GMCs collapse and form stars wherever gravitational forces can overwhelm the supportive effects provided by thermal pressure, magnetic fields and internal motions ("turbulence"). In practice, the bulk of star formation within molecular clouds is associated with dense gas where the Jeans mass and Jeans length are small (see Eqs. 1.1 and 1.2, Chap. 1). The characteristic scale of gravitational fragmentation (which gives rise to ‘pre-stellar cores’: see Chap. 1, Sect. 1.2) is somewhat less than a solar mass. Dense gas in GMCs is often organised into filamentary structures and cores and the protostars into which these evolve also trace a filamentary pattern (see for example Chap. 7, the right-hand panel of Fig. 7.1).

The evolution of dense self-gravitating gas from pre-stellar cores through to pre-main-sequence stars is usefully summarised in the famous cartoon of Shu et al. (1987) shown in Fig. 2.1. Roughly speaking the time spent in the pre-stellar/protostellar phase is of order $10^5$ years which equates roughly with the free-fall time for the densest regions within GMCs; on the other hand the overall lifetime of star-disc systems (a few Myr; Haisch et al. 2001) is of order the dynamical time of the entire GMC. The transformation of objects along the path shown in Fig. 2.1 thus occurs on timescales on which there is ample time for dynamical evolution. Observations of the stars and gas within star-forming regions (see e.g. Mathieu Chap. 11) thus do not just capture conditions at birth but also reflect a history of significant dynamical evolution.

In order to interpret such observations it is essential to perform simulations. Ideally these simulations should start with a GMC (or even start with the formation of the GMC from the diffuse ISM) and self-consistently form stars, thereafter tracking both continued star formation and the dynamical evolution of the gas and stellar components. In order to be realistic, magnetic fields in the gas should be included and the temperature of the gas (given its irradiation by the stars that form) should be modelled through radiative transfer calculations. At some point the residual gas is
also likely to be impacted by so-called mechanical feedback (i.e. the momentum input from winds, jets or supernovae). All these effects modify the location of the gas and its gravitational effects on the groupings of stars formed in the simulations. At some point, the gas is expelled from the vicinity of the stars and then—and only then—is it legitimate to treat the stars with purely stellar dynamical simulations.

Simulations that include all the effects listed above are currently computationally unfeasible and we instead need to make progress in a piecemeal fashion, gathering insights from simulations that focus on different aspects of the problem and which treat a different subset of physical ingredients. In this chapter we present a brief overview of the numerical techniques that are involved in modelling the formation of star clusters. We will start with the simplest (pure gravitational problem) and then work towards codes that can handle a larger range of physical effects.

2.1 The Pure Gravitational Problem

One approach to solving for the evolution of an ensemble of gravitationally interacting point masses is to regard the system as a fluid in six-dimensional phase space. In this case the fluid evolves according to the Fokker-Planck equation which is the collisionless Boltzmann equation including also source terms representing
the effect of gravitational encounters between individual stars. Monte Carlo codes (e.g. Hénon 1971; Freitag and Benz 2001) have been developed using this approach but are most appropriate to large-$N$ systems where the dominant stellar motion is composed of collisionless trajectories in the smoothed cluster potential and where ‘collisional effects’ (which in the stellar dynamical community usually refer to gravitationally focused encounters between stars rather than actual physical collisions) are rare. It is not however a good approach to small-$N$ systems where strong deflections are the norm. We will see later that the hierarchical nature of cluster assembly means that small-$N$ dynamics are relevant in the early evolutionary stages of even rather populous clusters. Henceforth we will instead concentrate on the alternative method of simulating stellar systems, i.e. by direct $N$-body integration: the interested reader is directed to reviews by Aarseth (2003) and Dehnen and Read (2011).

The $N$-body problem splits into two components: determining the potential given the instantaneous distribution of stellar mass points and then integrating the orbits of each star in this time-dependent potential. The most obvious way to determine the gravitational acceleration experienced by each star is through direct evaluation of each pairwise force, an operation that scales with particle number $N$ as $N^2$ and thus whose expense would prohibit the integration of populous systems. This difficulty is usually circumvented by the implementation of ‘tree gravity’ (Barnes and Hut 1986) in which particles are lumped together (for the purpose of evaluating the force on a given star) according to the angle that they subtend from the star (see Fig. 2.2). In this implementation, the contribution from close-by particles is evaluated directly whereas particles are increasingly grouped at larger distances. This computational economy is reflected in a more advantageous scaling with $N$ (i.e. as $N \ln N$): ‘tree gravity’ forms the basis not only of many $N$-body codes but also for the gravitational component of SPH codes, as described below.

