iVINE – Ionization in the parallel TREE/SPH code VINE: first results on the observed age-spread around O-stars

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ABSTRACT
We present a three-dimensional, fully parallelized, efficient implementation of ionizing ultraviolet (UV) radiation for smoothed particle hydrodynamics (SPH) including self-gravity. Our method is based on the SPH/TREE code VINE. We therefore call it iVINE (for Ionization + VINE). This approach allows detailed high-resolution studies of the effects of ionizing radiation from, for example, young massive stars on their turbulent parental molecular clouds. In this paper, we describe the concept and the numerical implementation of the radiative transfer for a plane-parallel geometry and we discuss several test cases demonstrating the efficiency and accuracy of the new method. As a first application, we study the radiatively driven implosion of marginally stable molecular clouds at various distances of a strong UV source and show that they are driven into gravitational collapse. The resulting cores are very compact and dense exactly as it is observed in clustered environments. Our simulations indicate that the time of triggered collapse depends on the distance of the core from the UV source. Clouds closer to the source collapse several 10^5 yr earlier than more distant clouds. This effect can explain the observed age spread in OB associations where stars closer to the source are found to be younger. We discuss possible uncertainties in the observational derivation of shock front velocities due to early stripping of protostellar envelopes by ionizing radiation.

Key words: radiative transfer – methods: numerical – stars: formation – H II regions – ISM: kinematics and dynamics – ultraviolet: ISM.

1 INTRODUCTION
As hydrodynamical simulations become more and more advanced, one of the key issues is the successful implementation of additional physics like the effects of radiation. Prominent applications are for example the re-ionization of the early Universe (for a comparison of methods see Iliev et al. 2006, and references therein).

In our present day universe ionizing radiation still plays a vital role. ultraviolet (UV) radiation from massive, young stars ionizes their surrounding. The hot, ionized gas then expands into the cold, neutral gas and thus drives shock fronts into the parental molecular clouds. Up to now, it is not fully understood if this violent feedback enhances or hinders star formation. Elmegreen & Lada (1977) proposed that the shock front builds up dense regions by sweeping up the cold gas, which then eventually collapse due to gravitational instability and form stars. This is called the ‘collect and collapse model’ (see also the review by Elmegreen 1998). Another situation arises when pre-existing, dense structures (e.g. molecular cloud cores) that are gravitationally marginally stable get compressed by the approaching front and start collapsing. This is commonly called radiation driven implosion (see e.g. Sandford, Whitaker & Klein 1982).

Observations provide widespread evidence for these scenarios (Sugitani et al. 1989, Hester et al. 1996). More recent observations indicate triggered star formation on the edges of H II regions for example in the Orion clouds (Stanke et al. 2002), the Carina nebula (Smith et al. 2000), M16 (Fukuda, Hanawa & Sugitani 2002), M17 (Jiang et al. 2002), 30 Dor (Walborn, Maíz-Apellániz & Barbá 2002) and the SMC (Small Magellanic Cloud; Gouliermis et al. 2008). Deharveng, Zavagno & Caplan (2005) report triggered star formation in samples of more distant H II regions. Besides these quite complex large-scale regions, there have been numerous observations of bright rimmed cometary globules. These are small isolated clouds with a clear head to tail structure with the dense heads pointing towards an ionizing source (Sugitani, Fukui & Ogura 1991). Their morphology enables a direct comparison to simulations. In particular, the properties of individual young stellar objects (YSOs) surrounding OB associations can be determined precisely. YSOs are observed in the mass range from T Tauri (0.1–3 M\(\odot\)) up to Herbig Ae Be (2–8 M\(\odot\)) stars (see e.g. Lee & Chen 2007; Snider et al. 2007). The velocity of the shock front triggering the star...
formation is calculated from the age difference of the stars and their relative distance. These estimates are in the range of a few km s\(^{-1}\) (e.g. Thompson et al. 2004; Getman et al. 2007).

Numerous simulations on the topic of cloud evaporation and sequential star formation have been performed. York, Bodenheimer & Tenorio-Tagle (1982) (and references therein) published a series of two-dimensional simulations on the gas dynamics of \(\text{HII}\) regions, especially on champagne flows, where a stream of hot gas breaks through the border of cold, confining gas. Subsequently, Elmegreen, Kimura & Tosa (1995) presented two-dimensional, grid-based simulations showing that the expansion of an \(\text{HII}\) region into the surrounding cloud can trigger star formation. Kessel-Deynet & Burkert (2003) demonstrated with a three-dimensional \(\text{SPH}\) code, that a marginally stable molecular core can be triggered into collapse when exposed to strong UV radiation. With a more detailed description of radiation implemented into an \(\text{SPH}\) code Miao et al. (2006) could reproduce the observed features of the Eagle Nebula, including the photodissociation regions and the temperature profile. Using a three-dimensional grid-based scheme, Mellema et al. (2006) simulated the \(\text{HII}\) region excavated by a point source of UV radiation. They find remarkably similar morphologies and physical properties when comparing their models to observations. Furthermore, simulations with an \(\text{SPH}\) code by Dale et al. (2005) and a grid code by Mac Low et al. (2007) showed that a turbulent interstellar medium surrounding an O-star allows the ionizing radiation to efficiently expel most of the nearby gas. Only the denser regions resist and continue to collapse.

However, none of the authors so far described ionizing radiation as an efficient trigger for star formation. There is only weak evidence by Dale, Clark & Bonnell (2007), that the external irradiation of a collapsing cloud by a point source can indeed increase the star formation efficiency from 3 to 4 per cent when compared to a control run without radiation. For a review of feedback processes, we refer the reader to Mac Low (2007). For completeness, we would like to refer to recently published implementations for ionizing radiation into an \(\text{SPH}\) code by Pawlik & Schaye (2008), where the photons of a source are followed along cones, and Altay, Croft & Pelupessy (2008), where the radiation is followed via a Monte Carlo ray-tracing scheme.

