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Development and Application of Numerical Modules for FLASH in Palermo: Two Astrophysical Examples

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Abstract. We collaborate with the Flash Center at the University of Chicago to help upgrading and to apply extensively the FLASH code to astrophysical problems. In particular, we have developed new modules for FLASH which extend the field of applicability of the code to some areas in astrophysics, like solar and stellar coronae, and supernova remnants. The new modules so far developed and tested describe: the non-equilibrium ionization effects of the most abundant elements in astrophysical plasmas, the thermal conduction and the viscosity according to the formulation of Spitzer (1962), and the radiative losses from an optically thin plasma according to the Raymond spectral code, and to Peres et al. (1982) for the chromosphere. We show some selected results for a coronal flare and for a supernova remnant, obtained with the version of FLASH 2.0 code including the new modules.

Key words. Hydrodynamics – Numerical Codes

1. Introduction

Recently, our group has started an intense collaboration with the Center for Astrophysical Thermonuclear Flashes (FLASH center), the University of Chicago, to upgrade, to test, and to apply extensively FLASH, an accurate numerical code for parallel computers capable of handling general compressible flow problems in astrophysical environments.

The FLASH center was founded in 1997 and it is sponsored by the Department of Energy of the US government in the framework of the ASCI (Accelerated Strategic

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Computing Initiative) program. Originally, the FLASH code has been developed to solve the long-standing problem of thermonuclear flashes on the surfaces of compact stars (e.g neutron stars and white dwarfs), and in the interior of white dwarfs (i.e., Type I supernovae). The main characteristic of the code is its modular design which permits the inclusion of additional physics and different solvers: users are allowed to configure initial and boundary conditions, change algorithms, and add new physics modules. The code parallelization is achieved using the Message-Passing Interface (MPI) library, allowing portability and scalability on a variety of different parallel computers. The code takes advantage of the PARAMESH library to handle adaptive mesh refinement (MacNeice et al. 2000), a copy of which is included with the FLASH source code.

In the framework of the collaboration between our group and the FLASH center, the SCAN (Sistema di Calcolo per l'Astrofisica Numerica) facility in Palermo is one of the test and development sites for FLASH in which the code has been ported to Compaq architectures. Our collaboration aims to upgrade, to test, and to apply extensively the code to astrophysical systems. A key task of our group is the development of new numerical modules extending the field of applicability of FLASH to other fields of astrophysics, such as the supernova remnants and flares in stellar coronae. An essential ingredient is the introduction of the treatment of non-equilibrium ionization (NEI) processes. The new modules so far developed and tested include:

1. the thermal conduction according to the formulation of Spitzer (1962);
2. the radiative losses from an optically thin plasma according to Raymond & Smith (1977) and Peres et al. (1982) for the chromosphere;
3. the viscosity according to the formulation of Spitzer (1962);
4. the non-equilibrium ionization effects of the most abundant elements in astrophysical plasmas.

In this project, the Palermo team takes advantage of its long experience in developing hydrodynamic codes for modeling astrophysical plasma and in optimizing the codes for efficient parallel execution on high performance computers. The group has recently acquired and uses, for the FLASH development, a high performance computing (HPC) cluster of 16 powerful alpha EV67 processors distributed in 4 compaq ES40 (interconnected with a highly efficient Memory Channel II), entirely dedicated to HPC projects.

2. Hydrodynamic modeling and non-equilibrium ionization

One of the research interests of our group is the study of the deviations from ionization equilibrium which may be present in astrophysical plasmas important for an accurate simulation of emitted spectra and thus for diagnostics. The effects of non-equilibrium ionization may be produced by a variety of processes, including plasma flows through steep temperature gradients or sudden variations of temperature. On the other hand, the analysis of UV and X-rays observations (e.g. spectral lines) is a powerful diagnostic tool of the physical conditions in astrophysical plasmas. Since any deviation from equilibrium may have a non-negligible effect on the UV and X-rays emitted spectrum, it is crucial to take into account this effect on the analysis and interpretation of the observations.

In this section we discuss two examples of application of the FLASH code with the new numerical modules developed in Palermo. In the first example we study the NEI effects induced during the evolution of a compact solar flare; and in the second one during the interaction of an old supernova shock front with an interstellar gas cloud.

