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The Paris-Durham shock code

Benjamin Godard

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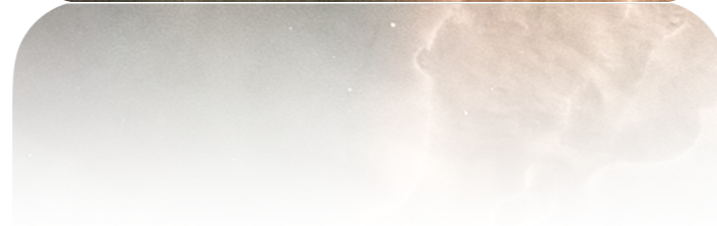
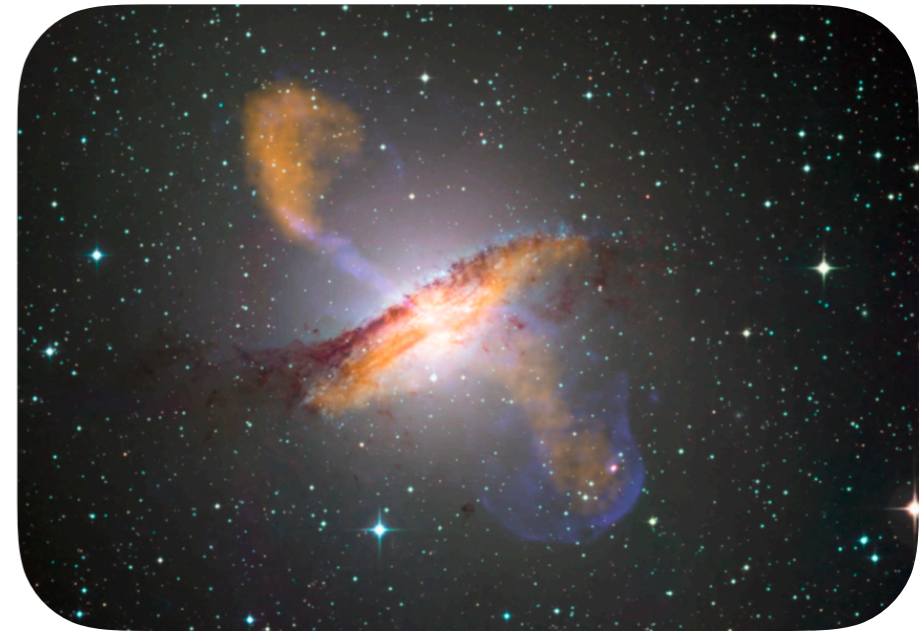
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The Paris-Durham shock code

Les Houches Interstellar Shock School

June 2022



Outline

- introduction
- assumptions
physics
- user guide
first steps
- services

1. Assumptions & physical ingredients
2. User Guide - first steps
3. Available services

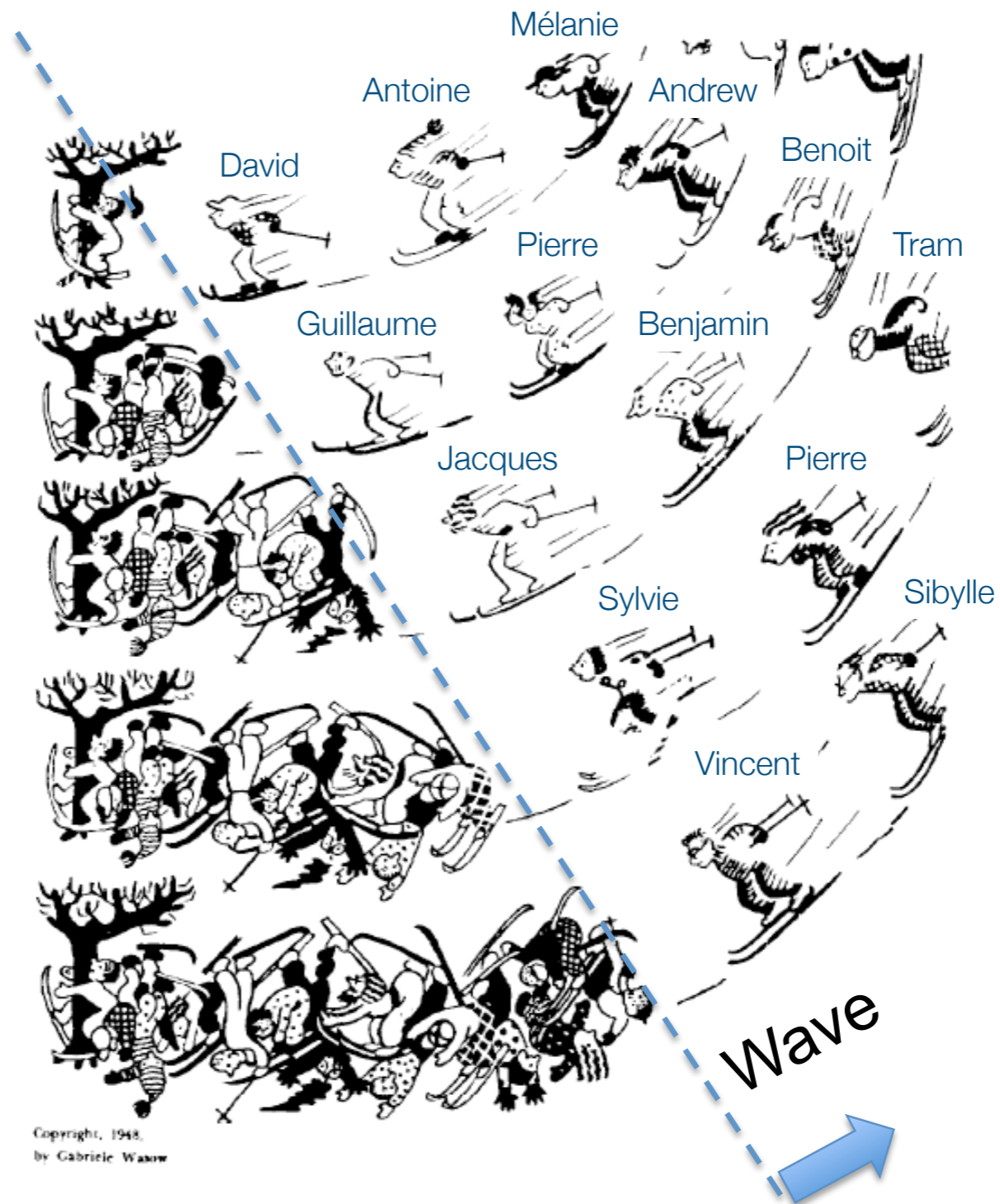
Introduction

Fortran code developed over 40 years

David Flower, Guillaume Pineau des Forêts, Tom Hartquist (1985)

Outline

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thermochemical structure of molecular shocks induced by

- interstellar turbulence, cloud collisions
- jets and bipolar outflows associated to star formation
- AGB winds
- evolved supernova remnants shells

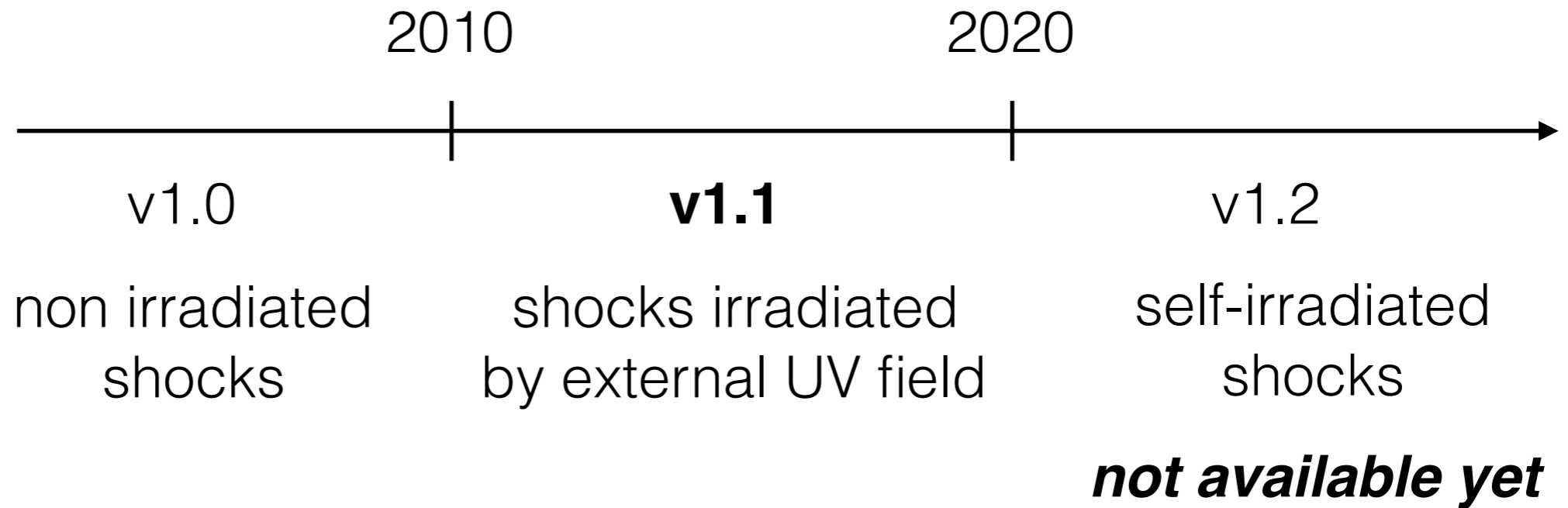
Goals

1. provide a tool to the community
2. understand the physics of shocks
3. interpret observations

Outline

- introduction
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Several public versions (<http://ism.obspm.fr>)



Services on the ISM platform: <https://ism.obspm.fr>

- download, documentation, tutorial
- help: support.shock.ism@obspm.fr (A. Gusdorf, S. Cabrit, B. Godard)
- tools for extracting and analyzing the results
- grids of precomputed models

