 yc = -xfocus * tan(theta)
42 zR = pi * w0^2 / las_lambda0
43 lfocus = xfocus / cos(theta)
44 wl = w0 * sqrt(1.0+(lfocus^2)/(zR^2))
45 w_y = wl / cos(theta)
46 r_curv = lfocus * (1.0+(zR^2)/(lfocus^2))
47 intensity_fac2d = 1.0 / sqrt(1.0+lfocus^2/zR^2) * cos(theta)
48 n_crit = critical(las_omega)
49 end:constant
50
51 begin:laser
52 boundary = x_min
53 amp = 1.8895615869e14
54 lambda = 1.0 * micron
55 pol_angle = 0.0 * pi
56 phase = -2.0*pi*(y-yc)*sin(theta)/las_lambda0 + pi/(las_lambda0)*((y-yc)*cos(theta))^2*1.0/
      r_curv - atan(((yc-y)*sin(theta)+lfocus)/zR)
57 profile = gauss(y, yc, sqrt(2)*w_y)
58 t_profile = gauss(time, 50*femto, w_time)
59 t_start = 0.0 * femto
60 t_end = 300 * femto
61 end:laser
62
63 begin:output
64 name = fields
65 file_prefix = field
66 dump_at_times = 50.00 * femto, 76.685127616 * femto, 103.370255232 * femto
67 grid = always + single
68 ex = always + single
69 ey = always + single
70 bz = always + single
71 dump_first = F
72 dump_last = F
73 restartable = F
74 end:output

```

**Listing A.3:** 2kppc

```

1 begin:control
2   nx = 1875
3   ny = 5000
4   x_min = 0 * micron
5   x_max = 15 * micron
6   y_min = -20 * micron
7   y_max = 20 * micron
8   t_end = 200 * femto
9   field_order = 2
10  stdout_frequency = 1
11  smooth_currents = T
12  dt_multiplier = 0.95
13 end:control
14
15 begin:boundaries
16   cpml_thickness = 16
17   cpml_kappa_max = 20
18   cpml_a_max = 0.2
19   cpml_sigma_max = 0.7
20   bc_x_min_field = cpml_laser
21   bc_x_max_field = cpml_outflow
22   bc_x_min_particle = thermal

```

```

23 bc_x_max_particle = thermal
24 bc_y_min_field = cpml_outflow
25 bc_y_max_field = cpml_outflow
26 bc_y_min_particle = thermal
27 bc_y_max_particle = thermal
28 end:boundaries
29
30 begin:species
31   name = electron
32   charge = -1.0
33   mass = 1.0
34   npart_per_cell = 2000
35   density = if((x gt 8 * micron) and (x lt 10 * micron) and (abs(y) lt 15 * micron), 100.0 *
36     n_crit, 0.0)
37   temp_ev = 100
38 end:species
39
40 begin:species
41   name = proton
42   charge = 1.0
43   mass = 1836.2
44   npart_per_cell = 100
45   density = density(electron)
46   temp_ev = 100
47 end:species
48
49 begin:laser
50   boundary = x_min
51   id = 1
52   fwhm_time = 30 * femto
53   t_0 = 60 * femto
54   w_0 = 0.5 * micron
55   pos = 0.0 * micron
56   focus = 8.0 * micron
57   intensity_w_cm2 = 1.0e20
58   lambda = 0.8 * micron
59   pol_angle = 0.0 * pi
60   t_start = 0.0 * femto
61   t_end = 300 * femto
62 end:laser
63
64 begin:subset
65   name = tenth
66   random_fraction = 0.1
67   include_species:electron
68   include_species:proton
69 end:subset
70
71 begin:output
72   name = particles
73   file_prefix = part
74   dt_snapshot = 10 * femto
75   particle_grid = tenth + single
76   px = tenth + single
77   py = tenth + single
78   pz = tenth + single
79   particle_weight = tenth + single
80   dump_first = F
81   dump_last = F
82   restartable = F
83 end:output

```

```

84 begin:output
85   name = fields
86   file_prefix = field
87   dt_snapshot = 10 * femto
88   grid = always + single
89   ex = always + single
90   ey = always + single
91   bz = always + single
92   dump_first = F
93   dump_last = F
94   restartable = F
95 end:output
96
97 begin:output
98   name = density
99   file_prefix = dens
100  dt_snapshot = 10 * femto
101  mass_density = always + single + species
102  charge_density = always + single + species
103  number_density = always + single + species
104  dump_first = F
105  dump_last = F
106  restartable = F
107 end:output
108
109 begin:output
110   name = diag
111   file_prefix = diag
112   dt_snapshot = 10 * femto
113   ekbar = always + single + species
114   ekflux = always + single + species
115   poynt_flux = always + single
116   temperature = always + single + species
117   total_energy_sum = always
118   dump_first = F
119   dump_last = F
120   restartable = F
121 end:output
122
123 begin:output
124   name = restart
125   file_prefix = r
126   dt_snapshot = 50.0 * femto
127   dump_first = F
128   dump_last = F
129   restartable = T
130 end:output

```



# Appendix B

## Code listings

Below, one can find the most important functions and methods that has been created within this work to provide some new functionalities and features into the code EPOCH. These serve mainly for the computations of laser fields at boundaries that are consistent with the Maxwell's equations using discrete Fourier transforms. Also, one can find the methods for the data manipulation and routines that interface corresponding C++ functions into the FORTRAN simulation code. Finally, the C++ and FORTRAN adaptors for ParaView Catalyst that enable in-situ visualization and diagnostics with a sample visualization Python script pipeline are all attached.

The following part is provided as it is, only with a short captions. It is mainly intended for those who are interested in the way of implementation and do not want to browse in the full source code, which can be found on the attached CD. Closer details are discussed in the third and fourth chapter of this work.

**Listing B.1:** Function performing forward fast Fourier transform using Intel® MKL library

```
1 std::vector<std::complex<double>> fft::mkl_fft_forward(std::vector<std::complex<double>> in) {  
2     DFTI_DESCRIPTOR_HANDLE desc;  
3     MKL_LONG status;  
4     DftiCreateDescriptor(&desc, DFTI_DOUBLE, DFTI_COMPLEX, 1, static_cast<MKL_LONG>(in.size()));  
5     DftiCommitDescriptor(desc);  
6     status = DftiComputeForward(desc, in.data());  
7     if(status != 0) {  
8         std::cerr << DftiErrorMessage(status) << std::endl;  
9         abort();  
10    }  
11    DftiFreeDescriptor(&desc);  
12    return in;  
13 }
```

**Listing B.2:** Function performing backward fast Fourier transform using Intel® MKL library

```
1 std::vector<std::complex<double>> fft::mkl_fft_backward(std::vector<std::complex<double>> in) {  
2     DFTI_DESCRIPTOR_HANDLE desc;  
3     MKL_LONG status;  
4     DftiCreateDescriptor(&desc, DFTI_DOUBLE, DFTI_COMPLEX, 1, static_cast<MKL_LONG>(in.size()));  
5     DftiCommitDescriptor(desc);
```