All of these studies demonstrate that there is a strong connection between the UV-radiative feedback from massive stars and the observed morphologies of the ambient molecular cloud gas. Yet, a quantitative discussion of the interaction between UV radiation and turbulent molecular clouds is still missing. To advance our understanding, we introduce IVINE, the fully parallel implementation of UV radiation in the parallel TREE-\text{SPH}-code VINE (Wetzstein et al. 2008; Nelson, Wetzstein & Naab 2008). This efficient tool permits high-resolution simulations of molecular clouds in the vicinity of strong UV sources such as an O-star or association.

The paper is structured as follows. The physical model and its implementation are described in Section 2, followed by a detailed comparison of the scheme with analytical results (Section 3). We apply the new method to the radiatively driven implosion of a marginally stable molecular cloud core and compare three simulations with different initial UV fluxes to observations (Section 4). In Section 5, we summarize and discuss the results.

2 NUMERICAL METHOD

As soon as a young massive star emits UV radiation, it ionizes its surrounding, creating an \(\text{HII}\) region. Initially, the ionization proceeds fast with a speed of this rarefied (or R-type) front of \(v_\text{R} \gg a_{\text{Hor}}\), where \(a_{\text{Hor}}\) is the sound speed of the hot, ionized gas. After a sound crossing time-scale, the hot gas reacts to its increased temperature and an isothermal shock front is driven into the cold surrounding medium. This dense (or D-type) shock travels at a much smaller speed \(v_\text{D} \approx a_{\text{Hor}}\). For a full textbook analysis of this evolution see for example Osterbrock (1989).

2.1 Description of radiation

To follow the evolution of the \(\text{HII}\) region of a young massive star in a numerical simulation, we use a prescription for the ionizing UV radiation similar to the one proposed by Kessel-Deynet & Burkert (2000) as presented before (Gritschneder et al. 2007). The flux \(J\) at any given position \(x\) is given by

\[
J(x) = J_{\text{Ly}} e^{-\tau_{\nu}(x)},
\]

where \(J_{\text{Ly}}\) is the Lyman continuum flux of the hot star. The optical depth \(\tau_\nu\) is given by the integral along the line of sight between the source of radiation and the position \(x\)

\[
\tau_\nu = \int_0^x k_\nu \rho \, dx,
\]

where \(k_\nu\) is the frequency weighted absorption coefficient

\[
k_\nu = \frac{\sigma_v n_\text{H}}{\rho},
\]

with \(n_\text{H}\) being the number density of neutral hydrogen and \(\rho\) the mass density of the gas. We assume the gas is pure hydrogen with a mean molecular weight of \(\mu = 1\). As the frequency dependent absorption cross-section \(\sigma_v\) peaks at the Lyman break, it is a valid assumption to take an average cross-section \(\bar{\sigma}\), thereby approximating the radiation to be monochromatic. Thus, every photon above the Lyman break is assumed to ionize one hydrogen atom.

We define the ionization degree \(\eta\) as

\[
\eta = \frac{n_e}{n},
\]

where \(n_e\) is the number density of electrons and \(n\) is the combined number density of protons and neutral hydrogen atoms. The time derivative of the ionization degree can be written as

\[
\frac{dn_e}{dt} = \frac{1}{n} \frac{dn}{dt} = \frac{1}{n} (I - R),
\]

with the ionization rate \(I\) given as

\[
I = \nabla J
\]

and the recombination rate \(R\) as

\[
R = n_e^2 \alpha_b = \eta n_e^2 \alpha_b.
\]

For the recombination coefficient \(\alpha_b\), we choose

\[
\alpha_b = \sum_{i=2}^{\infty} \alpha_i,
\]

where \(\alpha_i\) is the recombination probability for a level \(i\) of the hydrogen atom. The recombination of electrons and protons leads to a diffuse field of Lyman continuum photons, which in turn can again ionize a hydrogen atom. We neglect this effect under the assumption that every re-emitted photon is in turn immediately absorbed in the direct surrounding. This assumption, called ‘on the spot approximation’ is valid as long as the hydrogen density is high enough (e.g. Spitzer 1978), which is always true in the vicinity of the ionization front. Some fraction of the UV photons is absorbed by dust, and re-emitted in the infrared regime, leading to an effective lower
density throughout the entire simulation this guarantees that the bin size is always larger than the characteristic particle resolution. As soon as the ray approaches a density increase, the local \( d_{\text{part}} \) becomes smaller than \( \Delta y \) and \( \Delta z \). For

\[
\frac{d_{\text{part}}}{\Delta y} = \frac{d_{\text{part}}}{\Delta z} < \frac{1}{2}
\]

(12)

We refine the ray subsequently into four subrays to treat the ionization of high density regions correctly. Each of the subrays inherits the optical depth of the main ray. Currently, the code allows for five levels of refinement, thus increasing the effective bin resolution in each direction by a factor of 32. In principle, it would be possible to derefine the subrays by using the average optical depth of the four refined subrays for the derefined bin. We do not include this, since it would lead to an unphysical shading of lower density subrays as soon as they are combined with a high density subray due to an overestimation of the optical depth.

