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Numerical Solutions to Problems in Physics from Model to Model

Hierarchy of models

Models are the cornerstone of any scientific discipline not relying strictly on logic. In physics the present understanding of the world around us is based on a mosaic of models. Some models try to answer basic questions such as what are the governing forces of nature (e. g. general relativity [3]), or what are the building blocks of matter (e.g. the prediction of anti-particles [2]). From the fundamental models many more models are derived. These secondary models are often simplifications to the original models made by imposing additional assumptions (e. g. Newton's laws can be viewed as a simplification of general relativity). Models of this type are potentially well suited for describing smaller sub-sets of problems. A third category consists of models which rely more strongly on observations and where the connection to the underlying physical laws is more uncertain. These descriptive models often represent a first step towards a more fundamental understanding of the problems studied (e. g. stellar evolution models based on the Hertzsprung-Russel diagram [5]). All three classes of models are physical models whose primary task is to provide qualitative understanding of nature.

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Having a mathematical formulation of a physical model, we can hope to get quantitative information about processes in nature. Often mathematical models are an integral part of the corresponding physical models. Others are derived through strict manipulation of equations resulting in models which are not so easily tied to physical interpretations. Starting with observations, some mathematical models are established by simple functional fits to data. To be able to make predictions on the basis of a mathematical model, we usually have to solve a set of equations that describes the relation between relevant quantities. In some cases, it is both feasible and useful to solve the equations analytically. However, often the solutions to these equations can be so complicated that solving the equations numerically is the only option. For this we will need a third class of models, namely numerical models. Just as the mathematical models rely on the physical models, the numerical models rely on the mathematical models.

From an analytical to a numerical model

The main issue when designing a numerical model based on a mathematical or more precisely an analytical model, is often how descriptions based on continuous variables can be replaced by descriptions based on discrete variables. Assuming we restrict our attention to problems described by a temporal coordinate and a generalized spatial coordinate, we have to choose a method for discretizing time and space. Furthermore, we need to look at how the mathematical operations can be performed on a computer. This can be particularly challenging when dealing with quantities which can become arbitrarily large or which are stochastic. It is important to know what additional assumptions have been applied in order to construct the numerical model and to have a thorough understanding of how the solutions from the numerical model might differ from those of the corresponding analytical model as a result of these assumptions.

A solution at time *t0* can only influence the solution obtained at time *t1* if *t0* is less than *t1*. It is therefore a common approach to solve for time variations somewhat differently than space variations. Information on variation in space is generally stored by a large set of calculation points that cover the spatial domain. In contrast, information on variation in time is typically stored only for a few points in time. In solving for spatial changes, one of two different approaches is common:

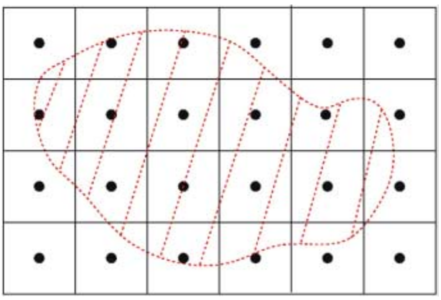

Figure 1. Illustration of the grid solver approach where the filled circles indicate calculation points, the red curve represents an isolated body of material.

(i) Grid solvers discretize space independently of whether the simulated regions contain any mass or not. A solver of this type must keep track of any material entering or leaving each grid cell (see Figure 1). Accurate estimates of higher order derivatives can be made[1]. Properties such as stability and accuracy of a particular solver are relatively easy to determine. Techniques for incorporating various boundary conditions are also well known. And in general, many different grid methods are available that have been developed and refined for decades.

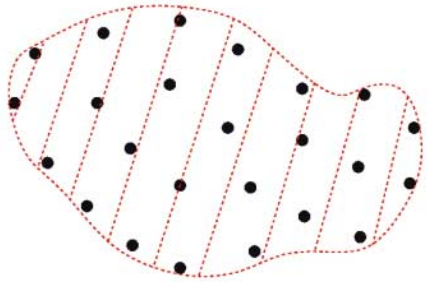

Figure 2. Illustration of the particle solver approach where the filled circles indicate calculation points ("particles"), red curve represents an isolated body of material.

(ii) Particle solvers discretize the material and neglect areas of vacuum. A solver of this type keeps track of how mass moves around by discretizing the material itself (see Figure 2). It is therefore well suited for describing complicated material flow (called advection), possibly with free surfaces and complex interfaces. Solvers of this kind use a more intuitive approach since we humans are more used to relating to the material that occupies space rather then space itself. Extensions to higher dimensional descriptions are easily facilitated with the particle approach.

Example: Plasma simulations of meteor ionization

In order to illustrate strengths and weaknesses of the grid and particle solver approach, we will take a look at a simulation of the interaction between the upper atmosphere and a 1m-sized meteor entering the atmosphere at a speed of roughly 40 km/s. In the interaction, atoms boiling off the surface of the meteor collide with the atmospheric gas causing originally neutral atoms to be split into negatively charged electrons and positively charged ions, creating what is known as a plasma around the meteor [4]. The plasma can generate electromagnetic waves, in addition to sound waves which can be generated by neutral gases as well. The simulation focuses on the plasma generated around the meteor, while the neutral particles in the atmosphere are assumed to originate

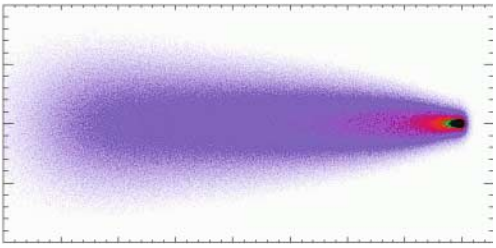

Figure 3. The density profile of the plasma generated around the meteor (Colours in decreasing density order: Black, green, red, purple, and white). The plotted frame has been rotated so that the meteor moves horizontally relative to the frame.

from a uniform, equilibrium background population. Figure 3 illustrates the plasma density profile in a two-dimensional simulation of the meteor. The plasma is generated close to the meteor head but subsequently spread out by elastic collision with the neutral background and by the electric forces.

The plasma density is only non-negligible in a fairly narrow field trailing the meteor head. Also, the generalized spatial coordinates in this simulation are a combination of the physical space coordinates and the velocity coordinates[2]. Free surfaces are therefore important features of this problem. Also, it is crucial to have an accurate treatment of advection. This points towards using particle solvers. However, the electric field generated by the plasma will extend into regions where the plasma density in practice is zero. Furthermore, to calculate the electric field, higher order derivatives must be calculated. This indicates that grid solvers are better suited for the problem. The current numerical model (known as Particle-In-Cell) combines grid and particle solvers [1]. The former approach describes the plasma itself and the advection of plasma. The latter approach describes the electric field resulting from the ever changing distribution of material. The coupling between the two approaches is done by projecting the particles onto a grid, thus achieving a hybrid description that takes advantage of both approaches.

Notes

1 As an example, the time derivative of a function f is in itself a function that describes how f varies in time. The second order derivative of f, correspondingly describes how the derivative of f varies in time.

2 This is known as a kinetic description where velocity is treated as an independent variable that cannot be expressed as a function of the physical space coordinates and time. This description takes into account that at any point in space and time, particles with widely different velocities can be found.

References

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