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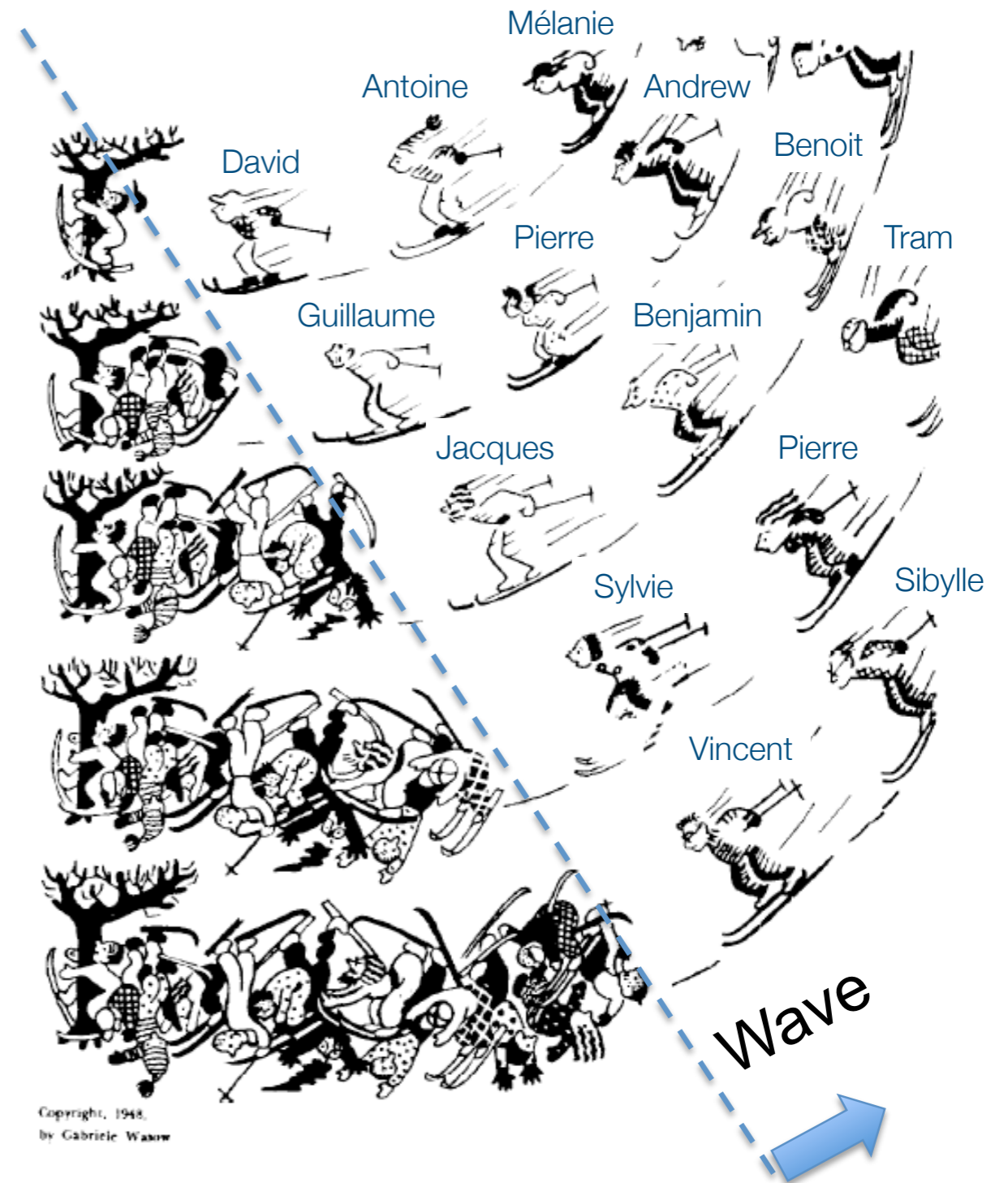
Introduction

non proprietary code under the GNU License

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- download
- run
- modify
- publish



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ASSUMPTIONS PHYSICAL INGREDIENTS

Assumptions & geometry

- in a perfect world
- 3D, time dependent shocks
 - non ideal MHD
 - with chemistry
 - excitation of chemical species
 - exact radiative transfer

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Assumptions & geometry

in a perfect world → 3D, time dependent shocks
→ non ideal MHD
→ with chemistry
→ excitation of chemical species
→ exact radiative transfer

requirements → orders of magnitude of scales
→ thousands of variables
→ non local code

⇒ out of reach of the most performant computers

⇒ need for simplifications

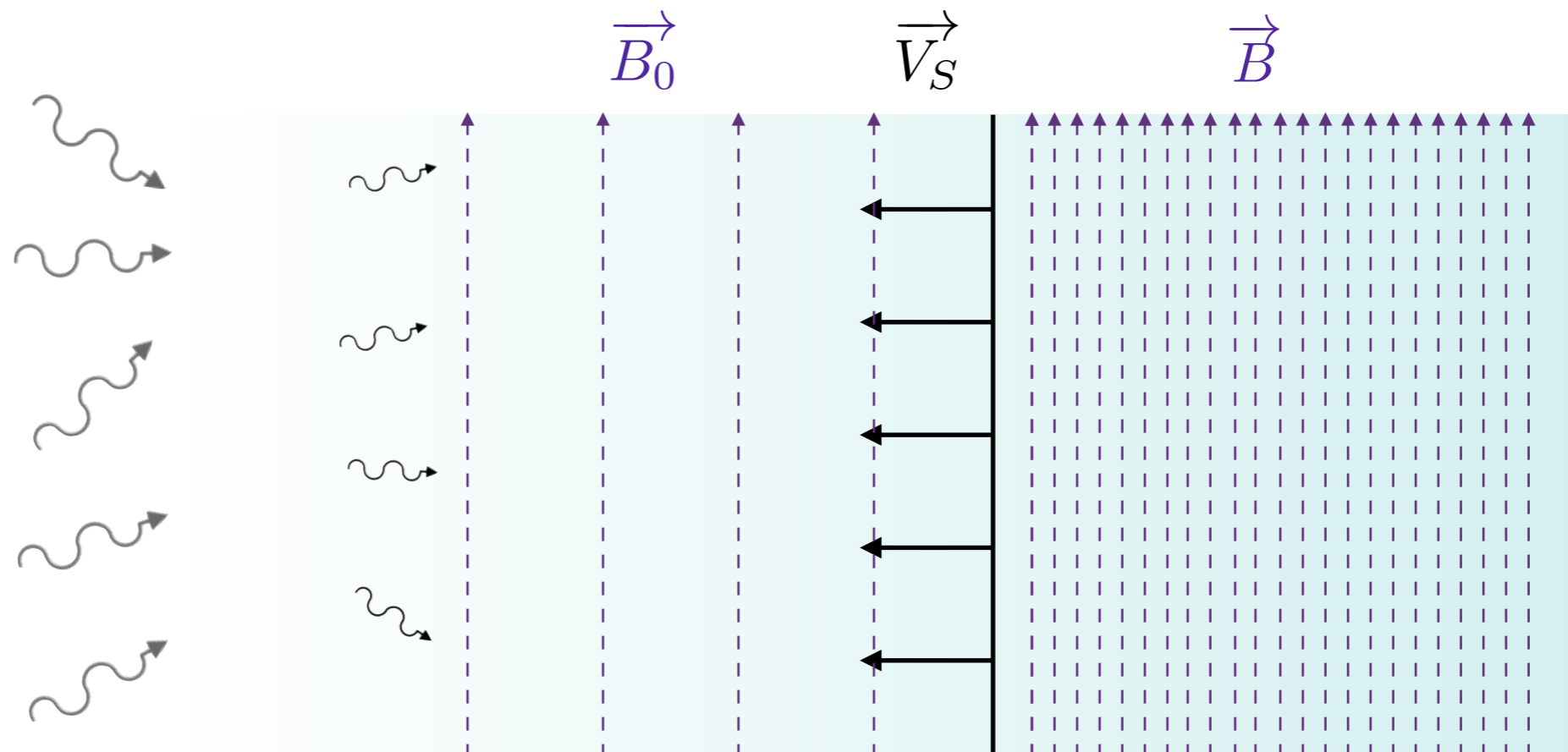
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Assumptions & geometry

main simplification hypotheses

1. plane parallel shock
2. at steady state $\partial/\partial t = 0$
3. propagating in a medium with an homogenous B_0 perpendicular to the propagation direction
4. illuminated upstream by an isotropic radiation field