Close encounters pose a particular problem for $N$-body codes, which can be seen by considering the case of two stars in a highly elliptical but marginally bound orbit. The total energy should of course be a fixed quantity around the orbit, but when the stars are at pericentre, this fixed total is given by the difference between two large numbers (the gravitational and kinetic energy). A small fractional error in either of these quantities can then produce a very large fractional error in the total energy, resulting, for example, in a situation where numerical errors can unbind an initially bound pair. Since this is deeply undesirable, it is preferable to stop particles getting very close to each other and this is often achieved by ‘softening’ the potential (i.e. modifying the potential for each pairwise interaction so that it tends to a finite value at zero separation and is significantly modified for separations on the order of a prescribed ‘softening’ length). The penalty paid for such softening is that results are unreliable at small scales and that two-body relaxation effects are somewhat suppressed (although not entirely, since the cumulative effect of large numbers of more distant, unsoftened, encounters are also important for two-body relaxation: see Heggie and Hut 2003). The alternative option (which is much less intuitively obvious) is the expedient of ‘Kustaanheimo-Stiefel (KS) regularisation’ (Kustaanheimo and Stiefel 1965) which is a coordinate transformation that—by removing the singularity at the origin—allows the integration of the two-body problem down to arbitrarily
Fig. 2.2  *Upper panel:* Computation of the force for one of 100 particles (asterisks) in two dimensions (for graphical simplicity) using direct summation: every line corresponds to a single particle-particle force calculation.  *Middle panel:* Approximate calculation of the force for the same particle using the tree code. Cells opened are shown as *black squares* with their centres $z$ indicated by *solid squares* and their sizes $w$ by dotted circles. Every *green line* corresponds to a cell-particle interaction.  *Lower panel:* Approximate calculation of the force for all 100 particles using the tree code, requiring 902 cell-particle and 306 particle-particle interactions ($\theta = 1$ and $n_{\text{max}} = 1$), instead of 4950 particle-particle interactions with direct summation.  Caption and figure from Dehnen and Read (2011)
small separations. Regularised codes switch to this integration regime as required; ‘chain regularisation’ is the application of this approach to the case of nested multiple systems (see Mikkola and Aarseth 1990, 1993, 2002).

2.2 Hydrodynamical Problems: A Quick Guide to SPH

We start by noting that hydrodynamic equations can be written in either Lagrangian or Eulerian form, which respectively follow the evolution of individual fluid elements or else trace the evolution with respect to a spatially fixed grid. Each of these approaches is associated with a class of numerical techniques. We shall start with Lagrangian codes of which the most well developed is that of ‘Smoothed Particle Hydrodynamics’, a technique that is widely applied to star and cluster formation simulations. The interested reader is referred to reviews by Monaghan (1992, 2005) and Springel (2010b).

The fundamental problem to be addressed by a Lagrangian code is how—when modelling a fluid as a set of discrete mass points—one can evaluate quantities such as the density and pressure since these are needed for the evaluation of hydrodynamical forces. One might, most simply, just place a ‘sampling volume’ around each particle and calculate the density as the number of particles in this volume divided by the volume. This quantity would however fluctuate as particles left and entered the sampling volume, making the density estimate a noisy quantity and thus rendering accelerations deriving from pressure gradients inaccurate. In SPH, this problem is handled by weighting the contribution of each particle within the sampling volume according to its distance from the particle in question, the weighting being controlled by a so-called ‘kernel function’. The spatial extent of the sampling volume is controlled by the SPH smoothing length, $h$; in modern implementations of SPH codes this is generally adaptive so as to ensure a roughly fixed number of particles within a ‘neighbour sphere’.

As mentioned above, gravity within SPH simulations is often handled with a tree formulation; gravitational softening is generally set equal to the SPH smoothing length and is thus adaptive. It is worth noting that in hybrid systems consisting of both gas and star particles, the accuracy of the stellar dynamics is therefore affected by the resolution of the gaseous component.

