Ionizing radiation in Smoothed Particle Hydrodynamics

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ABSTRACT

A new method for the inclusion of ionizing radiation from uniform radiation fields into 3D Smoothed Particle Hydrodynamics (SPH) simulations is presented. We calculate the optical depth for the Lyman continuum radiation from the source towards the SPH particles by ray-tracing integration. The time-dependent ionization rate equation is then solved locally for the particles within the ionizing radiation field. Using test calculations, we explore the numerical behaviour of the code with respect to the implementation of the time-dependent ionization rate equation. We also test the coupling of the heating caused by the ionization to the hydrodynamical part of the SPH code.

Key words: Methods: numerical – hydrodynamics – radiative transfer – HII regions

1 INTRODUCTION

Smoothed Particle Hydrodynamics (SPH) has become a numerical method widely used for addressing problems related to fluid flows in astrophysics. Due to its Lagrangian nature, it is especially well suited for applications involving variations by many orders of magnitude in density. Examples for this type of applications are simulations of the collapse of molecular clouds and the formation of a stellar cluster, as performed by Klessen, Burkert & Bate (1998). A comparison between grid based methods and SPH was performed by Burkert, Bate & Bodenheimer (1996) and Bate & Burkert (1997). They applied both methods to the numerically demanding problem of gravitational collapse and fragmentation of a slightly perturbed rotating cloud core with an r−2 density profile. Both methods yielded the same qualitative results. Bate (1998) performed the first calculation which followed the collapse of a molecular cloud core in 3 dimensions down to a protostellar object in hydrodynamical equilibrium, thus spanning 17 (!) orders of magnitude in density. Other applications include accretion processes in massive circumstellar disks (Bonnell & Bate 1994; Bate & Bonnell 1997), the collapse of cloud cores induced by shock waves (Vanhala & Cameron 1998) or colliding clumps (Bhattal et al. 1998), the precession of accretion disks in binary systems (Larwood & Papaloizou 1997), the dynamical behaviour of massive protostellar disks (Nelson et al. 1998), or the formation of large scale structure and galaxies in the early universe (Steinmetz 1996).

A variety of physical processes are at work in the interstellar medium, like magnetic fields, radiation or thermal conductivity, necessitating their inclusion into numerical codes. This has already been achieved to a large extent in grid based methods like the magneto-hydrodynamics codes ZEUS (Stone & Norman 1992) or NIRVANA (Ziegler, Yorke & Kaisig 1996), or codes including effects of IR and UV radiation (Yorke & Kaisig 1995; Sonnhalter, Preibisch & Yorke 1995; Richtling & Yorke 1998).

In contrast, the addition of physical processes to SPH codes is just at its beginnings. Extensions achieved so far are sophisticated equations of state (e.g. Vanhala et al. 1998) and self-gravity. Some efforts were made to make SPH faster and more accurate. The introduction of TREE algorithms (Barnes & Hut 1989; Press 1986; Benz et al. 1990) and the use of GRAvity PipE (GRAPE), a hardware device for fast computation of the gravitational N-body forces (Umemura et al. 1993; Steinmetz 1996), helped reducing the numerical effort for the gravitational force calculation and the determination of the nearest neighbours for each particle. Inutsuka (1993) presented a Godunov-like solver for the Eulerian equations in SPH thus enhancing the numerical treatment of shocks. The introduction of gravitational periodic boundaries (Hernquist, Bouchet & Suto 1991; Klessen 1997) allows the treatment of fragmentation and turbulence in molecular clouds without global collapse. The timestep problem which arises during isothermal collapse calculations at high densities is circumvented by the formation of sink particles, which substitute the innermost parts of the collapsing clump by one particle and accumulate the infalling mass and momenta (Bate, Bonnell & Price 1995).