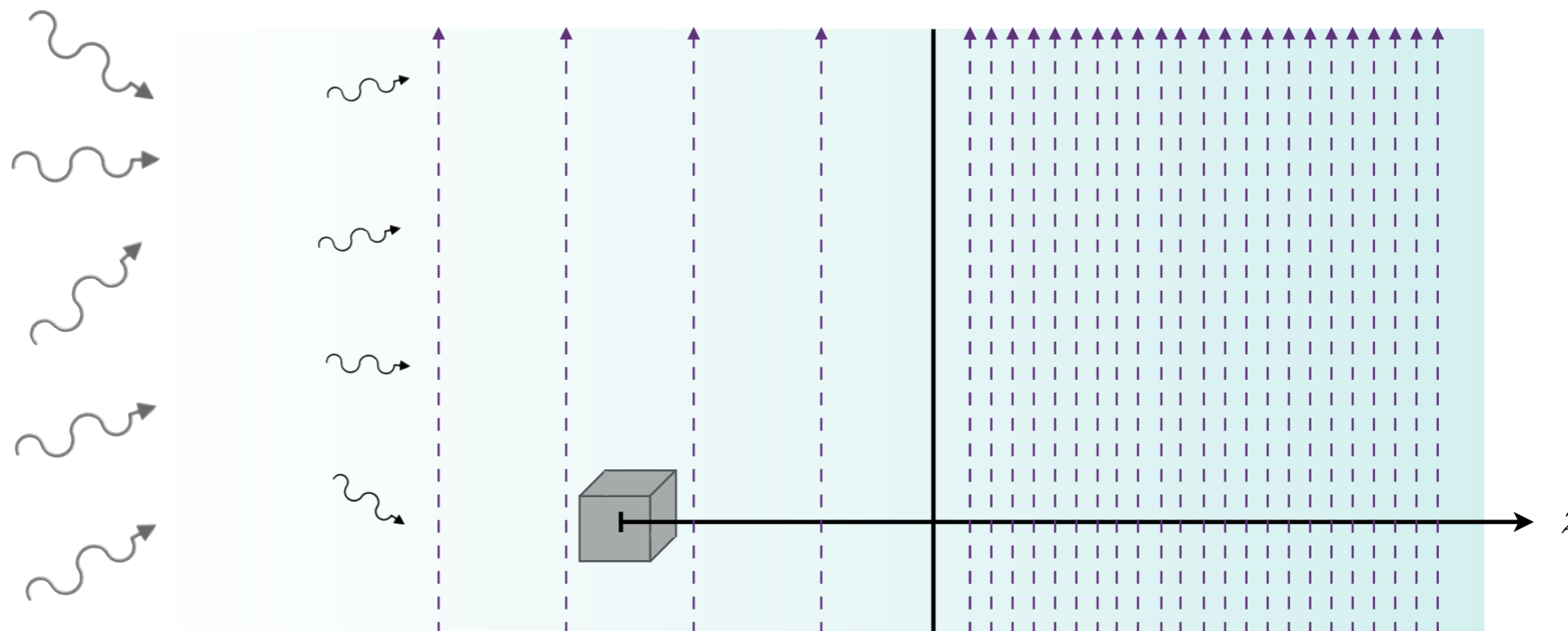


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Assumptions & geometry

in the reference frame of the shock wave



hundreds of variables

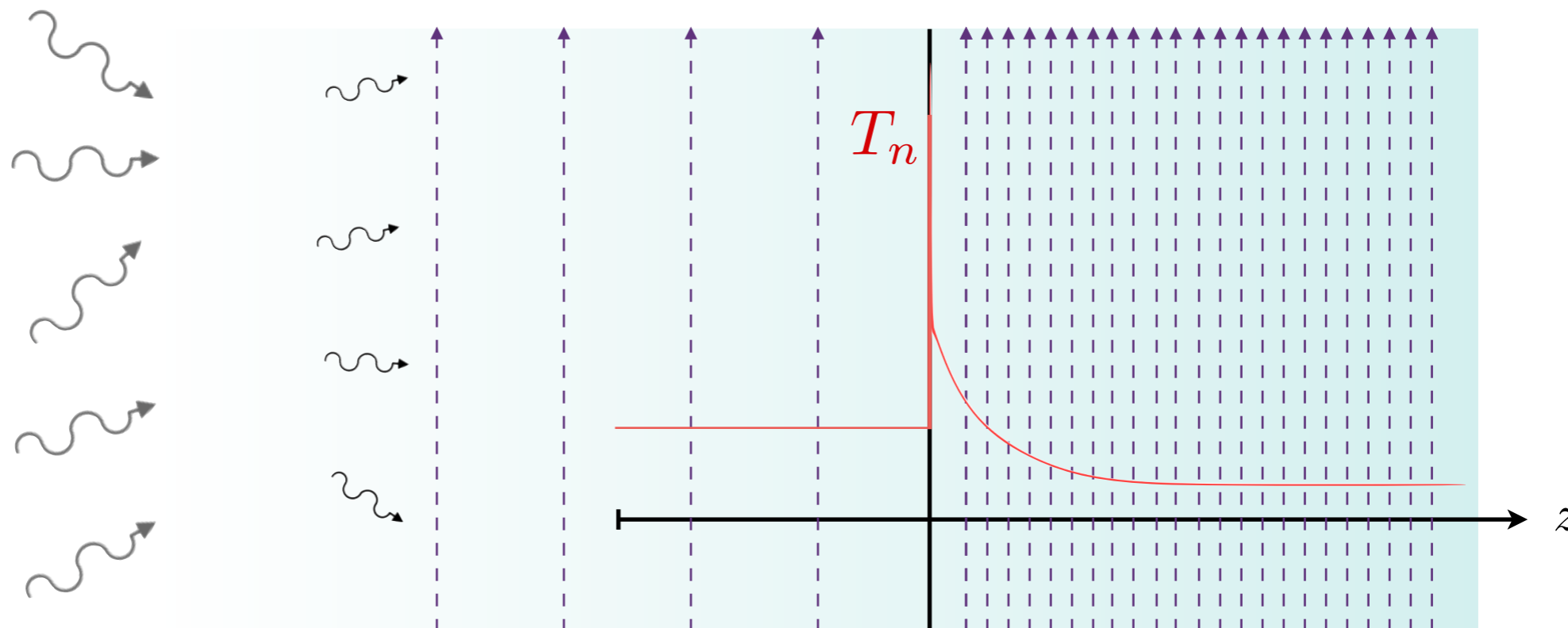
- dynamics V_n, n_n, ρ_n V_i, n_i, ρ_i
- thermal T_n T_i, T_e
- chemistry n_α
- H₂ excitation $n_{\text{H}_2^i}$

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Assumptions & geometry

in the reference frame of the shock wave



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hundreds of variables

- dynamics V_n, n_n, ρ_n V_i, n_i, ρ_i
- thermal T_n T_i, T_e
- chemistry n_α
- H₂ excitation $n_{\text{H}_2^i}$

set of equations

$$\frac{d}{dz} (n_n V_n) = N_n$$

$$\frac{d}{dz} (\rho_n V_n) = S_n$$

$$\frac{d}{dz} (\rho_n V_n^2 + n_n k T_n) = A_n$$

$$\frac{d}{dz} \left(\left(\frac{1}{2} \rho_n V_n^2 + \frac{\gamma}{\gamma-1} n_n k T_n \right) V_n \right) = B_n$$

$$\frac{d}{dz} (n_\alpha V_n) = C_\alpha$$

$$\frac{d}{dz} (n_{\text{H}_2^l} V_n) = C_l$$

$$\frac{d}{dz} (n_i V_i) = N_i$$

$$\frac{d}{dz} (\rho_i V_i) = S_i,$$

$$\frac{d}{dz} \left(\rho_i V_i^2 + n_i k (T_i + T_e) + \frac{B^2}{8\pi} \right) = A_i,$$

$$\frac{d}{dz} \left(\left(\frac{1}{2} \rho_i V_i^2 + \frac{\gamma}{\gamma-1} n_i k (T_i + T_e) + \frac{B^2}{4\pi} \right) V_i \right) = B_i + B_e$$

$$\frac{d}{dz} (n_\alpha V_i) = C_\alpha$$

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set of equations

$$\frac{d}{dz} (n_n V_n) = N_n$$

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$$\frac{d}{dz} (n_{\text{H}_2^l} V_n) = C_l$$

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$$\frac{d}{dz} (\rho_i V_i) = S_i,$$

$$\frac{d}{dz} \left(\rho_i V_i^2 + n_i k (T_i + T_e) + \frac{B^2}{8\pi} \right) = A_i,$$

$$\frac{d}{dz} \left(\left(\frac{1}{2} \rho_i V_i^2 + \frac{\gamma}{\gamma-1} n_i k (T_i + T_e) + \frac{B^2}{4\pi} \right) V_i \right) = B_i + B_e$$

$$\frac{d}{dz} (n_\alpha V_i) = C_\alpha$$

source terms

- chemical reactions
- fluid interactions
- heating and cooling processes
- H₂ (de-)excitation processes

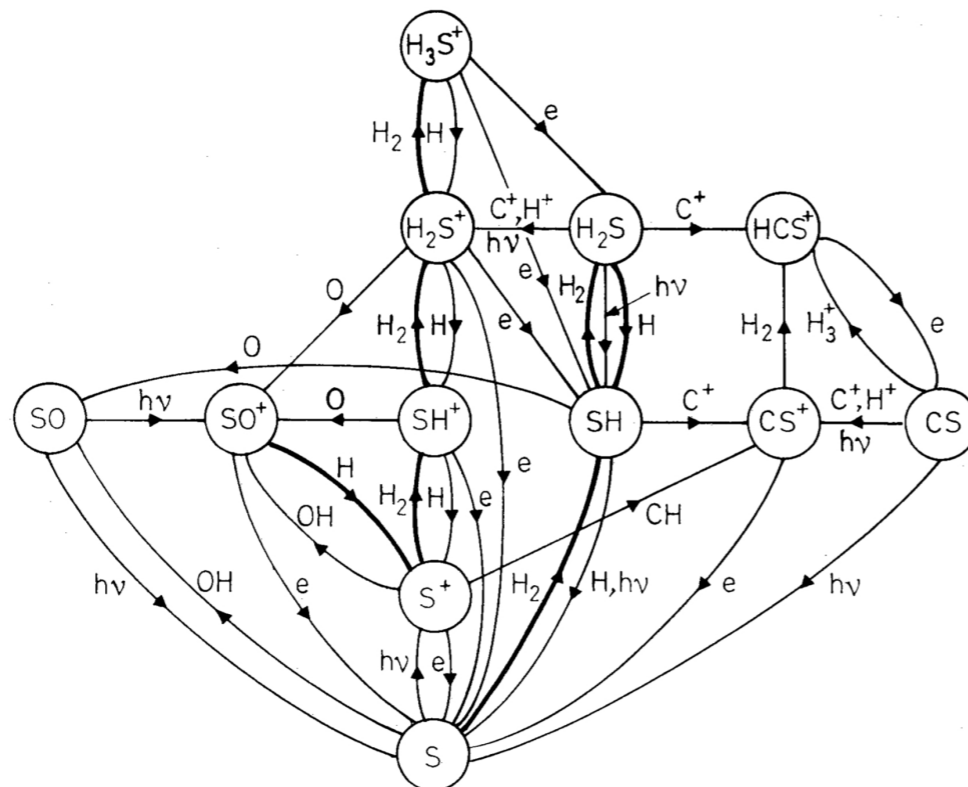
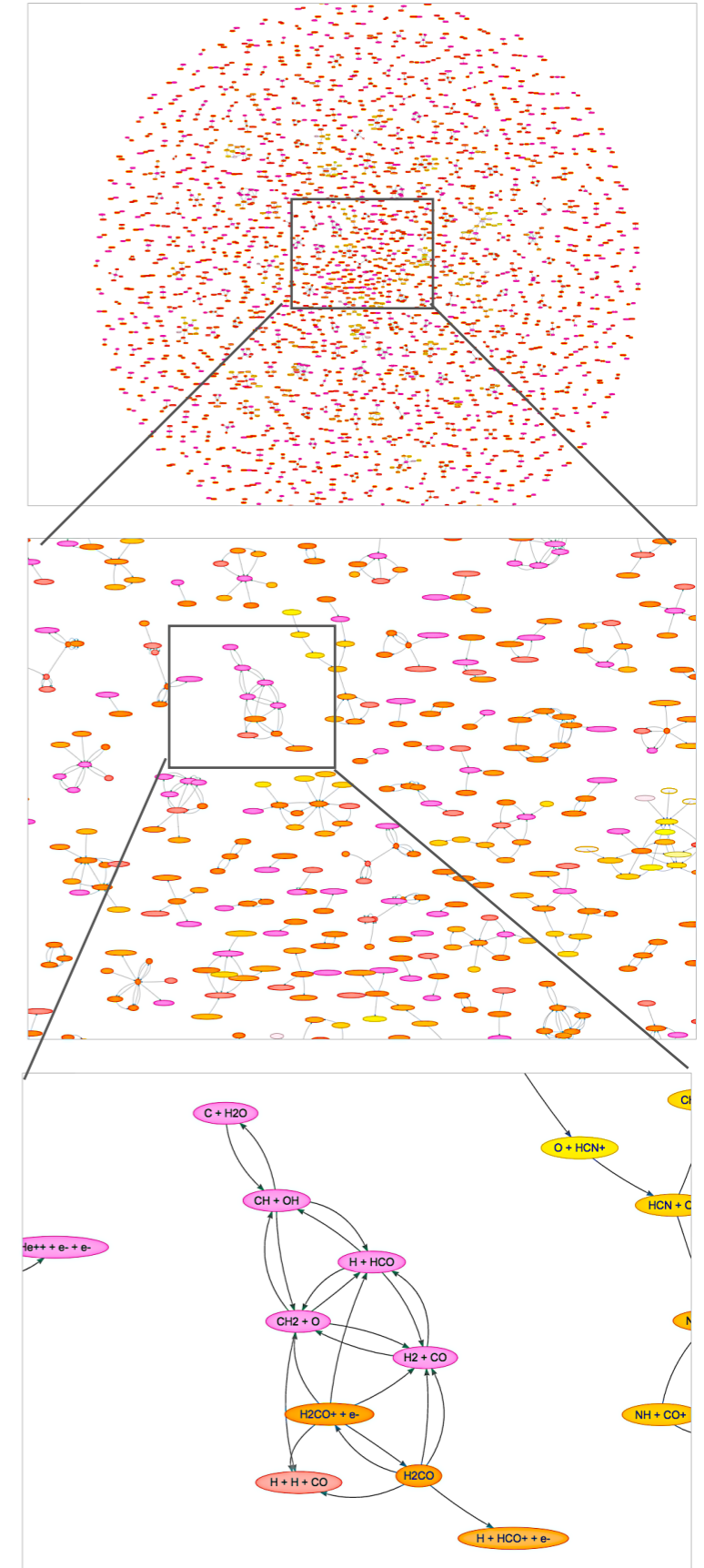
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Physical processes

gas phase chemistry

- 140 chemical species
- thousands reactions
 - ✓ photoionization
 - ✓ photodissociation
 - ✓ cosmic ray ionization
 - ✓ 2(3)-bodies reactions



