ISMServices

FIRST HANDS-ON SESSION WITH THE PARIS-DURHAM SHOCK CODE:

Non irradiated, stationary models

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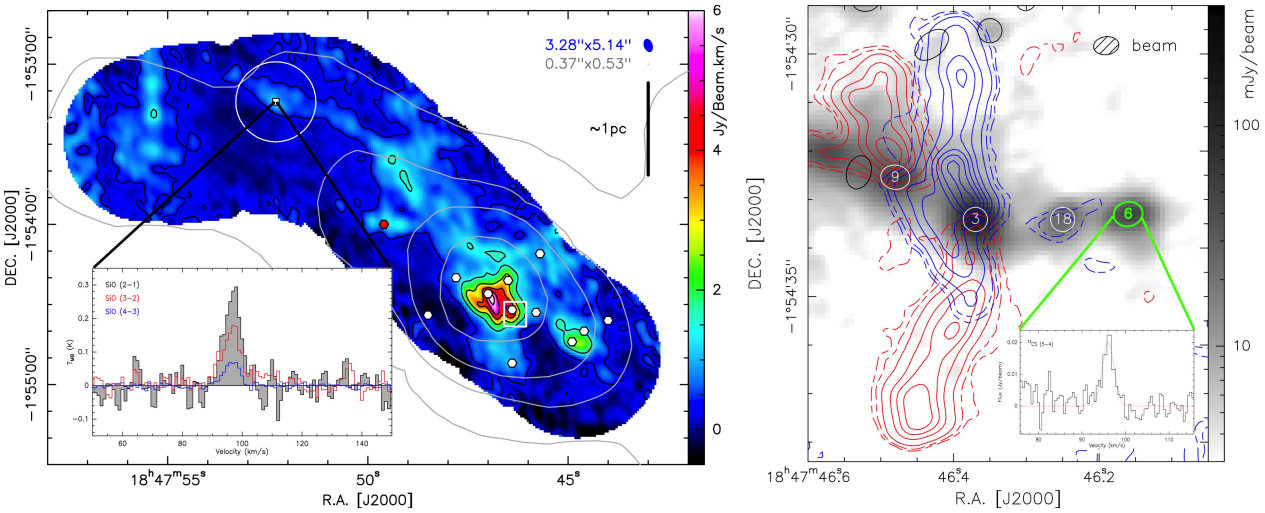

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Introduction

The Paris-Durham shock model is a code that simulates the propagation of hydrodynamical and magneto-hydrodynamical shock waves in the interstellar medium. It calculates the physical, chemical and dynamical structure of a shocked layer in interstellar conditions. The present version of the Paris-Durham shock code can be used to simulate the effects of the propagation of interstellar shock waves in the following conditions: pre-shock density of at least 10 to 10^8 cm^{-3}, and mininum and maximum shock velocity of sound velocity to 30 km s^{-1} for J-type models, and up to any velocity for C-type models. A new version of the code is under development to model J-type shocks with velocities up to 60 km s^{-1} (Lehmann et al., submitted). Further documentation and articles are available in https://ism.obspm.fr/.

Installing the Paris-Durham code

2.1 Downloading the source

Using your favourite web browser:

- go to https://ism.obspm.fr/ ;
- select Shock;
- click on the Download tab;
- click on the Download link of version Shock 1.1 rev 101.

2.2 Creating your workspace

Copy the 1.1 directory thus downloaded to your workspace. From now on we advise you to make it your working directory for all tasks related to the use of the Paris-Durham shock code.

2.3 Compiling the code

Compile the code and create the mhd_vode executable in the parent directory:

```
> cd 1.1
> cd bin
> make
```

Recommended. We recommend:

- to use the gfortran compiler. Other options are available in the Make file: pgf90 and ifort, but they are not maintained;
- to have a recent python distribution installed, either 2.7 or 3.x in order to benefit from the ready-to-use plotting routines we have prepared for this tutorial, provided on the ISM services wepage dedicated to shock models. The scipy and matplotlib libraries must be installed too;
- python-plotting routines are provided in the output directory.

