A new algorithm for modelling photoionizing radiation in smoothed particle hydrodynamics

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Accepted 2007 September 13. Received 2007 August 8; in original form 2007 May 23

ABSTRACT
We present a new fast algorithm which allows the simulation of ionizing radiation emitted from a point source to be included in high-resolution three-dimensional smoothed particle hydrodynamics simulations of star cluster formation. We employ a Strömgren volume technique in which we use the densities of particles near the line-of-sight between the source and a given target particle to locate the ionization front in the direction of the target. Along with one-dimensional tests, we present fully three-dimensional comparisons of our code with the three-dimensional Monte Carlo radiative transfer code, MOCASSIN, and show that we achieve good agreement, even in the case of highly complex density fields.

Key words: radiative transfer – methods: numerical.

1 INTRODUCTION
Smoothed particle hydrodynamics (SPH) is a powerful and flexible numerical technique which has been applied to numerous astrophysical problems. The wide applicability of SPH derives largely from the fact that it is intrinsically Lagrangian. This allows SPH to deal effortlessly with large density contrasts and obviates the need for a grid or mesh to be imposed on the simulation space, thus placing no restrictions on the symmetry of the problems which may be studied. SPH has been used to model circumstellar and circumbinary discs (Murray 1996; Speith & Kunze 2002), stellar collisions (Lombardi, Rasio & Shapiro 1996; Sills et al. 2002), the collapse of molecular cores (Bate 1998), the formation of star clusters (Klessen, Heitsch & Mac Low 2000; Bate, Bonnell & Bromm 2003) and galaxy formation (Kobayashi 2004). SPH is a proven tool for modelling gas dynamics, and hybridization with N-body codes allows the inclusion of gravity in SPH simulations, but such comparatively basic input physics limit the sophistication of the simulations that can be performed using SPH. Two problems that have been traditionally very difficult to solve in SPH are the inclusion of magnetic fields and the implementation of radiative transfer. Studies of all the systems mentioned above are likely to benefit considerably from the ability to model these phenomena.

In this paper, we describe a new algorithm designed to implement a very simple form of radiative transfer in the context of SPH simulations of the formation of star clusters. Massive stars inject energy and momentum into the ISM by a variety of means, and these feedback mechanisms have important consequences on a variety of size scales, from the photoevaporation of circumstellar discs around single or binary stars by ionizing radiation (Yorke & Welz 1996) to the inflation of galactic superbubbles by the combined action of the radiation, winds and supernova explosions of thousands of O-stars (Clarke & Oey 2002).

On a scale of a few parsec, midway between the extremes given above, feedback from massive stars is thought to have a profound impact on the evolution of star clusters (e.g. Lada, Margulis & Dearborn 1984; Elmegreen 1998; Tenorio-Tagle et al. 2003). Since most stars form in clusters (Clarke, Bonnell & Hillenbrand 2000), it is clear that the effect of stellar feedback acting on such scales is a crucial facet of the global star formation process. It has long been known that our galaxy is forming stars at only a fraction of the rate which would obtain if star formation were a process governed solely by gravity (Zuckerman & Evans 1974). It has also become clear that the majority of star clusters do not survive for long times as shown by, for example, Lada & Lada (2003) in our Galaxy, Bastian et al. (2005) in M51 and Goodwin & Bastian (2006) in a sample of extragalactic young massive clusters. Feedback from massive stars offers attractive solutions to both of these problems. The ionizing radiation and winds from massive stars drive powerful outflows into the gas around them. Such outflows can potentially remove enough mass from a protocluster on short time-scales, leaving it unbound; the rapid expulsion of gas inhibits the production of stars, making star formation a very inefficient process.

The influence of stellar feedback on star formation has been studied from a variety of theoretical angles. Goodwin (1997), Hills (1980), Geyer & Burkert (2001), Boily & Kroupa (2003) and Goodwin & Bastian (2006) investigated the effect of the removal of the gaseous content of protoclusters, although they did not model the mechanism of gas expulsion itself, treating it either as instantaneous
or as occurring on a prescribed time-scale. Several studies have investigated the dispersal of molecular clouds by photoionizing radiation. Whitworth (1979) used simple theoretical arguments to study the erosion of a molecular cloud by O-stars situated near the edge of the cloud. Tenorio-Tagle et al. (1986) used a one-dimensional Lagrangian finite-difference code to model the impact of photoionizing radiation on the residual gas in globular clusters and Franco & Garcia-Segura (1996) conducted two-dimensional grid-based simulations of the growth of H II regions. All the theoretical work described above makes use of some form of symmetry to simplify the problem. More recently, Goodwin & Whitworth (2004) adopted a fractal gas density distribution to mimic the asymmetries and inhomogeneities of star clusters. However, real protoclusters are inhomogeneous, anisotropic and dynamic environments. The only way in which to study ionizing feedback under realistic conditions is to perform fully three-dimensional numerical simulations, and SPH methods provide the ideal tool for this task. High-resolution SPH simulations are computationally very expensive and the addition of further physics inevitably results in further overheads. However, with the advent of fast parallel machines, such studies have now become technically feasible. Kessel-Deynet & Burkert (2000) were the first to attempt this with their studies of radiation-driven implosion of molecular cloud cores (Kessel-Deynet & Burkert 2003).