2.1. NEI effects induced by a solar flare

For our purposes, we model a coronal magnetic flux tube as a semicircular loop of semilength L and cross-sectional area uniform along the loop. The coronal loop contains low β plasma, and we assume that cross-field fluid motions and thermal conduction are negligible so that a one-dimensional description is adequate. The model takes into account the gravity stratification, the thermal conduction, the plasma viscosity[1], the radiative losses, the heating (via a phenomenological term), and the NEI effects. The fluid equations of mass, momentum, and energy conservation are in the form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v}\mathbf{v} + \nabla P = \rho \mathbf{g} + \nabla \cdot (\nu(T) \nabla \mathbf{v}) \quad (2)$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E + P)\mathbf{v} = \rho \mathbf{v} \cdot \mathbf{g} + \nabla \cdot (\kappa(T) \nabla T) + Q(s,t) - n_e n_H \Lambda(T) \quad (3)$$

$$\frac{\partial n_i^Z}{\partial t} + \nabla \cdot n_i^Z \mathbf{v} = R_i^Z \quad \begin{array}{l} (Z = 1, ..., N_{elem}) \\ (i = 1, ..., N_{ion}^Z) \end{array} \quad (4)$$

$$E = \epsilon + \frac{1}{2}|\mathbf{v}|^2 , \qquad P = (\gamma - 1)\rho\epsilon , \quad (5)$$

$$\kappa(T) = 9.2 \times 10^{-7} T^{5/2} , \quad (6)$$

$$\nu(T) = 1.25 \times 10^{-16} T^{5/2} \quad (7)$$

where ρ is the plasma mass density, $\mathbf{v}$ the plasma flow speed, t the time, P the pressure, g the component of gravity parallel to the field lines, ν the coefficient of plasma compressional viscosity (Spitzer 1962), T the temperature, E the total plasma energy (internal energy ϵ plus kinetic) per unit mass, $\kappa(T)$ the thermal conductivity in c.g.s units (Spitzer 1962), $Q(s,t)$ the phenomenological heating rate, n_e and n_H are the electron and hydrogen number density respectively, $\Lambda(T)$ is the radiative losses per unit emission measure (Raymond and Smith 1977), $\gamma = 5/3$ the ratio of specific heats, n_i^Z is the number density of the ion i of the element Z, N_{elem} is the number of elements, N_{ion}^Z the number of ionization states of element Z, and

$$R_i^Z = n_e [n_{i+1}^Z \alpha_{i+1}^Z + n_{i-1}^Z S_{i-1}^Z - n_i^Z (\alpha_i^Z + S_i^Z)] \quad (8)$$

where α_i^Z are the collisional and dielectronic recombination coefficients, and S_i^Z the collisional ionization coefficients (Summers 1974).

As in Peres et al. (1987), the phenomenological heating is prescribed as a constant and uniform component plus a transient component deposited on the top of the loop (see also Pallavicini et al. 1983):

$$Q(s,t) = E_H + H_0 \times g(s) \times f(t) \quad (9)$$

where E_H is the intensity of the constant and uniform component, H_0 the peak value of the transient component, $g(s)$ and $f(t)$ are the distribution along the loop coordinate s and time dependence of the transient heating defined as

$$g(s) = \exp[-(s - s_0)^2 / 2\sigma^2] , \quad (10)$$

$$f(t) = \begin{cases} 0, & t \le t^* \\ 1, & t^* < t \le t_0 \\ \exp[(t_0 - t)/\tau], & t > t_0 \end{cases} \quad (11)$$

where s_0, σ, t^*, t_0, and τ are the parameters characterizing the spatial and temporal dependence of the impulsive heating.

The FLASH code with the configuration described above has been used to model a compact flare observed with Solar

[1] Note that, in the current version of the FLASH code, Eq. 3 does not take into account the viscosity term, as its effect is assumed to be small. The results presented here, therefore, have to be considered preliminary.