The strength of SPH lies in its Lagrangian nature, which makes it especially attractive for problems involving gravitational collapse and star formation. Applications like e.g. by Klessen et al. (1997), which deal with the collapse and fragmentation of molecular clouds, neglect the feedback processes of newly born stars which act on their parental cloud through stellar winds, outflows and ionization. This simplification may be justified as long as the simulations deal with
collapse on timescales smaller than \(\approx 1\) Myr, on which single and binary stars or T Tau-like clusters are formed (Efremov \\& Elmegreen 1998). The case is different for larger timescales, on which OB subgroups and associations are formed. Neglecting feedback in these cases can lead to unphysical results, like a star formation efficiency of 100 per cent, since in the purely isothermal case all material will sooner or later be accreted onto the evolving protostellar cores. This is in strong contradiction to observations, which estimate a global star formation efficiency for ordinary molecular clouds of order 10 per cent (Wilking \\& Lada 1995). Another possible effect of feedback is the induction of star formation due to the compression of cloud material by shock waves and ionization fronts.

In this paper we discuss the implementation of the effects of ionizing UV radiation by massive stars into SPH calculations as a first step in order to perform collapse calculations on scales where OB-stars are formed in a more realistic way. This will in future applications allow us to assess questions like: How does the process of ionization by massive stars change the stellar initial mass function? What are the implications for the star formation efficiency? Can star formation be induced by ionization, and if yes, what are the time scales and the parameter space, for which induced star formation can be expected? These questions will be discussed in subsequent papers.

## 2 Physical Problem

We incorporate the effects of ionizing radiation from hot stellar photospheres into SPH by dividing the problem into three major substeps:

(i) calculation of the UV radiation field by solving the time-independent, non-relativistic equation of radiative transfer,

(ii) determination of the ionization and recombination rates from the local radiation field, density and ionization fraction,

(iii) advancing the ionization state of the particles in time by solving the time-dependent ionization rate equation.

### 2.1 Calculation of the UV radiation field

Given a planar infall of ionizing photons from a distant source onto the border of the volume of interest with a flux \(J_0\) Lyman continuum photons per time and square area, the resulting photon flux inside this volume is given by

\[
J(s) = J_0 \cdot \exp \left( -\tau(s) \right),
\]

where \(\tau(s)\) is the optical depth for the ionizing photons along the line of sight parallel to the infall direction of the photons, and \(s\) is the distance from the border of the integration volume along the line of sight:

\[
\tau(s) = \int_0^s \left[ \kappa \left( s' \right) + \kappa_d \left( s \right) \right] ds'.
\]  

(1)

We neglect the effect of ‘photon hardening’, i.e. the stronger absorption of weaker photons, and use an ‘effective’ absorption coefficient \(\kappa\), the mean of \(\kappa_\nu\) over frequency, weighted by the spectrum of the source \(S_\nu\):

\[
\kappa = n_H \cdot \sigma = n_H \cdot \int \frac{S_\nu(s)}{\sigma_{\text{tot}}} ds,
\]

(2)

where \(\sigma_\nu\) denotes the ionization cross section of hydrogen in the ground state and \(n_H\) the particle density of the H atoms.

The role of dust in HII regions and its effect on ionizing radiation is still very uncertain (Feldt et al. 1998). If dust is present, it will partially absorb UV photons, heat up and remit the energy in the IR regime. Its first order effect can be included easily under the assumption of a homogeneous distribution of the dust in the HII region. The corresponding contribution to the optical depth can be incorporated by adding the dust absorption coefficient at the Lyman border \(\kappa_d\) to the absorption coefficient in Eq. (1) \(\kappa_d\) depends on the dust model used and is regularly determined using Mie theory for grains with given distributions in size and shape. In this paper, we set \(\kappa_d\) to zero throughout.

We also neglect the diffuse field of Lyman continuum photons, which are being produced by recombinations of electrons into the ground level and which themselves possess sufficient energy for ionizing other H atoms. A thorough treatment of this radiation can only be achieved by detailed radiation transfer calculations as proposed e.g. by Yorke \\& Kaisig (1994). Instead we use the assumption of the validity of the ‘on the spot’ approximation as follows: due to the fact that the spectrum of the Lyman recombination photons as well as the the ionization cross section is strongly peaked at the Lyman border, a small amount of H atoms in the ionized region is sufficient to make the medium optically thick for the Lyman recombination photons. This leads to the absorption of these photons in the ultimate vicinity of their creation sites. As the creation of one photon is related to the creation of one H atom, its absorption leads to the destruction of one H atom. Thus the net effect of these photons on the local ionization structure is zero.