As well as having to model pressure and gravitational forces, SPH codes need also to include artificial viscosity terms, i.e. components of the equation of motion that depend on the relative mutual velocity of particles (in the absence of viscosity, approaching supersonic particles would simply ‘pass through’ each other and viscosity is required in order to instead attain the desired hydrodynamic behaviour—i.e. the generation of a shock). For our purpose here, the most important thing to note is the possibly undesirable consequence of artificial viscosity when it comes to modelling centrifugally supported discs around young stars. In most implementations of viscosity within SPH, increased viscous dissipation is activated in the case that particles within a neighbour sphere (i.e. within a distance $h$) have a supersonic mutual
relative velocity. However, in a Keplerian disc, the mutual velocity across a radial distance $h$ is $h\Omega$ where $\Omega$ is the local Keplerian angular velocity. On the other hand, hydrostatic equilibrium normal to the disc plane requires that the sound speed in the disc is given by $\sim H\Omega$ where $H$ is the disc vertical scale height. Thus supersonic relative motions within a neighbour sphere will be detected whenever $h > H$ and such a condition would, in default viscosity implementations, increase the levels of viscous dissipation (even though, in a shear flow, there is no shock and therefore such an enhancement is not necessary).

The reason why this enhancement of viscosity is undesirable is that it is associated with an increased (numerical) transport of angular momentum in the disc: mass will be transported radially through the disc and accrete on to the star by purely numerical effects. Such spurious accretion depletes circumstellar discs too rapidly and this then increases the accretion rate still further (because the declining surface density increases $h$ further). Although the effect of unwanted artificial viscosity in pure shear flows has been mitigated by the ‘Balsara switch’ (Balsara 1995), there is no universally accepted solution to the problem, since it does not allow the treatment of problems (such as those encountered when material accretes on to a disc) which combine both shocks and shear flows (see Cullen and Dehnen 2010; Morris and Monaghan 1997).

The reason why this point has been spelled out in some detail is that it represents a major shortcoming for the SPH simulations of star cluster formation that will be described later. When entire clusters are modelled, the resolution on the scale of individual discs is poor and numerical depletion of discs is likely. Disc evolution might not appear to be critical to the large-scale dynamics of the system, but it may in fact be important. For example the density and longevity of discs determines whether they are likely to fragment and produce low-mass companions; discs can also gravitationally influence neighbouring stars by gravitational drag. We will call attention several times to aspects of simulations which may be corrupted by this effect.

Despite this warning, SPH has many virtues. It obviously conserves total mass and—provided that interparticle forces are correctly symmetrised in the case of interactions between particles with different smoothing lengths (Price and Monaghan 2007)—it also conserves total momentum and total angular momentum to machine accuracy. In the absence of viscosity or cooling it also conserves total energy to machine accuracy. Its drawbacks (apart from the issue of angular momentum transport through artificial viscosity in shear flows highlighted above) concern its treatment of shocks and of fluid instabilities. In relation to shock modelling, it is often noted that Eulerian codes do a better job at producing sharp and narrow shock features. However, as noted by (Springel 2010b), the numerical shock width is always many orders of magnitude larger than the true width of the physical shock layer: what is more relevant is whether the properties of the post-shock flow are correct (which they are in SPH). Standard SPH however struggles with excessive mixing in the case of fluid instabilities involving interfaces between phases with a large contrast in density and temperature. Agertz et al. (2007) published a detailed analysis of how such mixing suppresses Kelvin-Helmholtz instabilities in SPH simulations: see
Price (2008) and Read et al. (2010) for partial fixes. We will not discuss this issue further here since it is of little relevance to the kinds of (single phase) simulations that we shall mainly be considering.

