First hands-on session with the Paris-Durham shock model

The Paris-Durham shock model is a code that simulates the propagation of hydrodynamical and magneto-hydrodynamical shock waves in the interstellar medium. The project is described further in http ://ism.obspm.fr where links to papers and documentation are given.

1 Installing the Paris-Durham code

Downloading the source. Using your favourite web browser :

- bullet go to 'https ://ism.obspm.fr/' ;
- select 'Shock' ;
- click on the 'Download' tab ;
- click on the 'Download' link of version Shock 1.1 rev 89.

Creating your workspace. Copy the directory 'Shock_1.1' thus downloaded to your workspace. From now on this will be your working directory for all tasks related to the use of the Paris-Durham shock code.

Compiling the code. Compile the code and create the 'mhd_vode' executable in the superior directory :
> *cd Shock_1.1*
> *cd bin*
> *make*

Running a test. Run a quick, meaningless and immediate test :
> *cd ../*
> *./mhd_vode*

2 Important input parameters and files

The list and brief description of input parameters can be found in the 'input_mhd.in' file located in the 'input' subdirectory. We highlight here some of the most important ones. In red are the ones that we'll modify during this first hands-on session.

Shock parameters. The shock parameters are the following :

- the shock type shock_type
- the number of fluids Nfluids
- the magnetic field parameter Bbeta
- the shock velocity Vs_km
- the initial drift velocity between the ion and neutral fluids DeltaVmin
- the pre-shock density nH_init
- the initial gas temperature Tn
- the initial value for the ortho-to-para ratio of H_2 op_H2_in

Environment parameters. The most important environment parameters are the following :

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

Excitation and cooling parameters. The most important 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
- the number of H_2 levels transitions into account 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

Numerical parameters. The most important numerical parameters are :

- the number of calculation steps Nstep_max
- the time of inclusion of the J contribution (for CJ-type models) timeJ
- the maximum shock duration duration_max
- a precision parameter for the computation Eps_V

Output specifications. The output specifications that we'll be using here are related to the unit of the data in the output ASCII files. All options are however kept in hdf5 format. The output files are described in section 3. These output specifications are :

- the data format in the 'mhd_speci.out' file : speci_out
- the data format in the 'H2_lev.out' file : H2_out
- the data format in the 'H2_line.out' file : line_out

Input files. The input files are 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, but also 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 total local density in the pre-shock region), and the list of chemical reactions that are taken into account in the model.

3 Output files

Output files. The output files are numerous, and are organized as follows :

- cooling.out contains the values of the molecular and atomic cooling (emissivity) due to the most relevant species at each point of the shock layer in (erg/s/cm^3) units ;
- 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 unimportant warning messages ;
- excit.out contains the final values to build the H2 excitation diagram associated to the shock layer ;

- fe_lines.out 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 contains the level density of the Fe levels at each point of the shock layer relative to ground state ;
- H2_lev.out contains the values of the density of each considered H_2 level in the unit chosen in the 'input_mhd.in' file (namely 'AD' : cm^{-3}, 'CD' : cm^{-2}, or 'ln(N/g)') ;
- H2_line.out contains the values of the (integrated) intensity of each considered H_2 line in the unit chosen in the 'input_mhd.in' file (namely 'local' : erg/s/cm^3, or 'integrated' : erg/s/cm^2/sr) ;
- info_mhd.out contains the information relevant to the inputs used in you run ;
- intensity.out contains the values of the integrated intensities of the most relevant atomic and ion lines at each point of the shock layer in (erg/cm^2/s/sr) units ;
- mhd_phys.out contains the values of physical/dynamical parameters at each point of the shocked layer ;
- mhd_speci.out contains the values of species abundances at each point of the shock layer in the unit chosen in the 'input_mhd.in' file (namely 'AD' : cm^{-3}, ''CD' : cm^{-2} or 'FD' : n(x)/nH) ;
- 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 a list of chemical species and corresponding abundances, for internal check-up/use only.

4 Running a model with the Paris-Durham code

4.1 Running a non-irradiated static model

Why is it necessary to run a static model ? When running a particular shock model with the Paris-Durham code, all the input parameters must be initialised. The initial value of a number of parameters are chosen by the user : the name of the 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 can be 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, the choice has been made to 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 the solar neighbourhood 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 abundance of all species included in the model. The specific 'species.in' to use for this step is contained in 'species.in_depl'. A particular chemistry network must be set, excluding specific grain processes that occur in shocks. This specific network is contained in 'chemistry.in_noadso'. At the end of the static run, the 'species.out' file from the run contains the values at the equilibrium and must be copied in the 'species.in' file before running a shock computation. 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.