To calculate the optical depth, we sort the particles within each bin according to their distance to the source and discretize into subsections of the size

\[
\Delta x_i = \frac{x_{i+1} - x_{i-1}}{2}
\]

(13)

Thus, \( \Delta x_i \) is the projected distance of a particle \( i \) to its direct neighbours closer and further away from the source, that is the length along the line of sight the particle occupies. We then calculate the optical depth \( \tau \) along each ray by summing up the individual optical depths \( \tau_i \) of each particle \( i \). The discrete value of \( \tau_i \) is given according to equation (2) as

\[
\tau_i = \sigma n_{\text{H,i}} \Delta x_i
\]

(14)

The number density \( n_{\text{H}} \) and the density \( \rho \) used to calculate the recombination rate (cf. equation 7) are simply given by the SPH density \( \rho_{\text{SPH}} \). From these quantities, the new ionization degree \( \eta \) is determined according to equation (2) by a Newton–Raphson iteration scheme. It converges with a precision of more than 0.1 per cent in less than 200 iterations. When the ionization degree reaches a value of \( \eta = 1 \times 10^{-3} \), we terminate the further calculation of this bin. This implementation is fully parallelized in OpenMP.

### 2.3 Modification of the time-step criterion

A detailed discussion of the different time-step criteria implemented in the underlying VINE code is given in Wetzstein et al. (2008). Note that our implementation of ionizing radiation is designed to be used in connection with individual particle time-steps (see Wetzstein et al. 2008, for details). To exactly follow the evolution of a particle during its ionization process, it is vital to use a small enough time-step. To do so, we decided to force every particle to a smaller time-step as soon as its ionization degree reaches \( \eta > 10^{-5} \), i.e. when the particle is going to be ionized. The new time-step is chosen by a modified Courant–Friedrichs–Lewy (CFL) condition according to

\[
\Delta t_{\text{new}} = \frac{a_{\text{cold}}}{a_{\text{hot}}} \Delta t_{\text{CFL}}
\]

(15)

where \( a_{\text{cold}} \) and \( a_{\text{hot}} \) are the fixed respective sound speeds of the cold and the ionized gas at \( T_{\text{cold}} \) and \( T_{\text{hot}} \). \( \Delta t_{\text{CFL}} \) is the individual time-step the particle would get assigned due to the CFL condition (see Wetzstein et al. 2008). This ensures that the hydrodynamical quantities are treated correctly even though the particle gets a boost in temperature. Therefore, we anticipate the subsequent acceleration due to the approaching ionization front by choosing already the much smaller time-step even though the particle is just ionized to 0.1 per cent. This criterion also ensures that the ionization degree is
followed accurately during the evolution of the later dense or D-type ionization front because \( v_D \) is always smaller than the sound speed of the hot gas \( v_D < a_{\text{hot}} \). Hence, this front will always be resolved by particles which have a small enough time-step to track the hot gas. In the beginning, the evolution of the faster R-type front (\( v_R \gg a_{\text{hot}} \)) can be followed by using a small enough initial time-step since this phase is quite short (\( \approx 5 \text{ kyr} \)).

The choice of a small initial time-step together with the modified CFL criterion ensures that the ionization degree \( \eta \) of a particle never changes by more than \( \pm 0.1 \) per time-step in all of our simulations. Thus, the ionization front can be followed in both stages (R- and D-type) precisely.

### 3 NUMERICAL TESTS

In order to validate the algorithm, we perform several tests. The first series of simulations addresses the evolution of the Strömgren solution and tests whether the time-dependent UV flux is treated correctly on all scales. In addition, we demonstrate the correct implementation of the refinement (Section 3.1). The second series of simulations (Section 3.2) is designed to demonstrate the correct interaction of ionizing radiation and hydrodynamics. In the end, the successful parallelization of the code is shown (Section 3.3).

#### 3.1 Ionization without hydrodynamics

##### 3.1.1 The Strömgren test – Ionization by a constant UV flux

When hydrodynamics is not taken into account, the homogeneous surrounding of an ionizing source will always converge towards an equilibrium between ionization and recombination. The volume of the ionized Strömgren sphere (Strömgren 1939) around an O-star is given by

\[
V = \frac{J_L}{\alpha_B n^2},
\]

assuming a monochromatic source with a constant UV-flux \( J_L \) given in photons per second. \( \alpha_B \) and \( n \) are again the recombination coefficient and the number density (for a textbook analysis see e.g. Shu 1991).

In the case of plane-parallel radiation, as discussed here, this volume is characterized by the length \( x_s \), which can be penetrated by the ionizing radiation. \( x_s \) is determined by the surface \( S \) on which the photon flux per area and time, \( F_{1,\text{Ly}} \), is impinging:

\[
x_s = \frac{V_s}{S} = \frac{F_{1,\text{Ly}}}{\alpha_B n^2}.
\]

The time evolution of the length \( x_s(t) \) of this region is given by the differential equation

\[
\frac{dx_s}{dt} n = F_{1,\text{Ly}} - x_s(t) \alpha_B n^2
\]

with the solution

\[
x_s(t) = x_s(1 - e^{-t/t_{\text{rec}}}),
\]

where \( t_{\text{rec}} = 1 / (n \alpha_B) \) is the recombination or Strömgren time-scale. The shape of the front is given by the ionization equilibrium equation

\[
n(1 - \eta) \int_{V_s} F_{\text{Ly}}, \sigma, \text{d}v = n^2 \eta^2 \alpha_B,
\]

which can be rewritten for the plane-parallel, monochromatic case in terms of the ionization degree (cf. equation 4) as

\[
\frac{dn}{dv} = \eta \frac{1 - \eta}{1 + \eta} n \sigma x_s.
\]

This equation can be solved numerically and gives the ionization degree \( \eta \) at any given position \( x \) for the chosen number density \( n \) and mean cross-section \( \sigma \).