2.3 Adding ‘More Physics’ to Hydrodynamical Codes

The description of molecular cloud parameters in Chap. 1 indicates that magnetic fields are an important ingredient and this has stimulated the development of MHD modules within SPH. Magnetic fields introduce extra terms in the momentum equation and need to be followed self-consistently in a manner that ensures that they satisfy the Maxwell equation specifying the ‘no magnetic monopoles’ requirement (i.e. \( \nabla \cdot B = 0 \)). At first sight, it would seem that this could be most readily achieved by adopting a vector potential (i.e. where \( B \) is set equal to \( \nabla \times A \) for some vector field \( A \)) since this automatically ensures that \( \nabla \cdot B = 0 \). Price (2010) found this approach to be inadvisable; an alternative approach is that of Euler potentials in which the magnetic field is set equal to the cross product of the gradients of two scalar fields (\( \alpha \) and \( \beta \); see Price and Bate 2007; Kotarba et al. 2009). What makes this approach so tractable is that in ideal MHD \( \alpha \) and \( \beta \) are conserved for each fluid element; in practice, however, the technique does not perform well in simulations of hydromagnetic turbulence (Brandenburg 2010) which is an important requirement for modelling star-forming clouds. Alternatively, other codes periodically ‘clean away’ non-zero values of \( \nabla \cdot B \) (see Rosswog and Price 2007; Dolag and Stasyszyn 2009).

An important requirement of all the simulations reported here is that they should be able to handle the conversion of distributed gas into ‘stars’ without having to perform computationally prohibitive and irrelevant modelling of the internal structure of the stars so created. This has led to the implementation of ‘sink particles’ which excise regions of collapsed gas from the domain of detailed computation and replace them with point masses with the same mass and momentum. The condition for sink creation is generally a threshold density of bound gas and the spatial extent of this region sets the initial sink radius. Thereafter particles are accreted onto the sink if they fall within the sink radius, are also bound and have low enough angular momentum that they would circularise within the sink radius. The mass and momentum of accreted sink particles is simply added to the ‘sink’.

Sink particles are relatively easy to incorporate in Lagrangian codes; the first implementation by Bate et al. (1995) opened up a generation of SPH star formation simulations on scales from binaries to entire clusters. In general they work well except for their influence on circumstellar discs: particles orbiting near the sink radius experience only spin-down torque from particles at larger radius (since the sink is devoid of SPH particles that interact hydrodynamically with gas beyond the sink) and hence the accretion of such particles is accelerated. This in turn accelerates the accretion of particles at larger radius. The net result of this is generally an unphysical depletion of gas in discs within a factor of a few times the sink radius (see Hubber et al. 2013c for details of an improved sink algorithm for disc applications).
So far, we have not specified how the gas temperature (which enters the hydrodynamic equations via the pressure) is assigned in SPH calculations. This can be set by solving the thermal equation (see below) or instead by simply prescribing a barotropic equation of state where pressure is expressed as a function of density. This latter expedient is computationally cheap and, if motivated by detailed simulations that do solve the full thermal equation, can provide a useful way of exploring cloud evolution in a semi-realistic manner. A commonly employed prescription is based on the detailed frequency dependent radiative transfer calculations of Masunaga and Inutsuka (2000), wherein the gas is assumed to be isothermal at densities less than $\rho_{\text{crit}} = 10^{-13} \text{g cm}^{-3}$ and ‘adiabatic’ ($p = K \rho^{7/5}$) at higher densities (where the gas becomes optically thick in the infrared and where cooling thus becomes inefficient). Note that ‘adiabatic’ is placed in inverted commas because this prescription is actually an isentropic equation of state (corresponding to reversible changes in the absence of cooling). In reality, gas that cannot cool should not be isentropic if it undergoes irreversible processes in shocks (i.e. the value of $K$ should actually increase). This assumption is however found to have a rather minor effect on simulation results (see Bate 2011).

A more accurate alternative, which is however more costly than imposing an equation of state, is to solve equations following the evolution of the thermal energy in both the gas and dust and the radiation field. These equations must take account of $pdV$ work, the flow of energy between matter and radiation (and between dust and gas by direct collisional interaction) and also the transport of radiation through the medium. This latter process should be modelled as a function of photon energy and thus becomes a particularly costly operation. A commonly used expedient is to apply a few simplifying assumptions: (a) the use of ‘grey’ opacities designed to model the propagation of radiative energy in a frequency averaged sense, (b) the imposition of thermal equilibrium between dust (the main opacity source at high densities and low temperatures) and gas (the main component by mass), and (c) the use of ‘flux-limited diffusion’ (Levermore and Pomraning 1981) to model radiation transport. This latter tends to the radiative diffusion approximation in regions of high optical depth (i.e. it models conditions where the radiation field is nearly isotropic and where the net flux results from gradients in temperature on length scales much larger than the photon mean free path). If however this formulation were (mis-)applied in regions of long photon mean free path, it could yield the unphysical result of radiative energy being advected at greater than the speed of light. The ‘flux-limiter’ prevents this and is formulated so that it caps the radiative flux as the product of the radiative energy density and the speed of light. ‘Flux-limited diffusion’ is thus a useful measure for modelling media that are largely optically thick and where one wants to avoid unphysically large energy fluxes in optically thin surface layers; it does not provide an accurate treatment of the cooling in these optically thin surface layers and should not be used in media that are largely optically thin (Kuiper et al. 2010; Owen 2012).