Optional. If you are familiar with working with HDF5 data and have no difficulty having different python distributions on your computer, we also advise you to install the 2.7 version, in addition to the following libraries: sys, h5py, votable, numpy, config, convert, util.

2.4 Running a test

In order to make sure that the `mhd_vode` executable is indeed an executable, run a quick, meaningless and immediate test:

```
> cd ../
> ./mhd_vode
```

If the code starts, a number of information will appear in the window where you launched it. At this stage, you can interrupt the run, and proceed to the following chapters.

Input parameters, input files, and output files

3.1 Input parameters and the `input_mhd.in` file

3.1.1 Introduction

The list and brief description of input parameters can be found in the `input_mhd.in` file located in the `input` subdirectory. This is also the file where you will modify the values according to the model that you want to run. We highlight here some of the most important inputs. Throughout this chapter, the most important files and parameters will be highlighted in this color.

Parameters of the following blocks will not be modified during this session:

- `Wind parameters`, that control the shock type `W`, that will not be touched on during this first hands-on session;
- `grain properties`, that control the properties of grains used in the code;
- `developer options`, that control various developer-level decisions related to quantities computed by the code.

3.1.2 Input file parameters

The input file parameters are the following:

- the name of the directory that will contain the output files of the run, `modele`;
- the name of the file containing the initial abundances of species for the run `specfile`;
- the name of the file containing the chemical network for the run you are about to launch `chemfile`;
- the name of the file containing the initial H_2 level populations, `h2exfile`;
- the name of the file containing the grid of position – radiation field, `gridfile`.

3.1.3 Shock parameters

The shock parameters are the following:

- the shock type `shock_type`;
- the number of fluids `Nfluids`;
- the magnetic field parameter `Bbeta`, that defines the initial transverse magnetic field strength in μG, equal to: `Bbeta` $\times \sqrt{n_{\rm H}(\rm cm^{-3})}$;
- the shock velocity `Vs_km`;

- the initial drift velocity between ion and neutral fluids `DeltaVmin`;
- the pre-shock proton density `nH_init`;
- the initial value of the gas temperature `Tn`;
- the initial value of the ortho-to-para ratio of H_2 `op_H2_in`.

The default, pre-shock proton density value is $n_{\rm H} = 10^4$ cm^{-3}.

3.1.4 Environment parameters

The environment parameters for this hands-on session are the following:

- the cosmic ray ionization rate `Zeta`;
- the radiation field intensity, expressed in Habing's unit `RAD`.

The other parameters of this block relate principally to the use of irradiated shock models. Their presentation is deferred to a next hands-on session.

The default values for the cosmic ray ionization rate and the radiation field intensity are respectively: `zeta`$= 5\times10^{-17}$ s^{-1} (a standard value for the dense ISM), and `RAD`$= 0$, corresponding to non-irradiated shocks.

3.1.5 Excitation and cooling parameters

The excitation and cooling parameters are the following:

- the molecular cooling calculation mode `Cool_KN`;
- the number of H_2 levels taken into account `NH2_lev` (important note: we advise you to use 150 H_2 levels for precise calculations);
- the number of H_2 lines (local or integrated) intensities written in output files (see section 3.3) `NH2_lines_out` ;
- the dataset of collisional rate coefficients between H and H_2 `H_H2_flag`;
- the H_2 formation scenarios option `iforH2`;
- the kinetic energy of the newly formed H_2 `ikinH2`;
- the option to include the H_2 levels pumping by UV photons `pumpH2`;
- the number of CO levels included in the radiative transfer calculation `NCO_lev` [obsolete].

3.1.6 Numerical parameters

The numerical parameters are:

- the option to select the kind of integration scheme used for the calculation `integ_type`;
- the maximum number of calculation steps `Nstep_max`;
- the time of inclusion of the J contribution for a non stationary CJ-type model `timeJ`;
- the maximum shock duration `duration_max`;
- the precision parameter used by fthe differential equation integrator `Eps_V`;
- the characteristic viscous length `XLL`.