Choosing the correct input parameter values. In the 'input_mhd.in' file, set :

- 'shock_type' to 'S1' ;
- 'Nfluids' to 1 ;
- 'Bbeta' to 1 ;
- 'Cool_KN' to 0 ;
- 'duration_max' to 1e10.

Choosing the correct chemistry and initial conditions. In the input directory :
> *cp chemistry.in chemistry.in-orig*
> *cp chemistry.in_noadso chemistry.in*
> *cp species.in_depl species.in*
> *cd ../*
> *./mhd_vode*

Very importante note. Launching a static model must be repeated each time you need to run a model with a different pre-shock density, ζ value, or radiation field value. A good reflex is to save the output thus created at the end of the run in a directory like 'output/static-nxx-zetaxx-gxx'.

4.2 Running a non-irradiated stationary J-type model

Choosing the correct input parameter values. In the 'input_mhd.in' file, set :

- 'shock_type' to 'J' ;
- 'Nfluids' to 1 ;
- 'Bbeta' to 0.1 ;
- 'Cool_KN' to 1 ;
- Nstep_max' to 25 000 ;
- 'duration_max' to 1e08.

Choosing the correct chemistry and initial conditions. In the input directory :
> *cp chemistry.in-orig chemistry.in*
> *cp ../output/static-n*xx-ζxx-*g*xx*/species.out species.in*
> *cd ../*
> *./mhd_vode*

Importante note. A good reflex is to save the output thus created at the end of the run in a directory like 'output/j-nxx-zetaxx-gxx-vxx-bxx'.

4.3 Running a non-irradiated stationary C-type model

Choosing the correct input parameter values. In the 'input_mhd.in' file, set :

- 'shock_type' to 'C' ;
- 'Nfluids' to 3 ;
- 'Bbeta' to 1 ;
- 'Cool_KN' to 1 ;
- Nstep_max' to 25 000 ;
- 'duration_max' to 1e08.

Choosing the correct chemistry and initial conditions. In the input directory :
> *cp chemistry.in-orig chemistry.in*
> *cp ../output/static-nxx-ζxx-gxx/species.out species.in*
> *cd ../*
> *./mhd_vode*

Importante note. A good reflex is to save the output thus created at the end of the run in a directory like 'output/c-nxx-zetaxx-gxx-vxx-bxx'.

5 An introductory hands-on session

5.1 Characterizing non-irradiated J-type models

0) Run the following J-type models : nHi = 10^4, 10^6 cm^{-3}, Vs = 10, 30 km s^{-1}.

1) Compare the temperature profiles for the models with nHi = 10^4, 10^6 cm^{-3} (mhd_phys.out).

2) What are the sound velocity and Mach numbers through the shock layer (mhd_phys.out) ?

3) Verify the Rankine-Hugoniot for each model (mhd_phys.out). Comments ?

4) For the models with nHi = 10^4 cm^{-3} and Vs = 10, 30 km s^{-1}, compare the H chemistry through the shock layer (mhd_speci.out).

5) For the model with nHi = 10^4 cm^{-3} and Vs = 30 km s^{-1}, what are the main coolants through the shock layer (cooling.out) ?

6) For the model with nHi = 10^4 cm^{-3} and Vs = 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) ?

7) For the models with nHi = 10^4 cm^{-3} and Vs = 10, 30 km s^{-1}, what is the maximum SiO fractional abundance in the shock (mhd_speci.out) ?

5.2 Characterizing non-irradiated C-type models

0) Run the following C-type models : nHi = 10^4 cm^{-3}, Bbeta = 1, 5, and Vs = 10, 15, 30 km s^{-1}.

1) Comment on the temperature profiles for the 15 km s^{-1} case (mhd_phys.out).

2) Compare the temperature profiles for the models with Bbeta = 1 (mhd_phys.out).

3) What are the sound velocity and Mach numbers through the shock layer for the models with Bbeta = 1 (mhd_phys.out) ?

4) Study the H chemistry through the shock layer for the models with Bbeta = 1 (mhd_speci.out).

5) For the model with nHi = 10^4 cm^{-3}, Bbeta = 1 and Vs = 15 km s^{-1}, what are the main coolants through the shock layer (cooling.out) ?

6) For the model with nHi = 10^4 cm^{-3}, Bbeta = 1 and Vs = 15 km s^{-1}, what are the contributions from the different forms of energy to the total energy flux through the shock layer (energetics.out) ?

7) For the model with nHi = 10^4 cm^{-3}, Bbeta = 1 and Vs = 15 km s^{-1}, build two diagrams, one with (Tn, the abundance of water, the total particle density and the fractional abundance of water through the shock), and one with (Tn, 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.