This assumption breaks down in regions next to OB stars, where due to the high UV flux the density of H atoms is not sufficient to make the medium optically thick to Lyman continuum photons. Next to ionization fronts, where the density of H atoms is much higher, the ‘on the spot’ assumption is nevertheless a good approximation. On further details refer to Yorke (1988).

### 2.2 Ionization and recombination rates

The ionization rate in the medium is given by the sinks of the UV radiation field, since every ionization leads to the absorption of one UV photon:

\[
\dot{I} = n_H \sigma J = -\nabla \cdot J,
\]

(3)

where \(J = J_0 \hat{e}_\nu\) is the flux vector in the direction \(\hat{e}_\nu\) of the line of sight.

The recombination rate can be estimated as:

\[
\mathcal{R} = n_e \alpha_B = n_x \alpha_{\text{eff}},
\]

(4)

with \(n\) being the particle density of H atoms and protons together, \(n_e\) the particle density of free electrons, \(x = n_e/n\) the ionization fraction and \(\alpha_B\) the effective recombination coefficient under assumption of validity of the ‘on the spot’ approximation. The recombination coefficient \(\alpha\) is given as the sum over the individual recombination coefficients \(\alpha_n\), where the electron ends up in the atomic level \(n\):
\[ \alpha = \sum_n \alpha_n. \]  

Under the assumption of the ‘on the spot’ approximation recombinations into the ground level do not lead to any net effect and thus \( \alpha_1 \) can be neglected in Eq. (2). The resulting net recombination rate which is used in Eq. (3) is commonly called \( \alpha_B \) after the nomenclature introduced by Baker & Menzel (1962):

\[ \alpha_B = \sum_{n=2}^{\infty} \alpha_n. \]

### 2.3 Ionization rate equation

Knowing the ionization and recombination rates, \( \mathcal{I} \) and \( \mathcal{R} \), the ionization fraction can be calculated from the ionization rate equation. The time dependency of the ionization fraction in the frame comoving with the corresponding particle, i.e. its Lagrangian formulation, is given by:

\[ \frac{d\alpha}{dt} = \mathcal{I} - \mathcal{R}. \]

### 2.4 Modeling the source

Since the spectral distribution of the UV radiation emitted by the photospheres of intermediate to high mass stars is very uncertain, we assume a black radiator with an effective temperature \( T_{\star} \).

### 3 NUMERICAL TREATMENT

We developed two different methods for the numerical treatment of time dependent ionization in the SPH calculations. Both have in common the method of finding paths from the ionizing source to the particles, along which the optical depth for the Lyman continuum photons can be calculated. They differ in the way the ionization rate is determined given the radiation field. Method A uses the SPH formalism to calculate the divergence of the radiation field in Eq. (3). In method B we adopt a different approach also used in grid methods, where we derive the ionization rate from the difference in the numbers of photons entering and leaving a particle.

### 3.1 Finding the evaluation points on the path towards the source

First, we specify the position, the rate of ionizing photons \( S_{\text{ion}} \) and \( \hat{s} \) (from Eq. (4)) of the source.

For each particle \( i \) we now proceed in the following way (see Fig. 1B): Given the list of nearest neighbours of particle \( i \), which has to be determined anyway for the SPH formalism, we look for the particle \( j \) in the list, closest to the line of sight defined by the smallest angle \( \Theta \) between the line connecting the particles \( i \) and \( j \) and the line of sight. We choose the angle between, not the distance from, the line of sight, since we are interested in controlling the error in the direction towards the source. This is not guaranteed by the latter criterion.

We store this particle in a list and determine the evaluation point \( S_k \) as the projected particle position on the line of sight. To determine the next evaluation point \( S_k \) even closer to the source we now repeat this method using the neighbor list of particle \( j \) and so forth until we reach the source.