```

6 status = DftiComputeBackward(desc, in.data());
7 if(status != 0) {
8 std::cerr << DftiErrorMessage(status) << std::endl;
9 abort();
10 }
11 DftiFreeDescriptor(&desc);
12 return in;
13 }
```

**Listing B.3:** Function performing forward fast Fourier transform using FFTW library

```

1 std::vector<std::complex<double>> fft::fftw_fft_forward(std::vector<std::complex<double>> in) {
2 fftw_plan p = fftw_plan_dft_1d(in.size(), reinterpret_cast<fftw_complex*>(in.data()),
3     reinterpret_cast<fftw_complex*>(in.data()), FFTW_FORWARD, FFTW_ESTIMATE);
4 fftw_execute(p);
5 fftw_destroy_plan(p);
6 return in;
```

**Listing B.4:** Function performing backward fast Fourier transform using FFTW library

```

1 std::vector<std::complex<double>> fft::fftw_fft_backward(std::vector<std::complex<double>> in) {
2 fftw_plan p = fftw_plan_dft_1d(in.size(), reinterpret_cast<fftw_complex*>(in.data()),
3     reinterpret_cast<fftw_complex*>(in.data()), FFTW_BACKWARD, FFTW_ESTIMATE);
4 fftw_execute(p);
5 fftw_destroy_plan(p);
6 return in;
```

**Listing B.5:** Function performing forward discrete Fourier transform without using any library

```

1 std::vector<std::complex<double>> fft::fft_forward(std::vector<std::complex<double>> in) {
2 std::vector<std::complex<double>> out(in.size());
3 for(auto j = 0; j < out.size(); j++) {
4 for(auto l = 0; l < out.size(); l++) {
5 out.at(j) += in.at(l) * exp(-2.0 * constants::pi * I * l * j / in.size());
6 }
7 }
8 return out;
9 }
```

**Listing B.6:** Function performing backward discrete Fourier transform without using any library

```

1 std::vector<std::complex<double>> fft::fft_backward(std::vector<std::complex<double>> in) {
2 std::vector<std::complex<double>> out(in.size());
3 for(auto j = 0; j < out.size(); j++) {
4 for(auto l = 0; l < out.size(); l++) {
5 out.at(j) += in.at(l) * exp(+2.0 * constants::pi * I * l * j / in.size());
6 }
7 }
8 return out;
9 }
```

**Listing B.7:** Method for performing discrete Fourier transform in time

```

1 void laser_bcs::dft_time(field_2d<std::complex<double>>& field) const {
2 #ifdef OPENMP
3 #pragma omp parallel for schedule(static)
```

```

4 #endif
5 for(auto j = 0; j < this->domain->Nx; j++) {
6 #ifdef USE_MKL
7 field.add_col(fft::mkl_fft_backward(field.get_col(j)), j);
8 #elif USE_FFTW
9 field.add_col(fft::fftw_fft_backward(field.get_col(j)), j);
10 #else
11 field.add_col(fft::fft_backward(field.get_col(j)), j);
12 #endif
13 }
14 field.multiply(this->domain->dt / (2.0 * constants::pi));
15 return;
16 }

```

**Listing B.8:** Method for performing inverse discrete Fourier transform in time

```

1 void laser_bcs::idft_time(field_2d<std::complex<double>>& field) const {
2 #ifdef OPENMP
3 #pragma omp parallel for schedule(static)
4 #endif
5 for(auto j = 0; j < this->domain->Nx; j++) {
6 #ifdef USE_MKL
7 field.add_col(fft::mkl_fft_forward(field.get_col(j)), j);
8 #elif USE_FFTW
9 field.add_col(fft::fftw_fft_forward(field.get_col(j)), j);
10 #else
11 field.add_col(fft::fft_forward(field.get_col(j)), j);
12 #endif
13 }
14 field.multiply(2.0 * (2.0 * constants::pi) / (this->domain->Nt * this->domain->dt));
15 return;
16 }

```

**Listing B.9:** Method for performing discrete Fourier transform in space

```

1 void laser_bcs::dft_space(field_2d<std::complex<double>>& field) const {
2 std::vector<std::complex<double>> row_global(this->domain->Nx_global);
3 std::vector<std::complex<double>> row_local;
4 for(auto j = 0; j < this->domain->Nt; j++) {
5 row_local = field.get_row(j);
6 MPI_Gatherv(row_local.data(), this->domain->Nx, MPI_CXX_DOUBLE_COMPLEX, row_global.data(), this->
    domain->counts.data(), this->domain->displs.data(), MPI_CXX_DOUBLE_COMPLEX, 0, MPI_COMM_WORLD
    );
7 if(this->domain->rank == 0) {
8 #ifdef USE_MKL
9 row_global = fft::mkl_fft_forward(row_global);
10 #elif USE_FFTW
11 row_global = fft::fftw_fft_forward(row_global);
12 #else
13 row_global = fft::fft_forward(row_global);
14 #endif
15 }
16 MPI_Scatterv(row_global.data(), this->domain->counts.data(), this->domain->displs.data(),
    MPI_CXX_DOUBLE_COMPLEX, row_local.data(), this->domain->Nx, MPI_CXX_DOUBLE_COMPLEX, 0,
    MPI_COMM_WORLD);
17 field.add_row(row_local, j);
18 }
19 field.multiply(this->domain->dx / (2.0 * constants::pi));
20 return;
21 }

```

**Listing B.10:** Method for performing inverse discrete Fourier transform in space

```

1 void laser_bcs::idft_space(field_2d<std::complex<double>>& field) const {
2 std::vector<std::complex<double>> row_global(this->domain->Nx_global);
3 std::vector<std::complex<double>> row_local;
4 for(auto j = 0; j < this->domain->Nt; j++) {
5 row_local = field.get_row(j);
6 MPI_Gatherv(row_local.data(), this->domain->Nx, MPI_CXX_DOUBLE_COMPLEX, row_global.data(), this->
    domain->counts.data(), this->domain->displs.data(), MPI_CXX_DOUBLE_COMPLEX, 0, MPI_COMM_WORLD
    );
7 if(this->domain->rank == 0) {
8 #ifdef USE_MKL
9 row_global = fft::mkl_fft_backward(row_global);
10#elif USE_FFTW
11 row_global = fft::fftw_fft_backward(row_global);
12#else
13 row_global = fft::fft_backward(row_global);
14#endif
15}
16MPI_Scatterv(row_global.data(), this->domain->counts.data(), this->domain->displs.data(),
    MPI_CXX_DOUBLE_COMPLEX, row_local.data(), this->domain->Nx, MPI_CXX_DOUBLE_COMPLEX, 0,
    MPI_COMM_WORLD);
17field.add_row(row_local, j);
18}
19field.multiply((2.0 * constants::pi) / (this->domain->Nx_global * this->domain->dx));
20return;
21}

```

**Listing B.11:** Method for dumping data into shared file