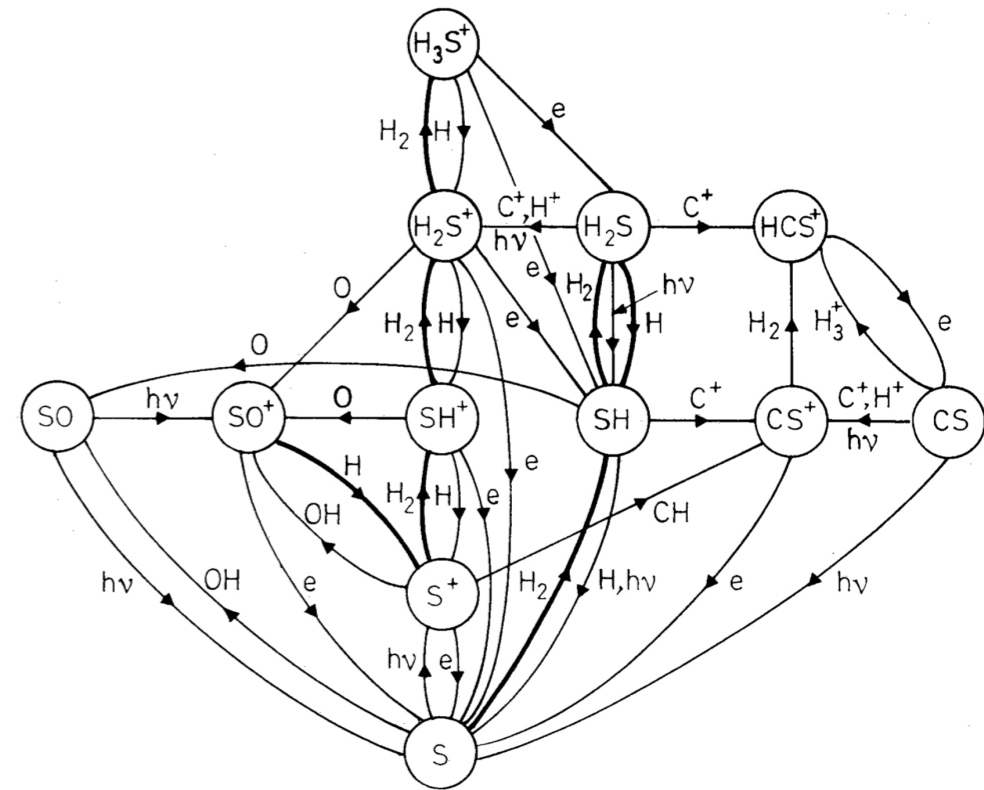
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Physical processes

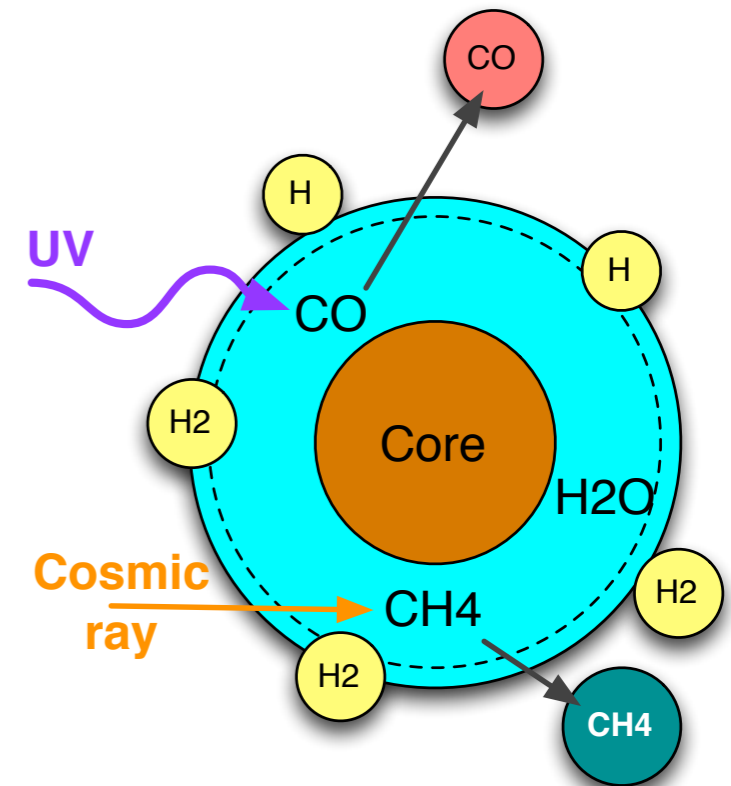
gas phase chemistry

- 140 chemical species
- thousands reactions
 - ✓ photoionization
 - ✓ photodissociation
 - ✓ cosmic ray ionization
 - ✓ 2(3)-bodies reactions



surface « chemistry »

- adsorption
- species hydrogenation on mantles
- desorption and sputtering



change in momentum

- viscous stress
- elastic scattering
 - ✓ ions - neutrals
 - ✓ electrons - neutrals
 - ✓ grains - neutrals

Outline

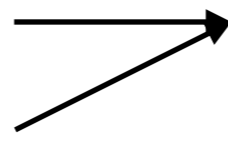
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change in momentum

- viscous stress
- elastic scattering
 - ✓ ions - neutrals
 - ✓ electrons - neutrals
 - ✓ grains - neutrals



heating / cooling

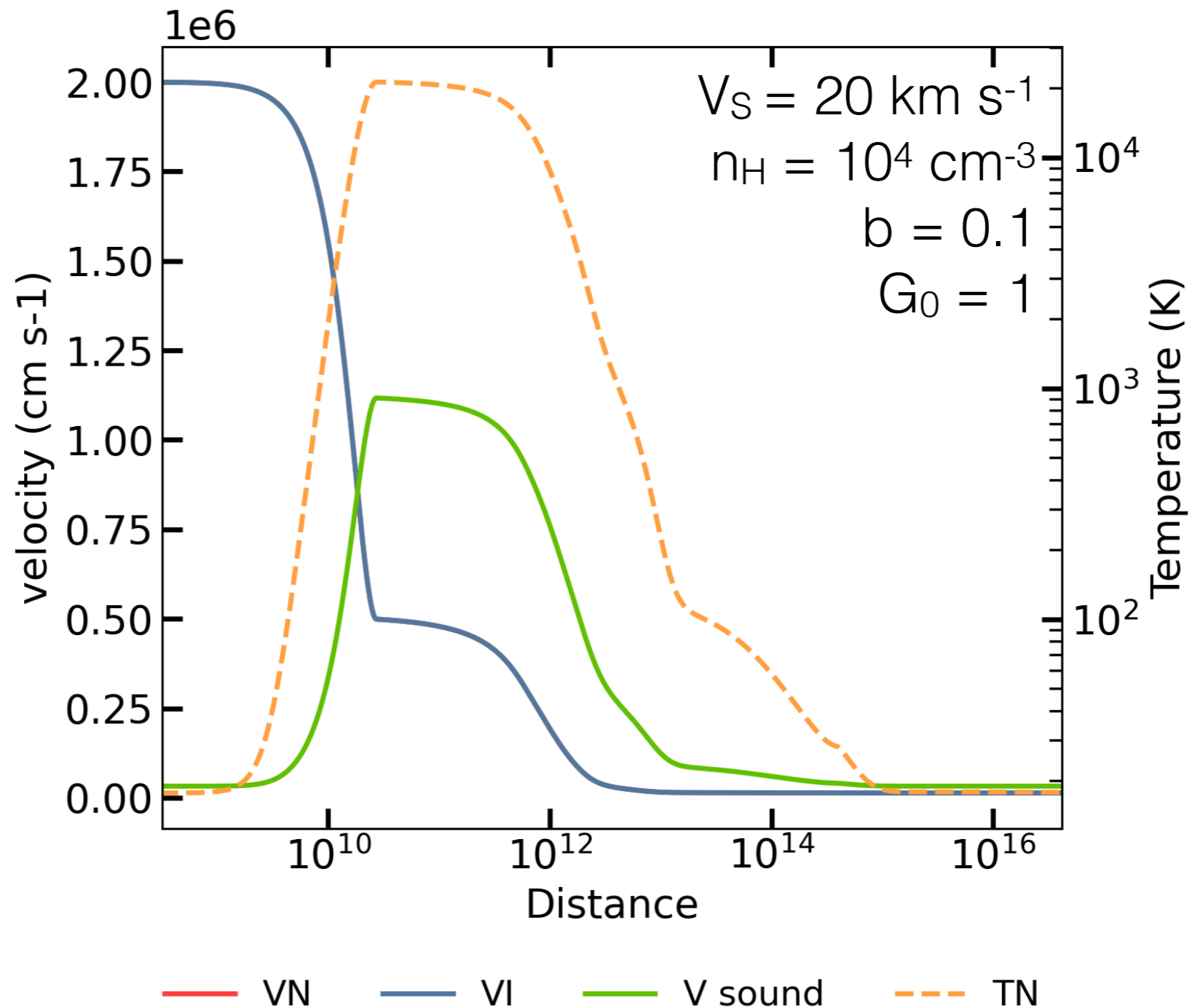
- fluid interactions
- ion-electron elastic scattering
- thermalization with grains
- photoelectric effect
- cosmic ray ionizations
- chemistry - exo(endo)thermicity
- collisional (de)excitation and radiative emission
 - ✓ atoms
 - H, C, C⁺, S, S⁺, N, N⁺, O, O⁺, Si, Si⁺
 - ✓ molecules
 - H₂, CO, ¹³CO, OH, H₂O, NH₃