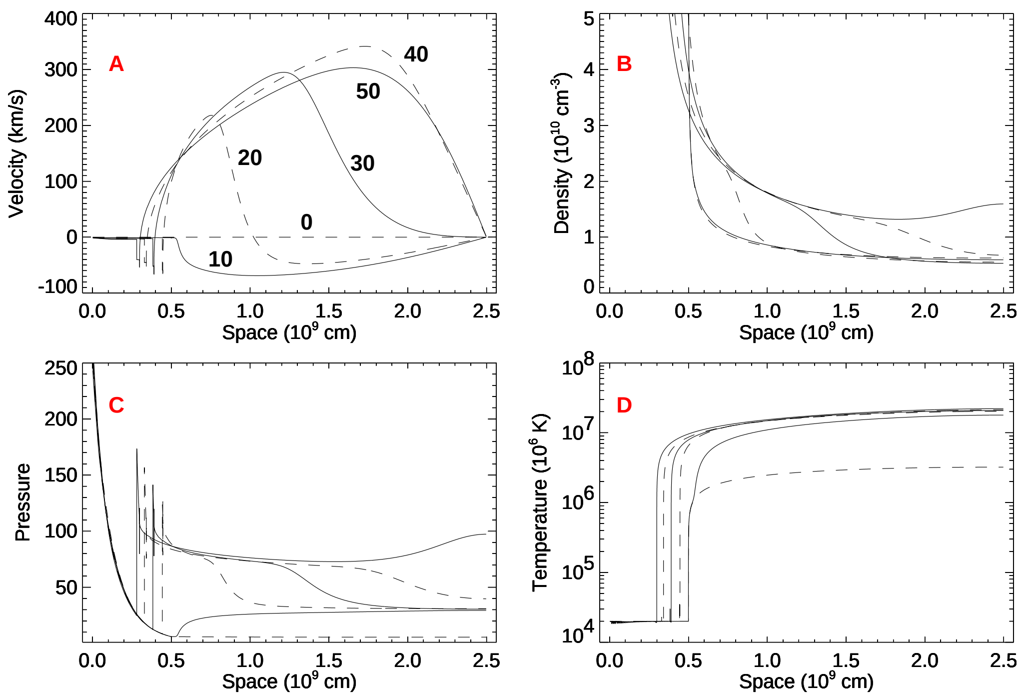

Fig. 1. Plasma velocity (A), density (B), pressure (C), and temperature (D) distributions along the loop from the chromosphere to the loop top sampled at the labeled times in seconds.

Maximum Mission (SMM) on November 12, 1980 and studied in detail by MacNeice et al. (1985), and Peres et al. (1987; see also Peres & Reale 1993). The flare evolution, therefore, is well known from these previous works and we focus only on the NEI effects.

We have adopted the boundary and initial conditions as well as the parameters characterizing the volumetric heating according to those adopted by Peres et al. (1987). In particular, we model a loop with semilength $L = 2.5 \times 10^9$ cm and with maximum temperature $T = 3.2 \times 10^6$ K and plasma pressure at the base of the transition region $P_0 = 6$ dyn cm^{-2} in the preflare conditions. The transient heating is located at the top of the loop ($s_0 = 2.5 \times 10^9$ cm, $\sigma = 5 \times 10^8$ cm) and is characterized by: $H_0 = 10$ erg cm^{-3} s^{-1}, $t^* = 0$, $t_0 = 180$ s, and $\tau = 60$ s; the uniform heating is defined by $E_H = 1.25 \times 10^{-2}$ erg cm^{-3} s^{-1}. The distributions of plasma velocity, density, pressure and temperature along the loop from the chromosphere to the corona, during the first minute of evolution, are shown in Fig. 1.

Fig. 1 shows that within the first 10 s from t^* the impulsive heating determines a rapid increase of the plasma temperature in corona to typical flare values ($T \sim 10^7$ K). As a consequence, the pressure increases in the corona, pushes plasma downwards and produces a downward motions. Simultaneously, a conduction front propagates downward to the chromosphere starting to heat it after approximately 10 s. The sudden heating of the chromospheric layers causes their rapid upward expansion determining a chromospheric evaporation. As

