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TESTS FOR COSMOLOGICAL RADIATIVE CODE COMPARISON PROJECT

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ABSTRACT

Below we describe the tests to be performed for the Cosmological Radiative Transfer Code Comparison Project.

Subject headings: H II regions—ISM: bubbles—ISM: galaxies: halos—galaxies: high-redshift—galaxies: formation—intergalactic medium—cosmology: theory—radiative transfer— methods: numerical

1. TESTS

Here we describe the tests to be performed, with their detailed parameters, geometry and setup. When constructing these problems, we aimed for the simplest, cleanest, but still cosmologically-interesting test problems. They were also chosen so as to test and compare the various important aspects of a radiative-transfer code, like tracking of both slow and fast I-fronts, the energy equation and temperature, formation of shadows, and, in Tests 5-7, the interaction with fluid flows and radiative feedback on the gas. For simplicity, in all tests below the gas is assumed to be hydrogen-only. In tests 1-4 the gas density distribution is fixed. Finally, a requirement in order to be included in the comparison is for each test to be done by at least two different codes, and preferably by three or more codes.

2. GENERAL INSTRUCTIONS

All test problems are to be solved in 3-D, with grid dimensions 128^3 cells (each coordinate running from 0 to 128). Ionizing sources are assumed to have a black-body spectrum with effective temperature $T = 100,000$ K (as expected for metal-free, massive Pop. III stars), except for Test 1 where the spectrum is monochromatic.

When you are finished with a test and ready to submit your results, please go to:

`www.cita.utoronto.ca/~iliev/workshop/form.html`

which provides a form for file submission. Since all files you submit would go to the same directory, please follow the following naming conventions:

The files should be called

`'Tnumber_grid_name.dat'`

and

`'Tnumber_front_name.dat'`

where 'name' is the name of your group or your code and 'number' is the test number, from 1 to 7, for the 3-D and 1-D data, respectively (e.g.

`'T2_grid_iliev.dat',`

etc.). Please sumbit ONE file with gridded data, containing all the output times.

All files should be provided as ASCII free-format single-precision (Real*4) files (gzipped or compressed), i.e. the 3-D data should be readable using:

```
do i=1,128
  do j=1,128
    do k=1,128
      read(*,*) all requested quantities
                in the order listed
    end do
  end do
end do
```

I-front positions and velocities vs. time along a given axis, which should be in three columns: t, x_I and v_I in units of Myr, kpc and km s^{-1}. The x_I should be the linearly-interpolated I-front position inside the cell, and v_I is finite-differenced from x_I.

The tests, data, results and the input data for Test 4 could be found at

`http://www.cita.utoronto.ca/~iliev/dokuwiki/doku.php?id=rt_comparison`

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2.1. *Pure radiative transfer tests*

2.1.1. *Test 1: Pure-hydrogen isothermal H II region expansion*

This test is the classical problem of an H II region expansion (Strömgren 1939; Spitzer 1978). A steady, monochromatic ($h\nu = 13.6$ eV) source emitting $\dot{N}_\gamma$ ionizing photons per unit time is turning on in an initially-neutral, uniform-density, static environment with hydrogen number density n_H. For this test we assume that the temperature is fixed at $T = 10^4$ K. There is a well-known analytical solution for the radius, r_I, and the velocity, $\mathrm{v_I}$, of the I-front, given by

$$r_I = r_\mathrm{S}\left[1-\exp(-t/t_\mathrm{rec})\right]^{1/3}. \tag{1}$$

$$\mathrm{v_I} = \frac{r_\mathrm{S}}{3t_\mathrm{rec}}\frac{\exp\left(-t/t_\mathrm{rec}\right)}{\left[1-\exp(-t/t_\mathrm{rec})\right]^{2/3}}. \tag{2}$$

$$\tag{3}$$

where

$$r_\mathrm{S} = \left[\frac{3\dot{N}_\gamma}{4\pi\alpha_B(T)n_\mathrm{H}^2}\right]^{1/3}, \tag{4}$$

is the Strömgren radius, obtained from

$$F = \int_0^{r_S} d\ell n_e n_H \alpha_B(T) \tag{5}$$

i.e. by balancing the number of recombinations with the number of ionizing photons arriving along a given LOS, where n_e is the electron density, and

$$t_\mathrm{rec} = [\alpha_B(T)n_\mathrm{H}]^{-1}, \tag{6}$$

is the recombination time. Here $\alpha_B(T)$ is the Case B recombination coefficient of hydrogen at temperature T in the ionized region. The H II region initially expands fast, then it slows considerably at $t \sim t_\mathrm{rec}$, as recombinations start balancing the ionizations as the H II region is closing on its Strömgren radius. At a few recombination times I-front stops at radius $r_I = r_S$ and in absence of gas motions remains static thereafter.