```

1 template <typename T>
2 void field_2d<T>::dump_to_shared_file(std::string name, int row_first, int row_last, int
    row_size_local, int row_size_global, int col_start) const {
3 MPI_File file;
4 MPI_Offset offset = 0;
5 MPI_Status status;
6 MPI_Datatype local_array;
7 int col_size = row_last - row_first;
8 const int ndims = 2;
9 std::array<int, ndims> size_global = {col_size, row_size_global};
10 std::array<int, ndims> size_local = {col_size, row_size_local};
11 std::array<int, ndims> start_coords = {0, col_start};
12 MPI_Type_create_subarray(2, size_global.data(), size_local.data(), start_coords.data(),
    MPI_ORDER_C, MPI_DOUBLE, &local_array);
13 MPI_Type_commit(&local_array);
14 std::vector<double> real_part(col_size * row_size_local);
15 for(auto i = std::make_pair(row_first, 0); i.first < row_last; i.first++, i.second++) {
16 for(auto j = 0; j < row_size_local; j++) {
17 real_part[i.second * row_size_local + j] = std::real(this->data[i.first * row_size_local + j]);
18 }
19}
20 MPI_File_open(MPI_COMM_WORLD, name.data(), MPI_MODE_CREATE|MPI_MODE_WRONLY, MPI_INFO_NULL, &file)
    ;
21 MPI_File_set_view(file, offset, MPI_DOUBLE, local_array, "native", MPI_INFO_NULL);
22 MPI_File_write_all(file, real_part.data(), col_size * row_size_local, MPI_DOUBLE, &status);
23 MPI_File_close(&file);
24 MPI_Type_free(&local_array);
25 return;
26}

```

**Listing B.12:** Extern C++ function to fill Fortran arrays with laser fields dumped in binary file

```

1 void populate_laser_at_boundary(double* field, int* id, const char* data_dir, int* timestep, int*
2     size_global, int* first, int* last) {
3     double num = 0.0;
4     std::string laser_id = std::to_string(*id);
5     std::string path(data_dir);
6     std::ifstream in;
7     in.open(path + "/laser_" + laser_id + ".dat", std::ios::binary);
8     if(in.is_open()) {
9         in.seekg(((*timestep) * (*size_global) + (*first) - 1) * sizeof(num));
10        for(auto i = 0; i < *last - *first + 1; i++) {
11            in.read(reinterpret_cast<char*>(&num), sizeof(num));
12            field[i] = num;
13        }
14    } else {
15        std::cout << "error: cannot read file " << path + "/" + filename + laser_id + ".dat" << std::endl
16        ;
17    }
18    return;
19 }
```

**Listing B.13:** Fortran interfaces for C++ library functions

```

1 INTERFACE
2
3 SUBROUTINE compute_laser_at_boundary(rank, nproc, laser_start, laser_end, &
4 fwhm_time, t_0, omega, pos, amp, w_0, id, L_min, L_max, L_focus, T_min, T_max, &
5 T_ncells, cpml_thickness, t_end, T_cell_size, L_cell_size, dt, output_path) bind(c)
6 USE, INTRINSIC :: iso_c_binding
7 IMPLICIT NONE
8 INTEGER(c_int), INTENT(IN) :: rank, nproc, id, T_ncells, cpml_thickness
9 CHARACTER(kind=c_char), DIMENSION(*), INTENT(IN) :: output_path
10 REAL(c_double), INTENT(IN) :: laser_start, laser_end, fwhm_time, t_0, omega, pos, &
11 amp, w_0, L_min, L_max, L_focus, T_min, T_max, t_end, T_cell_size, L_cell_size, dt
12 END SUBROUTINE compute_laser_at_boundary
13
14 SUBROUTINE populate_laser_at_boundary(field, laser_id, output_path, timestep, size_global, first,
15     last) bind(c)
16 USE, INTRINSIC :: iso_c_binding
17 IMPLICIT NONE
18 INTEGER(c_int), INTENT(IN) :: laser_id, timestep, size_global, first, last
19 CHARACTER(kind=c_char), DIMENSION(*), INTENT(IN) :: output_path
20 REAL(c_double), DIMENSION(*), INTENT(OUT) :: field
21 END SUBROUTINE populate_laser_at_boundary
22 END INTERFACE
```

**Listing B.14:** Fortran subroutines for Maxwell consistent computation of laser fields at boundaries

```

1 SUBROUTINE Maxwell_consistent_computation_of_EM_fields
2
3 TYPE(laser_block), POINTER :: current
4
5 current => laser_x_min
6 DO WHILE(ASSOCIATED(current))
7     CALL compute_laser_at_boundary(rank, nproc, current%t_start, current%t_end, &
8         current%fwhm_time, current%t_0, current%omega, current%pos, current%amp, current%w_0, &
9         current%id, x_min, x_max, current%focus, y_min, y_max, ny_global, cpml_thickness, t_end, &
10        dy, dx, dt, TRIM(data_dir)//C_NULL_CHAR)
```

```

11 current => current%next
12 ENDDO
13
14 current => laser_x_max
15 DO WHILE(ASSOCIATED(current))
16 CALL compute_laser_at_boundary(rank, nproc, current%t_start, current%t_end, &
17 current%fwhm_time, current%t_0, current%omega, current%pos, current%amp, current%w_0, &
18 current%id, x_min, x_max, current%focus, y_min, y_max, ny_global, cpml_thickness, t_end, &
19 dy, dx, dt, TRIM(data_dir)//C_NULL_CHAR)
20 current => current%next
21 ENDDO
22
23 current => laser_y_min
24 DO WHILE(ASSOCIATED(current))
25 CALL compute_laser_at_boundary(rank, nproc, current%t_start, current%t_end, &
26 current%fwhm_time, current%t_0, current%omega, current%pos, current%amp, current%w_0, &
27 current%id, y_min, y_max, current%focus, x_min, x_max, nx_global, cpml_thickness, t_end, &
28 dx, dy, dt, TRIM(data_dir)//C_NULL_CHAR)
29 current => current%next
30 ENDDO
31
32 current => laser_y_max
33 DO WHILE(ASSOCIATED(current))
34 CALL compute_laser_at_boundary(rank, nproc, current%t_start, current%t_end, &
35 current%fwhm_time, current%t_0, current%omega, current%pos, current%amp, current%w_0, &
36 current%id, y_min, y_max, current%focus, x_min, x_max, nx_global, cpml_thickness, t_end, &
37 dx, dy, dt, TRIM(data_dir)//C_NULL_CHAR)
38 current => current%next
39 ENDDO
40
41 END SUBROUTINE Maxwell_consistent_computation_of_EM_fields

```

**Listing B.15:** Fortran subroutines for populating laser sources at boundaries