8) For the models with Bbeta = 5, display the SiO fractional abundance profile (mhd_speci.out). Comments ?

9) Compare the temperature profiles of the models with nHi = 10^4 cm^{-3}, Vs = 15 km s^{-1} (mhd_phys.out). Comment on the influence of the magnetic field.

6 Running an irradiated stationary model

6.1 Running a static model to calculate initial conditions

Reminder : very importante note. Launching a static model must be repeated each time you need to run a model with a different pre-shock density, ζ value, or radiation field value. A good reflex is to save the output thus created at the end of the run in a directory like 'output/static-nxx-zetaxx-gxx'. In this section we describe how to calculate the initial conditions of an irradiated stationary model with a static calculation.

Choosing the correct input parameter values. In this case, the aim of the static calculation is to self-consistently calculate the physical and conditions in a buffer of gas that 'protects' the shocked region on the side of the pre-shock medium. The gas buffer represents a small photodissociation region of width A_v. The A_v value is chosen by the user, and the initial conditions for the shocked model will be collected for this value in the output files of the static model. To run this kind of calculation with the Paris-Durham model, in the 'input_mhd.in' file, set :

- 'shock_type' to 'PDR1' ;
- 'Nfluids' to 1 ;
- 'Vs_km' to a very small value, e.g. 0.01 km s^{-1}. The value must be small to get the conditions as close as possible to a static buffer of gas. The 'duration_max' value is chosen accordingly to ensure that the A_v width is reached within the calculation (see below for details on how to choose this 'duration_max' value) ;
- 'RAD' to the value of the radiation field intensity that you want to explore (Habing units) ;
- 'Av0' to a small value, e.g. 10^{-6} (this is the initial A_v value of the gas buffer) ;
- 'F_Av' to 1 to perform a self-consistent calculation of A_v in the gas buffer ;
- 'N_H2_0' to a small value, e.g. 10^{-6} (this is the initial N_{H2} value of the gas buffer) ;
- 'N_CO_0' to a small value, e.g. 10^{-6} (this is the initial N_{CO} value of the gas buffer) ;
- 'Cool_KN' to 0 ;
- 'NH2_lev' to 150 ;
- 'NH2_lines_out' to 200 ;
- 'duration_max' to a value that ensures that the desired width of the gas buffer is reached : 'duration_max' = L / v, where :

— v is the velocity of the gas buffer, i.e. 0.01 km s^{-1} = 10^3 cm s^{-1} ;

— L is the buffer width ∼ NH / nH ∼ [NH/Av] * Av / nH ∼ [5.34e-22]$^{-1}$ * Av / nH

overall : duration_max (yr) = 1.87e21 * [desired Av] / [1e3 * nH * 31.6e6]

- 'H2_out' to 'AD'.

Choosing the correct chemistry and initial conditions. In the input directory :
> *cp chemistry.in-orig chemistry.in*
> *cp species.in_ depl species.in*
> *cd ../*
> *./mhd_ vode*

6.2 Generating the correct input files and running an irradiated shock model

Generating the correct input files. In the output file of the freshly executed irradiated static calculation :
> *python fetch-inputs.py*
The 'fetch-inputs.py' routine collects all appropriate physical and chemical conditions from the output files of the irradiated static calculation, and create the corresponding input files for the irradiated shock calculation. The path to the output directory of the irradiated static models, the desired A_v value for the gas buffer (called 'Avin') and the 'RAD' value must be set at the beginning of the routine. In the output directory of the irradiated shock models, the following input files are created for the shock run :

- 'h2levels.in' that contains the initial values of H_2 level populations ;
- 'species.in' that contains the initial fractional abundances of the included species ;
- 'input_mhd_C.template' that is a template that can be used after changing the shock velocity value to perform an irradiated C-type shock calculation ;
- 'input_mhd_J.template' that is a template that can be used after changing the shock velocity value to perform an irradiated J-type shock calculation.

Running an irradiated shock calculation. In the case of a C-type shock run, in the input directory :
> *cp chemistry.in-orig chemistry.in*
> *cp ../output/static-n*xx*-zeta*xx*-g*xx*/species.in .*
> *cp ../output/static-n*xx*-zeta*xx*-g*xx*/h2levels.in .*
> *cp ../output/static-n*xx*-zeta*xx*-g*xx*/input_ mhd_ C.template input_ mhd.in*
> *cd ../*
> *./mhd_ vode*
(Mind the shock velocity value in the template 'input_mhd.in' file, and adapt to 'input_mhd_J.template' in case of a J-type calculation).