The numerical parameters for Test 1 are: computational box dimension $L = 6.6$ kpc, gas number density $n_H = 10^{-3}$ cm^{-3}, initial ionization fraction (given by collisional equilibrium) $x = 1.2\times10^{-3}$, $\dot{N}_\gamma = 5\times10^{48}$ photons s^{-1}. The source is at position $(x_s, y_s, z_s) = (1,1,1)$ cells (i.e. in the corner of the box). For these parameters the recombination time is $t_\mathrm{rec} = 3.86\times10^{15}$ s $= 122.4$ Myr. Assuming a recombination rate $\alpha_B(T) = 2.59\times10^{-13}\,\mathrm{cm^3 s^{-1}}$ at $T = 10^4$ K, then $r_S = 5.4$ kpc. The simulation running time is $t_\mathrm{sim} = 500$ Myr $\approx 4t_\mathrm{rec}$. The required outputs are the neutral fraction of hydrogen on the whole grid at times $t = 10, 30, 100, 200$, and 500 Myr, and the I-front position (defined by the 50% neutral fraction) and velocity vs. time along the x-axis.

2.1.2. *Test 2: H II region expansion: the temperature state*

Test 2 is essentially the same problem as in Test 1, but with varying gas temperature which is determined from the energy equation.

The initial conditions are as in Test 1 above, except the gas starts fully-neutral, the (pure-hydrogen) gas number density is $n_\mathrm{H} = 1\times10^{-3}\,\mathrm{cm^{-3}}$, and the initial gas temperature is $T = 100$ K.

The required outputs in this case are the H I fraction and the temperature on the whole grid at times $t = 10, 30, 100, 200$, and 500 Myr, and the I-front position and velocity (defined by the 50% neutral fraction) vs. time along the x-axis.

2.1.3. *Test 3: I-front trapping in a dense clump and the formation of a shadow.*

Test 3 involves propagation of a plane-parallel I-front and its trapping into a dense spherical clump. The condition for an I-front to be trapped by a dense clump of gas number density n_H can be expressed as follows (Shapiro et al. 2004). We define the Strömgren length $\ell_S(r)$ at impact parameter r again using equation (5), but in this case solving it for each impact parameter. We then can define the "Strömgren number" for the clump as $L_S \equiv 2r_\mathrm{clump}/\ell_S(0)$, where r_clump is the clump radius and $\ell_S(0)$ is the Strömgren length for zero impact parameter. If $L_S > 1$, then the clump is able to trap the I-front, while if $L_S < 1$, the clump would be ionized quickly by the passage of the I-front across it, which will not slow down enough to be trapped.

For a uniform clump equation (5) reduces to

$$\ell_S = \frac{F}{\alpha_H^{(2)} n_H^2}, \tag{7}$$

$$L_S = \frac{2r_\mathrm{clump}\alpha_H^{(2)} n_H^2}{F}. \tag{8}$$

The numerical parameters for Test 3 are as follows: ionizing photon flux is constant, $F = 10^6\,\mathrm{s^{-1}cm^{-2}}$, incident to the $y = 0$ box side, the hydrogen number density and temperature of the environment are $n_\mathrm{out} = 2\times10^{-4}\,\mathrm{cm^{-3}}$ and $T = 8{,}000$ K, while inside the clump they are $n_\mathrm{clump} = 200 n_\mathrm{out} = 0.04\,\mathrm{cm^{-3}}$ and $T_\mathrm{clump} = 40$ K. The box size is $x_\mathrm{box} = 6.6$ kpc, the radius of the clump is $r_\mathrm{clump} = 0.8$ kpc, and its center is at $(x_c, y_c, z_c) = (5, 3.3, 3.3)$ kpc, or $(x_c, y_c, z_c) = (97, 64, 64)$ cells.

For these parameters $\ell_S \approx 0.78(T/10^4 K)^{3/4}$ kpc, thus along the axis of symmetry the I-front should be trapped approximately at the center of the clump.

The required outputs are H I fraction and temperature at time $t = 1, 2, 3, 5$ and 15 Myr($\approx 5t_\mathrm{rec,clump}$) and the evolution of the I-front position and velocity along the axis of symmetry.

