

# Chapter 17

## Numerical Methods for Astrophysics

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### Chapter Outline

<b>1 Introduction</b>	<b>466</b>	4.1 Finite Difference Methods	469
<b>2 Astrophysical Scales for Astrophysical Phenomena</b>	<b>466</b>	4.2 Finite Volume Methods	470
2.1 Spatial Scales	466	4.3 Discontinuous Galerkin Method	471
2.2 Density and Temporal Scales	466	4.4 N-Body Method	472
<b>3 Equations Used in Astrophysical Modelling</b>	<b>467</b>	4.5 Grid-Free Method: Smoothed Particle Hydrodynamics	472
3.1 Source Terms	468	<b>5 High-Performance Computing</b>	<b>473</b>
3.2 Additional Force Terms	468	<b>6 Astrophysical Codes</b>	<b>473</b>
3.3 Equation of State	469	<b>7 Conclusion</b>	<b>475</b>
<b>4 Numerical Methods</b>	<b>469</b>	<b>Acknowledgement</b>	<b>475</b>
		<b>References</b>	<b>475</b>

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### ABSTRACT

The physical laws astrophysicists use to describe their phenomena are believed to have been understood in many cases. Thus modelling astrophysical phenomena is focussed on the numerical implementation of these models. The main issue astrophysicists have to overcome is the large range of spatial, temporal and density scales.

The models typically are the compressible inviscid Euler equations or magnetohydrodynamic equations in three space dimensions coupled with many source terms. The numerical methods used often are finite volume methods or particle methods. Numerical methods that deal with the large range of scales need to be addressed individually for each problem at hand. Examples of these methods are the introduction of subgrid scale models, using time implicit methods or moving mesh methods.

These notes are strongly indebted to discussions with Fritz Röpke from Heidelberg University and the Heidelberg Institute of Technological Science, <http://www.h-its.org/en/research/ps0/people/>.

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## 1 INTRODUCTION

Astrophysicists describe phenomena whose underlying physical laws they usually believe to have well understood. The objects they describe typically have a huge range of spatial and temporal and density scales. In addition, in these objects many physical mechanisms interact with each other in a nonlinear way.

Different from engineering the astrophysical objects are out of reach for direct experiments. All one usually has are observational data collected by observing the electromagnetic spectrum. The limitations of this can be seen by the example of a star, where direct observation of the physical processes inside the star are not possible.

This gives computations a special role in astrophysics. It takes the place of experiments in engineering by being able to study models with varying parameters. This requires the numerical solution of complex systems of nonlinear partial differential equations with complicated source terms.

## 2 ASTROPHYSICAL SCALES FOR ASTROPHYSICAL PHENOMENA

### 2.1 Spatial Scales

Let us first consider the vastly varying length scales in astrophysics (Fig. 1). Spatial scales of interest cover 27 orders of magnitude. Beginning with the size of a flame front inside an exploding supernova, which is of the size of centimetres, and moving next to the size of stars ( $10^{11}$  cm), and on to a solar system. Next in size consider the distance between solar systems (say  $10^{17}$  cm), where the interstellar medium is. The size of a galaxy, which contains roughly  $10^9$  solar systems, is about  $10^{23}$  cm. We continue on to the distance between galaxies ( $10^{24}$  cm), in between galaxies is the so-called intergalactic medium. Galaxies cluster in groups, say of size  $10^{25}$  cm. Clusters of galaxies are combined in superclusters ( $10^{27}$  cm). These are all part of the observable universe.

### 2.2 Density and Temporal Scales

In addition there are vastly varying density scales at which the physical processes take place. The intergalactic medium has a density of  $10^{-28}$  g cm<sup>-3</sup>, sun-type stars may have densities like 1 g cm<sup>-3</sup>, and neutron stars have densities like  $10^{14}$  g cm<sup>-3</sup>. This covers a range of 40 orders of magnitude, again illustrating the huge challenges this has for computations.