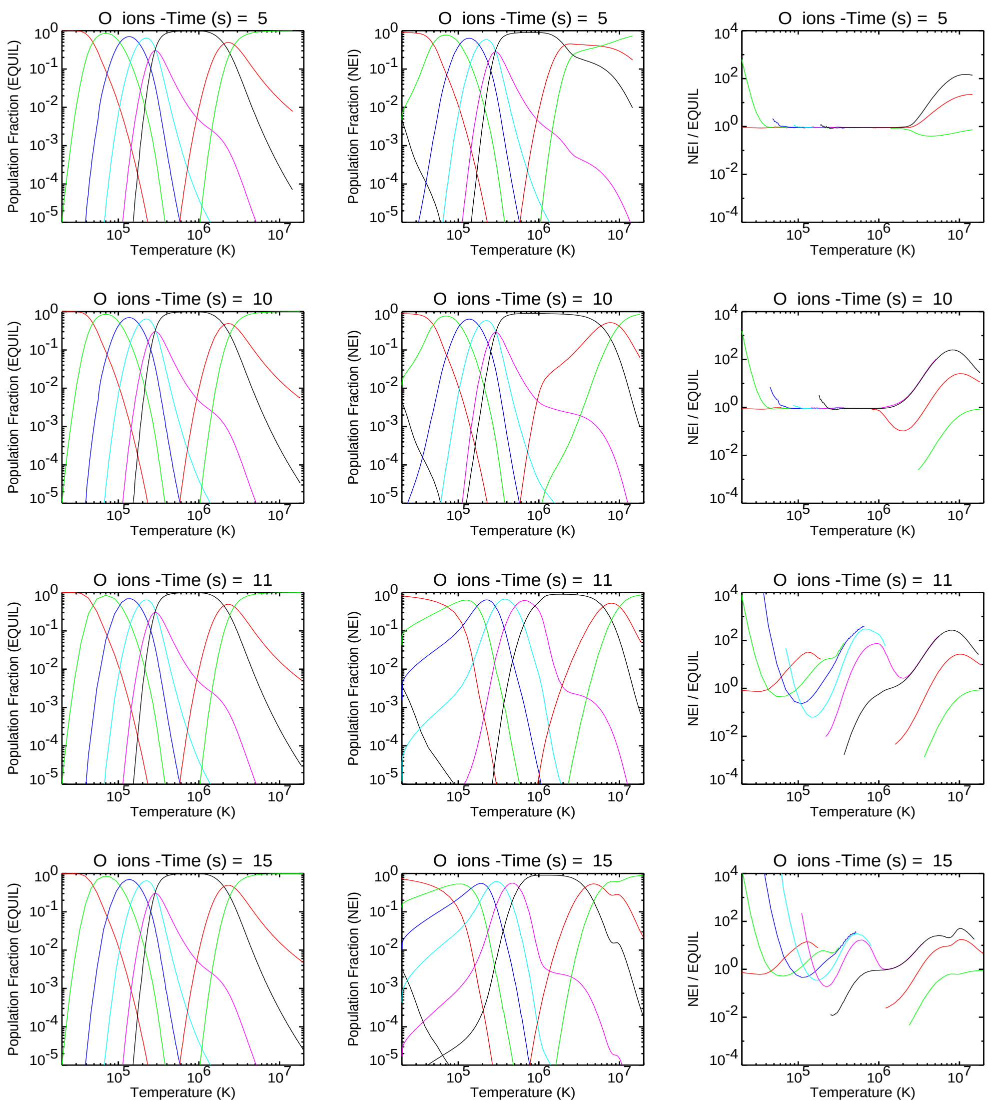

Fig. 2. Population fraction of Oxygen, n_i^O, vs. temperature along the loop. Panels from top to bottom are for increasing time (in seconds). Left panels show n_i^O assuming ionization equilibrium (EQUIL), central panels those in non-equilibrium of ionization (NEI), and the right panels the ratio of them (NEI/EQUIL).

a result the transition region drifts downwards (see Fig. 1).

There are, therefore, two main reasons to expect NEI effects: 1) the sudden temperature increase in corona, and 2) the violent flows carrying the cold plasma of the chromosphere through the transition region in the hot corona. As an example, in Fig. 2, we show the population fractions of Oxygen derived assuming ionization equilibrium, those in non-equilibrium of ionization and the ratio between the two, sampled at significant times. It is evident from the figure that both the local increase of temperature and the large plasma flows through the steep temperature gradients induced by the flare are responsible of non negligible NEI effects. In particular, before the chromospheric evaporation ($t \leq 10$ s) significant NEI effects are present in corona ($T > 10^6$ K) due to the temperature increase caused by the impulsive heating. During the chromospheric evaporation ($t > 10$ s) strong NEI effects are evident in the whole loop due to the rapid upward expansion of the upper chromospheric layers through the steep temperature gradient of the transition region, causing the presence of under-ionized plasma in corona.