In this paper, we present a fast and robust algorithm designed to simulate photoionization in SPH and describe tests performed to ensure that it produces accurate results. In Section 2, we give a brief overview of the physics of photoionization. In Sections 3 and 4, we describe how we have implemented the basic physics within the SPH formalism. In Section 5, we present one-dimensional tests of our algorithm and compare them to analytic solutions. In Section 6, we describe the comparison of the SPH algorithm to results generated with a fully three-dimensional Monte Carlo photoionization code. Our conclusions are presented in Section 7.

2 THE PHYSICS OF PHOTOIONIZATION

The idealized problem of the consequences of the sudden ignition of a source of ionizing photons inside a cloud of uniform-density H I has been well studied, first by Str"omgren (1939) and later by Kahn (1954).

Initially, the ample supply of ionizing photons causes an ionization front (IF) to progress radially outward from the source at a highly supersonic speed leaving behind it a spherical H II region. During this phase of its evolution, the IF is said to be of R-type. Geometrical dilution of the radiation field and the recombinations of ions and electrons within the H II region progressively reduce the photon flux arriving at the front and slow its progress into the neutral gas. If the neutral atomic gas has number density n_0, ionization of the gas will result in number densities of ions and electrons of n_i and n_e, respectively. If the gas is taken to be H I clearly n_i = n_e and if the gas is fully ionized, then n_e = n_o = n_0. The recombination rate per unit volume is then given by α n_e n_o, where α is a recombination coefficient. If the source’s ionizing photon luminosity is Q_H (measured in ionizing photons emitted per unit time, where any photon whose energy exceeds 13.6 eV is regarded as ionizing) and the surroundings are spherically symmetric, the flux F(r) arriving at a radius r is given by

\[ 4\pi r^2 F(r) = Q_H \int_{r'}^{\infty} r'^2 n_i^2 \alpha_B \, dr, \tag{1} \]

where n_0 has been taken to be constant during the initial phase of the H II region's development and α_B, taken to be 3.0 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}, is the temperature-dependent ‘case B’ recombination coefficient which neglects recombinations directly to the hydrogen ground state. The ionizing photons produced by such recombinations are assumed to be absorbed elsewhere in the H II region and not to make any contribution to the ionization equilibrium. This is commonly referred to as the ‘on-the-spot’ (OTS) approximation and is justifiable in cases where the optical depth of the H II region to secondary ionizing photons is smaller than the dimensions of the H II region. Yorke in Kudritzki, Yorke & Frisch (1988) shows that, for an O-star with an effective temperature of 40,000 K, the OTS approximation is valid throughout most of the H II region at the densities of interest here (> 10^4 \text{ cm}^{-3}).

As the IF proceeds into the neutral gas surrounding the source, the point is quickly reached where the integral on the right-hand side of equation (1) becomes equal to Q_H. The photon flux at this radius is then zero and the IF can proceed no further. The radius at which this happens is known as the Str"omgren radius, R_S, and is defined by integration of equation (1):

\[ R_S = \sqrt[3]{\frac{3Q_H}{4\pi\alpha_B n_0^2}}. \tag{2} \]

Since the ionized gas within the H II region is expected to reach an equilibrium temperature of ~10^4 K, whereas the ambient temperature of the neutral hydrogen in a typical giant molecular cloud is ~10 K, a very large pressure gradient then exists across the IF. This will cause the H II region to expand violently into the surrounding H I, driving a strong shock before it. This expansion is negligible during most of the initial phase described above, since the speed with which the IF propagates is much greater than the speed of sound in the ionized gas (~10 km s^{-1}). However, once the IF has slowed down to a speed of a few times the sound speed, the pressure-driven expansion of the H II region begins to dominate the evolution of the system. The IF is then said to be D-type.

By considering the jump conditions across both the shock front and the IF, Spitzer (1978) derived a simple expression for the time-dependence of the radius of the IF, R(t), during the expansion phase of the H II region

\[ R(t) = R_S \left(1 + \frac{7c_s t}{4R_S}\right)^{4/7}, \tag{3} \]

where c_s is the isothermal sound speed within the H II region.

3 BASIC STRÖMGREN VOLUME METHOD

We have conducted our simulations using a SPH code, fully described in Bate, Bonnell & Price (1995). The code is a hybrid N-body/hydrodynamic code, using a binary tree algorithm for gravitational calculations, and the SPH formulation to handle the gas dynamics. Particles are evolved on individual time-steps to improve efficiency. This code is a proven tool for studying clustered star formation (see e.g. Bonnell et al. 2001; Bonnell & Bate 2002; Bate et al. 2003) and is thus ideal for studying the problems outlined in the Introduction.