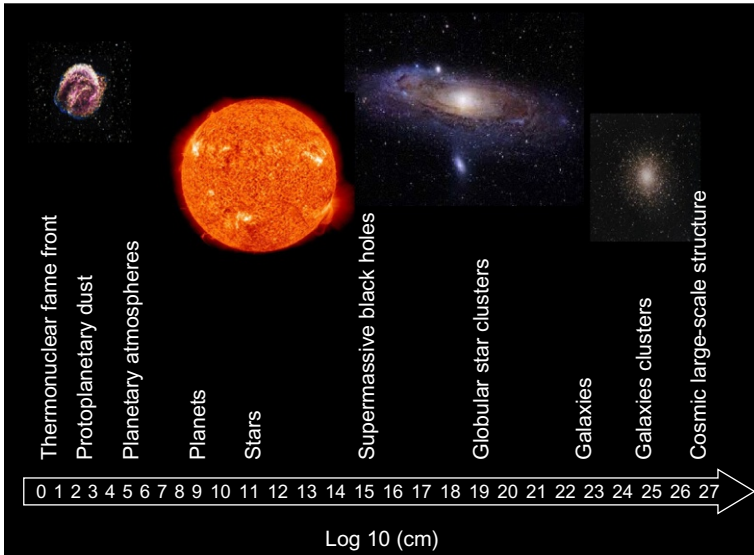


FIG. 1 Astrophysical length scales may vary vastly.

Temporal scales in astrophysics may vary about 20 orders of magnitude, from milliseconds to giga years.

For an individual object that gets studied the ranges of relevant scales for individual objects are narrower but still are very challenging.

### 3 EQUATIONS USED IN ASTROPHYSICAL MODELLING

Phenomena like the interstellar medium (ISM) seem predestined to be modelled microscopically. From a terrestrial point of view the ISM consists of the best vacuum a man made machine can produce, where individual molecules are separated by centimetres. One could be tempted to use Newton's law for each particle and plus a rule for their interaction. The problem is that in the expanse of the interstellar medium these would be so many particles that it is not feasible to follow them with a computer now and in the foreseeable future.

Thus one is forced to move from a microscopic level of description to a mesoscopic level of description, which will give rise to Boltzmann-type models. For certain regimes such models are actually used. Examples are the detailed modelling of the acceleration of cosmic rays at the shock fronts on remnants of supernovae explosions (Drury, 1983).

In other regimes the models are macroscopic fluid equations. These typically are balance laws based on the principles of conservation of mass, momentum and energy, see Eqs. (1)–(3).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad (1)$$

$$\frac{\partial(\rho v)}{\partial t} + \nabla \cdot \rho v v^T + \nabla p = 0 \quad (2)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (v(E+p)) = 0 \quad (3)$$

Here  $\rho$  is the density,  $v$  the velocity,  $p$  the pressure and  $E$  the total energy. These equations are supplemented by a relation between the pressure and the other dependent variables, see [Section 3.3](#). These are inviscid models, because the scale of the physical viscosity may easily be 20 orders of magnitude below the typically discretisation scale, and thus are impossible to resolve numerically.

In summary the mathematical models in astrophysics are typically partial differential equations. They may be Boltzmann-type equations, say in models where the evolution of the universe (that are solely based on the evolution of dark matter) is described. The mathematical models can also be macroscopic fluid dynamics equations, an example of which are systems of compressible inviscid flow equations describing the conservation of mass, balance of momentum and total energy.

Next we shall list examples of additional physical phenomena that at times need to be incorporated into these equations.

### 3.1 Source Terms

The balance of momentum and energy in some situations needs to be supplemented by source terms. Examples of these are chemical reactions, radiation and diffusion which may be anisotropic. Chemical reaction networks are very elaborate, and typically take place on different time scales than transport, they may, for example, take much longer. Energy transfer via radiation can be very important and may be numerically quite time consuming given all directions of the radiation and all its frequencies.

### 3.2 Additional Force Terms

The balance laws may be supplemented by forcing terms. One example is gravity. In the universe gravity plays a most important role, so there are instances where it needs to be modelled. Gravity is a phenomenon which influences the evolution everywhere. On smaller spatial scales and not such long temporal scales it is given by a fixed function. In general gravity is time and space dependent, and thus needs to be determined by separate equations. This equation typically lacks finite speed of propagation and this leads to additional numerical challenges.

The equations of reactive fluid dynamics with gravity are given in (4)–(7).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad (4)$$

$$\frac{\partial(\rho X_i)}{\partial t} + \nabla \cdot (\rho X_i v) = -\rho \omega_{X_i} \quad i = 1 \dots N - 1 \quad (5)$$

$$\frac{\partial(\rho v)}{\partial t} + \nabla \cdot \rho v v^T + \nabla p = -\rho \nabla \Phi \quad (6)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (v(E + p)) = \rho v \cdot \nabla \Phi + \rho S \quad (7)$$

Here  $\omega_{X_i}$  are the reaction rates,  $\Phi$  the gravitational potential, both are determined in separate systems of equations.  $S$  designates the energy transfer, again this may be given through a complicated mechanisms. Additional terms may be included to account for diffusion of energy, conduction or magnetic fields.