Shock types

if $V_S > \frac{B_0}{\sqrt{4\pi\rho_c}}$ \longrightarrow J-type shock

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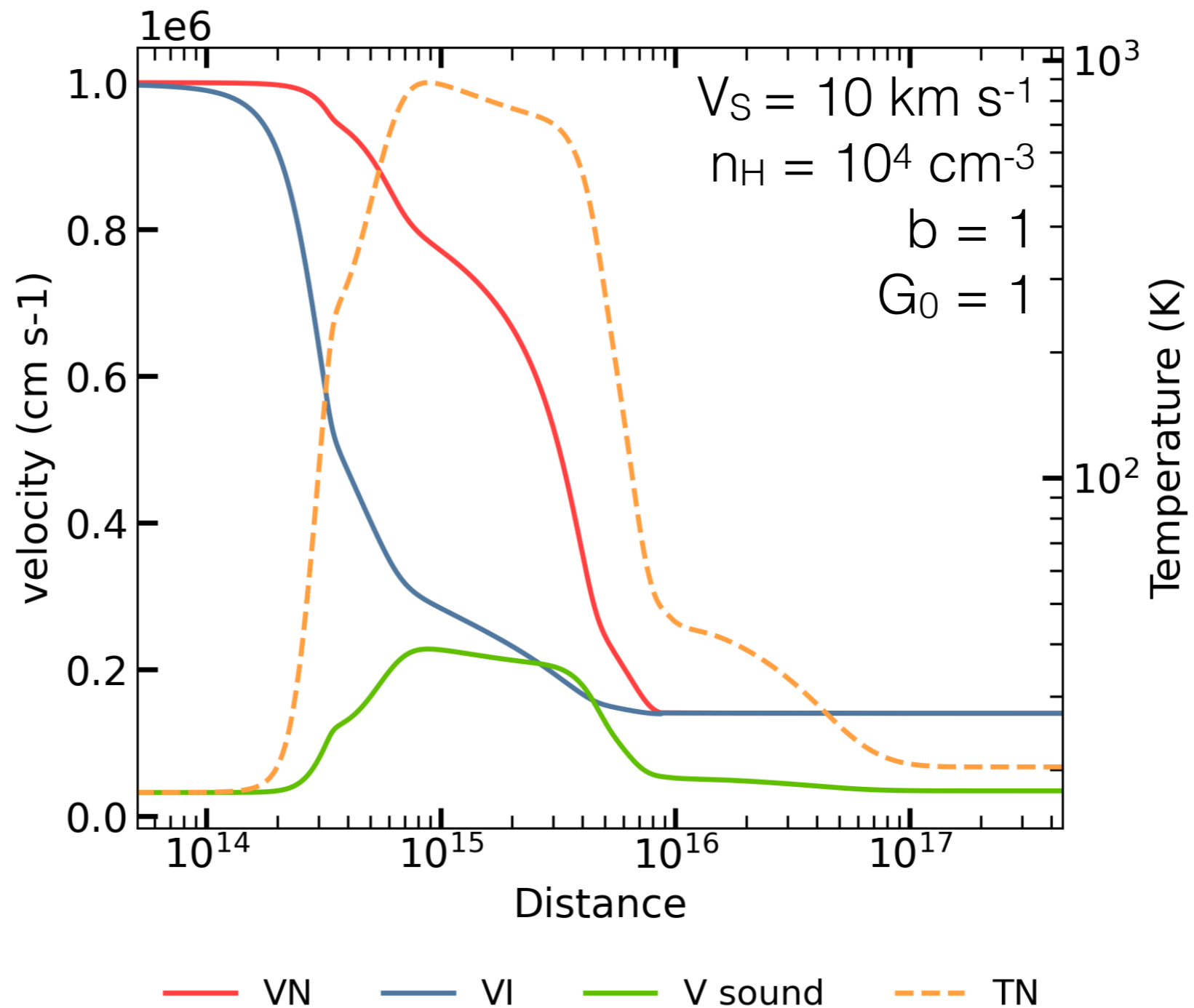


Shock types

if $V_S < \frac{B_0}{\sqrt{4\pi\rho_c}}$ & efficient cooling \longrightarrow C-type shock

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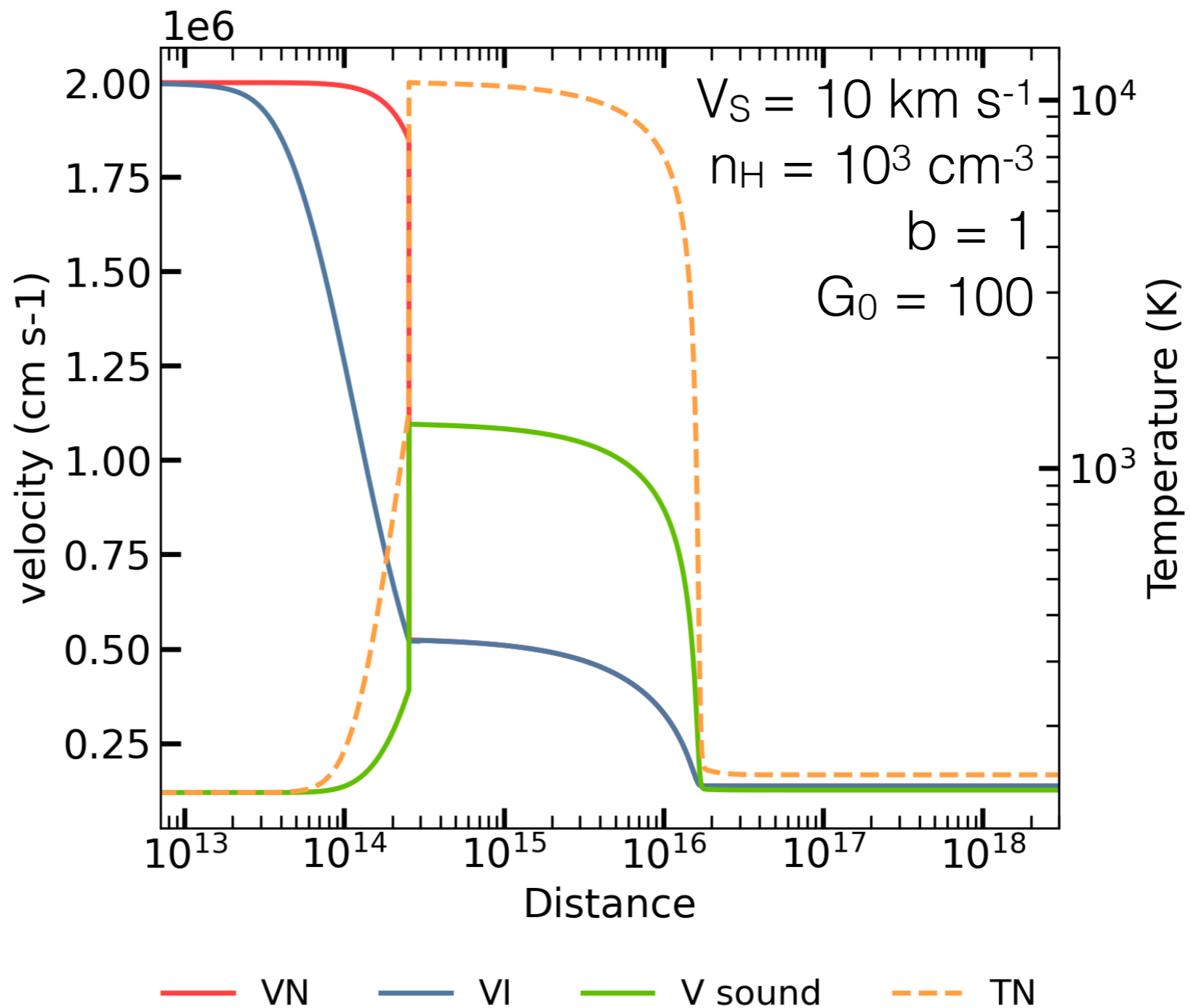


Shock types

if $V_S < \frac{B_0}{\sqrt{4\pi\rho_c}}$ & efficient cooling \longrightarrow C*-type shock
CJ-type shock

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domain of validity of preshock conditions

$$10^{-1} \text{ cm}^{-3} \leq n_{\text{H}} \leq 10^8 \text{ cm}^{-3}$$

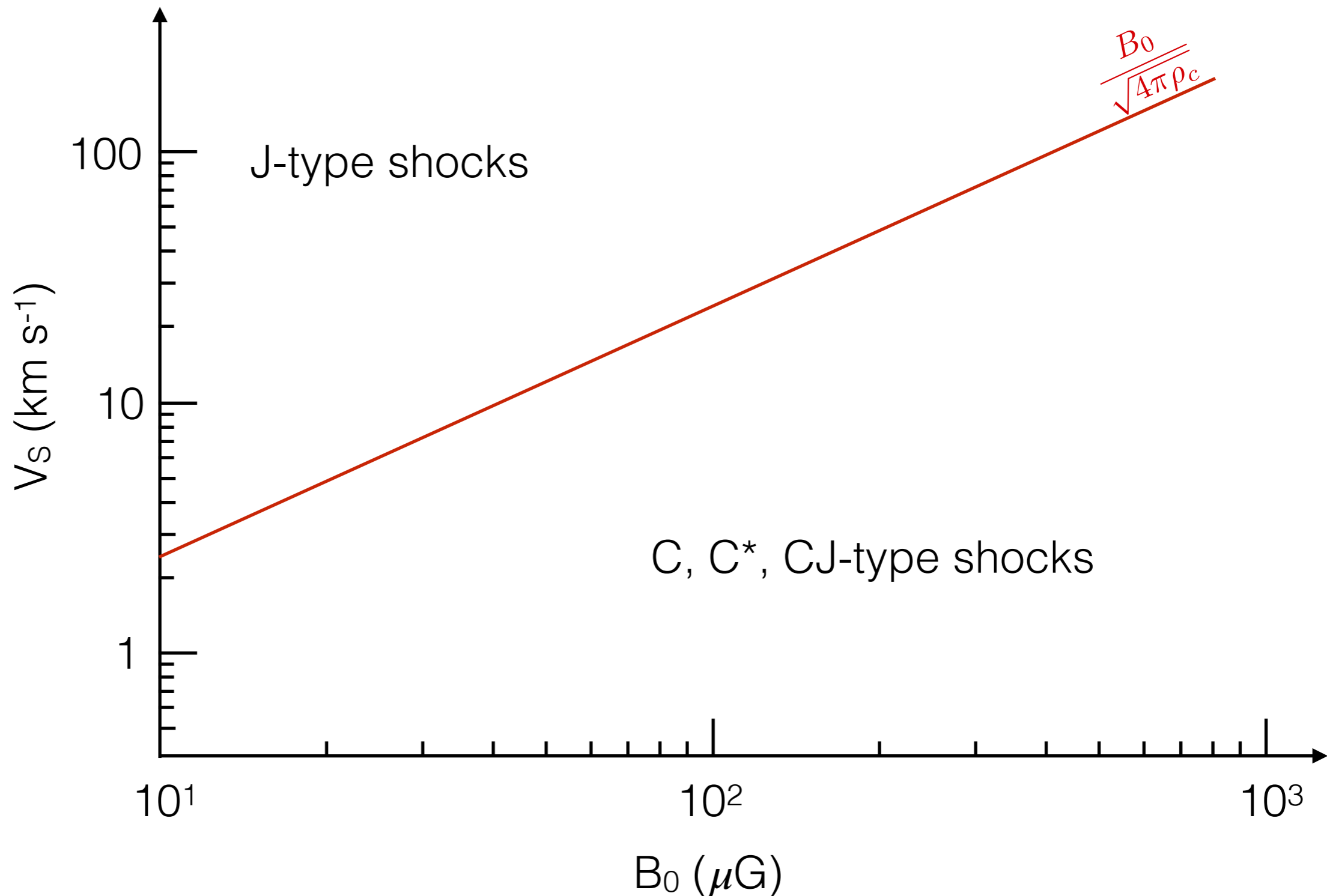
$$0 \leq G_0 \leq 10^4 \quad (\text{in unit of the Mathis ISRF})$$