The implementation of flux-limited diffusion is straightforward in grid-based codes but the evaluation of double derivatives in Lagrangian codes like SPH requires some care (see Whitehouse and Bate 2004; Whitehouse et al. 2005). For this reason approximate cooling prescriptions have been developed in SPH which evaluate a
cooling rate per particle based on the local temperature and an estimate of the local column density. This latter can be reasonably estimated from the local potential and density in the case of approximately spherical systems (Stamatellos et al. 2007; Forgan et al. 2009; Wilkins and Clarke 2012) or from the vertical component of the gravitational acceleration in the case of disc-like systems (Young et al. 2012).

In contrast to the Lagrangian codes discussed so far, Eulerian codes solve the hydrodynamic equations with respect to a grid. Fixed grid codes (such as ZEUS: Stone and Norman 1992) are however of limited utility in the case of star formation simulations due to the lack of predictable symmetry in the problem. It is generally impossible to predict at the outset of the simulation of a ‘turbulent’ cloud where and when high resolution will be required. Grid based codes have thus only become competitive with SPH codes in this field following the development of Adaptive Mesh Refinement (AMR) codes (Berger and Collela 1989; Bell et al. 1994). As the name suggests, these are able to map the simulation onto successively higher resolution meshes as locally required. As noted above, some problems (such as radiative transfer and the modelling of magnetic fields) are considerably easier in the case of Eulerian codes; moreover Eulerian codes perform better at modelling turbulent cascades over a significant dynamic range in size scales (Kritsuk et al. 2007; Lemaster and Stone 2008; Kitsionas et al. 2009, however see Price 2012 for a demonstration that SPH is also able to model the turbulent cascade provided that the artificial viscosity is appropriately reduced away from shocks). On the other hand, the use of Cartesian grids in AMR implies that spurious angular momentum transport can be problematical when modelling circumstellar discs. Moreover, the implementation of ‘sink’ particles is less straightforward than in the case of SPH.

Nevertheless the successful inclusion of moving sink particles in AMR (Krumholz et al. 2004: see Fig. 2.3) has allowed both SPH and AMR codes to tackle the same categories of problems. Despite well-publicised but unpublished claims from the AMR community that there were major numerical differences between star formation simulations conducted with AMR and SPH codes, subsequent calibration exercises have demonstrated generally fair agreement (Federrath et al. 2010; Junk et al. 2010; Price and Federrath 2010; Hubber et al. 2013b). We are now in the favourable situation, therefore, where simulation claims can be checked with two different classes of code. Within the last five years the debate within the numerical star formation community has therefore moved on from the purely technical issues of code comparison to a greater interest in the effect of varying the input physics.

An additional physical effect which is generally important in the case of high-mass star formation simulations is that of ionising radiation. This is most easily modelled in the case where densities are high enough for the ‘on-the-spot’ approximation to be valid: i.e. where it can be assumed that—whenever an ionising photon from a star is absorbed and then re-emitted due to recombination to the electronic ground state—it is then re-absorbed ‘on-the-spot’. If this is true then it is not necessary to follow this process in detail: eventually a recombination to an excited electronic state, followed by a further cascade to the ground state, will lead to the re-emission of non-ionising photons. The net effect of this series of events is thus that the ionising photon is finally ‘destroyed’ close to the point where it is first absorbed. In equilibrium one
can then balance the emission of ionising photons from the star into a given solid angle with the integrated rate of recombinations to excited electronic states (so-called ‘Case B’ recombinations). This means that for any snapshot of a hydrodynamical simulation one can define an ionised (‘Strömgren’) volume around an ionising source and set the temperature within this region to an appropriate value (∼10^4 K) accordingly. The necessity of computing recombination integrals makes this easier in grid codes, though Strömgren volume techniques have been successfully developed in SPH also (Kessel-Deynet and Burkert 2000; Dale et al. 2005). Comparison with Monte Carlo radiative transfer codes (which do not assume the validity of the ‘on-the-spot’ approximation) indicates fair agreement in the high-density environments surrounding newly formed massive stars (Dale et al. 2007). In lower density environments it is instead necessary to follow the propagation of ‘diffuse’ ionising
photons re-emitted by recombinations to the ground state. This has led to the development of other numerical techniques (see e.g. Petkova and Springel 2009, 2011 for the implementation of a variable Eddington factor approach in SPH simulations).