Stars are represented in the code by sink particles. A sink particle is a point mass with an accretion radius. Gas particles straying inside a sink particle’s accretion radius are accreted by the sink particle if they pass a series of the tests, the most obvious of which is whether or not the gas particle is gravitationally bound to the sink particle. If the gas particle passes the test, its mass, momenta and energy are added to those of the sink particle and the gas particle is removed from the simulation.
In previous simulations, the sink particles interact with the gas particles only via their gravitational fields and the accretion process described above. We have modified the code to treat one or more of the sink particles within a simulation as a source of radiation. The photoionization algorithm selects a gas particle as a target and determines whether or not enough ionizing photons from a given radiation source reach the target particle during the current time-step to ionize it (or, if it is already ionized, to keep it that way). Consistent with the physical assumptions described above, all gas particles in the simulation are regarded as being fully ionized or fully neutral. Once the ionization algorithm has decided which particles are ionized, these particles are heated to a temperature of $\sim 10^4$ K appropriate for the choice of $\sigma_R$, and control is returned to the dynamical portion of the code.

In a nebula consisting of pure hydrogen and characterized by conditions where the OTS approximation is valid, secondary ionizing photons do not contribute to the overall ionization equilibrium. The photons which do control the ionization balance are therefore the primary ionizing photons which travel radially outwards from the radiation source until they are absorbed. Since these photons follow purely radial trajectories through the gas, the fate of each photon is independent of those travelling along other radial trajectories. This has the consequence that, in a non-uniform cloud, each photon can be treated as though it were moving through a spherically symmetric cloud possessing whatever radial density profile exists along the photon’s direction of propagation. If the cloud in question is everywhere sufficiently dense that the OTS approximation holds, the ionization structure around a point source of radiation can then be found by a Strömgren volume method in which the distance from the source to the IP in any given direction can be found using the radial density profile in that direction. It is worth noting at this point that in the case of multiple ionizing sources with overlapping Strömgren spheres, the algorithm described above cannot reproduce the radiation field in the overlap region. The ionized mass will therefore be underestimated by the current methods. This may have important consequences in the case of crowded fields and therefore a new version of the photoionization algorithm is currently being developed and will be described in a forthcoming paper.

In a spherical cloud with an arbitrary radial density profile $\rho(r)$, equation (1) becomes

$$4\pi r^2 F(r) = \frac{Q_H}{m} - \int_{r=0}^{r=r'} r^2 n(r')^2 \alpha_g \, dr,$$

(4)

where the uniform number density $n_0$ has been replaced with a number density $n(r)$ which is a function of radius.

Hence, the flux arriving at any given particle can be found if the function $n(r)$ along the line-of-sight to that particle can be estimated. Kessel-Deynet & Burkert (2000) proposed an ingenious method by which the function $n(r)$ can be evaluated in SPH and make use of it here, with some modifications. The method is illustrated in Fig. 1. A target SPH particle is first selected and a line-of-sight from this target to the source is drawn. The target’s neighbours (those inside the dotted circle in Fig. 1) are fetched from the SPH code’s neighbour lists and the one closest to the line-of-sight is selected (labelled as point 4 in Fig. 1). The neighbours of the newly chosen particle to the line of sight. The position of the selected particle is then projected on to the line-of-sight to produce what Kessel-Deynet & Burkert (2000) term an evaluation point, labelled $r_3$, in Fig. 1. The neighbours of the newly chosen particle are then fetched and the selection process is repeated until the radiation source is reached. Once this process has been completed, Kessel-Deynet & Burkert (2000) then solve an equation for the rate of ionization of the target particle. Instead, we use the density profile determined by the process outlined above in a discretized version of equation (4) to decide whether the target particle receives enough radiation flux to ionize it, a faster and more robust method than that employed by Kessel-Deynet & Burkert (2000).

From the densities of the $N_{\text{LOS}}$ particles selected along the line-of-sight to the target, we know the value of $n(r)$ in a series of $N_{\text{LOS}}$ radial bins whose inner and outer radii are defined by the projected positions of the particles along the line-of-sight. We assume that the densities at these projected positions are simply the same as the densities of the relevant particle $i$, evaluated in the usual way as

$$\rho_i = m_i W(0, h_i) + \sum_{j=1}^{N_{\text{neigh}}} m_j W(r_{ij}, h_{ij}),$$

(5)

where $m$ denotes the mass of each particle and the sum runs over the $N_{\text{neigh}}$ neighbours of particle $i$ (defined as all other particles within two smoothing lengths, $2h$, of particle $i$). $W$ is the smoothing kernel, a function of the interparticle separations $r_{ij}$ and the average smoothing length $h_i$ of particle $i$ and each of its neighbours.