### 3.2 Calculating the optical depth and ionization rate for the particles

#### 3.2.1 Method A: SPH formalism method

Now the path from the source to particle \( i \) is known, and the integration of Eq. (1) can be discretized by using the evaluation points \( S_k \). The value for \( n_{\text{H}} \) can be estimated by using the SPH smoothing formalism:

\[ n_{\text{H}}(r) = \sum s_{\text{H},i} W(r - r_i), \]

where the sum runs over the particle corresponding to the evaluation point and its nearest neighbours. \( W \) is the weight factor for each neighboring particle provided by the smoothing kernel. We calculate the optical depth along the line of sight by applying the Trapezian Formula, until we reach particle \( i \):

\[ \tau_{k+1} = \tau_k + \frac{1}{2} \hat{s} (s_{k+1} - s_k) \left( n_{\text{H},k+1} + n_{\text{H},k} \right), \]

with \( s_k \) being the position of the evaluation point on the line of sight. Note that this treatment neglects the effects of scattering of the ionizing photons by recombination or dust.

The distance between two successive evaluation points is smaller or equal to the local smoothing length, which determines the largest distance of the particles included in the nearest neighbour list as well as the spatial resolution. This guarantees that the line of sight integration of Eq. (1) is discretized into a reasonable amount of substeps, consistent with the resolution given by the underlying particle distribution.

The flux of ionizing photons at the position of particle \( i \) in the direction of photon propagation \( \hat{e}_s \) is then given by:

\[ J_i = J_0 \cdot \hat{e}_s \cdot \exp (-\tau(s)). \]

With the ionizing flux known at the particle positions, the nabla operator in Eq. (3) can be calculated by the SPH formalism. It is given for each particle \( i \) as the sum over its neighbours:

\[ \mathcal{I}_i = - \sum \frac{n_{\text{H},i} J_{ji}}{\rho_i} \cdot \nabla_i W_{ji}. \]

Now we are able to solve Eq. (3) which we write as:

\[ \frac{d\alpha}{dt} = \mathcal{I}_i - n_{\text{H},i} \alpha_B. \]

The time scale for the establishment of ionization equilibrium is given by \( 1/(n_\alpha) \), which is regularly much shorter than the dynamical and gravitational timescales we are interested in. In order to avoid small timesteps arising from the usage of explicit methods, we use an implicit scheme. The first order discretization of Eq. (3) over a time interval \( \Delta t \) is given by:

\[ x_i^{n+1} = x_i^n + \Delta t \cdot (x_i^{n+1} - n_{\text{H},i}^{n+1} \alpha_B), \]

where the indices \( n \) and \( n+1 \) denote the values at the beginning and the end of the actual timestep \( \Delta t \), respectively. We already know all the values on the right hand side from advancing the particles by the SPH formalism, except the value
for $I_i^{n+1}$. Therefore a fully consistent implicit treatment is not feasible. We use the following guess for this value:

$$I_i^{n+1} = I_i^n \frac{1 - \exp\left(-n_i^{n+1} \sigma a_i^{n+1} (1 - x_i^n)\right)}{1 - \exp\left(-n_i^{n+1} \sigma a_i^{n+1} (1 - x_i^n)\right)}.$$  \hspace{1cm} (11)

In this equation, we assign an effective radius $a_i$ to each particle $i$ proportional to the mean particle separation, given by $a_i = (M_i/\rho_i)^{1/3}$. This is the estimate of the size of a region with the particle mass $M_i$ and density $\rho_i$. The factor with the exponentials on the right hand side accounts for the effect of higher absorption and hence ionization rate with decreasing ionization fraction.

We must use the effective radius $a_i$, instead of the smoothing length $h$, since the method works analogous to implementations in grid codes. In contrast to the SPH formalism, each particle now represents a volume of total mass $M_i$ and density $\rho_i$, in which ionizing radiation enters on one side and leaves on the opposite side. The size of this volume is given by $a_i$ as defined above. It is proportional to the particle spacing.

In contrast, $h_i$ differs from the mean particle separation as it is defined by the condition that there is a fixed number of neighbors $N_{\text{neigh}}$ of mass $M$ in the sphere with radius $2h_i$ and is thus given as

$$h_i = \left(\frac{3N_{\text{neigh}}M}{32\pi\rho}\right)^{1/3}.$$  

It depends on $N_{\text{neigh}}$ and can therefore not be used instead of $a_i$ in Eq. (11).