3.1.7 Output files specification parameters

Output files are available in ASCII and/or HDF5 formats. The ASCII-format output files are described in section 3.3. The corresponding output specifications are:

- the option to write HDF5 standard output files `F_W_HDF5_STD`;
- the option to write HDF5 standard output files `F_W_HDF5_CHE`;
- the option to write ASCII output files `F_W_ASCII` (for this hands-on session we advise you to use '1' for this value);
- the maximum number of points in HDF5 files, `Npthdf5`;
- the number of steps between 2 outputs, fof ASCII and HDF5 files, `Nstep_w`;
- the data format in the ASCII 'mhd_speci.out' file: `speci_out`;
- the data format in the ASCII 'H2_lev.out' file: `H2_out`;
- the data format in the ASCII 'H2_line.out' file: `line_out`;
- a flag for the output chemical analysis `flag_analysis` [obsolete].

3.2 Other input files

The other input files are also located in the `input` subdirectory. Three input files are of particular importance and will be modified during this first hands-on session: `input_mhd.in`, `species.in` and `chemistry.in`. They respectively contain the input parameters, the list of species and their initial abundances (defined as the ratio of the local density of the species divided by the local proton density in the pre-shock region, see note below), and the list of chemical reactions that are taken into account in the model. The choice of these files can be set either by modifying them manually (with `cp` instructions) either by modifying the selected file name in the `input_mhd.in` file (see the first block `input files` described above).

A variety of species can be found in the `species.in` file (and also in the `species.out` one, see section 3.3): atoms, molecules, ions, grains (neutral: `G`, positively or negatively charged `G+`, `G-`, Polycyclic Aromatic Hydrocarbons represented by the $C_{54}H_{18}$ molecule (neutral, positively and negatively charged), grain core species (denoted as `X**`, with X = O, Fe, Si, Mg, C), and grain mantle species (denoted as `X*`, with X = H_2O, O_2, CO, CO_2, CH_4, NH_3, CH_3OH, H_2CO, HCO_2H, OCS, H_2S, SiH_4, SiO, SiO_2, Fe).

Abundances are defined throughout this document as the ratio of the local density of the species divided by the local proton density in the pre-shock region. We **DON'T** define abundances as column density ratios, as observers usually do.

3.3 ASCII Output files

The ASCII output files are organized as follows:

- `check_isrf.out` contains the interstellar radiation field;
- `energetics.out` contains the values of mass, momentum, and energy fluxes contributions at each point of the shock layer respectively in g/s/cm^2, erg/cm^3, erg/s/cm^2 units;
- `err_cool.out` contains potential warning messages;
- `excit.out` contains the final values to build the H_2 excitation diagram associated to the shock layer;
- `fe_lines.out` is a currently deprecated file that contains the values of the integrated intensities of the Fe lines at each point of the shock layer in (erg/cm^2/s/sr) units;
- `fe_pops.out` is a currently deprecated file that contains the level density of the Fe levels at each point of the shock layer relative to ground state;
- `h2levels.out` contains H_2 level populations calculated at the last iteration of the run, in the format similar to the file indicated by `h2exfile` (see `input files` in section 3.1.2; in particular, at the end of the static calculation, `h2levels.out` can be used as an input for the subsequent shock run, similar to the `species.out` calculated at the end of the static calculation, see below and chapter 5);
- `H2_lev.out` contains the density (in cm^{-3}), column density (in cm^{-2}), or integrated $\ln(N/g)$ value of each considered H_2 level depending on the value of the `H2_out` variable, set in the `input_mhd.in` file (respectively `AD`, `CD`, or `ln(N/g)`);
- `H2_line.out` contains the values of the emissivity (in erg/s/cm^3) or integrated intensity (in erg/s/cm^2/sr) of each H_2 line, depending on the value of the `line_out` variable, set in the 'input_mhd.in' file (respectively `local` or `integrated`);
- `info_mhd.out` contains the information relevant to the inputs used in your run;
- `intensity.out` contains the integrated intensity values of the most relevant atomic and ion lines at each point of the shock layer in (erg/cm^2/s/sr) units;