To test the code, we ran three simulations.

(i) Case A: 125 k particles placed on a Cartesian grid.

(ii) Case B: 100 k particles placed randomly.

(iii) Case C: 250 k particles placed randomly.

For the cases B and C, the particles are placed randomly in the simulation box and then are allowed to relax with periodic boundaries and the inclusion of hydrodynamics for one crossing time-scale to dampen the numeric random noise. Thereafter, we switch off the hydrodynamics and compute the ionization. For all simulations, we used a mean density \( n = 10 \text{ cm}^{-3} \). The simulated volume is \( (2 \text{ pc})^3 \), the length the ionization can penetrate is set to \( x_s = 1 \text{ pc} \). The recombination coefficient and the absorption cross-section are set to typical values of \( \alpha_B = 2.7 \times 10^{-15} \text{ cm}^2 \text{ s}^{-1} \) and \( \sigma = 3.52 \times 10^{-18} \text{ cm}^2 \). For the above parameters, \( F_{1,\text{Ly}} = 8.33 \times 10^7 \text{ photons cm}^{-2} \text{ s}^{-1} \) and \( t_{\text{rec}} = 11.8 \text{ kyr} \). The simulations run up to \( t = 5 t_{\text{rec}} \) to allow for a quasi-equilibrium state to evolve.

In Fig. 1, the time evolution of the penetration length \( x_s(t) \) is shown. The position of the front is calculated by projection of the three-dimensional simulation along the \( y \) - and \( z \)-axis on to the \( x \)-axis. Note that the analytical solution (cf. equation 19) is based on the idealized assumption that the medium is fully ionized (\( \eta = 1.0 \)). However, the precise solution of equation (5) in equilibrium (\( dn/dt = 0 \)) is

\[
x_s(\eta^2) = \frac{V_s}{S} = \frac{F_{1,\text{Ly}}}{\alpha_B n^2}.
\]

In our simulations, \( x_s \eta^2 = 1 \text{ pc} \) is realized with \( x_s = 1.05 \text{ pc} \) and \( \eta = 0.976 \). We call this the exact solution whereas the solution assuming \( \eta = 1.0 \) will be referred to as classic solution. Our simulations converge very well towards the exact solution. Case A, where the particles are initially placed on a grid, slightly overestimates the final value of \( x_s \), while the low-resolution simulation (case B) underestimates it. Nevertheless, already with only 100 k this implementation shows a very good agreement with the analytical curve. In the high-resolution simulation (case C), the numerical result lies right on top of the predicted line.

Fig. 2 shows the ionized fraction \( \eta \) and the neutral fraction \( x = 1 - \eta \) after \( t = 5 t_{\text{rec}} \) at the end of the simulation. The numerical solution of equation (21) is evaluated for the exact solution with a
penetration length of $x_c = 1.05$ pc. As expected from Fig. 1, case A overestimates the front position, whereas case B underestimates it. Again the high resolution run C shows the best concordance and we can conclude that these results fit well within the range of the code comparisons done by Iliev et al. (2006). A more direct comparison to this work is not possible due to the plane-parallel nature of the test performed here.1

3.1.2 Ionization by a time-varying source

A more challenging test is the treatment of a time-varying source of ionization. Although this situation is not very realistic for an O-star it nevertheless provides a very good method to test the treatment of ionization. Although this situation is not very realistic for an O-star

Figure 2. Ionization degree $\eta$ ($\approx 1$ at $x/s = 0$) and neutral gas fraction $\chi = 1 - \eta$ versus position for the cases A (red), B (green) and C (blue). The dashed line represents the exact solution.

agreement with the exact solution, the resolution is high enough to keep the noise in the density distribution low and thus the position of the front is followed precisely.

3.1.3 Testing the refinement – Ionization by a constant source in a two-density medium

All tests up to now were independent of the implementation of refinement, since in a constant density medium each particle occupies roughly the same diameter $d_{\text{part}}$ (see Section 2.2). To verify the correct implementation of the refinement, we set up a simulation with a two-density medium. A lower density gas phase with $n_1 = 10$ cm$^{-3}$ is set up in the left half of the box and a higher density medium with $n_2 = 100$ cm$^{-3}$ is placed at the right half of the box. The density contrast is achieved via a different number of SPH particles in the different regions, the particle masses are equal in the entire simulation. The required flux to ionize the simulation domain up to a position $x$ can be calculated by linear superposition according to equation (22)

$$F_{\text{Ly}} = \alpha_B \left( x \right) n_1^2 + \alpha_B \left( x - x_1 \right) n_2^2,$$

where $n_1$ is the density of the low-density region. The simulation is set up with 550k randomly placed particles. The particle noise is reduced for both regions separately as described in Section 3.1.1. The resolution is high enough to keep the noise in the density distribution low and thus the position of the front is followed precisely.

Figure 3. Numerical simulation of an ionization front that moves with constant speed through a medium of constant density. Plotted is the position of the front in units of the box length versus the time in units of the crossing time for the three cases A (red), B (green) and C (blue).

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Nevertheless, the refinement has an important geometric effect, which becomes clear when assuming a density contrast with a discontinuity which is not aligned vertical to the impinging radiation. We perform a test with a diagonal density contrast between two regions with a number density of $n_{\text{low}} = 10$ cm$^{-3}$ and $n_{\text{high}} = 200$ cm$^{-3}$, respectively. Again the particles are placed randomly and the noise is reduced (see Section 3.1.1). A cubic domain of (0.5 pc)$^3$ including 25 k particles is shown in Fig. 4. In the unrefined case (left-hand side), the effect of the original bin size of $\approx 0.05$ pc can be clearly seen as step-like features. With refinement the density contrast of

1Note that in Fig. 2 the neutral fraction $\chi$ converges towards a value of $10^{-2}$ at $x = 0$ pc in both the simulations and the exact solution whereas in Iliev et al. (2006) $\chi$ is reaching much lower values. This is due to the fact that in our simulations the irradiated surface stays constant whereas when simulating a point source this surface and thus $\chi$ can get infinitesimally small.
be calculated from the corresponding sound speeds the ionized, the compressed and the undisturbed medium can then
tions as high as $10^8$.