One consequence of the discretization of the ionization rate equation is that the solution in ionized regions tends to oscillate around the equilibrium value. In order to avoid small timesteps arising from this, we set the ionization fraction $x$ of particles with an $x > 0.95$ to the equilibrium value $x_E$, which is defined by $dn_e/dt = 0$ in Eq. (3)

$$\frac{dx}{dt} = \frac{1}{n} \frac{dn_e}{dt} = \sigma(1 - x_E)J - nx_E^2 \alpha B = 0.$$  

With $k = \sigma J/(n\alpha B)$ follows that

$$x_E = \frac{1}{2} \left[(k^2 + 4k)^{1/2} - k\right].$$

This method works well in absolutely smooth, noise free particle distributions. However, if one wishes to initially distribute the particles randomly in space, one runs into problems. The sum in Eq. (3) is very sensitive to noisy particle distributions. Eventually the noise can be so high, that the error of the sum introduced by noise reaches the order of the sum itself. The ionization rate then locally drops below zero for some particles, which can only be avoided by smoothing the ionization rate spatially over several smoothing lengths. The result is poor resolution. We circumvent this problem in method B.

3.2.2 Method B: grid based method

In this case, a different method is used to discretize the calculation of the optical depth. We determine the positions of the evaluation points $i$ along the line of sight as described in Sect. 3.1 and calculate the hydrogen density $n_{H,1}$ at these positions using Eq. (3). The path is then divided into pieces with length $\Delta s_i = (s_i+1 - s_i-1)/2$, assuming a constant hydrogen density $n_{H,1}$ along each interval. The optical depth for one piece can then be approximated by

$$\Delta \tau_i = \sigma n_{H,1} \Delta s_i.$$  

These contributions to the optical depth are summed up until we reach the position located one effective radius $a_i$ before the position of particle $k$. A first order approximation for the ionization rate is now given by

$$I_k = \frac{J_0}{2a_k n_k} \exp \left(\tau_{k-a}\right) \left(1 - \exp \left(-\Delta \tau_k\right)\right),$$

where $\tau_{k-a} = \sum \Delta \tau_i$ denotes the optical depth one effective radius before the particle’s position and $\Delta \tau_k = 2a_k n_{H,k} \sigma$ the optical depth across the particle.

With the ionization rate derived above we solve the ionization rate equation as described for case A. One can easily show that Eqs. (11) and (11) now give the exact implicit first order discretization for Eq. (3). The solution now approximates the equilibrium value $x_E$ in the ionized regions without the instabilities mentioned in method A. It is not necessary to set $x$ artificially to $x_E$. 

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the source to $S_j$. Thus no integration is needed for this part of the path. One only has to make sure that $\tau_j$ is already known, i.e. that the line of sight integration for particle $j$ has been performed earlier. In this case, the average number of evaluation points $I$ per line of sight only depends on $\Theta_{\text{tol}}$ for large $N$. As shown in Fig. 3, $I$ becomes constant for large $N$ and decreases with increasing $\Theta_{\text{tol}}$. As soon as $I$ becomes independent of $N$ the total computational effort for all lines of sight together scales as $\propto N$.

We demonstrate the effects of using the tolerance angle on the accuracy of the ionization rate calculation in Fig. 3. Histograms are plotted for the errors in $I$ and $\tau$ for calculations with $\Theta_{\text{tol}} = 0.5^\circ, 1^\circ, 2^\circ$ and $90^\circ$ compared to $\Theta_{\text{tol}} = 0^\circ$. As the particle distribution we chose the evolved state of a numerical simulation which studies the compression and collapse of a dense clump within the UV field of an OB association using 200 000 particles. The results of this calculation will be presented elsewhere (Kessel & Burkert 1999). Note that $\Theta_{\text{tol}} = 90^\circ$ represents the worst case, since the tolerance angle criterion now is fulfilled for every particle with minimal $\Theta$ per search through the nearest neighbour list.