- `mhd_coldens.out` contains the values of species column densities at each point of the shocked layer;
- `mhd_phys.out` contains the values of physical/dynamical variables at each point of the shocked layer;
- `mhd_speci.out` contains the values of the density (in cm^{-3}), column density (in cm^{-2}), or abundance (defined as the ratio of the local density of the species divided by the local proton density, see note below) of all considered species at each point of the shock layer, depending on the value of the `speci_out` variable, set in the '`input_mhd.in`' file (respectively `AD`, `CD`, or `FD`);
- `populations.out` contains the level density of the most relevant atomic and ion levels at each point of the shock layer relative to ground state;
- `species.out` contains the abundance (see note below) of all considered species calculated at the last iteration of the run, in the format similar to the file indicated by `specfile` (see `input files` in section 3.1.2; in particular, at the end of the static calculation, `species.out` can be used as an input for the subsequent shock run, similar to the `h2levels.out` calculated at the end of the static calculation, see above and chapter 5);
- `thermal_balance.out` contains the values of the contribution of each mechanism included in the calculation of the thermal balance of the model (in $erg/s/cm^3$).

A variety of species can be found in the `species.in` file (and also in the `species.out` one, see section 3.3): atoms, molecules, ions, grains (neutral: `G`, positively or negatively charged `G+`, `G-`, Polycyclic Aromatic Hydrocarbons represented by the $C_{54}H_{18}$ molecule (neutral, positively and negatively charged), grain core species (denoted as `X**`, with X = O, Fe, Si, Mg, C), and grain mantle species (denoted as `X*`, with X = H_2O, O_2, CO, CO_2, CH_4, NH_3, CH_3OH, H_2CO, HCO_2H, OCS, H_2S, SiH_4, SiO, SiO_2, Fe).

Abundances are defined throughout this document as the ratio of the local density of the species divided by the local proton density in the pre-shock region. We **DON'T** define abundances as column density ratios, as observers usually do.

Running a non-irradiated static model

4.1 Why a static model ?

When running a particular shock model with the Paris-Durham code, all input parameters must be initialised. For a number of input parameters, the initial value is chosen by the user: the name of input files that will be used for the computation, shock parameters, environment parameters, grain properties, excitation and cooling options, numerical parameters, output specifications, and developer options. These choices are made in the `input_mhd.in` file, where all these parameters are listed and described, and where their initial value can be varied.

It is also necessary to compute the initial abundance of all species whose abundance is calculated by the code. To do this, we classically use initial values at the chemical equilibrium. The chemical equilibrium can be calculated by the Paris-Durham code. This is the purpose of the static run. Starting from solar neighbourhood elemental abundances and a fixed distribution over certain species for a given number of elements (H, C, O, N, S, Si, Mg, Fe), the static code calculates the equilibrium abundance of all species included in the model. Two options can be considered for this particular use of the code:

- if `RAD` $= 0$, i.e. one wants to run a non-irradiated shock model, the static model must be run in non-irradiated conditions. A specific chemical network must be used, and grain surface processes must be removed from the chemical network (the abundance of species on grain mantles is fixed). This is done by using `species.in_depl` as initial abundances file and `chemistry.in_noadso` as chemistry file;

- if `RAD` $\neq 0$, i.e. one wants to run an externally irradiated shock model, the static model must also be run in externally irradiated conditions. The `species.in` and `chemistry.in` input files can be used for the static run, that includes grain surface processes in the calculation of the equilibrium state. The description of such a run is deferred to a next hands-on session.

Note that the time necessary to reach the equilibrium is long, so the static computation must be made with a long enough `duration_max` parameter. The following paragraphs describe the procedure to launch a static model.