2.1.4. *Test 4: Multiple sources in a cosmological density field*

Test 4 involves the propagation of I-fronts from multiple sources in a fixed-density cosmological density field. The initial condition is provided by a time-slice (at redshift $z = 9$) from a cosmological N-body and gasdynamic simulation performed using the cosmological PM+TVD code by D. Ryu (Ryu et al. 1993). The simulation box size is $0.5h^{-1}$ Mpc, the resolution is 128^3 cells, 2×64^3 particles. The halos in the simulation box were found using friends-of-friends halo finder with linking length of 0.25. Initial temperature is fixed at $T = 100$ K. The ionizing sources are chosen to correspond to the 16 most massive halos in the box. The ionizing photon production rate for each source is constant and is assigned assuming that each source lives $t_s = 3$ Myr and emits $f_\gamma = 250$ ionizing photons per atom during its lifetime, hence

$$\dot{N}_\gamma = f_\gamma \frac{M\Omega_b}{\Omega_0 m_p t_s}, \tag{9}$$

where M is the total halo mass, $\Omega_0 = 0.27$, $\Omega_b = 0.043$, $h = 0.7$ and m_p is the baryon mass.

A file containing the density field (unformatted binary, in cm^{-3}, called 'density.bin'), should be read as:

```
parameter (ngrid=128)
real*4 redshift, dummy,
real*4 rho(ngrid,ngrid,ngrid)
open(unit=1,file='density.bin',
       form='unformatted',
       convert='big_endian')
read(1) redshift
read(1) dummy
do k=1,ngrid
   read(1) ((rho(i,j,k),i=1,ngrid),
                     j=1,ngrid)
end do
```

and a separate file (called 'sources.dat') containing the source positions (in cell units) and photon luminocities (in units of 10^{52} ionizing photons s^{-1}) is provided, to be read using:

```
integer nx(16),ny(16),nz(16)
real*4  phot_flux(16)
do i=1,16
   read(*,*) nx(i),ny(i),nz(i),phot_flux(i)
end do
```

For simplicity all sources are assumed to switch on at the same time. The boundary conditions are transmissive (i.e. any photons leaving the computational box are lost, rather than coming back in as in periodic boundary conditions). Codes that use periodic boundary conditions could do so, but please indicate that in a Readme file. The results from codes with periodic and transmissive boundary conditions would be compared separately. The evolution time is $t = 0.4$ Myr, and the required output is the neutral hydrogen fraction and temperature over the whole grid at times $t = 0.05, 0.1, 0.2, 0.3$ and 0.4 Myr.

2.2. *Radiative hydrodynamics tests*

2.2.1. *Test 5: Classical H II region expansion*

Consider an ionization front (I-front) created by an ionizing source emitting $\dot{N}_\gamma$ ionizing photons per second, which propagates into an initially-uniform gas distribution with gas number density n_0 and temperature T_0. I-fronts are classified based on their speed and the change in the gas density as it passes through the I-front, as follows (c.f. Kahn & Dyson 1965; Spitzer 1978). There are two critical speeds, R-critical speed, defined as $v_R = 2c_{s,I,2}$ and D-critical speed given by $v_D = c_{s,I,2} - (c_{s,I,2}^2 - c_{s,I,1}^2)^{1/2} \approx c_{s,I,1}^2/(2c_{s,I,2})$ where $c_{s,I,1} = (p_1/\rho_1)^{1/2}$ and $c_{s,I,2} = (p_2/\rho_2)^{1/2}$ are the isothermal sound speeds in the gas ahead and behind the I-front, respectively. The velocity of the I-front is given by the I-front jump condition (photon conservation) $v_I = F/n$, where n is the number density of the gas entering the front and F is the flux of ionizing photons at the I-front transition (which flux might be lower than the flux arriving from the source due to absorptions in the gas on the source side). We note that this jump condition is modified significantly for I-fronts moving with relativistic speeds with respect to the gas (Shapiro et al. 2005), which occurs in a number of astropysical and cosmological environments. However, we would not consider such cases here since currently few radiative transfer codes (and no radiative-hydrodynamics codes, to our knowledge) are able to handle such fast I-fronts.

When $v_I \geq v_R$ (e.g. close to the source, where the flux F is high) the I-front is of R-type (R-critical when $v_I = v_R$) and the gas passing through the front is compressed. R-type I-fronts always move supersonically with the neutral gas ahead, while with respect to the ionized gas behind the front can move either subsonically (strong R-type, highly compressive, but generally irrelevant to H II regions since it means that the isothermal sound speed behind the front is lower than the one ahead of it), or supersonically (weak R-type, resulting in only a slight gas compression as it passes through the front). When $v_I \leq v_D$ the I-front is of D-type (D-critical in the particular case of $v_I = v_D$). In this case the gas passing through the I-front always expands and the front is subsonic with respect to the gas ahead. With respect to the ionized gas behind, the I-front can be either supersonic (strong D-type), or subsonic (weak

D-type). When $v_D < v_{\rm I} < v_R$ the I-front is necessarily lead by a shock which compresses the gas entering the I-front sufficiently to guarantee that $v_{\rm I} \leq v_D$.