```

1 SUBROUTINE get_source_x_boundary(buffer, laser_id)
2 REAL(num), DIMENSION(:), INTENT(INOUT) :: buffer
3 INTEGER, INTENT(IN) :: laser_id
4 CALL populate_laser_at_boundary(buffer, laser_id, TRIM(data_dir)//C_NULL_CHAR, &
5 step, ny_global, ny_global_min, ny_global_max)
6 END SUBROUTINE get_source_x_boundary
7
8 SUBROUTINE get_source_y_boundary(buffer, laser_id)
9 REAL(num), DIMENSION(:), INTENT(INOUT) :: buffer
10 INTEGER, INTENT(IN) :: laser_id
11 CALL populate_laser_at_boundary(buffer, laser_id, TRIM(data_dir)//C_NULL_CHAR, &
12 step, nx_global, nx_global_min, nx_global_max)
13 END SUBROUTINE get_source_y_boundary

```

**Listing B.16:** Fortran adaptor for ParaView Catalyst

```

1 MODULE coprocessor
2
3 USE, INTRINSIC :: iso_c_binding
4 USE fields
5
6 IMPLICIT NONE
7
8 CONTAINS
9
10 SUBROUTINE init_coproc(step, time)

```

```

11 INTEGER, INTENT(in) :: step
12 REAL(num), INTENT(in) :: time
13 INTEGER :: ilen, i
14 CHARACTER(len=200) :: arg
15 CALL coprocessorinitialize()
16 DO i = 1, iargc()
17 CALL getarg(i, arg)
18 ilen = len_trim(arg)
19 arg(ilen+1:) = C_NULL_CHAR
20 CALL coprocessoraddpythonscript(arg, ilen)
21 ENDDO
22 CALL createinputdatadescription(step, time, "essential")
23 END SUBROUTINE init_coproc
24
25 SUBROUTINE run_coproc(step, time)
26 INTEGER, INTENT(in) :: step
27 REAL(num), INTENT(in) :: time
28 INTEGER :: flag, mytid, ntids, n, i, j
29 INTEGER, DIMENSION(6) :: local_extent, global_extent
30 INTEGER, DIMENSION(4) :: lim
31 REAL(num), DIMENSION(3*nx*ny) :: e_field, b_field
32 #ifdef OPENMP
33     INTEGER :: omp_get_thread_num, omp_get_num_threads, omp_get_max_threads
34     EXTERNAL :: omp_get_thread_num, omp_get_num_threads, omp_get_max_threads
35 #endif
36
37 local_extent = (/ nx_global_min, nx_global_max, ny_global_min, ny_global_max, 0, 0 /)
38 global_extent = (/ 1, nx_global, 1, ny_global, 0, 0 /)
39 lim = (/ 1 + ng, nx + ng, 1 + ng, ny + ng /)
40
41 CALL requestdatadescription(step, time, flag)
42 IF (flag /= 0) THEN
43     CALL buildgrid(rank, nproc, step, time, local_extent, global_extent, &
44     x(lim(1):lim(2)), y(lim(3):lim(4)), "essential"//C_NULL_CHAR)
45
46 !$omp parallel default (none) private(mytid,i,j,n) &
47 shared(ntids,lim,e_field,b_field,ex,ey,ez,bx,by,bz)
48 #ifdef OPENMP
49     mytid = OMP_GET_THREAD_NUM()
50     ntids = OMP_GET_NUM_THREADS()
51 #endif
52 DO j = 0, lim(4) - lim(3), ntids
53 n = (j+mytid)*(1 + lim(2) - lim(1))*3 + 1
54 IF(j + mytid <= lim(4)) THEN
55 DO i = 0, lim(2) - lim(1)
56 e_field(n + 0) = ex(lim(1) + i, lim(3) + j + mytid)
57 e_field(n + 1) = ey(lim(1) + i, lim(3) + j + mytid)
58 e_field(n + 2) = ez(lim(1) + i, lim(3) + j + mytid)
59 b_field(n + 0) = bx(lim(1) + i, lim(3) + j + mytid)
60 b_field(n + 1) = by(lim(1) + i, lim(3) + j + mytid)
61 b_field(n + 2) = bz(lim(1) + i, lim(3) + j + mytid)
62 n = n + 3
63 ENDDO
64 ENDIF
65 ENDDO
66 !$omp end parallel
67
68 CALL addfield(rank, e_field, "E (V/m)"//C_NULL_CHAR, 3, "essential"//C_NULL_CHAR)
69 CALL addfield(rank, b_field, "B (T)"//C_NULL_CHAR, 3, "essential"//C_NULL_CHAR)
70 CALL coprocess()
71 ENDIF
72 END SUBROUTINE run_coproc

```

```

73 SUBROUTINE finalise_coproc()
74 CALL coprocessorfinalize()
75 END SUBROUTINE finalise_coproc
76
77
78 END MODULE coprocessor

```

**Listing B.17:** C++ adaptor for ParaView Catalyst

```

1 #include "vtkCPDataDescription.h"
2 #include "vtkCPInputDataDescription.h"
3 #include "vtkCPPProcessor.h"
4 #include "vtkCPPythonScriptPipeline.h"
5 #include "vtkCPPythonAdaptorAPI.h"
6
7 #ifdef INSITU_DOUBLE_PREC
8 #include "vtkDoubleArray.h"
9 #else
10 #include "vtkFloatArray.h"
11 #endif
12
13 #include "vtkSmartPointer.h"
14 #include "vtkRectilinearGrid.h"
15 #include "vtkPointData.h"
16 #include "vtkImageData.h"
17 #include "vtkMultiBlockDataSet.h"
18 #include "vtkMultiPieceDataSet.h"
19
20 #include <iostream>
21 #include <fstream>
22 #include <vector>
23 #include <array>
24
25 #ifdef __cplusplus
26 extern "C" {
27 #endif
28 void createinputdatadescription_(int* step, double* time, const char* grid_name);
29 void buildgrid_(int* rank, int* size, int* step, double* time, int* local_extent, int*
   global_extent, double* x_coords, double* y_coords, const char* grid_name);
30 void addfield_(int* rank, double* input_field, char* name, int* components, const char* grid_name
   );
31 #ifdef __cplusplus
32 }
33 #endif
34
35 void createinputdatadescription_(int* step, double* time, const char* grid_name) {
36 if (!vtkCPPythonAdaptorAPI::GetCoProcessorData()) {
37 vtkGenericWarningMacro("unable to access coprocessor data");
38 return;
39 }
40 vtkCPPythonAdaptorAPI::GetCoProcessorData()->AddInput(grid_name);
41 vtkCPPythonAdaptorAPI::GetCoProcessorData()->SetTimeData(*time, static_cast<vtkIdType>(*step));
42 return;
43 }
44
45 void buildgrid_(int* rank, int* size, int* step, double* time, int* local_extent, int*
   global_extent, double* x_coords, double* y_coords, const char* grid_name) {
46 if (!vtkCPPythonAdaptorAPI::GetCoProcessorData()) {
47 vtkGenericWarningMacro("unable to access coprocessor data");
48 return;
49 }

```