A force may occur because of the presence of magnetic fields that exerts a force on an ionized gas. This force may be given by Maxwell's equations, which acts as a space and time-dependent force term acting on the balance laws. Under some idealizing assumptions Maxwell's equations can be incorporated into the balance laws (Besse et al., 2004; Klingenberg et al., 2017). These PDE models may have degeneracies. An example is the fact that there are no magnetic monopoles, which leads under some idealizing assumptions to a divergence-free constraint on the magnetic field.

### 3.3 Equation of State

The macroscopic balance laws (1)–(3) or (4)–(7) need to have a closure relationship. This typically is given by an equation of state. In astrophysics these can be quite complicated. At times they only exist as tabulated values. This may leads to challenges in the numerical implementation. Often algorithms are needed that do not depend in an essential way on standard equations of state.

## 4 NUMERICAL METHODS

Of the many numerical methods used in astrophysics we shall mention only the one's in the following sections. Examples of additional methods are spectral methods and Monte Carlo methods. In the textbook (Bodenheimer et al., 2006) these methods are explained.

### 4.1 Finite Difference Methods

Let us write (1)–(3) in the form  $v_t + f(v)_x + g(v)_y + h(v)_z = 0$ . Approximate space by a Cartesian mesh, where we shall seek approximate values of the

solution at the mesh points. A spatial discretization via a finite difference method will be of the form

$$f(v(t_n, x_j)_x) \approx \frac{1}{\Delta x} \left( \hat{f}(t_n, x_{j+\frac{1}{2}}) - \hat{f}(t_n, x_{j-\frac{1}{2}}) \right), \quad (8)$$

where  $\hat{f}$  is a numerical flux of  $f$ . The other two flux functions  $g$  and  $h$  get treated the same way. On a Cartesian mesh such schemes are easy to code and are computationally efficient. This first-order treatment can be made into a higher order discretization by using the assumption that away from a shock the solution is smooth. One now adapts the stencil to this smooth region and thus avoids interpolation across the jump discontinuity. This then allows one to approximate the conservative flux difference to higher order. This is done in such a way that the numerical solution does not introduce additional oscillations near the discontinuity. These are called the ENO and WENO method, see [Shu \(2003\)](#). This needs to be coupled to a stable higher order Runge–Kutta time discretization, see [Gottlieb et al. \(2001\)](#). On a Cartesian mesh (or a smooth curve-linear mesh), where one does not need grid refinement, these are very efficient methods.

In an astrophysical context there is a huge range of density scales. Thus on one side of a shock there may be an extremely low density. It is essential that the numerical oscillations do not give rise to a negative density. Thus these schemes need to be implemented in a way such that they ensures that the numerical approximation of density and temperature is guaranteed to stay positive, see [Zhang and Shu \(2012\)](#) and [Perthame and Shu \(1996\)](#).

## 4.2 Finite Volume Methods

When discretizing the systems of the conservation laws (1)–(3) or (4)–(7) from the previous chapter, typically a grid-based method is used. The method of choice used in astrophysics is a finite volume method. For a quick introduction to this, the book by [LeVeque \(1992\)](#) is nice, even though it is 25-year old. In [LeVeque \(2002\)](#), LeVeque gives a more comprehensive treatment.

To describe this method, first consider one-dimensional flow. Here one updates the mean values of the conserved variables in the control volume given by the intervals of the discretization. For this one integrates the equations on a control volume in space and time and uses the divergence theorem for the flux. Thus the update is achieved by computing the fluxes of the conserved quantities across the cell boundaries. This is done by solving a Riemann problem for the equations. In other words the method at its core requires the numerical solution of Riemann problems, see the comprehensive book by [Toro \(2009\)](#).

This leads to a first-order method in one space dimension. A second-order extension is achieved by considering piecewise linear reconstruction in the interval of discretization instead of piecewise constants when updating cell averages.

This can be made into a higher order nonoscillatory method (WENO), see, e.g., [Shu \(2003\)](#). Again the same comment as in the previous section holds: positivity of density and temperature are of essence. For one techniques to implement this, see [Hu et al. \(2013\)](#). An important ingredient in this implementation is the positivity-preserving method of the underlying first-order method. It boils down to positivity of the Riemann solver. For the Euler equations this was achieved for many Riemann solvers, for the equations of ideal MHD an approximate Riemann solver was found in [Bouchut et al. \(2007, 2010\)](#) and [Klingenberg and Waagan \(2010\)](#) with this useful property. It was then implemented in the astrophysics code FLASH (see [Section 6](#)), turning out to be useful, see, e.g., [Waagan et al. \(2011\)](#) and [Hill et al. \(2012, 2013\)](#).