In static medium and for fixed gas temperature the evolution of I-front radius, $r_{\rm I}$, and velocity, $v_{\rm I}$, are given by

$$r_{\rm I} = r_{\rm S}^0 \left[1-\exp(-t/t_{\rm rec})\right]^{1/3} . \tag{10}$$

$$v_{\rm I} = \frac{r_{\rm S}}{3t_{\rm rec}} \frac{\exp(-t/t_{\rm rec})}{\left[1-\exp(-t/t_{\rm rec})\right]^{2/3}} . \tag{11}$$

$$\tag{12}$$

where

$$r_{\rm S}^0 = \left[\frac{3\dot{N}_\gamma}{4\pi\alpha_B(T)n_{\rm H}^2}\right]^{1/3} , \tag{13}$$

is the Strömgren radius (assuming full ionization), which is reached when the number of recombinations in the ionized volume per unit time exactly balances the number of ionizing photons emitted by the source per unit time. The recombination time is given by the usual expression

$$t_{\rm rec} = [\alpha_B(T)n_{\rm H}]^{-1} . \tag{14}$$

Here $\alpha_B(T)$ is the Case B recombination coefficient of hydrogen at temperature T in the ionized region.

In the reality the gas is not static, which allows for a further evolution. The high gas pressure of the ionized and heated gas inside the H II region creates strong pressure forces outwards, and the I-front continues to expand even after the Strömgren sphere is reached. Analytical models predict that in this phase the I-front radius evolves approximately according to (c.f. Spitzer 1978)

$$r_I = r_{\rm S}^0 \left(1+\frac{7c_s t}{4r_{\rm S}^0}\right)^{4/7} , \tag{15}$$

where r_S^0 is the Strömgren radius and c_s is the sound speed in the ionized gas. The expansion finally stalls when a pressure equilibrium is reached. The predicted final H II region radius is

$$r_f = \left(\frac{2T}{T_e}\right)^{2/3} r_S^0, \tag{16}$$

where T is the temperature inside the H II region and T_e is the external temperature. In reality the evolution is of course more complicated, with non-uniform temperature inside the H II region, thick I-front with pre-heating due to large photons, etc., thus these analytical solutions should be considered just as a guideline for the expected behaviour, rather than an exact solution.

The numerical parameters for Test 5 are as follows, computational box size $L = 15$ kpc, gas number density $n_H = 10^{-3}$ cm^{-3}, initial ionization fraction $x = 0$, ionizing photon production of the source $\dot{N}_\gamma = 5\times10^{48}$ photons s^{-1}, and initial gas temperature $T_e = 100$ K. The source is at the $(0,0,0)$ corner of the box. Assuming that the temperature of the ionized gas is $T = 10^4$ K, and that the recombination rate is given by $\alpha_B(T) = 2.59\times10^{-13}\,{\rm cm^3 s^{-1}}$, we find $t_{\rm rec} = 3.86\times10^{15}\,{\rm s} = 122.4$ Myr and $r_S = 5.4$ kpc, $r_f \approx 185$ kpc. This final pressure-equilibrium radius is thus well outside our computational volume, which instead was chosen to resolve well the more physically-interesting transition from R-type to D-type, which occurs around r_S^0. The ionizing spectrum is 10^5 black-body. The simulation running time is $t_{\rm sim} = 500$ Myr $\approx 4t_{\rm rec}$. The required outputs are the neutral fraction of hydrogen, gas pressure and temperature on the whole grid at times $t = 10, 30, 100, 200$, and 500 Myr, and the I-front position (defined by the 50% neutral fraction) and velocity vs. time along the x-axis.

2.2.2. *Test 6: H II region expansion in $1/r^2$ density profile*

This test studies the propagation of an I-front created by a source emitting $\dot{N}_\gamma$ photons per unit time at the center of sperically-symmetric, steeply-decreasing density profile $n = n_0(r_0/r)^2$, with a flat core of gas number density n_0 and radius r_0. Inside the core the I-front evolution is described by equations 11 and 12. If the Strömgren radius in the core, $r_{S,0} = [3\dot{N}_\gamma/(4\pi\alpha_B(T)n_0^2)]^{1/3}$ is smaller than the core radius, r_0, the Strömgren sphere is reached within the core and the I-front never leaves the core, assuming no gas motions. On the other hand, if $r_{S,0} > r_0$ the H II region continues to expand and the I-front propagates down the density profile.