```

50 vtkCPPythonAdaptorAPI::GetCoProcessorData() -> SetTimeData(*time, static_cast<vtkIdType>(*step));
51 if (!vtkCPPythonAdaptorAPI::GetCoProcessorData() -> GetInputDescriptionByName(grid_name) -> GetGrid())
52 {
53     vtkCPInputDataDescription* idd = vtkCPPythonAdaptorAPI::GetCoProcessorData() ->
54         GetInputDescriptionByName(grid_name);
55     if (!idd) {
56         vtkGenericWarningMacro("cannot access data description to attach grid to");
57         return;
58     }
59     vtkSmartPointer<vtkRectilinearGrid> rectilinear_grid =
60     vtkSmartPointer<vtkRectilinearGrid>::New();
61     rectilinear_grid->SetExtent(local_extent);
62     int* ext = rectilinear_grid->GetExtent();
63     int dim[3] = {ext[1] - ext[0] + 1, ext[3] - ext[2] + 1, ext[5] - ext[4] + 1};
64
65 #ifdef INSITU_DOUBLE_PREC
66     vtkSmartPointer<vtkDoubleArray> x_array = vtkSmartPointer<vtkDoubleArray>::New();
67     vtkSmartPointer<vtkDoubleArray> y_array = vtkSmartPointer<vtkDoubleArray>::New();
68     double* x_c = x_coords;
69     double* y_c = y_coords;
70 #else
71     vtkSmartPointer<vtkFloatArray> x_array = vtkSmartPointer<vtkFloatArray>::New();
72     vtkSmartPointer<vtkFloatArray> y_array = vtkSmartPointer<vtkFloatArray>::New();
73     float* x_c = new float[dim[0]];
74     float* y_c = new float[dim[1]];
75     for(std::size_t i = 0; i < dim[0]; i++) {
76         x_c[i] = static_cast<float>(x_coords[i]);
77     }
78     for(std::size_t i = 0; i < dim[1]; i++) {
79         y_c[i] = static_cast<float>(y_coords[i]);
80     }
81 #endif
82     x_array->SetNumberOfComponents(1);
83     y_array->SetNumberOfComponents(1);
84     x_array->SetArray(x_c, static_cast<vtkIdType>(dim[0]), 1);
85     y_array->SetArray(y_c, static_cast<vtkIdType>(dim[1]), 1);
86     rectilinear_grid->SetXCoordinates(x_array);
87     rectilinear_grid->SetYCoordinates(y_array);
88
89     vtkSmartPointer<vtkMultiPieceDataSet> multi_piece = vtkSmartPointer<vtkMultiPieceDataSet>::New();
90     multi_piece->SetNumberOfPieces(*size);
91     multi_piece->SetPiece(*rank, rectilinear_grid);
92
93     vtkSmartPointer<vtkMultiBlockDataSet> grid = vtkSmartPointer<vtkMultiBlockDataSet>::New();
94     grid->SetNumberOfBlocks(1);
95     grid->SetBlock(0, multi_piece);
96
97     idd->SetWholeExtent(global_extent);
98     idd->SetGrid(grid);
99 }
100 return;
101 }
102
103 void addfield_(int* rank, double* input_field, char* name, int* components, const char* grid_name
104 ) {
105 if (!vtkCPPythonAdaptorAPI::GetCoProcessorData()) {
106     vtkGenericWarningMacro("unable to access coprocessor data");
107 }
108 vtkCPInputDataDescription* idd = vtkCPPythonAdaptorAPI::GetCoProcessorData() ->
```

```

109     GetInputDescriptionByName(grid_name);
110     vtkMultiBlockDataSet* multi_block = vtkMultiBlockDataSet::SafeDownCast(idd->GetGrid());
111     vtkMultiPieceDataSet* multi_piece = vtkMultiPieceDataSet::SafeDownCast(multi_block->GetBlock(0));
112     vtkRectilinearGrid* type = vtkRectilinearGrid::SafeDownCast(multi_piece->GetPiece(*rank));
113     if (!type) {
114         vtkGenericWarningMacro("no adaptor grid to attach field data to");
115         return;
116     }
117     if (idd->IsFieldNeeded(name)) {
118         int size = (*components)*type->GetNumberOfPoints();
119 #ifdef INSITU_DOUBLE_PREC
120         double* array = input_field;
121         vtkSmartPointer<vtkDoubleArray> field = vtkSmartPointer<vtkDoubleArray>::New();
122 #else
123         float* array = new float[size];
124         for(std::size_t i = 0; i < size; i++) {
125             array[i] = static_cast<float>(input_field[i]);
126         }
127         vtkSmartPointer<vtkFloatArray> field = vtkSmartPointer<vtkFloatArray>::New();
128 #endif
129         field->SetName(name);
130         field->SetNumberOfComponents(*components);
131         field->SetArray(array, static_cast<vtkIdType>(size), 1);
132         type->GetPointData()->AddArray(field);
133     }
134     return;
}

```

**Listing B.18:** Sample visualization pipeline using Python script

```

1 try: paraview.simple
2 except: from paraview.simple import *
3
4 from paraview import coprocessing
5
6 inputs = ['essential']
7 update_freq = 1
8 output_freq = 10000
9
10 def CreateCoProcessor():
11     def _CreatePipeline(coprocessor, datadescription):
12         class Pipeline:
13
14             essential = coprocessor.CreateProducer(datadescription, "essential")
15
16             multi_block_binary_writer = servermanager.writers.XMLMultiBlockDataWriter(Input=essential,
17                 DataMode='Appended', EncodeAppendedData=0, HeaderType='UInt32', CompressorType='ZLib')
18             coprocessor.RegisterWriter(multi_block_binary_writer, filename='full_grid_%t.vtm', freq=
19                 output_freq)
20
21         class CoProcessor(coprocessing.CoProcessor):
22             def CreatePipeline(self, datadescription):
23                 self.Pipeline = _CreatePipeline(self, datadescription)
24
25             coprocessor = CoProcessor()
26             freqs = {}
27             for name in inputs:
28                 freqs[name] = [update_freq]
29
29         coprocessor.SetUpdateFrequencies(freqs)
29         return coprocessor

```

```

30
31 coprocessor = CreateCoProcessor()
32 coprocessor.EnableLiveVisualization(True)
33
34 def RequestDataDescription(datadescription):
35     "Callback to populate the request for current timestep"
36     global coprocessor
37
38     if datadescription.GetForceOutput() == True:
39         for i in range(datadescription.GetNumberOfInputDescriptions()):
40             datadescription.GetInputDescription(i).AllFieldsOn()
41             datadescription.GetInputDescription(i).GenerateMeshOn()
42     return
43
44 coprocessor.LoadRequestedData(datadescription)
45
46 def DoCoProcessing(datadescription):
47     "Callback to do co-processing for current timestep"
48     global coprocessor
49
50 coprocessor.UpdateProducers(datadescription)
51 coprocessor.WriteData(datadescription);
52 coprocessor.WriteImages(datadescription, rescale_lookingtable=False)
53 coprocessor.DoLiveVisualization(datadescription, "visualization_node", 11111)

```

**Listing B.19:** EPOCH CMakeLists file to generate platform-specific build scripts