The particles which are most affected by the tolerance angle criterion lie next to the borders of shadows cast by optically thick regions, since here the path for the integration along the line of sight may be bent through the optically thick region, thus decreasing the ionizing flux artificially. In the opposite case, the path may lead around the opaque region, increasing the ionizing flux at the position of a particle in the shadow. These extreme cases lead to the tail in the error histograms in Fig. 3. Applying the tolerance angle criterion thus numerically blurs shadows.

The mean errors in $\tau$ are 1.3 per cent for $\Theta_{\text{tol}} = 0.5^\circ$, 2.2 per cent for $\Theta_{\text{tol}} = 1.0^\circ$, 3.4 per cent for $\Theta_{\text{tol}} = 2.0^\circ$ and 11.2 per cent for $\Theta_{\text{tol}} = 90^\circ$. The corresponding mean errors in $I$ are 2.8, 4.1, 5.7 and 13.3 per cent, respectively. For the remaining test cases presented in this paper the choice of $\Theta_{\text{tol}}$ has no effect, since they deal with one-dimensional problems, in which the optical depth is only a function of distance from the source. Applying the tolerance angle criterion only shifts the evaluation points from the lines of sight in directions perpendicular to these, along which there is no change in the optical depth. Indeed even the choice $\Theta_{\text{tol}} = 90^\circ$ gives the same results in the one-dimensional test cases as for $\Theta_{\text{tol}} = 0^\circ$. Thus the errors introduced by the angle criterion must be checked with problems in which this symmetry is broken and shadows are present, as the one mentioned above.

3.4 Smoothing the ionization front

For reasons of noise reduction we smooth the ionization front, which is not resolvable by the SPH representation, over a distance of the order of one local smoothing length. Nature provides a simple way for doing this. The width of the ionization zone is of the order of one photon mean free path length,

$$d = (\bar{\sigma} \cdot n_H)^{-1},$$  \hspace{1cm} (12)$$

where $\bar{\sigma}$ is the net absorption cross section for ionizing photons as defined in Eq. 8.

Since we cannot resolve the ionization region anyway, we are free to adjust $\sigma$ in a way that the width of the ion-
tronization of the order of $600 \text{ km s}^{-1}$, the thermalization timescale for the energies of the ejected electrons is far less than a year for densities of 1 particle cm$^{-3}$, which is many orders of magnitude smaller than the dynamical timescale. Thermalization thus occurs quasi instantaneously. This process runs even more rapidly for higher densities. Thus we are allowed to treat the gas behind the ionization front as thermalized.

We set the internal energy to:

$$e = x \cdot e_{10000} + (1 - x) \cdot e_{\text{cold}},$$

with $e_{10000}$ being the internal energy corresponding to a temperature of 10000 K for ionized hydrogen, and $e_{\text{cold}}$ to the internal energy for the 10 K cold, neutral gas. Note that this method does not properly treat recombination zones, since in this case one needs the correct inclusion of the heating and cooling processes in order to achieve the correct gas temperatures, sound velocities and pressures. Also, the equilibrium temperature in HII-regions can vary by 20 per cent from this value. These deviations can also only be taken into account by proper treatment of heating and cooling.

4 TESTS OF THE NUMERICAL TREATMENT

Although being of one-dimensional nature, the following test problems were performed fully in three dimensions.

4.1 Test 1: Ionization of a slab with constant density

With this problem we test the implementation of the time-dependent ionization rate equation by ionizing a slab of H I gas of constant density $n$ with ionizing radiation falling perpendicular onto one of the boundary surfaces. With hydrodynamics switched off, we let the ionization front traverse the slab with a constant velocity $v_t$. To achieve this, we have to vary the infalling photon flux with time. It is given by

$$J(t) = J_i + J_t = n v_i + n^2 \alpha B v_t t,$$

where the first term on the right hand side is the flux which provides the photons being absorbed in the ionization front. The second, time-dependent term equals the loss of photons on their way through the slab until they reach the front.