In the light of the above results, we expect that the emission in spectral UV and X-ray lines and bands can be strongly affected by non-equilibrium ionization during a flare. As a consequence, the interpretation of UV and X-ray data has to take into account the NEI effects.

2.2. Interaction of a supernova shock front and an interstellar cloud

It has long been suspected that one of the major reasons for the great morphological complexity of supernova remnants (SNR) is the inhomogeneity of the interstellar medium (ISM) into which the shock wave expands. One crucial point is the comparison of models results with the observations and, in particular, the accurate synthesis of the emission from the model results to be compared directly with the observational data.

In this context, we discuss the application of the FLASH code to study the non-equilibrium ionization effects induced during the interaction of the supernova shock front with an interstellar gas cloud. In fact, given the complex dynamics of the system, strong deviations from ionization equilibrium are expected.

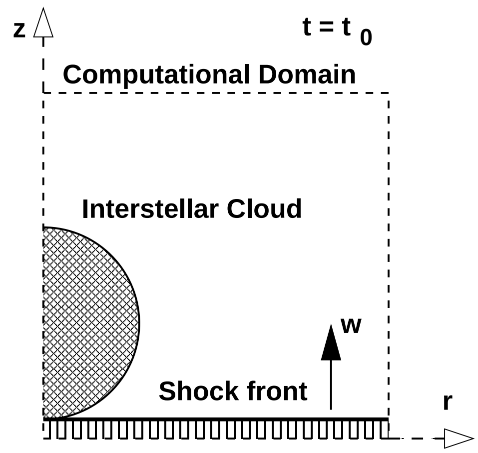

Fig. 3. Initial conditions for the cloud-shock interaction. At $t = t_0$ the cloud is centered at $r = 0$. The shock in the ISM is advancing upward with velocity w (see text). The dashed box marks our computational domain.

We consider a plane parallel supernova shock front interacting with a spherical isobaric interstellar cloud. The FLASH setup takes into account the NEI effects; the fluid equations of mass, momentum, and energy conservation are in the form:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} = 0 \tag{12}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \rho \mathbf{v}\mathbf{v} + \nabla P = 0 \tag{13}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E + P)\mathbf{v} = 0 \tag{14}$$

$$\frac{\partial n_i^Z}{\partial t} + \nabla \cdot n_i^Z \mathbf{v} = R_i^Z \quad \begin{matrix} (Z = 1, ..., N_{elem}) \\ (i = 1, ..., N_{ion}^Z) \end{matrix} \tag{15}$$

where R_i^Z is given by Eq. 8.

The interstellar cloud is assumed spherical with radius $r_{cloud} = 1$ pc, and uniform with mass density $\rho_{cloud} = 1.67 \times 10^{-24}$ gm cm^{-3} and temperature $T_{cloud} = 10^3$ K (see

Fig. 3). The cloud is in hydrostatic equilibrium with the ambient gas which is at constant temperature $T_{ism} = 10^4$ K and density $\rho_{ism} = 1.67 \times 10^{-25}$ gm cm^{-3}. The supernova shock front is modeled as a planar shock with a post-shock state defined as temperature $T_{sh} = 10^6$ K, plasma density $\rho_{sh} = \rho_{ism}\ (\gamma + 1)/(\gamma - 1)$ and flow velocity with respect to the undisturbed medium $v_{sh}^2 = c_s^2\ 2/(\gamma - 1)$. The shock front propagates in the ISM with velocity $w = v_{sh}(\gamma + 1)/2$ and, at time $t = t_0$, it starts the interaction with the cloud.

We adopted a 2-dimensional cylindrical (r, z) coordinate system: the horizontal direction is the cylindrical radial coordinate, r, and the vertical direction, running through the cloud center, is the z-coordinate. The equations are solved on a computational grid extending 10 pc in the r-direction and 5 pc in the z-direction. A reflecting boundary is assumed along the z-axis ($r = 0$), consistently with the symmetry. A constant inflow is assumed at the lower boundary ($z = 0$), and a zero-gradient outflow boundary at the upper ($z = 5$ pc), and left ($r = 10$ pc) boundaries, which allow plasma to flow off the edge of the computational grid.