$$10^{-17} \text{ s}^{-1} \leq \zeta_{\text{H}_2} \leq 10^{-15} \text{ s}^{-1}$$

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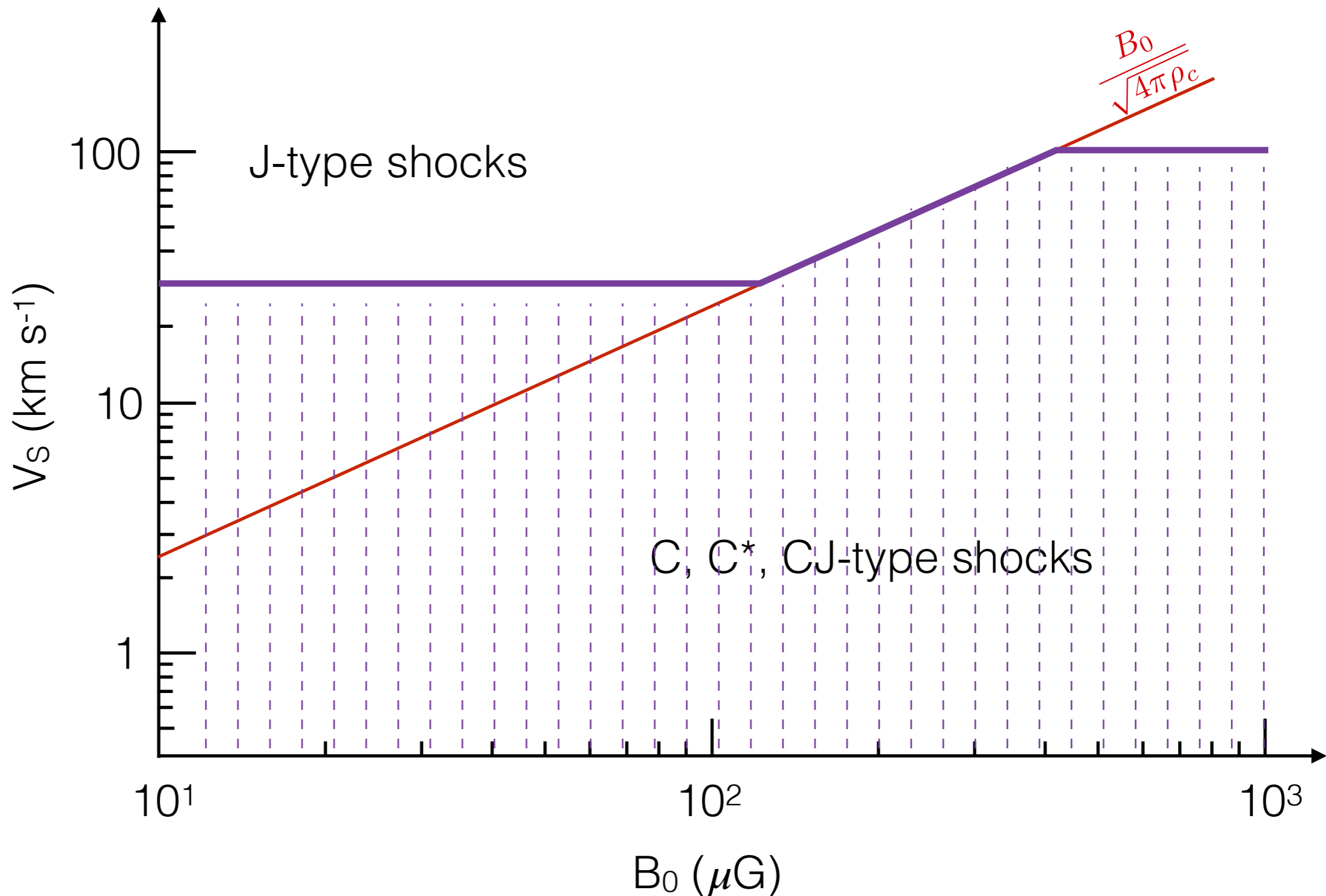
domain of validity of shock velocity



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domain of validity of shock velocity



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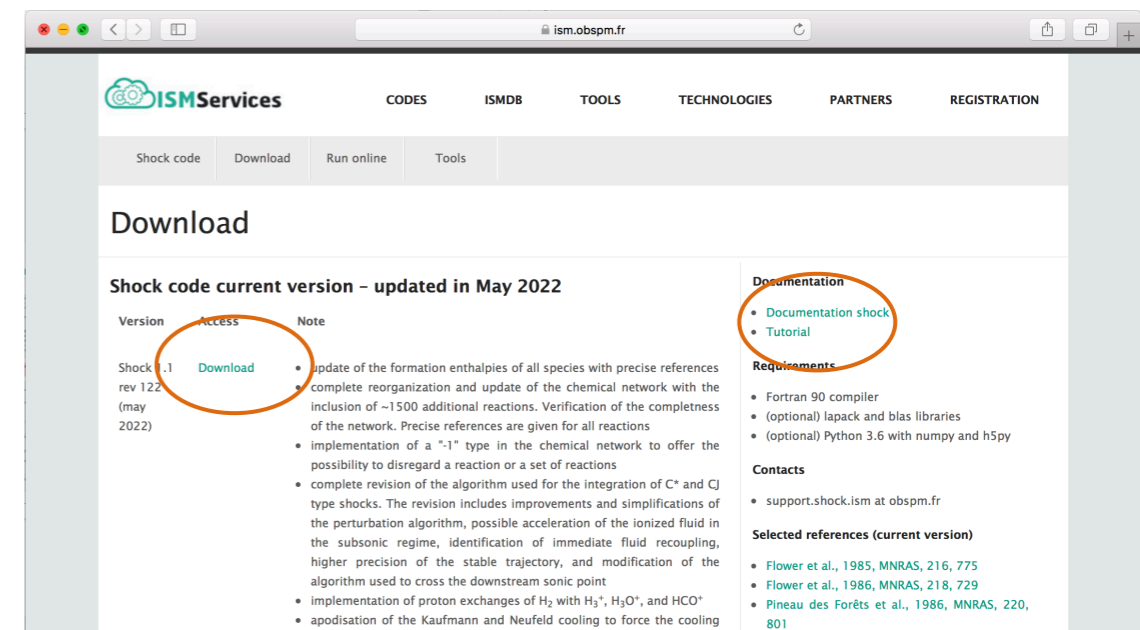
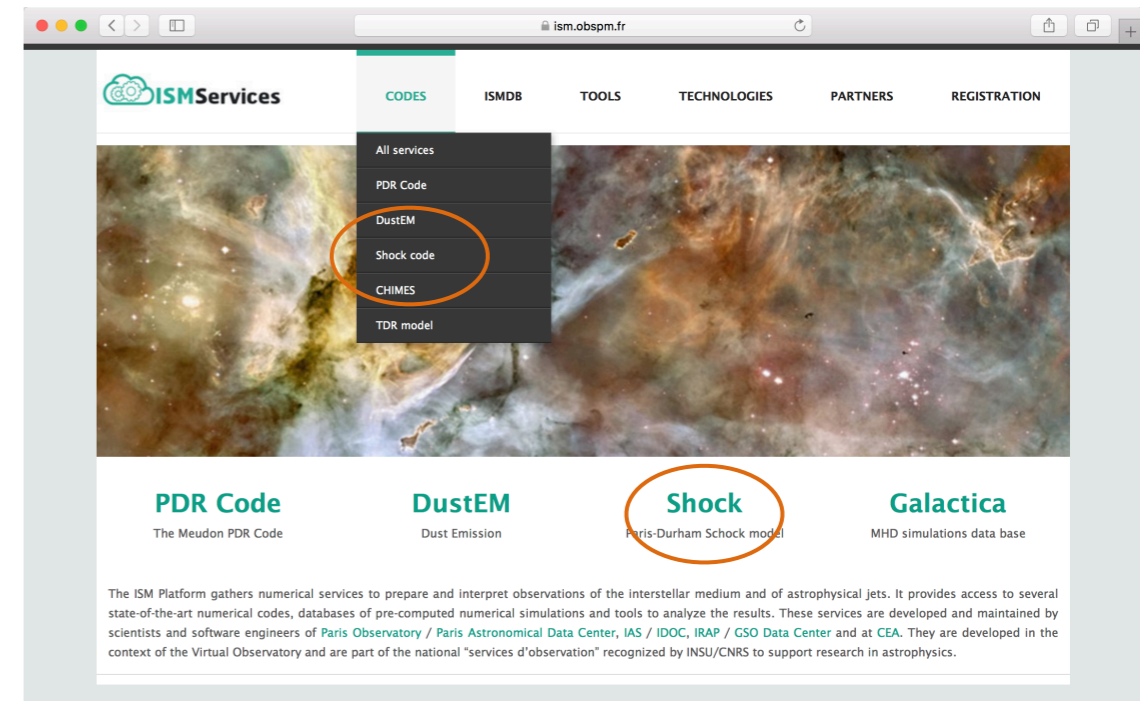
USER GUIDE FIRST STEPS

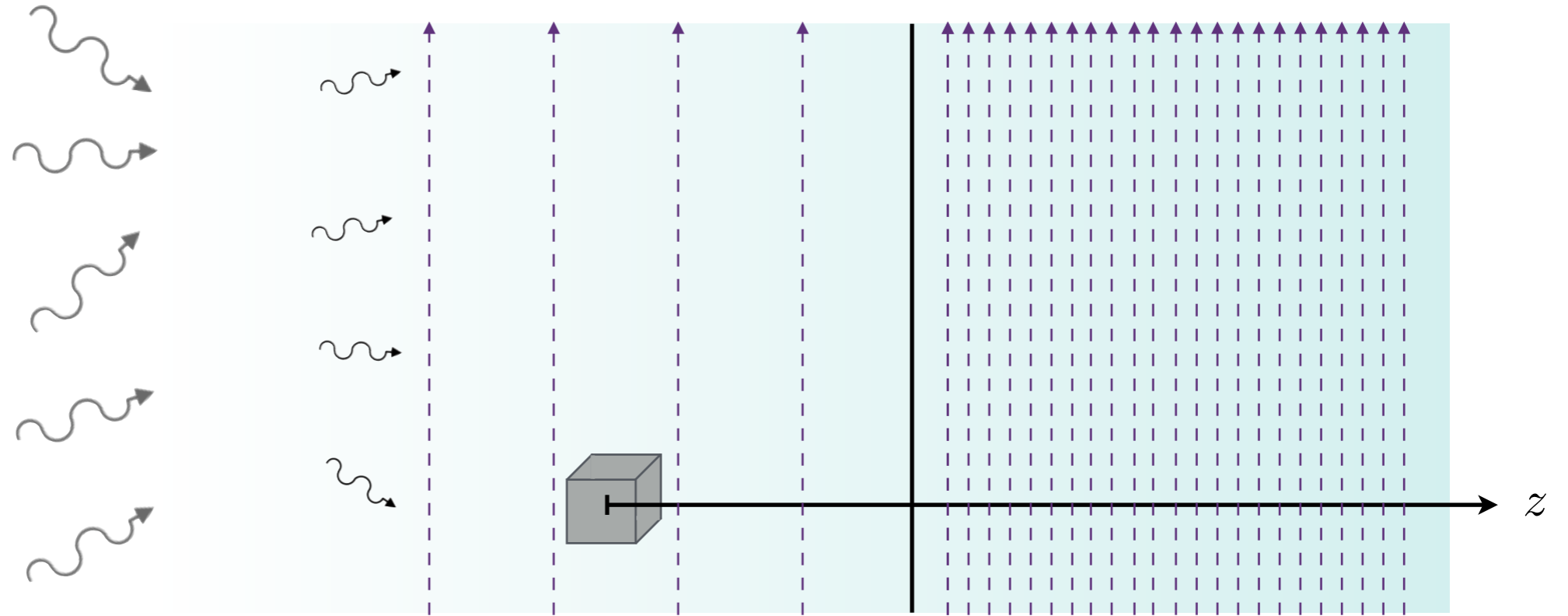
ISM platform

Outline

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- user guide first steps
- services

