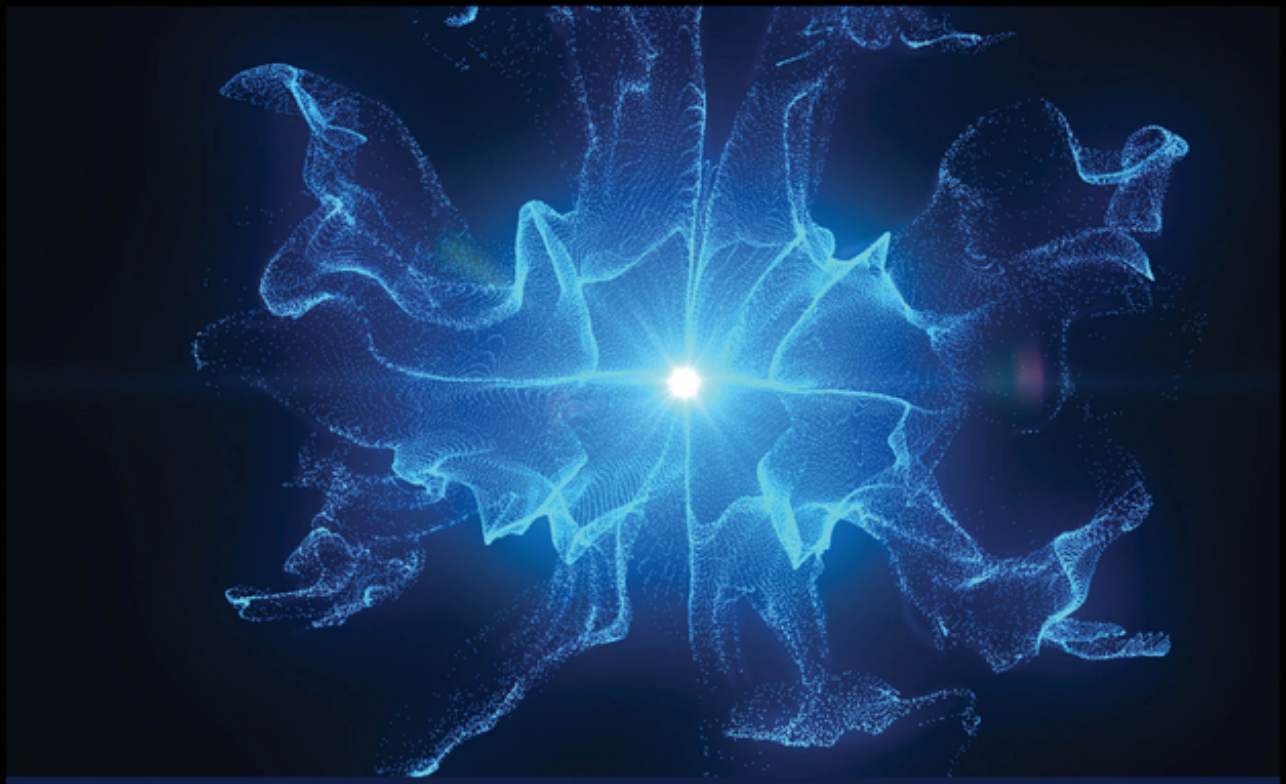

GEOFFREY J. PERT

MODELLING AND SIMULATION IN PLASMA PHYSICS FOR PHYSICISTS AND MATHEMATICIANS

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Modelling and Simulation in Plasma Physics for Physicists and Mathematicians

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Preface

This volume is the fruit of a career embracing the development of computational modelling from the 1960s to the present, mainly involving plasma physics. The author has been active as both user and developer of sophisticated computer models for plasma over the past 50 years, starting in the late 1960s. This book is intended as a continuation of our earlier study of the fundamental principles underlying the present understanding of the physics of plasmas and ionised gases in laboratory environments. The author started to study plasma using computational models over 50 years ago and has maintained an activity at the forefront of the field.

The theoretical development of the behaviour of such systems involves complex sets of equations whose calculation is beyond current analytic methods. As a consequence, the theory has increasingly relied on computational modelling methods. These generally involve complex programmes with many interacting elements. The development of these codes has relied heavily on some standard procedures, whose foundations were developed in the early days of computational techniques by pioneers such as von Neumann, Richtmyer, Metropolis and Harlow principally at Los Alamos. Building on these methods has resulted in effective methods for solving the partial differential equations involved in studying the dynamics of plasmas, such as computational fluid dynamics, Monte-Carlo, finite-difference methods. In this text, we review these methods applied to the multiple problems involved in solving the behaviour of plasma systems.