Alternatively, we could estimate the densities at the evaluation points by performing an SPH density estimation of the form

$$\rho_k = \sum_{j=1}^{N} m_j W(r_{kj}, h_j),$$

(6)

where the sum instead runs over all $N$ SPH particles that overlap the $k$th evaluation point, $r_{kj}$ is the distance of each of these particles from the evaluation point and $h_j$ is the individual smoothing length of each particle. However, identifying the $N$ particles is not trivial;
some but not all are likely to be neighbours of the $k$th particle on the line-of-sight to which the evaluation point belongs. Finding them is therefore time-consuming and we find that in any case it makes very little difference to the results; the density of the $k$th particle is almost always a good estimator of the density at the $k$th evaluation point.

We now rewrite equation (4) as $4\pi r^2 F(r) = Q_{\text{H}} - I(r)$ and approximate the integral $I(r)$ by a sum as follows:

\[ I(r) = \sum_{i=1}^{N_{\text{los}}} r_i^2 (n(r_i))^2 \alpha_B \Delta r_i. \tag{7} \]

The inner radius of bin $i$ is defined by the radial position of particle $i - 1$ projected on to the line-of-sight, $r(i - 1)$, and the outer radius of bin $i$ by the projected radial position of particle $i$, $r(i)$. The width of each bin is then $r(i) - r(i - 1) = \Delta r_i$. $(n(r_i))$ is the average number density of the two SPH particles whose positions define the bin, $(n(i) + n(i - 1))/2$. The density of the point mass, used in calculating the number density of the first bin, is taken to be zero. Once the sum has been calculated, $I(r)$ can be subtracted from the source luminosity $Q_{\text{H}}$ to obtain the flux of photons arriving at the target particle. We can then determine the particle’s ionization state during the current time-step.

### 4 IMPROVEMENTS OVER THE BASIC STRÖMGREN VOLUME METHOD

Although the method described above is adequate for the simulation of the growth of a spherical H II region in a uniform motionless cloud, our code is also intended for use in highly inhomogeneous and dynamic situations. It is highly likely under such circumstances that neutral gas may enter the H II region from outside, in an accretion flow, for example, and that ionized gas may either leave the H II region or be otherwise cut-off from the supply of photons required to prevent it from recombining. We have therefore improved upon the basic Strömgren volume method to cope with these eventualities.

#### 4.1 Neutral gas inside the H II region

Modifying the above method to account for the photons required to ionize neutral material which has entered the H II region (perhaps via an accretion flow) or to grow the H II region from scratch (the R-type phase of the IF’s evolution) is not difficult. If we introduce an ionization fraction $x_i$ (still taken to be either 0 or 1) for each particle, then we can rewrite equation (7) as

\[ I(r) = \sum_{i=1}^{N_{\text{los}}} r_i^2 (n(r_i))^2 \alpha_B \Delta r_i + \sum_{i=1}^{N_{\text{los}}} r_i^2 (n(r_i))(1 - x_i) \frac{\Delta r_i}{\Delta t}. \tag{8} \]

The first term in the equation, the flux required to keep pace with the recombinations in ionized gas, is always present. The second term allows for the possibility that some flux may be consumed by ionizing the gas from a neutral state first, and makes the expression time-dependent. The term $\Delta r_i/\Delta t$ is the discretized speed at which the IF propagates. The time-step on which the algorithm evolves the IF, $\Delta t$, is usually set to the shortest dynamical time-step in use by the SPH code at the time, so that the H II region is updated whenever any SPH particles are updated. If this time-step is very short, the flux arriving at a given target particle may not be sufficient to ionize it immediately, in which case the flux is banked – allowed to accumulate until the particle can be ionized. Particles with banked flux are not heated above the neutral gas temperature.

#### 4.2 Ionized gas straying outside the H II region

Ionized material that is for some reason deprived of photons will recombine and eventually cool. To allow for this eventuality, ionized particles which are receiving no ionizing flux are flagged and monitored by a neutralization routine. This routine reduces the ionization fraction of such particles according to their local recombination time-scale, $(an)^{-1}$. If the ionization fraction of a particle drops below a half, it is assumed to become fully neutral.

Kessel-Deynet & Burkert (2000) note that cooling recently recombined gas instantaneously back down to the original ambient gas temperature is not a good treatment of the physics of recombination, since recombined gas, although neutral, is likely to still be hot. Neutralized particles are therefore passed on to a cooling routine which assigns them new temperatures according to the cooling curve described by Schmutzler & Tscharnuter (1993) until they reach a temperature of 100 K, at which point they are returned to the initial average gas temperature (usually 10 K).