- download from the platform ism.obspm.fr
code, documentation, tutorial
- untar and compile
fortran compiler (gfortran)
`cd bin/`
`make`
- prepare the input files
type of model
output options
- run the model
- analyse the results
plotting routines
IDAT, chemistry analyser

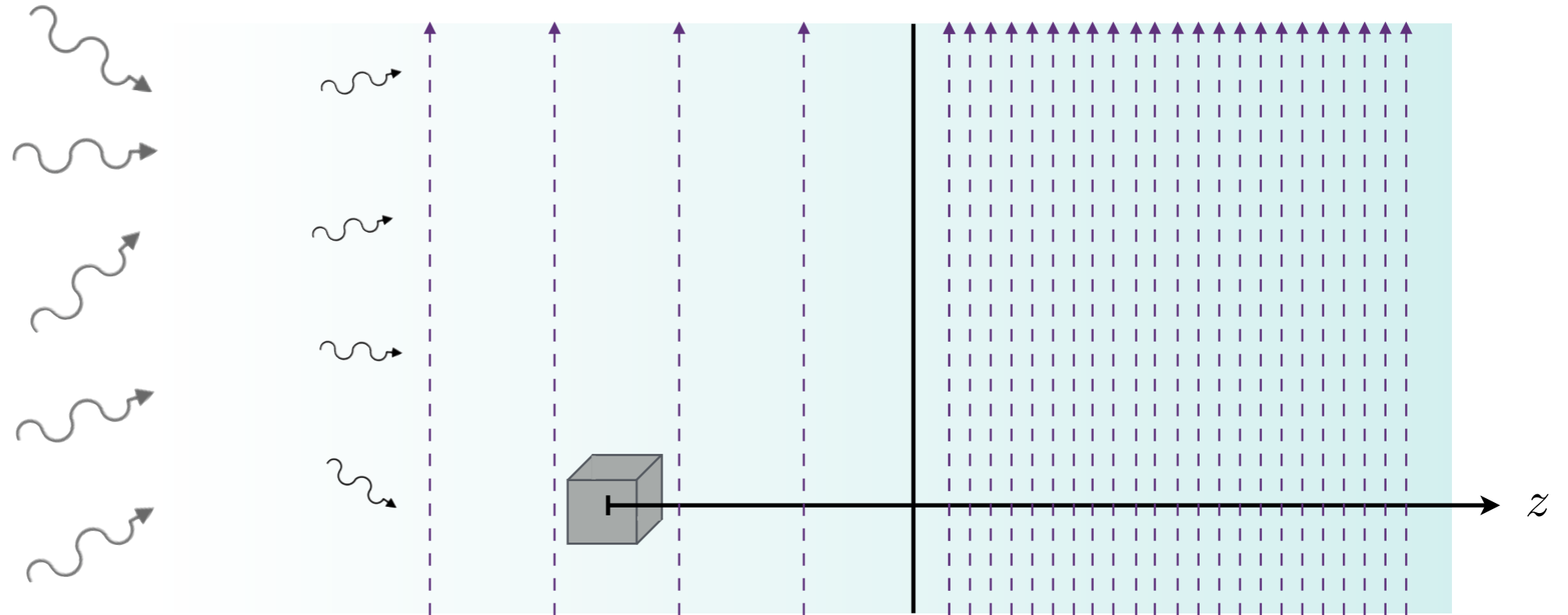




What initial conditions for all variables (T_n, n_α, \dots) ?

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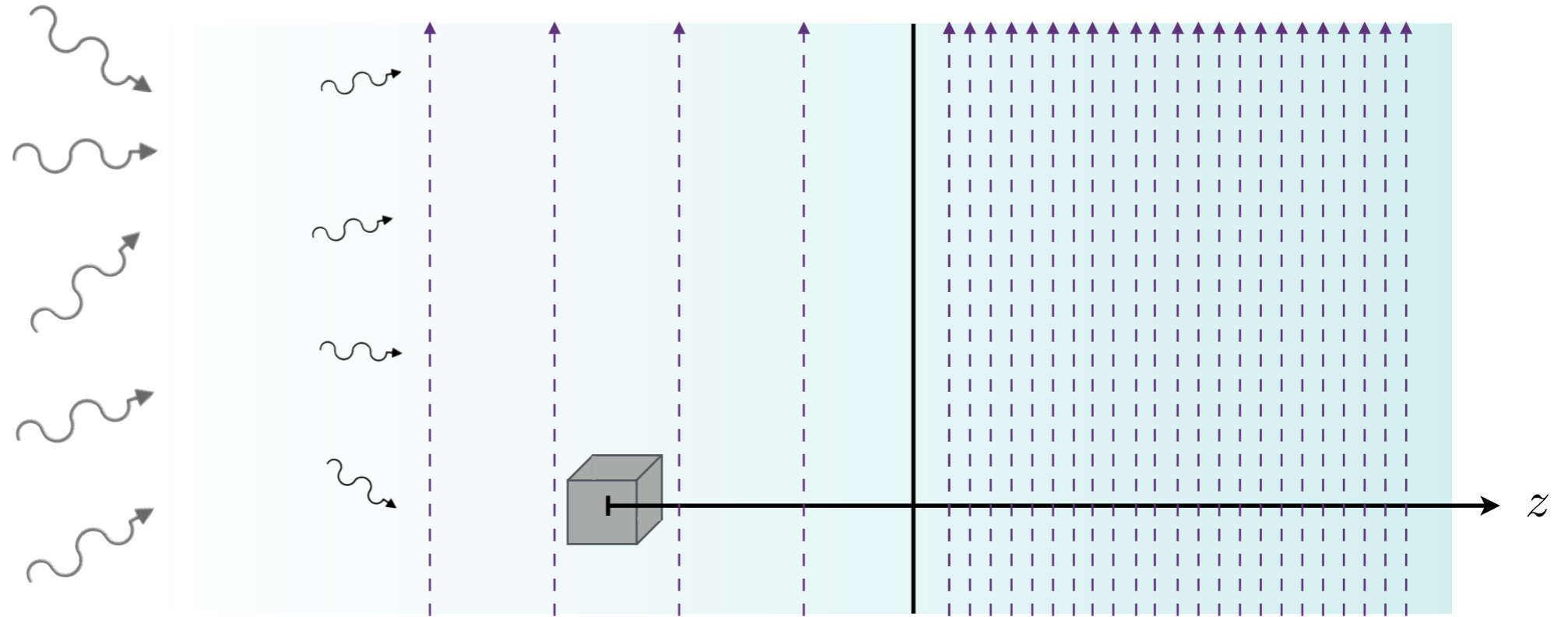


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What initial conditions for all variables (T_n, n_α, \dots) ?

- option A - set by hand \rightarrow more than 200 parameters



What initial conditions for all variables (T_n, n_α, \dots) ?

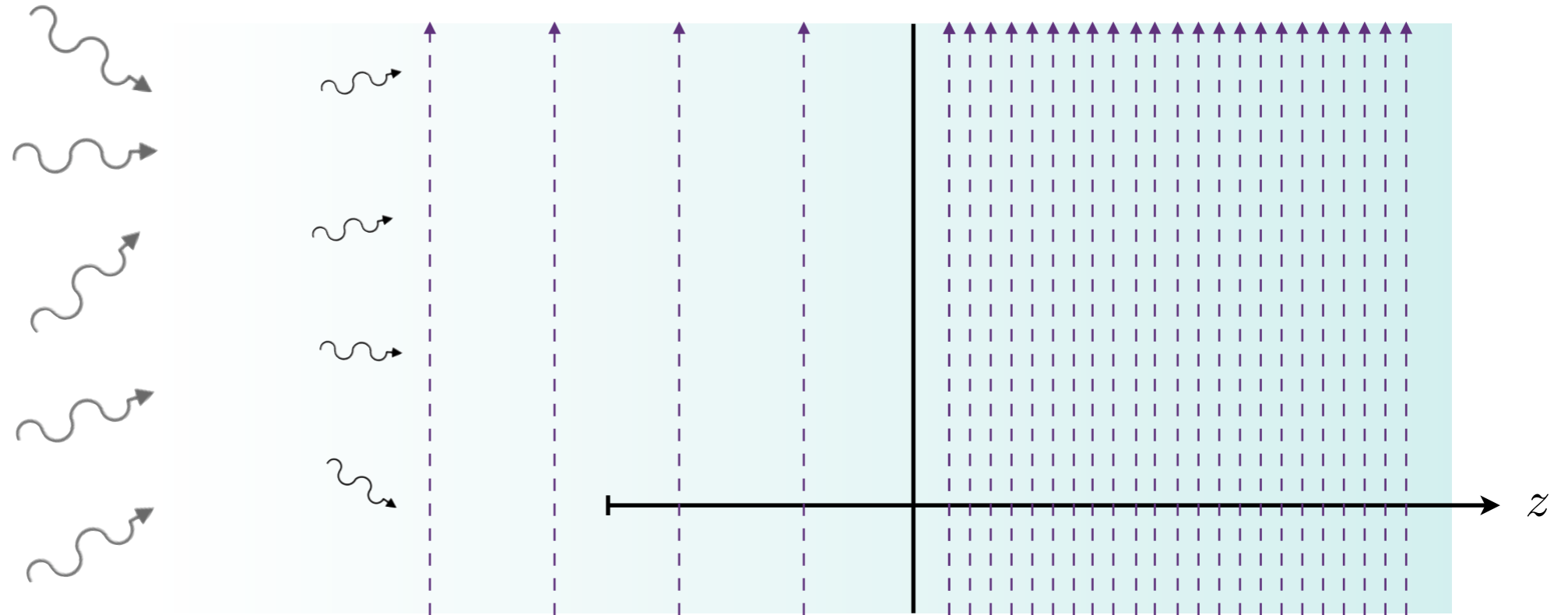
- ~~option A - set by hand \rightarrow more than 200 parameters~~
- option B - compute the equilibrium thermochemical state of the preshock

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Outline

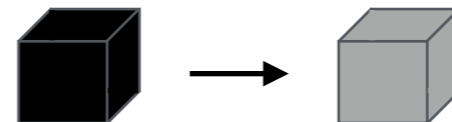
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Running a shock model is a two step process

1. first, run the code to compute the preshock conditions
use the Paris-Durham shock code with no dynamics

THIS IS NOT A SHOCK !