4.2 Choosing the input parameters for a non-irradiated static run

We detail here the procedure to run a static model, with the following characteristics: pre-shock proton density $n_{\mathrm{H}} = 10^4$ cm^{-3}, cosmic ray ionization rate $\zeta = 5 \times 10^{-17}$ s^{-1}, and no external irradiation (`RAD` = 0). In the `input_mhd.in` file, set the following values:

```
!---- input files ----
...
species.in_depl          ! specfile
chemistry.in_noadso      ! chemfile
...
!---- shock parameters ----
S1                       ! shock_type
1                        ! Nfluids
1.00E+04                 ! nH_init
...
!---- environment ----
5.00E-17                 ! Zeta
...
0.00E+00                 ! RAD
...
!---- excitation & cooling ----
0                        ! Cool_KN
...
150                      ! NH2_lev
200                      ! NH2_lines_out
...
!---- numerical parameters ----
...
1.00E+09                 ! duration_max
...
!---- output specifications ----
...
FD                       ! speci_out
AD                       ! H2_out
local                    ! line_out
...
```

Then, from the input directory:

```
> cd ../
> ./mhd_vode
```

4.3 A very important note

Filing system. Launching a static model must be repeated each time you need to run a model with a different pre-shock density `nH_init` ($n_{\rm H}$), cosmic ray ionization rate `zeta` (ζ), or radiation field `RAD` value. A good reflex is to save the output created at the end of the run in a directory with a self-explanatory name like `output/static-n`xx`-zeta`xx`-rad`xx (`output/static-n1e4-z5em17-rad0` for the above example).

Running a non-irradiated, stationary shock model

5.1 Running a non-irradiated stationary J-type model

We detail here the procedure to run a stationary J-type shock model, with the following characteristics: pre-shock proton density $n_{\rm H} = 10^4$ cm^{-3}, shock velocity $v_{\rm s} = 15$ km s^{-1}, transverse magnetic field (in μG, defined by `Bbeta` $\times\sqrt{n_{\rm H}(\rm cm^{-3})}$) of 10 μG, cosmic ray ionization rate $\zeta = 5 \times 10^{-17}$ s^{-1}, and no external irradiation (`RAD` = 0). In the `input_mhd.in` file, set the following values:

```
!---- input files ----
...
output/static-n1e4-z5em17-rad0/species.out      ! specfile
chemistry.in                                    ! chemfile
output/static-n1e4-z5em17-rad0/h2levels.out     ! h2exfile
...
!---- shock parameters ----
J                       ! shock_type
1                       ! Nfluids
1.00E-01                ! Bbeta
1.50E+01                ! Vs_km
1.00E+04                ! nH_init
...
!---- environment ----
5.00E-17                ! Zeta
...
0.00E+00                ! RAD
...
!---- excitation & cooling ----
1                       ! Cool_KN
...
150                     ! NH2_lev
200                     ! NH2_lines_out
...
!---- numerical parameters ----
...
1.00E+07                ! duration_max
...
!---- output specifications ----
...
FD                      ! speci_out
AD                      ! H2_out
local                   ! line_out
...
```