#### 4.3 The ionization code’s decision tree

Once the flux reaching a given target particle has been determined, taking into account the consumption of photons by neutral material lying on the line-of-sight from the source, the ionization state of the target particle is determined using the decision tree illustrated in Fig. 2. Note that in this tree, the approximation is made that if the flux reaching an ionized particle is non-zero, that particle remains ionized. It could be argued that the flux must in fact be sufficient to exceed the recombination rate in the particle. However, in all cases, the fluxes calculated by the code are those reaching the centres of particles and the decrement in flux incurred between the particle edge and its centre is taken account of. The only particles for which this assumption is questionable are those at the IF. For a given ionized particle $i$ at the IF, a non-zero flux reaches the centre of particle $i$ but zero or ‘negative’ flux reaches the next particle further out along the line-of-sight to the source, $j$. This means that the true IF lies somewhere between the centres of $i$ and $j$ and thus somewhere inside both particles (recall that SPH particles overlap one another). The decision to keep $i$ ionized and $j$ neutral introduces an error in the location of the IF along the line-of-sight on which $i$ and $j$ lie of $\sim \Delta x$, consistent with the accuracy to which any spatial quantity can be meaningfully determined in SPH.
5 ONE-DIMENSIONAL TESTS

The most basic tests one can perform with our hybrid hydrodynamics/ionization code are to follow the approach to the Strömgren radius and the subsequent expansion of the H II region.

The sudden ignition of a source of $Q_H$ ionizing photons per second in a uniform cloud of atomic number density $n_0$ leads to the highly supersonic expansion of an R-type IF. The expansion velocity of the front can be derived by considering the rate of fresh ionizations at the front. If the IF has an instantaneous radius $R_I$ and the flux reaching the front is $F_t$, we may write

$$\frac{dR_I}{dt} = \frac{F_t}{4\pi n_0 R_I^2} = \frac{1}{4\pi n_0 R_I^2} \left( Q_H - \frac{4}{3} \pi n_0^2 R_I^2 \alpha_I \right).$$

(9)

This can easily be integrated and combined with equation (2) to yield

$$R_I(t) = R_S (1 - \exp[-n_0 \alpha_I t])^{1/3}.$$  

(10)

In Fig. 3, we show the results of the ignition of an ionizing source in a uniform cloud, following the approach of the IF to the Strömgren radius. As in all one-dimensional tests presented here, the SPH particles were initially distributed on a uniform hexagonal close-packed grid. To study the approach to the Strömgren radius, the heating of ionized particles was disabled and the time-step on which the code dumps output was set to a very small value. The radius of the H II region was then estimated from each output dump. If a number of points are distributed randomly in a sphere of radius $R$, the average distance of the points from the centre of the sphere $\bar{r}$ is given by $\bar{r} = 3/4R$. We therefore estimated the radius of the H II region by finding the average distance of all ionized particles from the radiation source and multiplying by $4/3$. We see that the agreement between the SPH results and the analytic solution is excellent.

As the IF approaches the Strömgren radius, its velocity slows towards the speed of sound in the neutral material surrounding the H II region. The IF then transitions to its D-type phase according to equation (3) (Spitzer 1978). To test the ability of our code to replicate the Spitzer solution at different numerical resolutions, we constructed three spherical clouds of identical mass $M_{\text{cld}}$ and radius $R_{\text{cld}}$, containing ionizing sources of identical luminosities $Q_H$, but built from different numbers of particles. Since the Strömgren radius in the three clouds is the same, the initial H II regions in the clouds contain different numbers of particles. We chose $M_{\text{cld}} = 1700 M_\odot$, $R_{\text{cld}} = 1\text{ pc}$, $Q_H = 10^{49} \text{ s}^{-1}$, so that $n_0 = 1.65 \times 10^4 \text{ cm}^{-3}$ and $R_S = 0.1 \text{ pc}$. We chose particle numbers $N_{\text{part}}$ of $10^9$ (high resolution run HR), $10^8$ (medium resolution run MR) and $10^7$ (low resolution run LR), so that the initial Strömgren radii contain, respectively, 1000, 100 and 10 particles.

It is not a priori obvious what the minimum requirement to resolve an H II region in SPH might be. To resolve an object in SPH is usually taken to require at least the average number of particles contained within the SPH smoothing kernel (usually 50). Bate & Burkert (1997) found that, to resolve gravitational fragmentation correctly required that a Jeans mass contain at least 100 particles (twice the canonical resolution limit). However, Hubber, Goodwin & Whitworth (2006) find that even seriously underresolving the Jeans mass (with <10 particles) does not result in spurious fragmentation. Our run LR also underresolves the H II region, in the sense that 10 particles are well below the canonical SPH resolution limit, meaning that the H II region may behave unpredictably.