Figure 4 shows the resulting evolution of temperature and mass density, at six different times; $t = 0$ marks the beginning of the shock-cloud interaction. After the SN shock front strikes the cloud, a shock is transmitted into the cloud, and a bow shock is reflected back into the intercloud medium. The shock transmitted into the cloud has a temperature of $\sim 10^5$ K. The bow shock reflected back into the intercloud medium undergoes the so-called conical self-reflection (Tenorio-Tagle & Rozyczka 1984). The flow around the cloud converges on the z axis, and the shock deposits vorticity (Klein et al. 1995). The cloud is gradually destroyed by the combined action of the Kelvin-Helmholtz and Rayleigh-Taylor instabilities.

The dynamics of the system leads the population fractions of the elements out of ionization equilibrium. A useful way to evaluate where and to what extent the deviations from equilibrium are important is considering the normalized difference D between the population fraction of a given element computed taking into account the NEI effects, N_{nei}, and that computed assuming ionization equilibrium, N_{eq}:

$$D = \frac{N_{nei} - N_{eq}}{N_{nei} + N_{eq}}\ . \tag{16}$$

negative values of D mark zones in which the population fraction of an element N_i^Z is overestimated assuming equilibrium, and the opposite for positive values of D.

As an example, Fig. 5 shows the normalized difference D computed for O V at the six different times sampled in Fig. 4. Assuming ionization equilibrium, the population fraction of O V is underestimated in the zones marked in white and overestimated in those marked in black. The figure shows that NEI effects are important along the whole evolution of the SN shock-cloud interaction. In particular, Kelvin-Helmholtz and Rayleigh-Taylor instabilities are responsible for significant NEI effects at the cloud border and the shock transmitted into the cloud leads to NEI effects inside the gas cloud.

3. Summary

Our group in Palermo is collaborating with the FLASH center, the University of Chicago, to update and test FLASH, an accurate numerical code for astrophysical plasma. In this paper, we have discussed two examples of application of FLASH with new numerical modules developed by our group and included in the last release of FLASH (2.1). These modules extend the field of applicability of the code to some areas in astrophysics, from solar and stellar coronae, to supernova remnants, and to galaxy clusters halos.

Among other modules, we have developed one which allows to study the deviations from equilibrium ionization induced by sudden variations of temperature or by