At low densities, typical of most terrestrial plasma, the space charge field between the positively charged ions and negatively charged electrons is sufficiently strong at quite small separations that the two ionic species are 'tied' together, and the plasma behaves as a single fluid. In this case, the fluid has the particularly simple equation of state of a monatomic polytropic gas, with polytropic index $\gamma = 5/3$. In the absence of external magnetic fields, and when the ion and electron densities and temperatures are equal, the plasma dynamics may be treated as a standard gas by the well-established routines of compressible gas dynamics. The early sections see Chapter 1 of this book are therefore devoted to a review of the development of computational gas dynamics. The distinctive application to magneto-hydrodynamics is considered later. We note however that energy transfer and consequent equilibration is much slower between electrons and heavy particles and that consequently the energy balance of each particle must be treated separately.

The modelling described above is known as the *continuum approximation*, which yields a method of sampling the pseudo-distribution function of the computed plasma. The output is the local thermodynamic state and fluid mean velocity.

Alternatively, we may sample the spatial and temporal velocity of a representative group of particles by calculating the dynamics of a group and the electromagnetic fields associated with them. Such an approach is known as a *particle method*, of which particle-in-cell is the most important.

The development of small, inexpensive yet powerful personal computers and laptops has allowed modelling simulations of complex interactive systems at a scale that a decade ago required the use of large multi-processor vector and parallel processing computer machines. Correspondingly, the expected accuracy, number and complexity of different elements treated in a single computer run have greatly increased. The laboratory facilities and manpower required to run such codes have increased and the costs correspondingly have grown markedly. Thus, we have the situation where we can perform the most accurate calculations which can be compared directly with experiment but at a high price and as a result, only at a limited number of facilities. Alternatively, we can relax the accuracy and perform representative calculations using desktop computers. The enormous increase in CPU power and memory has allowed the most complex calculations that were possible in the 1960s and 1970s to be performed on top-of-the-range desktop and laptop machines. As a consequence, many of the routines developed in the earliest days of computational physics can now be used as the foundation for practical desktop calculations. A very useful reference for these programmes is the set of annual texts 'Methods in Computational Physics'.[1] It is this latter requirement that this book will address. We will not consider the most sophisticated models or the construction of an accurate picture, but only the elements which tied together enable us to easily run and manipulate programmes, thereby allowing us to quickly identify the basic scaling of potential plasma configurations, i.e. as a design tool.

Like many aspects of kinetic physics, there are simplifications that make theoretical studies tractable, for example the markedly different time scales in the Bogobuliev treatment of gas kinetic theory and the Chapman–Enskog approximation in gas transport theory (§4.5 4.11). In this case, it is the different scales relative to the Debye length, where scale lengths are short compared to the Debye length or plasma frequency.

It is a requirement for the existence of the electric field cancellation associated with the Debye length that the plasma be dilute, i.e. the number of electrons contained within the Debye sphere is large. This requirement ensures that the electron distribution in the neighbourhood of any charge imbalance is Maxwellian. The Debye length is then the distance over which the field exists given by

$$\lambda_D = \sqrt{\frac{\epsilon_0 k T}{n_e e^2}} \tag{1}$$

We define a number of parameters which characterise the condition of the plasma from the Debye length.

- The Debye parameter is defined by

$$N_d = \frac{4\pi}{3} n_e \lambda_D^3$$

1 Methods in Computational Physics, edited by B. Alder, S. Fernbach and M. Rotenberg: published by Academic Press, New York, 1963–1977.

- The plasma or Spitzer parameter by

$$\Lambda = 4\pi n_e \lambda_D^3 = 3N_D$$

  The Spitzer parameter plays an important role as the cut-off for long-range weak collisions. It differentiates between the effects of single strong collisions and weak multiple ones – weak multiple collisions being $\ln \Lambda$ times more effective than strong.
- Characteristic times are defined by the plasma frequency

$$\omega_p = \sqrt{\frac{n_e e^2}{\epsilon_0 m_e}}$$

  The plasma frequency and the Debye length are related by $\Lambda_D \, \omega_p = \overline{v}_e$ an average electron velocity.

Laboratory plasma physics in almost all experimental configurations involves dilute plasma with a relatively large plasma parameter ($\ln \Lambda \gtrapprox 10$) whose values greatly limit the range of practical computational complexity. Values outside this range tend to be limited to astronomical plasma.