In Fig. 4, we plot the time-evolution of the IF radius in our three models together with the Spitzer solution for comparison. In these simulations, we found that estimating the radius of the IF using the average distance of the ionized particles from the source did not work well because of radial sloshing of the hot gas inside the H II region. Instead, we computed the radius of the shock by finding the average separation from the radiation source of the $N_{\text{part}}/10^3$ densest particles – this number of particles proved to be large enough to give a reasonably noise-free result. We see that the three SPH models agree very well both with each other and with the Spitzer solution, at least for the evolution of the H II region from $R_S$ to $\sim 10R_S$. Even the low-resolution calculation gives reasonable agreement with the analytical solution over the range of radii considered. For this simple problem at least, our implementation can faithfully follow the evolution of an H II region which would be considered severely underresolved by the usual SPH resolution criteria.
6 COMPARISON WITH A THREE-DIMENSIONAL MONTE CARLO PHOTOIONIZATION CODE

Since we intend to use our ionization code in situations where the gas density distribution is highly inhomogeneous, one-dimensional tests can only take us so far. In order to perform a more stringent test than those presented in the previous section, we therefore selected a very complex density distribution derived from a three-dimensional simulation of clustered star formation, and compared the H II regions generated by our code and by the fully three-dimensional Monte Carlo photoionization and radiative transfer code, MOCASSIN (Ercolano et al. 2003; Ercolano, Barlow & Storey 2005). This code adopts a stochastic approach to the transfer of radiation by simulating the individual processes of absorption and re-emission of radiation quanta as they leave an ionization source and diffuse through a gas. The polychromatic nature of both the primary (stellar) and the secondary (diffuse) components of the radiation field is accounted for self-consistently as the photon trajectories are computed and the ionization and thermal structure of the nebula established. All relevant atomic physics processes are included and the atomic data base is updated regularly, currently using a combination the Chianti V5 (Landi et al. 2006) data base for collision strengths, transition probabilities and energy levels of heavy metals, the opacity project for photoionization cross-section and a new calculation of the H I, He II and He III free–bound continua presented by Ercolano & Storey (2006).

Dust grains mixed with gas inside the ionized regions may also affect the global ionization structure of the gas. The grains compete with the gas for the absorption of UV radiation, hence reducing the flux available for the photoionization of atom and ions. This can be self-consistently accounted for by MOCASSIN (Ercolano et al. 2005), but not by the SPH ionization algorithm, since the amount of radiation subtracted from the field, and thus available to the gas, depends heavily on a number of variables, including the local dust-to-gas ratio, the grain chemistry and size distribution, as well as the shape of the local radiation field, which cannot be obtained by the SPH ionization algorithm. In order to be able to compare the outputs from the two codes, we did not include any dust in the MOCASSIN calculation, nevertheless we point out that the ionized masses thus obtained may be slightly overestimated.

We chose to compare MOCASSIN and the SPH ionization algorithm under realistic astrophysical conditions. The gas distribution selected for the comparison was drawn from an SPH simulation of the collapse of a molecular cloud originally performed by Bonnell & Bate (2002) and repeated by Dale et al. (2005), who modelled the effect on the cloud and the stellar cluster formed by it of the ionizing radiation from the single O-star born at the cluster centre (using the code described here). Three views of the gas distribution are shown in the top panels of Fig. 5. The ionizing source is at the centre of the image, at the intersection of several dense filaments of gas. The density structure of the cloud is evidently highly inhomogeneous – maximum and minimum densities are \(2 \times 10^7\) and \(2 \times 10^1\) cm\(^{-3}\), respectively, with mean and median densities of \(2 \times 10^4\) and \(4 \times 10^2\) cm\(^{-3}\), respectively (these densities are derived from the densities of the SPH particles). Note that, as well as exhibiting a very large dynamic range, these densities are sufficiently high that the OTS approximation will hold. Modelling photoionization in this highly inhomogeneous (and, from the source’s point of view, highly anisotropic) environment is clearly very challenging.

MOCASSIN is a grid-based code, in which a ‘mother-grid’ of arbitrary resolution is defined; any cell in this grid may be further divided into a finer subgrid of arbitrary resolution, so that arbitrary gas distributions can be efficiently represented in the code with adequate detail. SPH is a gridless method, representing gas distributions by an ensemble of overlapping particles of (usually) equal mass, but...
Figure 6. Comparison of H II regions generated by the SPH ionization code and the MOCASSIN radiative transfer code of Ercolano et al. Shown are column density maps of the H II region produced by the two codes as viewed along the x- (leftmost two panels), y- (central two panels) and z-axes (rightmost two panels).

varying radius (the smoothing length). We therefore devised a method to interpolate the SPH gas distribution on to a grid suitable for use by MOCASSIN and subdivided in such a way that the resolution of the grid was everywhere as close as possible to the resolution of the SPH particle ensemble. We first generated a uniformly spaced 63^3 mother-grid with cell size $d_{\text{max}}$ filling the same volume as the SPH particle distribution. Each SPH particle was then located in the grid and the smoothing length of the smallest particle $h_{\text{min}}$ (if any) in each mother-grid cell determined. If for any cell $d_{\text{max}} > 2h_{\text{min}}$, the cell is subdivided into $(1 + \text{INT}(d_{\text{max}}/(2h_{\text{min}})))^3$ cells. Finer subdivision of grid cells, for example, by $h_{\text{min}}$ or $h_{\text{min}}/2$ did not result in a significant improvement in the interpolation accuracy. This procedure resulted in the division of 223 of the 250 047 mother-grid cells into subgrids. Once the simulation volume is suitably partitioned, the mass of each cell is calculated by finding all $N_{\text{cell}}$ SPH particles overlapping the centre of the cell, estimating the density at that point using equation (6) with the sum running from 1 to $N_{\text{cell}}$, and multiplying the density estimate by the cell volume.