Then, from the input directory:

```
> cd ../
> ./mhd_vode
```

5.2 Running a non-irradiated stationary C-type model

We detail here the procedure to run a stationary C-type shock model, with the following characteristics: pre-shock proton density $n_{\rm H} = 10^4$ cm^{-3}, shock velocity $v_{\rm s} = 15$ km s^{-1}, transverse magnetic field (in μG, defined by `Bbeta` $\times \sqrt{n_{\rm H}(\rm cm^{-3})}$) of 100 μG , cosmic ray ionization rate $\zeta = 5 \times 10^{-17}$ s^{-1}, and no external irradiation (`RAD` = 0). In the `input_mhd.in` file, set the following values:

```
!---- input files ----
...
output/static-n1e4-z5em17-rad0/species.out      ! specfile
chemistry.in                                    ! chemfile
output/static-n1e4-z5em17-rad0/h2levels.out     ! h2exfile
...
!---- shock parameters ----
C                       ! shock_type
3                       ! Nfluids
1.00E+00                ! Bbeta
1.50E+01                ! Vs_km
1.00E+04                ! nH_init
...
!---- environment ----
5.00E-17                ! Zeta
...
0.00E+00                ! RAD
...
!---- excitation & cooling ----
1                       ! Cool_KN
...
150                     ! NH2_lev
200                     ! NH2_lines_out
...
!---- numerical parameters ----
...
1.00E+07                ! duration_max
...
!---- output specifications ----
...
FD                      ! speci_out
AD                      ! H2_out
local                   ! line_out
...
```

Then, from the input directory:

```
> cd ../
> ./mhd_vode
```

5.3 Filing system

Filing system. A good reflex is to save the outputs thus created at the end of the run in a directory with a self-explanatory name, like respectively `output/j-n1e4-b0p1-v15-z5em17-rad0` and `output/c-n1e4-b1p0-v15-z5em17-rad0` for the above examples.

The tutorial

The tutorial consists of a list of questions. The answers to the question should be based on figures, that will be produced from the input files indicated in this colour in each question.

6.1 Static model

❏ 0 – Run a static model with the following characteristics: pre-shock proton density $n_{\rm H} = 10^4$ cm^{-3}, cosmic ray ionization rate $\zeta = 5 \times 10^{-17}$ s^{-1}, and no external irradiation (`RAD` = 0).

❏ 1 – Plot the temperature, total density, H_2 and H densities as functions of time (`mhd_phys.out`).

❏ 2 – Plot the abundances of electrons, ions, H^+, C^+, S^+, PAH^-, PAH^+, and HCO^+ as functions of time (`mhd_speci.out`).

a) Is the chemical equilibrium reached after 10^9 yrs ? What is the equilibrium temperature ?

b) What are the molecular fraction and ionization fraction in this gas ? What are the main charge carriers ?

❏ 3 – Plot the abundance of C^+, C, CO, CH_3OH and HCO^+ as functions of time (`mhd_speci.out`). Plot the abundances of H_2O, OH, O, CO, CH_3OH and HCO^+ as functions of time (`mhd_speci.out`). Are the elemental abundances of C and O conserved ? What are the dominant carriers of C and O at equilibrium ?

❏ 4 – Plot the conserved quantities ($n_{\rm i} - n_{\rm e}$, elemental abundances, total PAH abundance...; `mhd_speci.out`). Are evolutionary trends consistent for these quantities ?

Abundances are defined throughout this document as the ratio of the local density of the species divided by the local proton density in the pre-shock region. We **DON'T** define abundances as column density ratios, as observers usually do.

6.2 Stationary J-type models

❏ 0 – Run stationary J-type models with the following characteristics: pre-shock proton density $n_{\rm H} = 10^4, 10^6$ cm^{-3}, transverse magnetic field strength of 10 μG, shock velocity $v_{\rm s} = 10, 30$ km s^{-1}, cosmic ray ionization rate $\zeta = 5 \times 10^{-17}$ s^{-1}, and no external irradiation (`RAD` = 0).

❏ 1 – Compare the temperature profiles of all these models (`mhd_phys.out`).

a) What are the shock timescales ? What is the sizes of the shocked layers ?

b) What are the maximum temperatures reached within the shock layers ?

❏ 2 – What are the sound velocity and Mach numbers through the shock layers (`mhd_phys.out`) ?

❏ 3 – For the models with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 10, 30$ km s^{-1}, study and compare the H chemistry through the shock layer (`mhd_speci.out`).

❏ 4 – For the models with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 10, 30$ km s^{-1}, plot the abundances of electrons, ions, H^+, C^+, S^+, PAH^-, PAH^+, and HCO^+ as functions of time (`mhd_speci.out`). What is the evolution of the molecular fraction and ionization fraction in these shocks ? What are the main charge carriers ?

