Stability of expanding ionization fronts

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1 Objectives

- Study expansion of H II regions in power-law density profiles, compared to analytic solutions.
- Investigate stability of ionization fronts, using different algorithms and numerical resolutions.

2 Introduction

Whalen & Norman (2008, hereafter WN08) study D-type ionization front (I-front) expansion and stability in 2D and 3D simulations, following earlier 2D simulations by García-Segura & Franco (1996, hereafter GSF96). We will follow this work, using the setup for simulation “S22” from these two papers. It consists of a monochromatic source of ionizing photons that photoionizes a spherically-symmetric gas cloud with a constant density core and $1/r^2$ envelope. They find strong I-front instability develops close to the star, approximately at the core radius. The instability grows as the I-front expands down the density gradient (see Figs. 2 and 5 in WN08 and Fig. 7 in GSF96). Initially this calculation was done in two dimensions (spherical polars $(r, \theta)$), but WN08 also extended this calculation to three dimensions (also spherical coordinates). Both GSF96 and WN08 found that the neutral gas must be able to cool efficiently for instability to set in.

This problem is similar to Test 6 in Iliev et al. (2009), except on a much smaller scale and with stronger cooling from solar-metallicity gas. It is somewhat complicated by the fact that the heating and cooling prescriptions have a strong effect on results. In particular, the expansion velocity depends mainly on the temperature of the ionized gas, and the shell stability depends crucially on the ability of the shocked gas to cool. For this reason it is important that all contributors use microphysics prescriptions that are as similar as possible (see below). It is also possible to contribute results using the native thermal physics module in the codes being used, but there is no guarantee that they will be published because they are more difficult to compare with each other.

3 Test description

The test can be run with either the two-temperature isothermal (TTI) or the non-equilibrium (NEQ) thermal physics modules. We set the equilibrium temperature of the ionized gas to $T_i = 10^4$ K and of the neutral gas to $T_n = 10^2$ K. We assume the gas contains $1/11$ He by number, so the hydrogen number density $n_H$ is given by $n_H = 0.714 \rho/m_p$, where $\rho$ is the mass density, $m_p$ is the proton mass, and $10/14 \approx 0.714$. We assume that He is inert (i.e. never ionized).

The radiation source has an ionizing photon luminosity $Q_0 = 10^{48}$ s$^{-1}$ and is located at the origin. The initially static density field has $n_H = 10^4$ cm$^{-3}$ (or mass density $\rho = 2.338 \times 10^{-20}$ g cm$^{-3}$) for $r < 0.2$ pc and $n_H(r) = n_H(0)(r/0.2$ pc$)^{-2}$ for $r \geq 0.2$ pc. The initial conditions have gas temperature 100 K everywhere, following the model S22 of GSF96. The initial H$^+$ fraction is $x(r, t = 0) = 10^{-5}$. The simulation is run for 0.25 Myr, and gravity is not included. Note that
the initial conditions are not in pressure equilibrium so the cloud will expand somewhat even without photoionization, but always with \( v \ll 1 \text{ km s}^{-1} \).

### 3.1 SPH setup

We recommend that contributors use \( 10^6 - 10^7 \) particles for 3D simulations (certainly no more than \( 256^3 \)), within a radius of 2.048 pc. Lower dimensionality simulations can also be run. If a high resolution run is supplied, please also send a lower resolution run (e.g. with 8× fewer particles).

### 3.2 Grid setup

The grid domain should be \((x, y, z) \in [-2.048, 2.048] \text{ pc}\), but there is no constraint on the dimensionality and geometry of the grid. In addition, feel free to simulate only an octant or quadrant of the full space. For ease of analysis, we request (as for SPH setup) that the total number of grid zones be limited to a maximum of \( 256^3 \), although these zones can be distributed in whatever way one wants. If a high resolution run is supplied, please also send a lower resolution run (e.g. with 8× fewer grid zones).