A simple check reveals that the total mass in our SPH particle distribution is 514.8 $M_\odot$, compared to 513.3 $M_\odot$ in the adaptive grid, implying that our interpolation method is adequate. In Fig. 5, we compare column density maps, as seen along the three principal axes, of the SPH particle distributions (top row) and the density grids created for MOCASSIN (bottom row). We see that the MOCASSIN grids appear to reproduce the morphology of the SPH particle distribution very well. It should be noted that, in order to facilitate visualization, the information contained by each subgrid and SPH particle has been averaged and mapped on to a uniform pixel map, so that the resolution of the figures shown is much lower than that actually used in our calculations.

To compare the H II regions generated by the two codes, we placed sources emitting $Q_\text{H} = 10^{49}$ (ionizing) photons s$^{-1}$ at position (0, 0, 0) in both simulation volumes. The modifications described in Section 4 were disabled, so that the SPH code was operating in a pure Strömgren volume mode. We first used extremely metal poor abundances for the MOCASSIN run. The general H II region morphologies predicted by the two codes are shown in Fig. 6 and are in good agreement, although a closer look will reveal low-density ionized protrusions in the SPH maps that are absent or much less accentuated in the MOCASSIN maps. The MOCASSIN maps also have generally sharper edges than do the SPH maps. Given that MOCASSIN treats the diffuse radiation field, whereas the SPH algorithm does not, this is the opposite of what one might expect. However, we found that the gas densities in this problem are large enough that the diffuse field is insignificant. The sharper H II regions produced by the Monte Carlo code are a consequence of the intrinsic fuzziness of SPH particles. The SPH code is obliged to ionize whole SPH particles, whereas, since every particle is represented by at least eight (and usually more) cells in the MOCASSIN grid, the Monte Carlo code is able to resolve the edge of the H II region somewhat better than the SPH code. In terms of total ionized mass fractions predicted, however, the morphological discrepancies seem to have little significance, with total ionized masses being predicted by the SPH algorithm and the MOCASSIN code of 20.9 and 20.5 $M_\odot$, respectively. The extra features appearing in the SPH maps in fact tend to be of much lower densities. The qualitative morphological differences but quantitative agreement may be caused by the inherently poorer resolution of low-density regions by the SPH code, or it may be an artefact of the interpolation of the Lagrangian SPH mass distribution on to a set of Eulerian grids. However, it is more probable instead that temperature effects may be the dominant cause, as described in the next section.

6.1 Temperature-dependence of the recombination coefficient

The isothermal nature of the SPH ionization algorithm introduces some uncertainty in the calculation of the ionized region due to the temperature dependence of the recombination coefficient. The
MOCASSIN model presented here, where the gas temperatures are calculated self-consistently with the ionization structure, shows that the ionized region of such a complex density field is far from being isothermal. The temperature structure of the ionized region is illustrated in Fig. 7 as the histogram of mass fraction (black solid line) and the cumulative mass fraction (red dashed line) of material at a given temperature. It is clear that the success of the SPH algorithm to calculate the correct ionized mass of the grid relies on the careful choice of the value of the recombination coefficient, and implied gas temperature. For a density inhomogeneous pure hydrogen nebula of arbitrary geometry, the total ionized volume is obtained from the solution of

$$\int_V n_e n_\alpha(T) \, dV = Q_H,$$  \hfill (11)

where, for almost complete ionization, $n_\alpha = n_e \approx n_H$, the hydrogen number density. The total ionized mass of a region under such assumptions, therefore, strongly depends on the recombination rate averaged temperature, defined as

$$\langle T [n_H^2] \rangle = \frac{\int_V n_e^2 T \, dV}{\int_V n_e^2 \, dV}. \hfill (12)$$

The MOCASSIN calculations yield $\langle T [n_H^2] \rangle = 9120$ K, which is very close to the value 8950 K implied by the choice of $\alpha_B = 3.0 \times 10^{-13}$ cm$^3$ s$^{-1}$ in the SPH calculation. The proximity of these two temperatures allowed for the excellent agreement in the global ionized masses calculated by the two codes. As anticipated in the previous section, however, the detailed ionized volume shapes do show some differences suggesting that the temperature structure along a given line of sight may deviate from that implied in the SPH.