For the initial setup we place a number $N$ of particles randomly into a slab with length-to-height and length-to-width ratios of 10. Subsequently we let the particle distribution relax by evolving it isothermally within the slab, adding a damping term to the force law. This is necessary to diminish the numerical noise which was introduced by the random distribution. We now have an ensemble of the particles which does not possess any privileged directions and which represents a gas of constant density and temperature. We use this distribution as our starting configuration. From now on we keep the particles fixed in space and switch off hydrodynamics.

The test was performed for a total number of $N = 2000, 16000$ and 128000 particles. Since the spatial resolution for SPH calculations scales as $N^{-1/3}$ (with number of neighbours $N_{\text{neigh}}$ per particle fixed), this yields an increase of linear resolution of a factor of two from one simulation to the simulation with next higher resolution. The results of these tests are shown in Fig. 5.
The mean relative errors between the theoretical result and the calculations decrease linearly with increasing resolution, consistent with our first order discretization of both the line of sight integration and the time dependent ionization equation. The error also decreases with time as the representation of the ionization front gets thinner and thinner compared to the already ionized region. The spread in the errors for $N = 16000$ and $N = 128000$ results from the fact that in these cases the numerical solution oscillates around the theoretical solution, sometimes being larger than the latter, sometimes smaller.

4.2 Test 2: Ionization of a slab with density gradient

We proceed as in test 1, with the difference that we choose a slab with a constant density gradient in the direction of photon propagation. We choose the time dependence of $J$ such that the ionization front should travel through the gas with constant $v_i$. $J$ is given by:

$$J(t) = n_0 v_i + \left( \alpha_B n_0^2 + \frac{d}{dx} n_i \right) v_i t + \alpha_B n_0 \frac{d}{dx} n_i v_i^2 t^2 + \alpha_B \left( \frac{d}{dx} n_i \right)^2 v_i^3 t^3,$$

where $n_0$ denotes the density at the surface where the radiation penetrates the slab and $\frac{d}{dx} n_i$ is the density gradient.

In Fig. 6 we plot the ionized mass for the theoretical solution and the numerical simulations against time. The numerical results converge against the theoretical solution with increasing resolution. The deviations at $t > 0.9$ are caused by the ionization front reaching the rear boundary of the slab.

Note that the version of SPH used in this paper is not able to follow ionization fronts exactly which travel faster than one local smoothing length per time step. This must be taken into account during the timestep determination. In applications with fast ionization fronts (typically R-type fronts in the early phases of the evolution of HII-regions) this criterion can lead to very small timesteps and thus to a high amount of CPU time needed. A version which circumvents this problem is being developed.

4.3 Test 3: Coupling of ionization and hydrodynamics

For this test we adopt the problem mentioned by Lefloch & Lazareff (1994). A box filled with atomic hydrogen of particle density $n_0 = 10 \text{ cm}^{-3}$ and temperature $T_{\text{cold}} = 100 \text{K}$ is exposed to ionizing radiation, with the photon flux increasing from zero linearly with time with a rate $d\Phi/dt = 5.07 \cdot 10^{-2} \text{ cm}^{-2} \text{s}^{-2}$. There exists an analytical solution to this problem, which is self similar in the sense that physical...
values at position $x$ measured in the direction of the photon flow at time $t$ are only functions of $x/t$. This means: the structure is stretched with time. The convergence of the code towards the correct solution with increasing resolution can be tested in one calculation, since for all appearing structures the ratio between structure sizes and smoothing lengths increases linearly with time.

The resulting structure is the following: an isothermal slab of their calculations, from which they derived their result: ionizing radiation infall from the left. Solid line: analytical result. Ratio of the thickness of the swept-up layer to the current local smoothing length for different resolutions: dotted 6, dashed 12, dash-dot 20. Corresponding times in code units: 0.34, 0.70, 0.93, 1.0.