Eq. (12) and the geometrical bias is already negligible (Fig. 4,
travelling at a constant speed. The number densities
linearly with time. This leads to a hydrodynamical shock wave
area of constant density is ionized by a photon flux which increases
This test was originally proposed by Lefloch & Lazareff (1994). An

3.2 Ionization with hydrodynamics

3.2.1 Steady propagation of an ionizing front

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20 leads to one level of refinement (since $d_{\text{par}}/\Delta y \approx 1/2.7$, cf. equation 12) and the geometrical bias is already negligible (Fig. 4,

right-hand side). In the simulations, in Section 4, all five levels of
refinement lead to spatial resolution of the radiation in our simulations
as high as $10^{-3}$ pc, therefore the radiation does not produce
any unphysical geometrical effects.

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Figure 4. Effect of the refinement on a diagonal density step. Plotted are the
SPH particles in a (0.5 pc)$^3$ volume projected along the $z$-axis. Red: ionized
particles ($\eta > 0.1$), black: unionized particles. Left-hand side: without the
inclusion of refinement. Right-hand side: with the inclusion of one level of
refinement.

\[ \frac{n}{n_0} = \frac{a_0^2}{a_0^2} = \frac{a_0^2}{a_0^2} = \frac{a_0^2}{a_0^2} = \frac{a_0^2}{a_0^2} \]  
(26)

since the compressed and the neutral medium have the same
temperature and thus the same sound speed. At the isothermal shock,
the jump conditions are

\[ u_i (u_i - u_i) = a_0^2, \]
(27)

\[ \frac{n}{n_0} = \frac{u^2}{u_0^2}, \]
(28)

where $u_i$ is the gas velocity just inside the shock. With the approxi-
mation of a thin shock it can be assumed that the ionization front
and the shock front have the same speed $u_i = u_i$. For a detailed
derivation of the jump conditions see for example Shu (1991).
Introducing the time derivative of the ionizing flux $C = dF/dt$, the
speed of the front can be calculated similar to equation (17):

\[ u_i = \frac{Ca_B}{n_0^2} (= u_i). \]
(29)

The jump conditions can then be rewritten to give the following
relations:

\[ n_i = n_i \frac{a_0^2}{a_0^2} = n_0 \left( \frac{C}{\alpha B n_0^2} \right)^{1/5}, \]
(30)

\[ n_i = n_i \frac{a_0^2}{a_0^2} = \frac{n_0 C^2}{\alpha B n_0^2}, \]
(31)

To compare directly to previous results, we used the initial condi-
tions by Lefloch & Lazareff (1994). The density is $n_0 = 100$ cm$^{-3}$,
the temperature is $T_{\text{cold}} = 100$ K. The flux increases linearly with
time at a constant rate of $dF/dt = 5.07 \times 10^{-6}$ cm$^{-2}$ s$^{-1}$, starting

Figure 5. Number density versus position for the steady propagation of an
ionizing front. The dashed line shows the classic solution, obtained by using
a value of $T_{\text{hot,a}} = 10^4$ K for the hot gas. The solid line corresponds to
the analytic solution for a more realistic value of $T_{\text{hot,c}} = 9200$ K for the
hot gas. Blue and green lines show the simulations at different resolutions.

\begin{align*}
    u_1 &= u_s - \frac{a_0^2}{u_0}.
\end{align*}
(32)
Table 1. Comparison of analytical and numerical results for the test including hydrodynamics and ionization. The iVINE data is obtained from the 2 million particle run, the errors given are 1σ. The grid data is taken from Lebloch & Lazareff (1994), the swil data from Kessel-Deynet & Burkert (2000). The analytical values differ from the previous work due to a higher accuracy in our calculations.

|                | Classic | Exact | Grid | swil | iVINE |
|----------------|---------|-------|------|------|-------|
| $n_c$ (cm$^{-3}$) | 147     | 137   | 169  | 155  | 138 ± 6 |
| $n_i$ (cm$^{-3}$) | 0.734   | 0.747 | 0.748| 0.75  | 0.743 ± 0.01 |
| $u_0$ (km s$^{-1}$) | 3.48    | 3.37  | 3.36 | 3.43  | 3.34 ± 0.18 |
| $u_i$ (km s$^{-1}$) | 3.24    | 3.12  | –    | –    | 3.13 ± 0.04 |

3.3 Performance

To test the performance of the parallel iVINE code with increasing number of processors, we choose the simulation described in Section 4 at a later stage and compute one time-step on different numbers of CPUs. The parallel scaling of the various parts of the underlying VINE code is discussed in detail in Nelson et al. (2008). For our test, we use a SGI Altix 3700 Bx2 supercomputer. In total, the ionization uses only a few percent of the total computational time. The precise values range from 2.32 per cent on two CPUs to 2.70 per cent on 16 CPUs and 2.86 per cent on 32 CPUs.

When refinement is used, these values change to 8.52 per cent on 2 CPUs and 8.73 per cent on 32 CPUs. Although the ionization takes up relatively more time in this case, the difference in the calculation time between the numbers of CPUs gets smaller. This is to be expected, as the refinement is calculated inside the bins and part of the implementation is parallelized very efficiently (each bin is independent of the other bins).