The temperature at any point in the ionized region is determined by the balance between the heating, dominated by the mean energy of the photoelectrons absorbed by H and He, and cooling, which, when metals are present, is dominated by collisionally excited emission lines (particularly infrared fine-structure lines of [O III]). In the absence of metals, which is the case here, the cooling is dominated by collisionally excited Lyα, which is much less efficient at removing energy from the system, therefore metal-rich regions show lower overall temperatures and steeper temperature gradients than their pure-H counterparts. This less-efficient cooling is also the cause of the significant quantity of H II at $T \sim 20000$ K shown in Fig. 7. Metallicity will therefore influence the temperature structure, and consequently the ionized mass of a region. This is likely to be the most important in metal-rich nebulae and can be taken into account in the SPH ionization algorithm by choosing a different recombination coefficient appropriate for each case. A good estimate of the appropriate $\alpha_B$ can be obtained by running snapshots of the evolving density structure calculated by the SPH code at some representative ages through a three-dimensional photoionization code, such as MOCASSIN, to self-consistently calculate the temperature and ionization structure and thus obtain the recombination-rate average temperature for the grid. The recombination coefficient to be used by the SPH ionization code will therefore be that calculated at the recombination-rate averaged temperature found. Although fully parallel, MOCASSIN is relatively computationally expensive to run, in the sense that it may require a computational time to converge which is comparable to that required by the SPH code to integrate for one dynamical time. The CPU time required by MOCASSIN depends on the number of frequency bins used and the number of atomic species modelled — the model presented here required ~40 CPU hours to converge, compared to ~50 h required to integrate the SPH model cluster for a dynamical time. However, running MOCASSIN a handful of times per dynamical time to re-estimate the average recombination coefficient should be sufficient.

We should finally note that the range of gas temperature obtained throughout the ionized region may indeed affect the hydrodynamical evolution of the system (the SPH ionization algorithm assigns the same gas temperature to all ionized particles). We defer the investigation of these potentially important effects to future work.

### 6.2 Effects of dust

None of the calculations presented here includes the effects of dust, which would in reality also act as a sink of ionizing photons — for example, Wood & Churchwell (1989) suggest that up to 90 per cent of the stellar flux in an H II region may be absorbed by dust. It is not clear what effect dust would have on the morphology of complex H II regions such as those studied here. If the dust distribution closely follows that of the gas, the effect would essentially be to shrink the H II region but to preserve its shape. This effect could be approximately modelled by modifying the recombination coefficients used in the codes. However, if the dust and gas are not strongly correlated, two different radiative transfer problems must be solved simultaneously. In this, the coupling of the radiative transfer solutions to the hydrodynamic evolution of the system in question is much more complicated, and we do not attempt to address this problem here.

### 7 CONCLUSIONS

We presented the results of tests of a new fast algorithm for simulating ionizing radiation from point sources in the context of SPH simulations. The method we use is essentially a Strömgren volume technique. We use a method similar to that presented in Kessel-Deynet & Burkert (2000) to estimate the density profiles along lines of sight to individual SPH particles before performing a Strömgren integral to calculate how much flux, if any, reaches that particle. We improved on the simple Strömgren volume method by including in the flux calculation the flux required to ionize any neutral material lying on the path to the target particle. This modification is relevant in problems where the dynamical time-scales can be as short as the time-scale required to ionize the gas, which can be the case in accretion flows. We also developed a method to allow ionized particles which are somehow deprived of their photon supply to recombine and cool using an optically thin cooling curve. This modification is also important in dynamical applications where gas can move out of an H II region, or be shadowed by dense material intervening between it and the radiation source.

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We conducted simple one-dimensional tests in which we showed that the algorithm was able to reproduce the IF’s R-type phase, in which it approaches the Strömgren radius at a very high velocity, and the D-type phase in which the H II region expands thermally at supersonic but ever-decreasing speed. We showed that the SPH code is able to reproduce the D-type expansion phase well even when the number of particles inside the H II region is well below the canonical SPH resolution limit.

Having demonstrated that the algorithm is able to reproduce the analytical solutions to simple problems, we compared the results generated in a highly inhomogeneous and anisotropic gas distribution to the output from MOCASSIN, a much more sophisticated Monte Carlo photoionization and radiative transfer code. We found that, for an appropriate choice of the recombination coefficient $\alpha_B$, the two codes agreed very well, to within 2 per cent, on the quantity of gas that should be ionized, and agreed reasonably well on the morphology of the H II region. We conclude that the algorithm is adequate for modelling photoionization in SPH simulations of star formation with very complex gas distributions.

ACKNOWLEDGMENTS

JED is supported by the Wenner-Gren Foundation and also gratefully acknowledges many useful discussions with Matthew Bate while in the process of devising the algorithm presented here.

BE was partially supported by Chandra grants GO6-7008X and GO6-7009X.

The authors would also like to thank the referee, Ant Whitworth, for a very thorough report.

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