```

1 cmake_minimum_required(VERSION 3.1)
2 project(EPOCH_2D)
3 enable_language(CXX Fortran)
4
5 set(CMAKE_MODULE_PATH ${CMAKE_SOURCE_DIR}/cmake)
6 set(CMAKE_Fortran_MODULE_DIRECTORY ${CMAKE_SOURCE_DIR}/obj)
7 set(CMAKE_ARCHIVE_OUTPUT_DIRECTORY ${CMAKE_SOURCE_DIR}/lib)
8 set(EXECUTABLE_OUTPUT_PATH ${CMAKE_SOURCE_DIR}/bin)
9
10 find_package(MPI REQUIRED)
11 find_package(SDF REQUIRED)
12
13 include_directories(${MPI_Fortran_INCLUDE_PATH})
14 include_directories(${SDF_Fortran_INCLUDE_PATH})
15 include_directories(src/include)
16
17 execute_process(COMMAND ./src/gen_commit_string.sh)
18 execute_process(COMMAND grep -oP "(?=<COMMIT=)[^ ]+" ./src/COMMIT OUTPUT_VARIABLE COMMIT)
19 execute_process(COMMAND date +%s OUTPUT_VARIABLE DATE)
20 execute_process(COMMAND uname -n OUTPUT_VARIABLE MACHINE)
21
22 add_definitions('-D_COMMIT="${COMMIT}"')
23 add_definitions('-D_DATE=${DATE}')
24 add_definitions('-D_MACHINE="${MACHINE}"')
25
26 if(NOT CMAKE_BUILD_TYPE AND NOT CMAKE_CONFIGURATION_TYPES)
27 message(STATUS "Setting build type to 'Release', Debug mode was not specified.")
28 set(CMAKE_BUILD_TYPE Release CACHE STRING "Choose the type of build." FORCE)
29 # Set the possible values of build type for cmake-gui
30 set_property(CACHE CMAKE_BUILD_TYPE PROPERTY STRINGS "Debug" "Release")
31 endif()
32
33 if(${CMAKE_Fortran_COMPILER_ID} MATCHES "Intel")
34 set(CMAKE_Fortran_FLAGS_RELEASE "-O3 -xHost -no-prec-div -fno-math-errno -unroll=3 -qopt-

```

```

      subscript-in-range -align all")
35 set(CMAKE_Fortran_FLAGS_DEBUG "-O0 -nothreads -traceback -flichtconsistency -C -g -heap-arrays 64 -
   warn -fp-stack-check -check bounds -fpe0")
36 elseif(${CMAKE_Fortran_COMPILER_ID} MATCHES "GNU")
37 set(CMAKE_Fortran_FLAGS_RELEASE "-O2 -fimplicit-none -ffixed-line-length-132")
38 set(CMAKE_Fortran_FLAGS_DEBUG "-O0 -g -Wall -Wextra -pedantic -fbounds-check -ffpe-trap=invalid,
   zero,overflow -Wno-unused-parameter")
39 elseif(${CMAKE_Fortran_COMPILER_ID} MATCHES "PGI")
40   set(CMAKE_Fortran_FLAGS_RELEASE "-r8 -fast -fastsse -O3 -Mipa=fast,inline -Minfo")
41   set(CMAKE_Fortran_FLAGS_DEBUG "-Mbounds -g")
42 elseif(${CMAKE_Fortran_COMPILER_ID} MATCHES "G95")
43   set(CMAKE_Fortran_FLAGS_RELEASE "-O3")
44   set(CMAKE_Fortran_FLAGS_DEBUG "-O0 -g")
45 elseif(${CMAKE_Fortran_COMPILER_ID} MATCHES "XL")
46   set(CMAKE_Fortran_FLAGS_RELEASE "-O5 -qhot -qipa")
47   set(CMAKE_Fortran_FLAGS_DEBUG "-O0 -C -g -qfullpath -qinfo -qnosmp -qxflag=dvz -Q! -qnounwind -
   qnunroll")
48 else()
49 message(STATUS "No optimized Fortran compiler flags are known")
50 message(STATUS "Fortran compiler full path: " ${CMAKE_Fortran_COMPILER})
51 set(CMAKE_Fortran_FLAGS_RELEASE "-O2")
52 set(CMAKE_Fortran_FLAGS_DEBUG "-O0 -g")
53 endif()
54
55 if(${CMAKE_CXX_COMPILER_ID} MATCHES "Intel")
56 set(CMAKE_CXX_FLAGS_RELEASE "-O3 -std=c++11 -no-prec-div -ansi-alias -qopt-prefetch=4 -unroll-
   aggressive -m64")
57 set(CMAKE_CXX_FLAGS_DEBUG "-O0 -std=c++11 -g -traceback -mp1 -fp-trap=common -fp-model strict")
58 elseif(${CMAKE_CXX_COMPILER_ID} MATCHES "GNU")
59 set(CMAKE_CXX_FLAGS_RELEASE "-O2 -std=c++11 -msse4 -mtune=native -march=native -funroll-loops -
   fno-math-errno -ffast-math")
60 set(CMAKE_CXX_FLAGS_DEBUG "-O0 -std=c++11 -g -pedantic -Wall -Wextra -Wno-unused")
61 elseif(${CMAKE_CXX_COMPILER_ID} MATCHES "PGI")
62   set(CMAKE_CXX_FLAGS_RELEASE "-std=c++0x")
63   set(CMAKE_CXX_FLAGS_DEBUG "-std=c++0x")
64 elseif(${CMAKE_CXX_COMPILER_ID} MATCHES "G95")
65   set(CMAKE_CXX_FLAGS_RELEASE "-std=c++0x")
66   set(CMAKE_CXX_FLAGS_DEBUG "-std=c++0x")
67 elseif(${CMAKE_CXX_COMPILER_ID} MATCHES "XL")
68   set(CMAKE_CXX_FLAGS_RELEASE "-qlanglvl=extended0x")
69   set(CMAKE_CXX_FLAGS_DEBUG "-qlanglvl=extended0x")
70 else()
71 message(STATUS "No optimized C++ compiler flags are known")
72 message(STATUS "C++ compiler full path: " ${CMAKE_CXX_COMPILER})
73 set(CMAKE_CXX_FLAGS_RELEASE "-O2 -std=c++11")
74 set(CMAKE_CXX_FLAGS_DEBUG "-O0 -std=c++11 -g")
75 endif()
76
77 set(SOURCES
${CMAKE_SOURCE_DIR}/src/epoch2d.F90
${CMAKE_SOURCE_DIR}/src/boundary.f90
${CMAKE_SOURCE_DIR}/src/fields.f90
${CMAKE_SOURCE_DIR}/src/laser.F90
${CMAKE_SOURCE_DIR}/src/particles.F90
${CMAKE_SOURCE_DIR}/src/shared_data.F90
)
78
79 set(FOLDERS deck housekeeping io parser physics_packages user_interaction)
80 foreach(FOLDER ${FOLDERS})
81 file(GLOB TMP ${CMAKE_SOURCE_DIR}/src/${FOLDER}/*)
82 list(APPEND SOURCES ${TMP})
83 endforeach()

```