This test shows that the additional cost of our implementation of ionizing radiation in SPH is always much smaller than the cost for other implemented physics, like gravity and hydrodynamics. In particular, our new ray-tracing scheme shows a substantial speedup compared to the algorithm by Kessel-Deynet & Burkert (2000), where the path finding alone took up about 50 per cent of the total computational time (Kessel-Deynet 1999). Another drawback of their approach is that for every particle the optical depth is calculated along a path towards the source until a particle closer to the source with an already calculated optical depth is found. This is a highly serial approach and thus the scheme of Kessel-Deynet & Burkert (2000) does not lend itself easily to an efficient parallelization.

4 RADIATION DRIVEN IMPLOSION

As a first application of iVINE, we model the radiation driven implosion of an otherwise stable molecular cloud core. This approach is very similar to Kessel-Deynet & Burkert (2003) but at 10 times higher mass resolution. A marginally stable Bonnor–Ebert sphere (BES) (Bonner 1956) with a radial pressure profile defined by

$$\frac{1}{r^2} \frac{d}{dr} \left( \frac{r^2 d\rho}{\rho dr} \right) = -4\pi G \rho \quad (33)$$

is exposed to UV radiation from a nearby source. The temperature of the sphere is $T = 10$ K, the peak density is $n_{max} = 10^7$ cm$^{-3}$, and the gas is initially at rest (i.e. no turbulence). The total mass contained in the sphere is $96 M_\odot$ and the radius is 1.6 pc. We embed the sphere into cold gas (10 K) with a constant density corresponding to the cut-off-density at the edge of the sphere. These simulations where performed with $2.2 \times 10^6$ particles resulting in a particle mass of 7.2 $\times 10^{-5}$ $M_\odot$. Self-gravity is included. The cooling time-scale ($t_{cool} < 0.3$ kyr) is much shorter than any other time-scale involved in our simulations (e.g. the crossing time-scale of the hot gas is $t_{cross} \approx 70$ kyr). Thus, we treat the non-ionized gas with an isothermal equation of state ($\gamma = 1$). The ionized gas is assigned a temperature according to equation (9) with $T_{ion} = 10^4$ K and $T_{cool} = 10$ K and then treated isothermally as well.

The artificial viscosity and the criteria for the individual time-steps are the same as in Section 3.2.1 ($\alpha = 1$, $\beta = 2$, $\tau_{acc} = 1$, $\tau_{CFL} = 0.3$ and $r_{pole} = 0.15$). In addition, we use a multipole acceptance criterion (MAC) for the TREE based calculation of gravitational forces according to Springel, Yoshida & White (2001) as implemented by Wetzstein et al. (2008) with a TREE accuracy parameter of $\theta = 5 \times 10^{-7}$. The implementation of the SPH smoothing kernel and the gravitational softening length in VINE are equal at all times. The number of neighbours is set to $n_{neigh} = 50 \pm 20$. The hydrodynamical boundaries are periodic in the y- and z-direction, and open in the x-direction. This resembles the situation around a massive O-star where the material is allowed to move freely in the radial direction while at the sides similar material is existing. Gravitational forces are calculated by just taking into account the self-gravity of the gas and no external or boundary effects. This is reasonable as the total simulation time (<600 kyr) is much shorter than the free-fall time ($t_{ff} \approx 1.5$ Myr). In the simulations, the radiation is impinging from the left-hand side. We perform three different simulations, differentiated by the penetration length in the surrounding medium relative to the box size $C = x_0/s_{box}$.

(i) Simulation high flux (HF):

$F_0 = 9.0 \times 10^8$ photons cm$^{-2}$ s$^{-1}$ $\Rightarrow C \approx 1.0$.

(ii) Simulation intermediate flux (IF):

$F_0 = 4.5 \times 10^8$ photons cm$^{-2}$ s$^{-1}$ $\Rightarrow C \approx 0.5$.

(iii) Simulation low flux (LF):

$F_0 = 9.0 \times 10^7$ photons cm$^{-2}$ s$^{-1}$ $\Rightarrow C \approx 0.1$.

This corresponds to the molecular cloud being placed inside (HF), at the border (IF) and outside (LF) of the Strömgren sphere. The evolution of the BES for all three cases is shown in Fig. 6.

4.1 Dynamical evolution

The general evolution of a simulation of this kind is as follows. As soon as the simulation starts, a R-type ionization front is driven into the medium. As it can be expected from Section 3.1.1, the front reaches the Strömgren radius $x_0$ of the diffuse gas within a few recombination time-scales ($x_{rec} \approx 5$ kyr). After a sound crossing time-scale ($t_{cross} \approx 70$ kyr), the hot gas reacts to its change in pressure and starts to drive a shock front into the cold gas – a D-type front evolves. This front will affect the morphology of the BES. In the following, we describe the individual cases in more detail.

4.1.1 Simulation HF

Due to the HF (see Fig. 6, first column), the R-type front is able to propagate very far into the simulation domain. A bow-like shock structure around the edge of the BES evolves ($t \approx 100$ kyr). The shock front running into the denser parts of the cloud is slowed down, so that the front starts to ‘wrap around’ the cloud. Soon, the two flanks are approaching each other while the centre of the shock is held back by the dense innermost region (Fig. 6, third row, first column, $t \approx 100$ kyr). As the two sides finally collide an elongated filament forms which is gravitationally unstable. In Fig. 7, we show

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Figure 6. Time evolution of the driven collapse of a BES ionized by a source with HF (first column), IF (second column) and LF (third column). The simulation volume is a cube with sides 4 pc long, the UV radiation is impinging from the left-hand side. Colour coded is the density of the central cold gas slab. Yellow arrows denote the velocities of the hot gas, black arrows the motion of the cold gas. Density and velocities are averaged across a slice of 0.125 pc in the $z$-direction. Each row shows the three simulations at a different time.
arys are justified by the fact that the molecular cloud is completely bound. Otherwise the gas could stream away freely. However, these bounds are due to the periodic boundaries on the upper and lower edge.