In absence of gas motions the I-front evolution has (a quite complex) analytical form for abitrary source flux and gas profile parameters. There is a simpler solution in a special case, when $\dot{N}_\gamma = 16\pi r_0^3 n_0^2 \alpha_B/3$, in which case the I-front radius evolution once it leaves the core is given by

$$r_I = r_0(1+2t/t_{\rm rec,core})^{1/2}, \tag{17}$$

where $t_{\rm rec,core}$ is the recombination time in the core (Mellema et al. 2006). Similar solutions exist for the case of relativistic I-fronts (Shapiro et al. 2005). The case with hydrodynamic gas motions is more complicated and does not allow for an exact, closed-form analytical solution, but there are detailed semianalytical solutions available (Franco et al. 1990).

The proposed numerical parameters for Test 6 are as follows: computational box dimension $L = 0.8$ kpc, $n_0 = 3.2$ cm^{-3}, $r_0 = 91.5$ pc, zero initial ionization fraction, $\dot{N}_\gamma = 10^{50}$ photons s^{-1} and initial temperature $T = 100$ K everywhere. The source position is at the corner of the computational volume $(x_s, y_s, z_s) = (0,0,0)$. For these parameters the I-front is expected to convert from R-type to D-type inside the core. Once the I-front reaches the core edge it should accelerate again to higher speeds as it propagates down the steep density slope. The recombination time in the core is $t_{\rm rec,core} = 0.04$ Myr. The simulation running time is $t_{\rm sim} = 75$ Myr. The required outputs are the neutral fraction of hydrogen, the gas number density and temperature on the whole grid at times $t = 1, 3, 10, 25$ and 75 Myr, and the I-front position (defined by the 50% neutral fraction) and velocity vs. time along the x-axis.

2.2.3. *Test 7: Photoevaporation of a dense clump*

Test 7 involves the propagation of a plane-parallel I-front, its trapping in a dense spherical clump and the subsequent photoevaporation the clump. This problem has been studied e.g. in relation to the photoveporation of clumps in planetary nebulae (Mellema et al. 1998). The condition for an I-front to be trapped by a dense clump of gas number density n_H can be expressed as follows (Shapiro et al. 2004). We define the Strömgren length $\ell_S(r)$ at impact parameter r again using equations (11) and (12), but in this case solving it for each impact parameter. We can then define the “Strömgren number” for the clump as $L_S \equiv 2r_{\rm clump}/\ell_S(0)$, where $r_{\rm clump}$ is the clump radius and $\ell_S(0)$ is the Strömgren length for zero impact parameter. If $L_S > 1$, then the clump is able to trap the I-front, while if $L_S < 1$, the clump would be ionized quickly by the passage of the I-front across it, which will not slow down enough to be trapped.

For a uniform clump equation (13) reduces to

$$\ell_S = \frac{F}{\alpha_H^{(2)} n_H^2}, \tag{18}$$

$$L_S = \frac{2r_{\rm clump}\alpha_H^{(2)} n_H^2}{F}. \tag{19}$$

The numerical parameters for Test 7 are as follows (the same as for Test 3 in Paper I): ionizing photon flux is constant, $F = 10^6\,{\rm s}^{-1}{\rm cm}^{-2}$, incident to the $y = 0$ box side, the initial hydrogen number density and temperature of the environment are $n_{\rm out} = 2\times10^{-4}\,{\rm cm}^{-3}$ and $T = 8,000$ K, while inside the clump they are $n_{\rm clump} = 200 n_{\rm out} = 0.04\,{\rm cm}^{-3}$ and $T_{\rm clump} = 40$ K. The box size is $x_{\rm box} = 6.6$ kpc, the radius of the clump is $r_{\rm clump} = 0.8$ kpc, and its center is at $(x_c, y_c, z_c) = (5, 3.3, 3.3)$ kpc, or $(x_c, y_c, z_c) = (97, 64, 64)$ cells.

With gasdynamical evolution the dense clump initially traps the I-front, but as the heated and ionized gas is evaporated and expands towards the source, its recombination rate decreases and it attenuates the ionizing flux less. As a consequence, the I-front slowly eats through the clump until it photoevaporates completely.

The required outputs are H I fraction, the gas pressure and temperature at times $t = 1, 5, 10, 25$ and 50 Myr and the evolution of the I-front position and velocity along the axis of symmetry.

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