### 3.3 Seed perturbations

For now, please add some density perturbation to the data, e.g., white noise at a fractional level of 1%. During the workshop we will discuss how to force a certain mode to grow, for example by imposing a non-linear density perturbation according to a spherical harmonic pattern on a spherical shell near the Strömgren radius, \( R_s \).

### 3.4 Data

Participants should provide outputs from each simulation containing:

1. **position**: components for each dimension in cm, measured from the radiation source, with zeros for unused second or third dimensions.
2. **density** (g cm\(^{-3}\)),
3. \( \text{H}^+ \) fraction,
4. **pressure** (dyne cm\(^{-2}\)),
5. **temperature** (K), and
6. **velocity components** for each dimension (cm s\(^{-1}\)), again with zeros for unused dimensions.

Outputs should be taken at 0.025, 0.05, 0.1, 0.15, 0.2, and 0.25 Myr. Please use ASCII text, in a similar format as for the D-type expansion of H\( \text{II} \) regions test:

```
XX0.1000000E-100XX0.1000000E-100XX0.1000000E-100XX0.1000000E+102XX0.1000000E+102...
```

where \( X \) is a space. It doesn’t have to be exactly this; if you only have two digits in the exponent then that is also ok, and lower case ‘e’ of ‘d’ instead of ‘E’ is not a problem. The key points are (0) use CGS units! (1) use exponential notation with plenty of significant figures, (2) use spaces (not tabs
Figure 1: **Left:** Radius of the I-front as a function of time for 1D simulations using the TTI and NEQ thermal physics modules, with 128 and 2048 grid zones (as indicated in the legend). The analytic approximation given by Eq. (3) is also plotted. **Right:** Maximum density in the shell as a function of time for the same simulations, plus higher resolution runs with 4096 and 16384 grid zones, as indicated.

or commas) to separate quantities, and (3) include columns for unused dimensions of position and velocity.

If the data are already in a format that can be read and plotted using VisIt\(^1\) with a standard file plugin then that would be useful to have as well as the text files.

Please do not send your data by email. Contact jmackey@astro.uni-bonn.de and we will work something out.

### 4 Example results for 1D evolution

Analytic solutions were developed by Franco et al. (1990), but only for the case where the core radius, \(r_c\) (here \(r_c = 0.2 \text{ pc}\)), satisfies \(r_c < R_S\), where \(R_S\) is the Strömgren radius. For our test, \(R_S = 0.067 \text{ pc}\), so these solutions are not applicable. The standard D-type expansion solution applies as long as the shell remains in the constant density core, and similar considerations can give a solution at later times. We assume as before that the H\(\text{II}\) region maintains constant density and temperature, and use the strong shock jump conditions to relate the interior thermal pressure to the shell expansion velocity, \(v_{sh}\). Photon conservation gives the shell radius in terms of the core number density \(n_H(0)\),

\[
\frac{n_H(0)}{n_i(t)} = \left(\frac{r_{sh}(t)}{R_S}\right)^{3/2},
\]

where \(n_i(t)\) is the H number density within the H\(\text{II}\) region and \(r_{sh}(t)\) is the shell radius, both of which are changing with time. Total (ram plus thermal) pressure balance through the shell gives

\[
n_H(0) \left(\frac{r_{sh}(t)}{r_c}\right)^{-2} v_{sh}^2(t) \approx n_i(t)a_i^2,
\]

where \(a_i\) is the isothermal sound speed in ionized gas. This gives the solution

\[
r_{sh}(t) \approx r_c \left(1 + \frac{3R_S^{3/4}a_i}{4r_c^{7/4}}[t - t_c]\right)^{4/3},
\]

\(^1\)https://wci.llnl.gov/codes/visit/
Figure 2: Resolution study for 2D axisymmetric simulations of the S22 simulation, using the TTI microphysics with PION after 0.2 Myr of evolution. Each quadrant shows the same simulation but run with 128 grid zones (top right), 256 (bottom right), 512 (bottom left), and 1024 (top left). We plot $\log n_H$ (with $n_H$ in units of $\text{cm}^{-3}$) on the colour scale indicated in the legend. The black contour shows where the ionization fraction $x = 0.5$.

where $t_c$ is the time at which $r_{sh}(t_c) = r_c$. For the parameters we use in this test, $a_i = 11.1 \text{ km s}^{-1}$ and $t_c = 0.0197 \text{ Myr}$.