Another physical effect associated with massive star formation is that due to powerful stellar winds. This has been incorporated into SPH simulations by Dale and Bonnell (2008) through the injection of momentum into those particles that define a wind ‘working surface’ around the star (see Fig. 2.4), while Rogers and Pittard (2013) have recently followed wind feedback from clusters using AMR. Algorithms dealing with each of these additional physical effects are naturally tested against analytic solutions where available (for example the case of steady momentum injection into a uniform medium; Ostriker and McKee 1988). Although agreement in these situations is encouraging, it is regrettable that there are no analytic solution treating the highly inhomogeneous conditions encountered in star formation simulations (and in real molecular clouds). This means that code intercomparison becomes of particular importance for these problems.

We end this summary of the numerical tools for star formation simulations with a brief look to the future. Recently, Springel (2010a) has developed the hybrid Eulerian-Lagrangian code ‘AREPO’ which solves the fluid equations on a moving Voronoi mesh. The superiority of this approach with respect to conventional SPH simulations
has been demonstrated for a range of cosmological problems (Sijacki et al. 2012): in particular AREPO suppresses the spurious mixing between hot and cold phases that be-devils cosmological simulations modelled with conventional SPH. It remains to be seen whether there are commensurate advantages to such an approach when applied to the very different regimes encountered in star formation simulations; these differences are both physical and numerical, since cosmological simulations are—by necessity—typically less well resolved than the star formation simulations we discuss here. (Note that despite the advantages of AREPO mentioned above, there are some downsides—for example it does not strictly conserve total angular momentum, in contrast to conventional SPH.)

A development of more obvious relevance to star formation simulations is the capacity to combine high-accuracy \( N \)-body dynamics with simulations that also model the gas phase (the use of low accuracy integrators and softened gravitational potentials in SPH means that the gravitational dynamics of ‘sinks’ are not treated with the same degree of accuracy as in conventional \( N \)-body codes). On the other hand, \( N \)-body codes model the effect of gas only via the influence of prescribed gravitational potentials. This task—of combining high accuracy \( N \)-body dynamics with hydrodynamic simulations in which the gas is a ‘live’ component—is currently under way in several groups (see Hubber et al. 2013a).

More broadly, the ‘AMUSE’ initiative (Astrophysical Multipurpose Software Environment) seeks to combine suites of ‘community software’ (e.g. \( N \)-body codes, hydrodynamics codes, radiative transfer codes, stellar evolution codes) linked by a Python user script (see http://amusecode.org/). It will remain to be seen in the coming years whether the sort of complex hybrid problems encountered in star formation simulations are best served by such generic linkage of well-tested codes or whether it is more efficient to develop hybrid codes that are optimised for specific applications.

### 2.4 Summary

In this chapter we have reviewed the main numerical techniques employed in the simulations that will be discussed in following chapters, providing a brief overview of \( N \)-body codes and both grid-based and Lagrangian hydrodynamical codes. We have placed particular emphasis on those aspects of the numerical implementation that are important in the context of cluster formation simulations, emphasising in particular the problematical feature of disc evolution that is accelerated by numerical viscosity. We have also discussed the range of ways that so-called ‘additional physics’ (e.g. magnetic fields in addition to thermal and mechanical feedback) have been incorporated in such codes. This chapter is designed to give the non-specialist an overview of the state-of-the-art and an awareness of how numerical issues may influence the outcome of cluster formation simulations.
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