❏ 5 – For the models with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 10, 30$ km s^{-1}, plot the abundance of C^+, C, CO, CH_3OH and HCO^+ as functions of time (`mhd_speci.out`). Plot the abundances of H_2O, OH, O, CO, CH_3OH and HCO^+ as functions of time (`mhd_speci.out`). Are the elemental abundances of C and O conserved ? What are the dominant carriers of C and O at equilibrium ?

❏ 6 – For the models with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 10, 30$ km s^{-1}, plot the abundance of Si^+, Si, and SiO as functions of time (`mhd_speci.out`). What is the dominant carrier of silicon ?

❏ 7 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 30$ km s^{-1}, verify the Rankine-Hugoniot equations (`mhd_phys.out`).

❏ 8 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 30$ km s^{-1}, plot the total heating rate (sum of `line_rad_tot` + `chem_DE_tot` + `elast_scat_tot` + `exch_eint_tot` + `therm_grain_tot` + `mech_trsf_tot`) as functions of time or distance (`thermal_balance.out`). How does the sign of this term evolve over time ? Is it coherent with the evolution of the temperature plotted before ? What physical processes are mostly responsible for the heating and cooling over the trajectory ?

A bit of deciphering (all heating/cooling terms are in erg cm^{-3} s^{-1}):

```
line_rad_tot    ! total radiative heating/cooling
chem_DE_tot     ! total chemical heating/cooling
elast_scat_tot  ! total elastic scat heating/cooling
exch_eint_tot   ! total heat exchange
therm_grain_tot ! total heating/cooling by thermalization with grains
mech_trsf_tot   ! total mechanical heating/cooling
```

❏ 9 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 30$ km s^{-1}, decompose the line_rad_tot term in atomic (`line_rad_n_atoms` + `line_rad_i_atoms` + `line_rad_e_atoms`) and molecular contributions (`line_rad_n_molec` + `line_rad_i_molec` + `line_rad_e_molec`), then further decompose these terms (`thermal_balance.out`). Identify the processes cooling the gas between 1e-3 and 1e3 yr.

A bit of deciphering (all heating/cooling terms are in erg cm^{-3} s^{-1}):

```
line_rad_n_atoms ! radiative heating/cooling of
                 ! neutral fluid  by all atoms
line_rad_i_atoms ! radiative heating/cooling of
                 ! positively charged fluid  by all atoms
line_rad_e_atoms ! radiative heating/cooling of
                 ! negatively charged fluid  by all atoms
line_rad_n_molec  ! radiative heating/cooling of
                 ! neutral fluid  by all molecules
line_rad_i_molec ! radiative heating/cooling of
                 ! positively charged fluid  by all molecules
line_rad_e_molec ! radiative heating/cooling of
                 ! negatively charged fluid  by all molecules
```

❏ 10 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 30$ km s^{-1}, decompose the `mech_trsf_tot term` (`thermal_balance.out`). What are the most important processes heating the gas over its trajectory ?

❏ 11 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 30$ km s^{-1}, what are the contributions from the different forms of energy to the total energy flux through the shock layer (`energetics.out`)?

Abundances are defined throughout this document as the ratio of the local density of the species divided by the local proton density in the pre-shock region. We **DON'T** define abundances as column density ratios, as observers usually do.

6.3 Stationary C-type models

❏ 0 – Run stationary C-type models with the following characteristics: pre-shock proton density $n_{\rm H} = 10^4$ cm^{-3}, transverse magnetic field strength of 100 and 500 μG, shock velocity $v_{\rm s} = 10, 15, 30$ km s^{-1}, cosmic ray ionization rate $\zeta = 5 \times 10^{-17}$ s^{-1}, and no external irradiation (`RAD` = 0).

❏ 1 – Compare the temperature profiles of all these models (`mhd_phys.out`).

a) What are the shock timescales ? What is the size of the shocked layers ? Comment on the influence of the magnetic field.

b) What are the maximum temperatures reached within the shock layer ? Comment on the influence of the magnetic field.