The core always forms at the very tip of the filament. This filament at the final stage of our simulations. In comparison runs without self-gravity the two shock fronts cross each other and the cloud disperses. With the inclusion of self-gravity the filament becomes gravitational unstable and is triggered into collapse. In fact the core fragments into several objects, as will be discussed in a subsequent paper. The resolution limit according to Bate & Burkert (1997) is $n_{\text{max}} = 2 \times 10^{10} \text{ cm}^{-3}$ in these simulations. As soon as this limit is reached the local Jeans mass is smaller than the mass of 100 particles and artificial fragmentation can occur. Thus, we stop the simulations at this point.

### 4.1.2 Simulation IF

With an IF the R-type front penetrates much less into the gaseous medium (see Fig. 6, second column). Thus, the front does not wrap around the sphere as much as in Simulation HF. As soon as the hot gas reacts to its increased temperature a flattened shock wave in front of the BES. This shock sweeps away much more material than in the high and IF cases, where the material is concentrated in the centre. Nevertheless, as the shock propagates further the very centre of the sphere gets compressed and becomes gravitationally unstable. In contrast to Simulations HF and IF, there is no sign of fragmentation in the unstable region.

### 4.1.3 Simulation LF

The very LF in this case only leads to a R-front which barely reaches the sphere (see Fig. 6, third column). Therefore, the D-front starts as a nearly plane-parallel shock wave in front of the BES. This shock sweeps away much more material than in the high and IF cases, where the material is concentrated in the centre. Nevertheless, as the shock propagates further the very centre of the sphere gets compressed and becomes gravitationally unstable. In contrast to Simulations HF and IF, there is no sign of fragmentation in the unstable region.

### 4.2 Structure, collapse time-scales and final mass assembled

A close look at the final structure of the collapsing filaments of the three simulations (Fig. 7) reveals that in all three simulations the core forms at the tip of an elongated filament, which might be eroded in the future. This matches exactly the observed head to tail structure described in Section 1. The core regions have an extent of just 0.02–0.05 pc, which corresponds very closely to, for example, the findings of Motte & André (2001) in the Perseus star cluster. They observe eight Class 0 protostars with compact envelopes ($R_{\text{max}} < 10^4 \text{ au} \approx 0.05 \text{ pc}$). In addition, they are denser by a factor of 3–12 than it would be expected from the standard collapse model, which would suggest densities of $n \approx 10^6 \text{ cm}^{-3}$ (see e.g. Walch et al., in preparation). Motte & André (2001) suggest that this higher densities are due to external disturbances initiating the collapse, which agrees very well with our simulations. Following the observations, we define a core as all material with a density higher than $n_{\text{crit}} = 10^7 \text{ cm}^{-3}$ in a region of $R_{\text{crit}} = 0.02 \text{ pc}$ (which is roughly a Jeans length at a density of $n_{\text{crit}}$) around the peak density.

We plot the evolution of the maximum density in Fig. 8. In all three simulations after the first phase of compression by the hot gas a metastable phase at densities between $10^6 \text{ cm}^{-3}$ and $10^7 \text{ cm}^{-3}$ can be seen. This fits very nicely to the structure of observed cores described above. The duration of this phase depends on the initial flux (HF: 90 kyr, IF: 155 kyr, LF: 290 kyr). In addition, we find evidence that the filaments collapse earlier in the cases with a higher flux. The collapse happens at $t = 200, 280$ and 600 kyr in Simulation HF, IF and LF, respectively. Observations of triggered star formation tend to show the same trend (see Lee et al. 2005; Ikeda et al. 2008) – each other similar to Simulation HF and the central region becomes unstable and fragments (see Fig. 7).

### Figure 7

Final stage of the three simulations. Colour coded is the density in the central slab. Yellow arrows denote the velocities of the hot gas, black arrows the motion of the cold gas. Density and velocities are averaged across a slice of 0.0625 pc in the $z$-direction. The time of the collapse as well as the displacement of the fragment clearly depend on the initial flux. Furthermore, the velocity of the cold gas (black arrows) is decreasing with decreasing flux. The very LF in this case only leads to a R-front which barely reaches the sphere (see Fig. 6, third column). Therefore, the D-front starts as a nearly plane-parallel shock wave in front of the BES. This shock sweeps away much more material than in the high and IF cases, where the material is concentrated in the centre. Nevertheless, as the shock propagates further the very centre of the sphere gets compressed and becomes gravitationally unstable. In contrast to Simulations HF and IF, there is no sign of fragmentation in the unstable region.

### Figure 8

The maximum number density versus time for the three different simulations. In the higher flux cases HF and IF, the collapse happens much earlier than in the LF case LF. The dash–dotted line represents the resolution limit as given by Bate & Burkert (1997).
the younger the star, the further it is away from the ionizing source. This cannot be explained by just attributing it to the speed of the R-type front. As seen in Section 3.1.1, the crossing time for the R-type front is of the order of a few kyr, whereas any observed age spread is of the order of several hundred kyr. To explain this huge spread the position of the density enhancement relative to the Str"omgren radius has to be considered. As we show decreasing the flux and thereby increasing the distance to the source can delay collapse and star formation by 0.08–0.4 Myr.