The short Debye length in experimental situations has another important effect, namely since electric fields are screened out by the electron mobility it follows from Poisson's equation that the space charge $\sigma \approx 0$, i.e. that the plasma is quasi-neutral. This has a very important consequence on the plasma dynamics, namely the plasma behaves as a single fluid, with the electrons and ion tied together by their mutual electric field. We may therefore treat the simulation of the plasma using a single fluid model with two separate energy relations if the electron and ion temperatures are unequal. We will therefore examine in detail the computer models for fluid simulation.

The quasi-neutral behaviour of the plasma results in the density of ions and electrons being equal. However, it does not prevent the mobile electrons from carrying current and generating magnetic fields, behaviours taken into account in the magneto-hydrodynamics relationships.

It follows from the small value of the Debye length that the plasma (or Spitzer) parameter is small. Consequently, the fraction of weak multi-particle collisions compared to strong single interactions is small. This result ensures the effectiveness of multiple weak particle interactions in cell models, where the interaction occurs via the self-generated fields rather than direct collisions.

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I am grateful to several people who have contributed to the work reported in this book:

Firstly, my many graduate students and research fellows who have acted as 'guinea pigs' for many of the methods and routines described;
Secondly, my editorial team at Wiley who saved the day when my health failed;
Finally, my colleague and friend Prof G. J. Tallents for enabling me to maintain a continued interaction with the real world of experimental physics.

Preamble

Plasma is defined as a conducting fluid. As such, it is an extensive state of matter within the universe, generally consisting of a fully ionised gas. It is found in many situations both cosmically and terrestrially. In this work, we will be principally concerned with only terrestrial applications, related to controlled fusion research. This encompasses magnetically and inertially confined plasma, together with magnetospheric and applied (engineering) applications.

Experimental studies of plasma in these regimes involves large and complex apparatus, such as tokamaks and high-power lasers. As a result, theoretical studies play an important role. Again, since the plasma is a material state with a large number of degrees of freedom, theoretical study generally falls into one of two methodologies:

1) **Analytic studies**: These are relatively simple models which can be described by a limited number of parameters and involve a restricted number of coupled equations. They generally describe fundamental activity within the plasma, for example Landau damping.
2) **Computer simulation**: These are more complex models attempting to give an accurate picture of the behaviour of plasma in an experimental environment. The large number of coupled equations demands the application of substantial computer power and storage. Originally this required top-of-the-range machines, but increasingly simple desktop personal computers have had sufficient power to perform substantial realistic simulations. A major advance has been the development of parallel processing systems, essentially a series of coupled PCs operating simultaneously in parallel.

The nature of the theoretical model is determined by the environment in which it is applied. This is characterised by the scale of the system ℓ with respect to the Debye length λ_D. Again the models fall into one of two classes:

1) Debye length small ($\ell \gg \lambda_D$). In this case, the inter-particle electrostatic forces dominate the motion of the charged particles, whose overall motion is, in turn, dominated by their mutual coupling. This is the region of collective motions characterised by plasma waves. In the context of plasma theory, it is a regime of individual single-particle motion generally known as *particle-in-cell*. At this level of approximation, the self-consistent inter-particle fields are treated directly through Maxwell's equations.
   This level of approximation corresponds to dilute plasma where the plasma parameter (namely the ratio of the Debye length to electron mean separation) and is the normal plasma state [see (Pert 2021; §1.3.2)].

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2) Debye length large ($\ell \ll \lambda_D$). The space charge fields established by even a relatively small, spatial charge separation are so large that no space charge density can exist ($\sigma \approx 0$). The negative electrons and positive ions therefore tend to move as a single unit with mass approximately equal to the ion mass ($m \sim m_i$), i.e. the plasma dynamics are that of a single fluid. In this regime, the plasma is described by standard fluid mechanics, and the simulation follows the methods of computational physics fluid dynamics (CFD).
   Under this level of approximation, the basic equations are supplemented by two further conditions.
   a) If the characteristic time scale of the plasma development is long compared to the mean free time (ion/electron collision time), the heavy particles (ions) and electrons are in thermal equilibrium. The particle energy is equilibrated and the energy is calculated by a single first law of thermodynamics relation – *single fluid model*.
   b) On the other hand, if equilibration is slow, the energy relation for the heavy particles and ions must be calculated separately with an equalisation term between the two – *two fluid model*.
      Finally, if there are magnetic fields produced by plasma currents or by external fields or pressure gradients, transport coefficients and energy relations are modified. The magnetic fields can be calculated from the Faraday and Biot–Savart laws. When magnetic fields are important, the *magneto-hydrodynamic approximation* (MHD) may be valid.