```

91 option(OPENMP "Enable multithreading using OpenMP directives." OFF)
92 option(PER_SPECIES_WEIGHT "Set every pseudoparticle in a species to represent the same number of
93     real particles." OFF)
94 option(NO_TRACER_PARTICLES "Don't enable support for tracer particles." OFF)
95 option(NO_PARTICLE_PROBES "Don't enable support for particle probes." OFF)
96 option(PARTICLE_SHAPE_TOPHAT "Use second order particle weighting." OFF)
97 option(PARTICLE_SHAPE_BSPLINE3 "Use fifth order particle weighting." OFF)
98 option(PARTICLE_ID "Include a unique global particle ID using an 8-byte integer." OFF)
99 option(PARTICLE_ID4 "Include a unique global particle ID using an 4-byte integer." OFF)
100 option(PARTICLE_COUNT_UPDATE "Keep global particle counts up to date." OFF)
101 option(PHOTONS "Include QED routines" OFF)
102 option(TRIDENT_PHOTONS "Use the Trident process for pair production." OFF)
103 option(PREFETCH "Use Intel-specific 'mm_prefetch' calls to load next particle in the list into
104     cache ahead of time." OFF)
105 option(PARSER_DEBUG "Turn on debugging." OFF)
106 option(PARTICLE_DEBUG "Turn on debugging." OFF)
107 option(MPI_DEBUG "Turn on debugging." OFF)
108 option(SIMPLIFY_DEBUG "Turn on debugging." OFF)
109 option(NO_IO "Don't generate any output at all. Useful for benchmarking." OFF)
110 option(COLLISIONS_TEST "Bypass the main simulation and only perform collision tests." OFF)
111 option(PER_PARTICLE_CHARGE_MASS "specify charge and mass per particle rather than per species."
112     OFF)
113 option(PARSER_CHECKING "Perform checks on evaluated deck expressions." OFF)
114 option(USE_INSITU "Link epoch with ParaView Catalyst." OFF)
115 option(INSITU_DOUBLE_PREC "Double precision for data exported insitu." OFF)
116 option(TIGHT_FOCUSING "Maxwell consistent computation of EM fields at boundary for tight-focusing
117     ." OFF)
118
119 if(OPENMP)
120 message(STATUS "Option 'OPENMP' enabled")
121 add_definitions("-DOPENMP")
122 if(${CMAKE_Fortran_COMPILER_ID} MATCHES "Intel")
123 set(CMAKE_Fortran_FLAGS_RELEASE "${CMAKE_Fortran_FLAGS_RELEASE} -fopenmp")
124 set(CMAKE_Fortran_FLAGS_DEBUG "${CMAKE_Fortran_FLAGS_DEBUG} -fopenmp")
125 elseif(${CMAKE_Fortran_COMPILER_ID} MATCHES "GNU")
126 set(CMAKE_Fortran_FLAGS_RELEASE "${CMAKE_Fortran_FLAGS_RELEASE} -fopenmp")
127 set(CMAKE_Fortran_FLAGS_DEBUG "${CMAKE_Fortran_FLAGS_DEBUG} -fopenmp")
128 else()
129 message(STATUS "Fortran OpenMP compiler flag not known.")
130 endif()
131 if(${CMAKE_CXX_COMPILER_ID} MATCHES "Intel")
132 set(CMAKE_CXX_FLAGS_RELEASE "${CMAKE_CXX_FLAGS_RELEASE} -fopenmp")
133 set(CMAKE_CXX_FLAGS_DEBUG "${CMAKE_CXX_FLAGS_DEBUG} -fopenmp")
134 elseif(${CMAKE_CXX_COMPILER_ID} MATCHES "GNU")
135 set(CMAKE_CXX_FLAGS_RELEASE "${CMAKE_CXX_FLAGS_RELEASE} -fopenmp")
136 set(CMAKE_CXX_FLAGS_DEBUG "${CMAKE_CXX_FLAGS_DEBUG} -fopenmp")
137 else()
138 message(STATUS "C++ OpenMP compiler flag not known.")
139 endif()
140 endif()
141
142 if(TIGHT_FOCUSING AND NOT FFT_LIBRARY)
143 message(STATUS "No FFT library specified. Setting FFT library to 'none'.")
144 set(FFT_LIBRARY none CACHE STRING "Choose the FFT library." FORCE)
145 set_property(CACHE FFT_LIBRARY PROPERTY STRINGS "FFTW" "MKL" "None")
146 endif()
147
148 if(PER_SPECIES_WEIGHT)
149 message(STATUS "Option 'PER_SPECIES_WEIGHT' enabled")
150 add_definitions("-DPER_SPECIES_WEIGHT")
151 endif()

```

```

149 if (NO_TRACER_PARTICLES)
150 message(STATUS "Option 'NO_TRACER_PARTICLES' enabled")
151 add_definitions("-DNO_TRACER_PARTICLES")
152 endif()
153
154 if (NO_PARTICLE_PROBES)
155 message(STATUS "Option 'NO_PARTICLE_PROBES' enabled")
156 add_definitions("-DNO_PARTICLE_PROBES")
157 endif()
158
159 if (PARTICLE_SHAPE_TOPHAT)
160 message(STATUS "Option 'PARTICLE_SHAPE_TOPHAT' enabled")
161 add_definitions("-DPARTICLE_SHAPE_TOPHAT")
162 endif()
163
164 if (PARTICLE_SHAPE_BSPLINE3)
165 message(STATUS "Option 'PARTICLE_SHAPE_BSPLINE3' enabled")
166 add_definitions("-DPARTICLE_SHAPE_BSPLINE3")
167 endif()
168
169 if (PARTICLE_ID)
170 message(STATUS "Option 'PARTICLE_ID' enabled")
171 add_definitions("-DPARTICLE_ID")
172 endif()
173
174 if (PARTICLE_ID4)
175 message(STATUS "Option 'PARTICLE_ID4' enabled")
176 add_definitions("-DPARTICLE_ID4")
177 endif()
178
179 if (PARTICLE_COUNT_UPDATE)
180 message(STATUS "Option 'PARTICLE_COUNT_UPDATE' enabled")
181 add_definitions("-DPARTICLE_COUNT_UPDATE")
182 endif()
183
184 if (PHOTONS)
185 message(STATUS "Option 'PHOTONS' enabled")
186 add_definitions("-DPHOTONS")
187 endif()
188
189 if (TRIDENT_PHOTONS)
190 message(STATUS "Option 'TRIDENT_PHOTONS' enabled")
191 add_definitions("-DTRIDENT_PHOTONS")
192 endif()
193
194 if (PREFETCH)
195 message(STATUS "Option 'PREFETCH' enabled")
196 add_definitions("-DPREFETCH")
197 endif()
198
199 if (PARSER_DEBUG)
200 message(STATUS "Option 'PARSER_DEBUG' enabled")
201 add_definitions("-DPARSER_DEBUG")
202 endif()
203
204 if (PARTICLE_DEBUG)
205 message(STATUS "Option 'PARTICLE_DEBUG' enabled")
206 add_definitions("-DPARTICLE_DEBUG")
207 endif()
208
209 if (MPI_DEBUG)

```