We comment that in astrophysics one tends to not consider discretizations beyond second order. The reason for not going beyond second order is the generally held belief in this community that for a finite volume method the increased computational complexity for higher order methods is computationally more expensive than using a finer grid for a second-order method. In addition the PDE models in astrophysics are believed to be an approximation to the physical phenomenon that may not warrant a more precise resolution. In recent attempts in [Schaal et al. \(2015\)](#) and [Bauer et al. \(2016\)](#), where a third-order method has been introduced based on a different numerical method (the discontinuous Galerkin method, see the following section), the efficiency of the method seems to point towards the potential usefulness of higher order methods in astrophysics.

The second-order finite volume method in one space dimension is then extended to three space dimensions by using dimensional splitting in case that one uses a Cartesian grid (which is typically done). For an unstructured three-dimensional grid, where the grid boundaries are planar, the finite volume method is used by updating cell averages using the fluxes across all the cell faces. Across each cell face one solves a one-dimensional Riemann problem in the normal direction.

One reason for the success of the finite volume method in astrophysics is that it has been typically used on a Cartesian grid combined with adaptive mesh refinement, where the mesh adapts dynamically in space and time. Early on the ideas of [Berger and Colella \(1989\)](#) caught hold and proved successful.

### 4.3 Discontinuous Galerkin Method

This is a method based in the weak formulation of the flow equations. The Galerkin approach approximates the infinite-dimensional function spaces in the weak formulation by finite-dimensional function spaces, say by polynomials. Space is discretized into cells that may form an unstructured grid. In the discontinuous Galerkin approach the polynomial approximation in neighbouring cells need not be continuous across cell boundaries. Conservation is maintained by computing the flux across cells with (an approximate) Riemann

solvers. For the explicit time discretization a Runge–Kutta method is typically used. For a nice survey of the method by C.-W. Shu the reader is referred to [Shu \(2014\)](#). This method can be made positivity-preserving thanks to [Zhang and Shu \(2010, 2012\)](#).

This method has the big advantage to be of any order of accuracy, the triangulation may be of arbitrary shape and the method is extremely local in its data communication, making it ideal for extremely parallel computer architectures.

This method is still rather new for computational astrophysicists. Because its potential has been in shown recently (see [Bauer et al., 2016](#); [Klingenberg et al., 2015](#); [Schaal et al., 2015](#)) we included it in this survey.

#### 4.4 N-Body Method

This refers to the classical problem of solving  $N$  bodies located at  $x_i$  with mass  $m_i$  that mutually attract themselves under Newtonian gravitation

$$\frac{d^2x_i}{dt^2} = -\sum_{j=1, j \neq i}^N \frac{Gm_j(x_i - x_j)}{|x_i - x_j|^3}.$$

These are used to model the evolution of star clusters with a large amount of stars. In another application by modifying the gravitational potential this may model dark matter by considering dark matter as a collisionless gas modelled as many small particles. For this problem the complexity of summing  $N^2$  particles is reduced to  $N \log N$  by taking account of particles far away in an approximate way. For details, see, e.g., [Springel \(2005\)](#).

#### 4.5 Grid-Free Method: Smoothed Particle Hydrodynamics

This method was originally devised by [Monaghan and Gingold \(1983\)](#). It is a Lagrangian method where one writes the equations of hydrodynamics in Lagrangian form. Then one collects the fluid in packets, called particles with a given mass. These then get moved in a way inspired by the N-body method. The equations of motion of the particles are

$$\frac{dx_i}{dt} = v_i \tag{9}$$

$$\frac{dv_i}{dt} = -\frac{1}{\rho_i} \nabla p_i \tag{10}$$

where  $\rho_i$  is the density,  $p_i$  assigned to each so-called fluid particle. The idea now is to represent the particles in a smoothed out form by convolving it with a compactly supported smooth kernel, see [Monaghan \(1982\)](#). The density, pressure and temperature at a point are then determined by summing over all particles that make contributions to this point. The spatial derivatives of



these quantities can then be determined by the derivatives of the smooth kernel due to integrating the convolution by parts.

These methods have proved quite popular in the numerical astrophysical community. Their advantage is that they run quite stable, their disadvantage is that they tend to smear out shocks quite a bit. A nice review by Dan Price can be found here ([Price, 2004](#)).

## 5 HIGH-PERFORMANCE COMPUTING

Astrophysicist make extensive use of supercomputers. Still their problems typically are so computationally expensive that even these huge computational resources need to be used in a most efficient manner.

These include

- Vector processing, where the same operations are applied to whole arrays.
- Parallelization, where many computations are performed simultaneously. Here one has to distinguish between a shared and distributed memory systems. In the former all processors access a common physical memory, in the latter each processor has it own local processor.