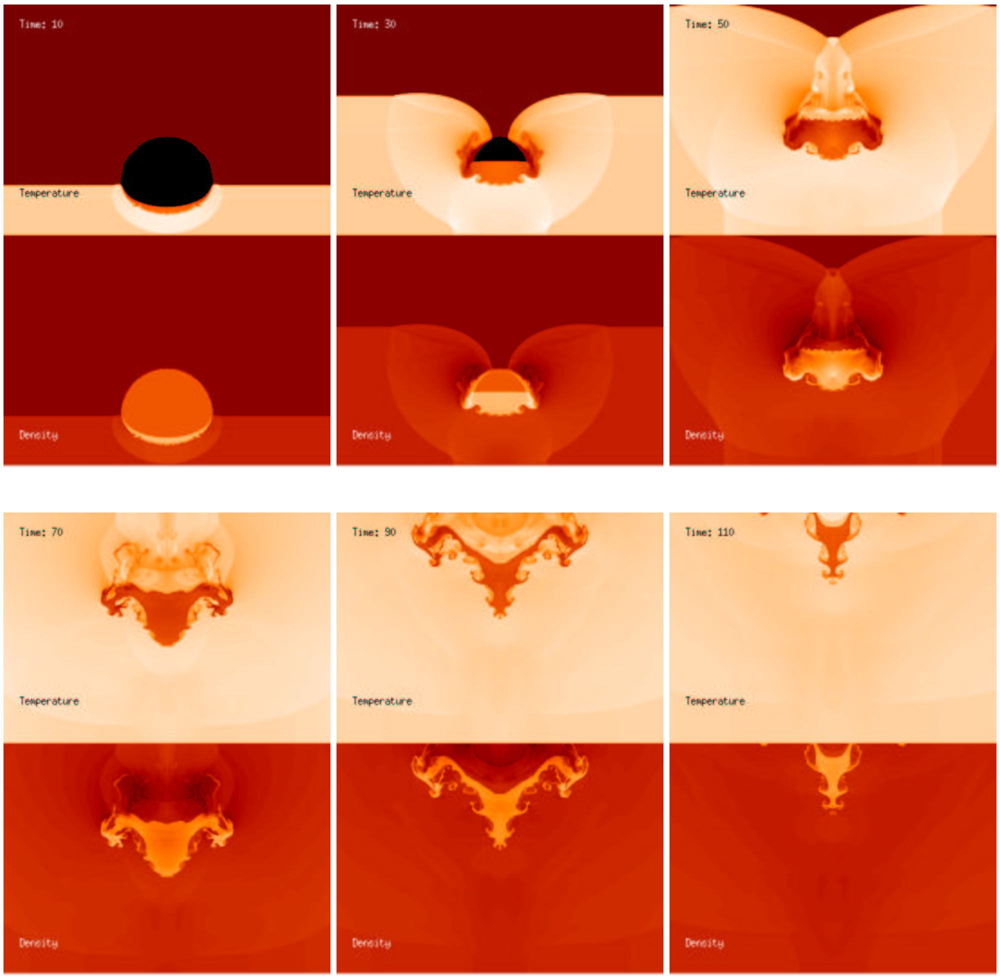

Fig. 4. Evolution of temperature and mass density during the SN shock-cloud interaction, sampled at the labeled times in units of 10^{10} sec, namely from 10×10^{10} sec to 110×10^{10} sec in steps of 20×10^{10} sec.

violent flows of plasma through steep temperature gradients. The accurate analysis of NEI effects may be crucial in the data interpretation in the light of the recent UV and X-ray missions.

In the first example considered, we have analyzed the NEI effects induced during the evolution of a compact solar flare and we have shown that these effects are strong at least within the first minute of the evolution due to both local variations of temperature and large plasma flows through the transition region (chromospheric evaporation). In the second example, we have studied the NEI effects induced during the interaction of a SN shock front with an interstellar gas cloud. Also in this case, we have found that the dynamics of the system induce strong deviations from ionization equilibrium due to the shock transmitted into the cloud but also due to the dy-

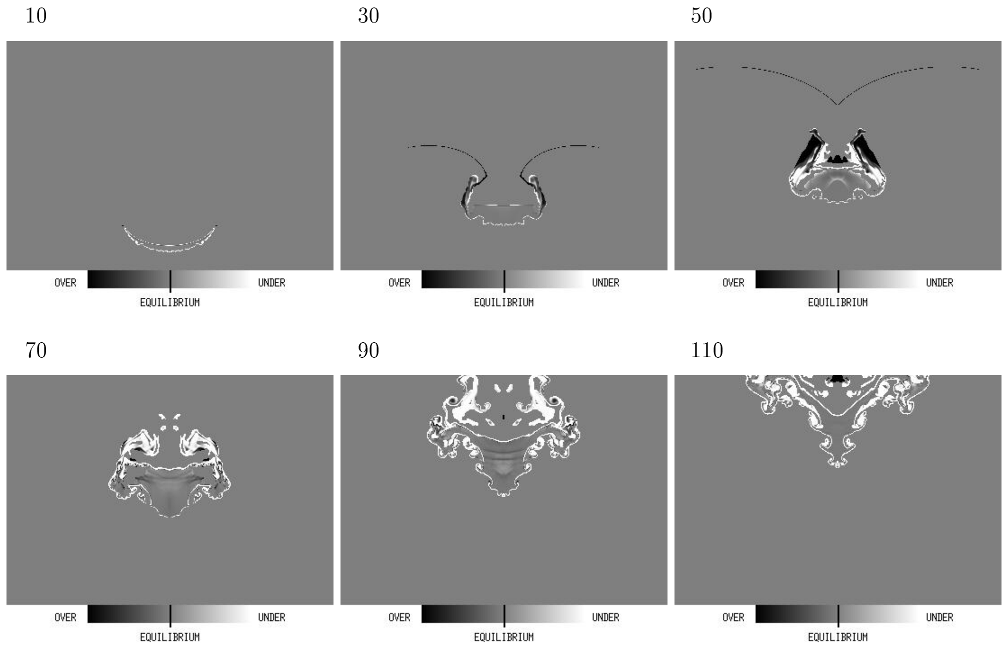

Fig. 5. Evolution of the normalized difference D (see text) sampled at the labeled times in units of 10^{10} sec (from 10×10^{10} sec to 110×10^{10} sec in steps of 20×10^{10} sec).

namical instabilities developed at the cloud border.

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