```

211 message(STATUS "Option 'MPI_DEBUG' enabled")
212 add_definitions("-DMPI_DEBUG")
213 endif()
214
215 if(SIMPLIFY_DEBUG)
216 message(STATUS "Option 'SIMPLIFY_DEBUG' enabled")
217 add_definitions("-DSIMPLIFY_DEBUG")
218 endif()
219
220 if(NO_IO)
221 message(STATUS "Option 'NO_IO' enabled")
222 add_definitions("-DNO_IO")
223 endif()
224
225 if(COLLISIONS_TEST)
226 message(STATUS "Option 'COLLISIONS_TEST' enabled")
227 add_definitions("-DCOLLISIONS_TEST")
228 endif()
229
230 if(PER_PARTICLE_CHARGE_MASS)
231 message(STATUS "Option 'PER_PARTICLE_CHARGE_MASS' enabled")
232 add_definitions("-DPER_PARTICLE_CHARGE_MASS")
233 endif()
234
235 if(PARSER_CHECKING)
236 message(STATUS "Option 'PARSER_CHECKING' enabled")
237 add_definitions("-DPARSER_CHECKING")
238 endif()
239
240 if(USE_INSITU)
241 message(STATUS "Option 'USE_INSITU' enabled")
242 find_package(ParaView 5.2 REQUIRED COMPONENTS vtkPVPythonCatalyst)
243 include(${PARAVIEW_USE_FILE})
244 file(GLOB ADAPTOR ${CMAKE_SOURCE_DIR}/src/adaptor/*)
245 list(APPEND SOURCES ${ADAPTOR})
246 add_definitions("-DINSITU")
247 if(NOT PARAVIEW_USE_MPI)
248 message(SEND_ERROR "ParaView must be built with MPI enabled")
249 endif()
250 if(INSITU_DOUBLE_PREC)
251 message(STATUS "Option 'INSITU_DOUBLE_PREC' enabled")
252 add_definitions("-DINSITU_DOUBLE_PREC")
253 endif()
254 endif()
255
256 if(TIGHT_FOCUSING)
257 message(STATUS "Option 'TIGHT_FOCUSING' enabled")
258 file(GLOB FOCUSING ${CMAKE_SOURCE_DIR}/src/focusing/interface.f90)
259 list(APPEND SOURCES ${FOCUSING})
260 include_directories(${MPI_CXX_INCLUDE_PATH})
261 add_definitions("-DTIGHT_FOCUSING")
262 set(FOCUS_SRC
263 ${CMAKE_SOURCE_DIR}/src/focusing/main.cpp
264 ${CMAKE_SOURCE_DIR}/src/focusing/domain_param.cpp
265 ${CMAKE_SOURCE_DIR}/src/focusing/laser_param.cpp
266 ${CMAKE_SOURCE_DIR}/src/focusing/global.cpp
267 ${CMAKE_SOURCE_DIR}/src/focusing/laser_bcs.cpp
268 )
269 include_directories(${CMAKE_SOURCE_DIR}/src/focusing/inc)
270 if(${FFT_LIBRARY} MATCHES "FFTW")
271 if(OPENMP)
272 message(SEND_ERROR "Multi-threaded FFTW routines are not supported. Disable OpenMP.")

```

```

273 endif()
274 message(STATUS "FFT library: FFTW")
275 message(STATUS "Option 'USE_FFTW' enabled")
276 add_definitions("-DUSE_FFTW")
277 find_package(FFTW REQUIRED)
278 include_directories(${FFTW_INCLUDES})
279 endif()
280 if(${FFT_LIBRARY} MATCHES "MKL")
281 if(NOT ${CMAKE_CXX_COMPILER_ID} MATCHES "Intel")
282 message(SEND_ERROR "MKL library can be used only with Intel compilers")
283 endif()
284 message(STATUS "FFT library: MKL")
285 message(STATUS "Option 'USE_MKL' enabled")
286 add_definitions("-DUSE_MKL")
287 set(CMAKE_CXX_FLAGS_RELEASE "${CMAKE_CXX_FLAGS_RELEASE} -mkl")
288 set(CMAKE_CXX_FLAGS_DEBUG "${CMAKE_CXX_FLAGS_DEBUG} -mkl")
289 set(CMAKE_Fortran_FLAGS_RELEASE "${CMAKE_Fortran_FLAGS_RELEASE} -mkl")
290 set(CMAKE_Fortran_FLAGS_DEBUG "${CMAKE_Fortran_FLAGS_DEBUG} -mkl")
291 endif()
292 if(${FFT_LIBRARY} MATCHES "None")
293 message(STATUS "FFT library: None")
294 endif()
295 add_library(focus ${FOCUS_SRC})
296 if(${FFT_LIBRARY} MATCHES "FFTW")
297 #if(OPENMP)
298 # target_link_libraries(focus LINK_PUBLIC ${FFTW_LIBRARIES} ${FFTW_LIBRARIES_OMP})
299 #else()
300 target_link_libraries(focus LINK_PUBLIC ${FFTW_LIBRARIES})
301 #endif()
302 endif()
303 set_target_properties(focus PROPERTIES LINKER_LANGUAGE CXX)
304 endif()
305
306 add_executable(epoch2d ${SOURCES})
307 target_link_libraries(epoch2d LINK_PRIVATE ${MPI_Fortran_LIBRARIES} ${SDF_Fortran_LIBRARIES})
308 if(USE_INSITU)
309 target_link_libraries(epoch2d LINK_PRIVATE vtkPVPythonCatalyst vtkParallelMPI)
310 endif()
311 if(TIGHT_FOCUSING)
312 target_link_libraries(epoch2d LINK_PRIVATE ${MPI_CXX_LIBRARIES} focus)
313 endif()
314 set_target_properties(epoch2d PROPERTIES LINKER_LANGUAGE Fortran)

```

# Appendix C

## CD content

All the stuff created during the work. Nothing more, nothing less. Enjoy.

directory/file	specification
master_thesis/	directory containing this document and all related sources
epoch/	directory containing EPOCH source code (cloned on 15-04-2017)
scripts/	directory containing scripts intended for post-processing of simulation data