In the future the architecture of supercomputers will rely heavily on massive parallelization with reduced communication between nodes. This will have to be taken into account when devising numerical methods in astrophysics for them to take advantage of this development. An example if a method with such potential is the discontinuous Galerkin method.

## 6 ASTROPHYSICAL CODES

Numerical astrophysicists spend the majority of their effort running numerical experiments with existing codes. Thus these codes play a big role in the field. After a code has been developed and is used to publish simulations it is then typically made publicly available by its authors. A site to share these codes after they are made publicly available is the *Astrophysics Source Code Library* (<http://ascl.net>).

Here we shall give a small list of some of the codes available, the selection biased by the experience of the author. All codes mentioned below are designed for three space dimensions.

- *GADGET*  
This was developed by [Springel \(2005\)](#) to solve the evolution of gravity (dark matter) in the universe. Gravity is modelled as a collisionless fluid and solved by an N-body method. This gets coupled to a discretization of hydrodynamics via the smoothed particle hydrodynamics (SPH) method.

See here <http://www.mpa-garching.mpg.de/gadget/> for more details.

- *AREPO*

This was developed by [Springel \(2010\)](#) to solve hydrodynamics (HD) or magnetohydrodynamics (MHD) coupled to gravitation. The HD and MHD equations are solved via a finite volume method with an innovative moving mesh method. The reason for moving the mesh is to have a numerical method that can achieve approximate Galilean invariance. The evolution of the gravity (dark matter) is solved as in GADGET.

See here [www.h-its.org/tap-software-de/arepo-code/](http://www.h-its.org/tap-software-de/arepo-code/) for more details. This code will be made publicly available in the future.

- *ENZO*

This code was developed among others by Abel, Bryant and Norman ([Oshea et al., 2005](#)). It solves hydrodynamics with gravitation as used in models to describe the evolution of the universe. It is based on a Cartesian grid with adaptive mesh refinement.

See here <http://enzo-project.org/> for more details.

- *NIRVANA*

This was developed by [Ziegler \(2005\)](#) to solve ideal magnetohydrodynamics with self-gravitation. It is based on a central scheme.

See here <http://www.aip.de/Members/uziegler/nirvana-code/> for more details.

- *FLASH*

[Fryxell et al. \(2000\)](#) wrote a code for reactive hydrodynamics using a finite volume method based at its core on the PPM method of [Colella and Woodward \(1984\)](#).

See here <http://flash.uchicago.edu/site/flashcode/> for more details.

- *PLUTO*

One of the developers of this code is [Mignone et al. \(2007\)](#). It uses a finite volume method to solve hydrodynamics and ideal magneto hydrodynamics, both nonrelativistic and relativistic.

See here <http://plutocode.ph.unito.it/> for more details.

- *ATHENA*

This code is developed by the group of [Stone et al. \(2008\)](#). It solves the equations of ideal MHD using a finite volume method on a Cartesian mesh. The authors strongly believe in the constrained transport method to enforce the divergence-free constraint on the magnetic field, ensuring that there are no magnetic monopoles.

See here <https://trac.princeton.edu/Athena> for more details.

- *RAMSES*

This code was developed by [Teyssier \(2002\)](#). It solves the equations of ideal MHD (using a second-order finite volume method) under the influence of self-gravity (using an N-body code). It is based on a Cartesian grid with a tree based adaptive mesh refinement.

See here <http://www.ics.uzh.ch/~teyssier/ramses/RAMSES.html> for more details.

- *SLH*

This code was developed under the supervision of Fritz Röpke, see [Miczek et al. \(2015\)](#) and [Barsukow et al. \(2016\)](#). It solves the Euler equations with gravity and incorporates a general nuclear reaction network. This allows it to model the evolutions of stars. Their numerical method has an efficient solver for implicit time integration, thus being able to solve both low and high Mach number flows correctly.

See here <http://slh-code.org> for more details. This code will be made publicly available in the future.

## 7 CONCLUSION

The challenges of numerical methods in astrophysics are due to their huge range of scales. This warrants extremely robust numerical methods. Examples are very low densities, which numerically are not allowed to deviate below zero, or shocks at very high Mach numbers that need to be computed in stable manner. In addition the subject naturally solves its problems in three space dimensions, which sometimes challenges numerical methods inherently designed for one space dimensions.

This survey gave only a very partial view of the subject. A more comprehensive view, albeit written by astrophysicists, can be found in [Bodenheimer et al. \(2006\)](#). A collection of lectures on computational astrophysics can be found in the Saas Fee notes ([LeVeque et al., 2006](#)), still useful, even though they are almost 20-year old.

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