By the early 1960s, the basic equations describing the motion of plasma had been well established and it was clear that in the fluid regime, plasma acted as a continuum and could be described by modified fluid dynamics equations. Under these conditions, computational methods based on CFD were appropriate. By the end of the 1960s to the early 1970s these were well established.

On the other hand, in the particle regime, the dynamic equations of motion are simply established based on Newton's laws of motion and Maxwell's laws of electromagnetism. The scale of modelling was however limited by the speed and storage of the basic computer.

The development of small, inexpensive yet powerful personal computers and laptops has allowed modelling simulations of complex interactive systems at a scale that a decade ago required the use of large multi-processor vector and parallel processing computer machines. Correspondingly, the accuracy, number and complexity of different elements treated in a single computer run have greatly increased. The laboratory facilities and manpower required to run such machines have increased and the costs correspondingly have grown markedly. Thus, we have the situation where we can perform the most accurate calculations which can be compared directly with experiment but at a high price and as a result only at a limited number of facilities. Alternatively, we can relax the accuracy and perform representative calculations using desktop computers. The enormous increase in CPU power and memory has allowed the most complex calculations that were possible in the 1960s and 1970s to be performed on top-of-the-range desktop and laptop machines. As a consequence, many of the routines developed in the earliest days of computational physics can now be used as the foundation for practical desktop calculations. A very useful reference for these programmes is the set of annual texts 'Methods in Computational Physics'.[1] It is this latter requirement that this book will address. We will not consider the

1 Alder, Fernbach and Rotenberg (1963–1977).

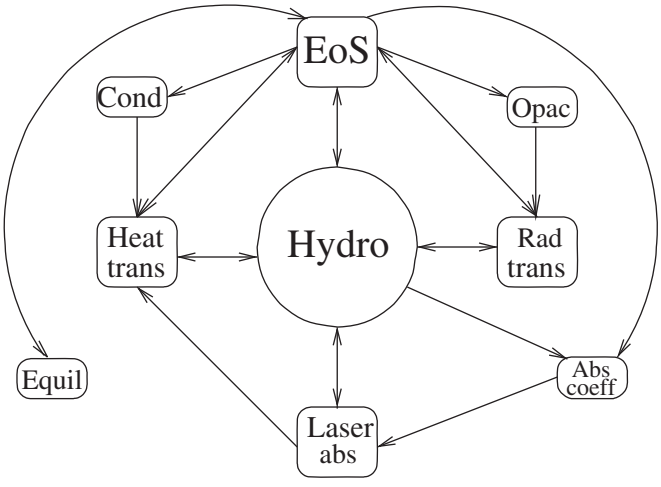

Figure I Sketch to illustrate the key interactions in the simulation of a laser–plasma interaction indicating how different physical processes interact.

most sophisticated models, which generally require a high-end parallel machine for the construction of an accurate picture, but only the elements which tied together enable us to easily run and manipulate programmes, thereby allowing us to quickly identify the basic scaling of potential plasma configurations i.e. as a design tool. As a particular case, it is convenient to imagine the plasma formed by the interaction of a powerful laser beam with a solid target (see Pert, 2013). Many of the elements and the interactions involved in such a model are identified schematically in Figure I.

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Part I

Continuum Methods

1

Foundations of Computational Fluid Mechanics

1.1 Basic Concepts of Fluid Mechanics

Computational fluid dynamics attempts to solve the dynamical structures of systems within the fluid approximation, namely when the behaviour of the fluid is dominated by collisions between the constituent molecules. This implies that the mean free path is everywhere smaller than the characteristic dimensions of the problem, and that the mean collision interval short compared to the characteristic time so that the system may be treated as a continuum and individual molecular motions are treated by averaging. These averaging techniques may be applied to plasma when the Debye length is small and the averaging leads to the magneto-hydrodynamic (MHD) approximation (Pert, 2021). The derivation and validity of the dynamical MHD equations are developed in Pert (2021). Only plasma within the MHD approximation will be treated here. The collision-free model of plasma are fully treated in Section 8.1 and in more detail by Birdsall and Langdon (1991) and Hockney and Eastwood (1988).