In IC 1396N, Getman et al. (2007) report a T Tauri (Class II and Class III stars) population with ages $\approx 0.5–1$ Myr. In addition, 0.3–0.5 pc further away from the ionizing source HD 206267 (an O6.5f-type star), there is an embedded population of Class 0/I protostars with ages $\approx 0.1$ Myr. This can be compared to our simulations, where for example Simulation IF represents gas clumps closer to the source which start to form stars 0.3 Myr earlier than Simulation LF. So at the time the embedded stars start to form in Simulation LF the stars of Simulation IF would be no longer embedded and represent the Class II/III stars population. In fact, in our simulations, the spread of a few hundred kyr is smaller than in the observations. This difference could be attributed to the classification of the protostars as discussed below.

Besides the age-spread one can look at the velocities of the front and core. From Fig. 6, it can be seen that the shock front travels with a speed of $3$–$7$ km s$^{-1}$, depending on the initial flux. Most observational estimates provide a front speed $<1$ km s$^{-1}$ (Thompson et al. 2004), leading to a difference of almost an order of magnitude between observations and simulations which has been noted before (see e.g. Getman et al. 2007). The age estimates of the YSOs are mainly based on their classification by the spectral energy distribution (SED). A Class 0/I object is deeply embedded, therefore the short micrometer wavelengths are much weaker due to absorptions in the envelope when compared to Class II/III objects. This allows for a clear distinction between both types for example in the Infrared Array Camera (IRAC) [3.6]–[4.5] versus [5.8]–[8] colour diagram as shown by Hartmann et al. (2005). We suggest that in the case of triggered star formation, the ionizing radiation could strip the envelope of a YSO, thereby unveiling the central object in short micrometer wavelengths. Thus, the observed Class II/III SED could be caused by a much younger Class 0/I protostar with a removed envelope. This would reduce the estimated age spread, thereby increasing the estimated speed of the shock front and finally leading observations and simulations to agree. This assumption will be subject to further examination.

A dependence on distance is also seen for the velocities of the cold filaments [see the velocities of the cold gas (black arrows) in Fig. 7]. The precise velocities of the cores in the Simulations HF, IF and LF are 8.4, 7.6 and 5.1 km s$^{-1}$, respectively. Again, the closer the core is to the OB-association the higher is its velocity. Although the cores themselves have bulk velocities which are slightly higher (by about 0.5–1 km s$^{-1}$) than the rest of the filament. However, this effect may get weaker as the core gets slowed down while sweeping up the rest of the filament.

The final mass assembled does not show a dependence on the initial distance. In Simulation HF, the core consists of 6.0 $M_\odot$ in Simulation IF of 7.4 $M_\odot$ and in Simulation LF of 2.8 $M_\odot$. The filaments as a whole have masses of 61.5 $M_\odot$, 75.3 $M_\odot$ or 67.4 $M_\odot$, respectively. It is obvious that the most effective scenario is Simulation IF. Here, the ionization encompasses most of the sphere and thus the shock front is not nearly as plane parallel as in Simulation LF and does not sweep away as much material. On the other hand, less material gets evaporated by the ionization since the flux is lower than in Simulation HF. Overall the final masses of the collapsing cores fit the observations well. Assuming a star formation efficiency of 30 per cent (see e.g. Lada et al. 2008), we find masses from 0.84 to 2.2 $M_\odot$ which agrees with the observed range from classical T Tauri up to Herbig Ae/Be stars (see e.g. Lee & Chen 2007; Snider et al. 2007).

5 SUMMARY AND DISCUSSION

We present iVINE, a new implementation of UV radiation into the TREE-SPH code VINE. It uses a plane-parallel geometry which renders the code most suitable to perform high-resolution studies of the small scale effects of, for example, ionization and turbulence in the surrounding of young massive stars. It is efficiently parallelized and very fast, as only 2–8 per cent of the total computational time is used for the calculation of ionization. The comparison with analytic solutions shows that iVINE treats time-dependent ionization as well as the resulting heating effects precisely and convergently.

We base our numerical implementation of ionizing radiation on several assumptions. First, we use a simplified prescription for the radiative transfer by for example assuming a monochromatic flux. Secondly, we neglect UV absorption by dust, which would lower the total UV flux. Thirdly, we do not include a full treatment of recombination zones. In our simulations, the ionized gas which gets shaded is assumed to recombine immediately. In addition, the gas in the shaded regions does not get heated by irradiation from the hot gas surrounding it. These effects require a precise time-dependent treatment of heating and cooling processes by ionization and recombination as well as a treatment for the scattering of photons. An implementation of this effect is planned in a future version of the code.

As an application, we investigate radiation driven implosion of a marginally stable BES. We show that these spheres are indeed driven into gravitational collapse. The resulting cores are in the observed mass range. They are more compact and a factor of $\approx 10$ more dense than it would be expected in a more quiescent environment. This fact fits very well with the observations of star formation in a clustered environment. By comparing simulations with three different UV fluxes, we show that there is a clear dependence of the final mass and the age of the collapsed core on the position of the pre-existing density enhancement relative to the Str"omgren radius. Our findings that the onset of star formation is delayed by 0.08–0.4 Myr, depending on the position, are in good agreement with observations of the age spread in bright rimmed clouds. The velocity of the triggering shock is an order of magnitude higher than the observational estimates. This discrepancy has been noted before. We suggest that this can be attributed to the ionizing radiation stripping the envelope from a Class 0/I star. Thereby, it might be classified as an Class II/III star, leading to an higher age spread between the observed objects. Correcting for this effect would increase the estimated velocity of the shock front and thus lead simulations and observations towards agreement.

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