❏ 2 – What are the sound velocity and Mach numbers through the shock layers (`mhd_phys.out`) ?

❏ 3 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, study and compare the H chemistry through the shock layer (`mhd_speci.out`).

❏ 4 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, plot the abundances of electrons, ions, H^+, C^+, S^+, PAH^-, PAH^+, and HCO^+ as functions of time (`mhd_speci.out`). What is the evolution of the molecular fraction and ionization fraction in these shocks ? What are the main charge carriers ?

❏ 5 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, plot the abundance of C^+, C, CO, CH_3OH and HCO^+ as functions of time (`mhd_speci.out`). Plot the abundances of H_2O, OH, O, CO, CH_3OH and HCO^+ as functions of time (`mhd_speci.out`). Are the elemental abundances of C and O conserved ? What are the dominant carriers of C and O at equilibrium ?

❏ 6 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, plot the abundance of Si^+, Si, and SiO as functions of time (`mhd_speci.out`). What is the dominant carrier of silicon ?

❏ 7 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, verify the Rankine-Hugoniot equations (`mhd_phys.out`).

❏ 8 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, plot the total heating rate (sum of `line_rad_tot` + `chem_DE_tot` + `elast_scat_tot` + `exch_eint_tot` + `therm_grain_tot` + `mech_trsf_tot`) as functions of time or distance (`thermal_balance.out`). How does the sign of this term evolve over time ? Is it coherent with the evolution of the temperature plotted before ? What physical processes are mostly responsible for the heating and cooling over the trajectory ?

A bit of deciphering (all heating/cooling terms are in erg cm^{-3} s^{-1}):

```
line_rad_tot    ! total radiative heating/cooling
chem_DE_tot     ! total chemical heating/cooling
elast_scat_tot  ! total elastic scat heating/cooling
exch_eint_tot   ! total heat exchange
therm_grain_tot ! total heating/cooling by thermalization with grains
mech_trsf_tot   ! total mechanical heating/cooling
```

❏ 9 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, decompose the line_rad_tot term in atomic (`line_rad_n_atoms` + `line_rad_i_atoms` + `line_rad_e_atoms`) and molecular contributions (`line_rad_n_molec` + `line_rad_i_molec` + `line_rad_e_molec`), then further decompose these terms (`thermal_balance.out`). identify the processes cooling the gas over the entire trajectory.

A bit of deciphering (all heating/cooling terms are in erg cm^{-3} s^{-1}):

```
line_rad_n_atoms ! radiative heating/cooling of
                 ! neutral fluid  by all atoms
line_rad_i_atoms ! radiative heating/cooling of
                 ! positively charged fluid  by all atoms
line_rad_e_atoms ! radiative heating/cooling of
                 ! negatively charged fluid  by all atoms
line_rad_n_molec ! radiative heating/cooling of
                 ! neutral fluid  by all molecules
line_rad_i_molec ! radiative heating/cooling of
                 ! positively charged fluid  by all molecules
line_rad_e_molec ! radiative heating/cooling of
                 ! negatively charged fluid  by all molecules
```

❏ 10 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, decompose the `mech_trsf_tot term` (`thermal_balance.out`). What are the most important processes heating the gas over its trajectory ?

❏ 11 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, what are the contributions from the different forms of energy to the total energy flux through the shock layer (`energetics.out`)?

❏ 12 – For the model with $n_{\rm H} = 10^4$ cm^{-3} and $v_{\rm s} = 15$ km s^{-1}, and transverse magnetic field strength of 100 μG, build two diagrams: one with ($T_{\rm n}$, the abundance of water, the total particle density and the fractional abundance of water through the shock), and one with ($T_{\rm n}$, the column density of water, the total particle column density and the fractional column density of water through the shock) (`mhd_speci.out`). Comment on the differences. In principle, you are now able to understand the following remark:

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