The key underlying equation of motion in the MHD equations are those of compressible fluid mechanics: MHD requiring the introduction of additional effects. Making use of the concept of time splitting discussed earlier these additional behaviours may be treated by separate additional routines. The key fluid routines thus form a basic core to which additional physics is tied. It is therefore appropriate to examine with some care the treatment of the compressible fluid initially and subsequently the additional terms.

Compressible fluid is described by its thermodynamic state and by the velocity of flow. These values must be specified at each point within the flow field. The thermodynamic state is specified by two state variables (e.g. pressure p and density ρ), the remainder being then known from the equation of state. The velocity is defined by the three-vector components v. There are thus five independent quantities, which vary in space $\mathbf{r}$ and time t, and must be determined subject to the constraints on the system. The equations of fluid mechanics contain five equations, which are simply the basic conservation laws of physics applied to moving fluid, whose derivation is well known (Pert, 2013).

Typical problems investigated using these basic fluid techniques include aerodynamics (e.g. aeronautical design or car design), meteorology, oceanography and plasma dynamics.

Let us now examine the characteristic structure of compressible fluid mechanics which, as we shall see, are hyperbolic in form, which leads to problems in formulating numerical approximations.

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1.2 The Basic Equations of Fluid Mechanics

1.2.1 Eulerian Frame

The simplest co-ordinate system, and in many cases the simplest, in which to define the flow of fluid is the stationary one which is relative to the laboratory, known as the Eulerian frame.

In the laboratory (or Eulerian) frame, the general equations of fluid mechanics can be written in several forms, of which the general conservation form is most appropriate for a general discussion (Pert, 2013). In Cartesian tensor form, these are:

$$\frac{\partial}{\partial t}\left[\rho\right] + \frac{\partial}{\partial x_j}\left(\rho v_j\right) = 0 \tag{1.1a}$$

$$\frac{\partial}{\partial t}\left[\rho v_i\right] - \frac{\partial}{\partial x_j}\pi_{ij} = 0 \tag{1.1b}$$

$$\frac{\partial}{\partial t}\left[\rho\left(\epsilon + \frac{1}{2}v^2\right)\right] + \frac{\partial}{\partial x_j}\left[\rho v_j\left(h + \frac{1}{2}v^2\right)\right] + \frac{\partial}{\partial x_j}q_j = 0 \tag{1.1c}$$

where ϵ is the specific internal energy of the fluid, $h = \epsilon + p/\rho$ the specific enthalpy and $\mathbf{q}$ the heat flux vector. $\boldsymbol{\pi}$ is the momentum flux tensor

$$\pi_{i,j} = \rho\, \mathrm{v}_i\, \mathrm{v}_j - \tau_{i,j} \tag{1.2}$$

$\tau_{i,j}$ is the total stress tensor

$$\tau_{i,j} = \sigma_{i,j} - p\,\delta_{i,j} \tag{1.3}$$

where σ_{ij} is the viscous stress tensor and $\delta_{i,j}$ the Kronecker delta (1 if $i = j$ and 0 otherwise).

The heat flow vector may be written in terms of the temperature T gradient and the thermal conductivity (κ)

$$\mathbf{q} = \kappa \nabla T \tag{1.4}$$

The temperature is determined from the equation of state in the form $T(\rho, \epsilon)$.

In the laboratory (or Eulerian) frame, the general equations of fluid mechanics can be written in several forms, of which the general conservation form is most appropriate for a general discussion (Pert, 2013).

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) && = 0 \\
&\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot \underline{\boldsymbol{\pi}} && = 0 \\
&\frac{\partial}{\partial t}\left[\rho\left(\epsilon + \frac{1}{2}\mathrm{v}^2\right)\right] + \nabla \cdot \left[\rho \mathbf{v}\left(h + \frac{1}{2}\mathrm{v}^2\right)\right] + \nabla \cdot \mathbf{q} && = 0
\end{aligned} \tag{1.5}$$

where ϵ is the specific internal energy of the fluid, $h = \epsilon + p/\rho$ the specific enthalpy, and q_i the heat flux vector. π_{ij} is the momentum flux tensor

$$\pi_{i,j} = \rho\, \mathrm{v}_i\, \mathrm{v}_j - \tau_{i,j} \tag{1.6}$$

$\tau_{i,j}$ is the total stress tensor

$$\tau_{i,j} = \sigma_{i,j} - p\,\delta_{i,j} \tag{1.7}$$