Test simulations have been performed with PION (Mackey, 2012) on a 1D uniform grid on $r \in [0, 2.048] \text{ pc}$ with various spatial resolutions from 64 to 16384 grid zones. The evolution of $r_{sh}$ (as traced by the I-front at its inner edge) is plotted in the left panel of Fig. (1) for 128 and 2048 grid zones, using both NEQ and TTI thermal physics, and compared to Eq. (3). The low resolution simulations expand somewhat slower than predicted, but the higher resolution simulations agree almost exactly with the predictions. The resolution dependence is not a concern because the numerical thickness of the shell at low resolution is significantly larger than the difference. Other quantities such as kinetic energy and momentum of the gas, ionized and neutral gas mass in $r \leq 2.048 \text{ pc}$, show similarly good convergence. Only the peak density in the shell shows strong resolution effects, shown in the right panel of Fig. (1). This is because the shell is not well resolved in any of the simulations at early times, and at no time for the lowest resolution simulations.
5 Example results for multidimensional evolution

GSF96 and WN08 showed that simulation S22 should be unstable to I-front instability when the neutral gas can cool efficiently (so that the shocked shell is thin). We want to study this in detail with multi-dimensional simulations using as many different codes, geometries, and algorithms as possible. Results from 2D simulations with PION are plotted in Fig. (2) for simulations using $128^2$, $256^2$, $512^2$, and $1024^2$ grid zones on a uniform axisymmetric grid (cylindrical coordinates $(z, R) \in [0, 2.048]$ pc) using the TTI microphysics approximation.

The lowest resolution simulation stays stable, but this is an artefact because the shocked shell is numerically broadened. With $256^2$ grid zones the shell begins to become unstable at about $\theta = 45^\circ$, and less so at $\theta \approx 0^\circ$ and $90^\circ$. This is because PION uses a short characteristics raytracer which has zero diffusivity at these special angles and non-zero diffusivity at all other angles. The errors in the scheme are then largest at either side of these angles, so instability is seeded most effectively here. At higher resolution, the instability also seeds itself earliest at these angles, so the I-front distortion is largest here, but all other angles are also unstable. These simulations certainly have not converged numerically, because 1D simulations show that we would need at least $16384^2$ grid zones to resolve the shell structure at late times (and even more to resolve it at early times).

Fig. (3) plots the same results, but this time using the NEQ microphysics routines. The basic picture is the same, but here the details of the instability are somewhat different. This is to be expected because the thermal physics of the shell is what determines stability. The median I-front and shell
Figure 4: Median radius of the I-front (left) and shell (right) as a function of time for 2D simulations with different spatial resolutions (indicated) using the NEQ microphysics module. For the 1024\textsuperscript{2} simulation the maximum and minimum radius are also plotted as errorbars on top of the median value. A high-resolution 1D simulation is overplotted for comparison.

radius are plotted as a function of time in Fig. (4). The shell is defined as gas with \( x < 0.01 \) and with a radial velocity \( > 1 \text{ km s}^{-1} \). While the median radii are compatible with the lower-resolution 2D results and with the 1D result, the scatter introduced by the unstable shell is very large.

3D results with PION look basically similar to 2D using 128\textsuperscript{3} and 256\textsuperscript{3} grid zones in an octant of the full domain (with reflective boundary conditions). Specifically the shell is completely stable with 128\textsuperscript{3} and develops some instability at 45\textdegree\ to the grid axes with 256\textsuperscript{3}. It is clear that this is purely a numerical resolution effect, so it will be very interesting to see what happens with other simulation codes, especially those using other coordinate systems and SPH codes that have high resolution near the core of the cloud.

References