![Figure 7. Velocity profile for test case 3 and different resolutions. Unit of the x-axis normalized to the position of the shock front. Ionizing radiation infall from the left. Solid line: analytical result. Ratio of the thickness of the swept-up layer to the current local smoothing length for different resolutions: dotted 6, dashed 12, dash-dot 20. Corresponding times in code units: 0.34, 0.70, 0.93, 1.0.](image)

The method presented in this paper allows the treatment of the dynamical effects of ionizing radiation in SPH calculations. Thus the study of astrophysical problems arising from ionization, like the impact of ionizing radiation from newly born stars onto the evolution of their parental molecular clouds or the more consistent treatment of heating by OB associations in galaxy dynamics calculations are now feasible for the first time with SPH in 3 dimensions. We use the same method as described in Sect. 4.3 to produce the initial conditions. No gas is allowed to enter or leave the surface.

Table 1 lists the result of this comparison. The SPH calculation slightly underestimates $V_4$ and $V_5$, as is also observed for the grid code. The errors of order 5 per cent are comparable to those achieved by Lefloch & Lazareff (1994).

In the early phases, i.e. low resolution, the poor treatment of the ionization front leads to irregularities in the ionized region and thus produces sound waves travelling back and forth between the boundary to the left and the ionization front (Figs. 4, 5), which decrease in power as time increases, i.e. at higher resolution. With increasing resolution, i.e. increasing ratio of layer thickness to smoothing length, the representation of the dense layer and the shock front improves (Figs. 6, 7).

![Figure 8. Density of the layer for test case 3. Unit of the x-axis normalized to the position of the shock front. Ionizing radiation infall from the left. Solid line: analytical result. Ratio of the thickness of the swept-up layer to the current local smoothing length for different resolutions: dotted 6, dashed 12, dash-dot 18, dash-dot-dot-dot-dot 20. Corresponding times in code units: 0.34, 0.70, 0.93, 1.0.](image)

Table 1. Comparison of analytical and numerical results for test case 3.

| Parameter | Value |
|-----------|-------|
| $n_i$ ($\text{cm}^{-3}$) | 0.756 |
| $n_e$ ($\text{cm}^{-3}$) | 1.59 $\cdot$ 10$^2$ |
| $V_4$ ($\text{km s}^{-1}$) | 3.71 |
| $V_5$ ($\text{km s}^{-1}$) | 3.48 |

| Parameter | Value |
|-----------|-------|
| $n_i$ ($\text{cm}^{-3}$) | 0.75 $\pm$ 0.05 |
| $n_e$ ($\text{cm}^{-3}$) | 1.55 $\pm$ 0.05 $\cdot$ 10$^2$ |
| $V_4$ ($\text{km s}^{-1}$) | 3.67 $\pm$ 0.05 |
| $V_5$ ($\text{km s}^{-1}$) | 3.36 |

5 SUMMARY

The method presented in this paper allows the treatment of the dynamical effects of ionizing radiation in SPH calculations. Thus the study of astrophysical problems arising from ionization, like the impact of ionizing radiation from newly born stars onto the evolution of their parental molecular clouds or the more consistent treatment of heating by OB associations in galaxy dynamics calculations are now feasible for the first time with SPH in 3 dimensions. We demonstrate that the code is able to treat time-dependent ionization, the related heating effects and hydrodynamics correctly. Our first applications, detailed calculations of photoionization induced collapse in molecular clouds and results...
Ionizing radiation in SPH

Figure 9. Velocity profile for test case 3. Unit of the x-axis normalized to the position of the shock front. Ionizing radiation infall from the left. Solid line: analytical result. Ratio of the thickness of the swept-up layer to the current local smoothing length for different resolutions: dotted 6, dashed 12, dash-dot 18, dash-dot-dot 20. Corresponding times in code units: 0.34, 0.70, 0.93, 1.0.

obtained from them, will be presented in a subsequent paper.

To allow the correct treatment of recombination zones, one has to include the effects of time dependent heating and cooling processes by ionization and recombination, emission of forbidden lines and thermal radiation from dust. Another important aspect which was neglected here is the effect of the diffuse Lyman continuum recombination field. It can lead to the penetration of regions shielded from the direct ionizing radiation by the ionization front, which is e.g. seen in calculations of photoevaporating protostellar disks (Yorke & Welz 1996; Richling & Yorke 1998). An implementation of these processes into our SPH code is planned in the future.

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