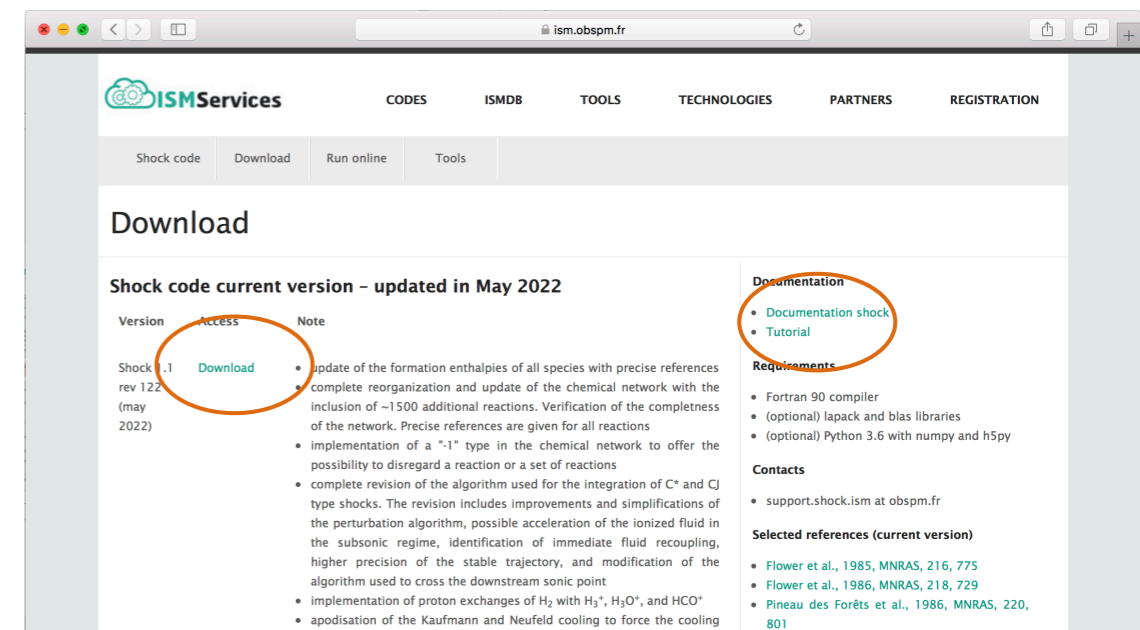
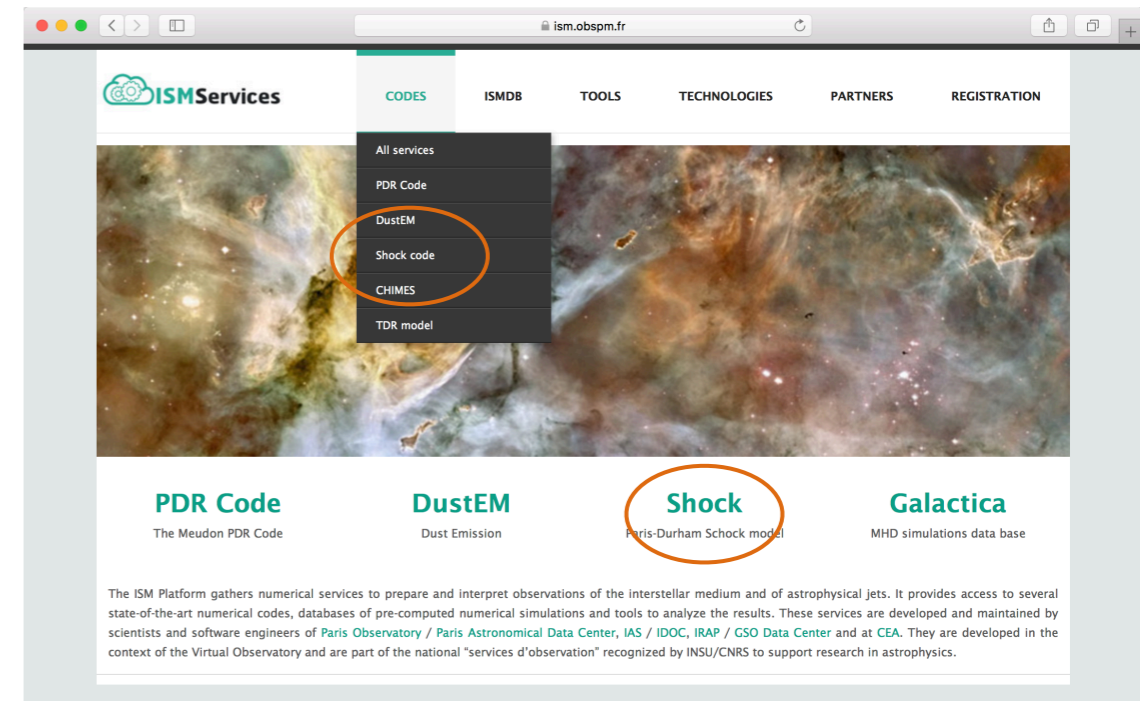
2. use the final conditions of the preshock run as initial conditions of the shock

ISM platform

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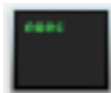



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IDAT, chemistry analyser



Architecture of the code

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	AnalysisTools	→	IDAT / Chemistry Analyser
	bin	→	Makefile & binary files
	Doc_quickstart.html	→	online documentation
	Doc_tutorial.html	→	online tutorial
	GPL_Licence	→	GNU License
	input	→	input files
	mhd_vode	→	executable
	mtx	→	LAPACK library
	output	→	output files
	src	→	sources files


Architecture of the code


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Inputs

 input

 Aij_H2.in




H₂ lines

 chemistry_..._all.in




chemical networks

 coeff_..._H2.in



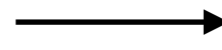
H₂ excitation data

 coeff_SiO.in



SiO excitation data

 cross_sections




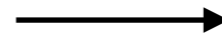
photoreac cross sections

 gamma_eFe



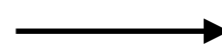
Fe excitation data

 Grains



grain data

 H2_levels_Evj.in



H₂ levels

 input_mhd.in



main input file

 species_...in



list of species

 TechConfig



HDF5 configuration

 UVdata




H / H₂ / CO UV lines

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Inputs

 input

 Aij_H2.in



H₂ lines

 chemistry_..._all.in



chemical networks

 coeff_..._H2.in



H₂ excitation data

 coeff_SiO.in



SiO excitation data

 cross_sections



photoreac cross sections

 gamma_eFe



Fe excitation data

 Grains



grain data

 H2_levels_Evj.in



H₂ levels

 input_mhd.in



main input file

 species_...in



list of species

 TechConfig



HDF5 configuration

 UVdata



H / H₂ / CO UV lines

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Main input file : `input_mhd.in`

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```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1  !---- input files -----
2  example_preshock           ! modele   : output files radix-
3  species_2022_05.in_depl    ! specfile  : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile  : chemistry file (reaction
5  none                       ! h2exfile  : h2* file (if none, populat
6  none                       ! gridfile  : file containing the grid
7  !---- shock parameters -----
8  S1                         ! shock_type : 'C' or 'J', Isoprotonic o
9  1                          ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                   ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                   ! Vs_km     : shock speed (km/s)-
12 1.00E+03                   ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                   ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                   ! Tn        : initial gas temperature (
15 3                          ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                   ! Zeta      : cosmic ray ionization rate
18 1                          ! F_ISRF    : radiation field spectrum -
19 0.00E+00                   ! RAD       : radiation field intensity
20 1.00E-01                   ! Av0       : initial extinction (magnit
21 0                          ! F_COUP_RAD : perform a full coupling w
22 0                          ! F_AV      : integrate Av or not-
23 0                          ! F_invAv   : use grain coefficients to
24 5.34D-22                   ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                   ! N_H2_0    : column density of H2 buffe
26 1.00E+06                   ! N_CO_0    : column density of CO buffe
27 3.50E+00                   ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                          ! F_TGR     : compute grain temperature
30 15                         ! Tgrains   : initial grain temperature
31 1.00E-06                   ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                   ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                   ! alph_mrn  : grain MRN index-
34 2.00E+00                   ! rho_grc   : grain core volumic mass (
35 1.00E+00                   ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                          ! ieqth     : thermal Balance (1 : solve
38 0                          ! Cool_KN   : Kaufman & Neufeld cooling
39 100                        ! NH2_lev   : number of H2 levels includ
40 100                        ! NH2_lines_out : maximum number of H2 l
41 BOTH                      ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                          ! iforH2    : formation on grain model
43 2                          ! ikinH2    : kinetic energy of H2 newly
44 0                          ! pumpH2    : H2 pumping by UV photons
45 50                         ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                          ! integ_type : linear (0) or logarithmic
48 30000                     ! Nstep_max  : maximum number of integrat
49 9.99E+99                   ! timeJ      : shock age (years)-
50 1.00E+06                   ! duration_max : maximum shock duration
51 1.00E-07                   ! Eps_V      : precision of computation-
52 1.00E+14                   ! XLL        : characteristic viscous leng
53 !---- output specifications -----
54 0                          ! F_W_HDF5_STD : write HDF5 standard outp
L: 3 C: 28 (none) Unicode (UTF-8) Unix (LF) Saved: 18/05/2022 14:54:42 8 396 / 790 / 85
```

Main input file : `input_mhd.in`

```

1  !---- input files -----
2  example_preshock           ! modele   : output files radix-
3  species_2022_05.in_depl   ! specfile : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5  none                       ! h2exfile : h2* file (if none, populat
6  none                       ! gridfile : file containing the grid
7  !---- shock parameters -----
8  S1                          ! shock_type : 'C' or 'J', Isoprotonic o
9  1                           ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                    ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                    ! Vs_km     : shock speed (km/s)-
12 1.00E+03                    ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                    ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                    ! Tn       : initial gas temperature (
15 3                            ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                    ! Zeta      : cosmic ray ionization rate
18 1                            ! F_ISRF    : radiation field spectrum -
19 0.00E+00                    ! RAD       : radiation field intensity
20 1.00E-01                    ! Av0       : initial extinction (magnit
21 0                            ! F_COUP_RAD : perform a full coupling w
22 0                            ! F_AV      : integrate Av or not-
23 0                            ! F_invAv   : use grain coefficients to
24 5.34D-22                    ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                    ! N_H2_0    : column density of H2 buffe
26 1.00E+06                    ! N_CO_0    : column density of CO buffe
27 3.50E+00                    ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                            ! F_TGR     : compute grain temperature
30 15                           ! Tgrains   : initial grain temperature
31 1.00E-06                    ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                    ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                    ! alph_mrn  : grain MRN index-
34 2.00E+00                    ! rho_grc   : grain core volumic mass (
35 1.00E+00                    ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                            ! ieqth     : thermal Balance (1 : solve
38 0                            ! Cool_KN   : Kaufman & Neufeld cooling
39 100                          ! NH2_lev   : number of H2 levels includ
40 100                          ! NH2_lines_out : maximum number of H2 l
41 BOTH                         ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                            ! iforH2    : formation on grain model
43 2                            ! ikinH2    : kinetic energy of H2 newly
44 0                            ! pumpH2    : H2 pumping by UV photons
45 50                            ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                            ! integ_type : linear (0) or logarithmic
48 30000                       ! Nstep_max : maximum number of integrat
49 9.99E+99                    ! timeJ     : shock age (years)-
50 1.00E+06                    ! duration_max : maximum shock duration
51 1.00E-07                    ! Eps_V     : precision of computation-
52 1.00E+14                    ! XLL       : characteristic viscous leng
53 !---- output specifications -----
54 0                            ! F_W_HDF5_STD : write HDF5 standard outp

```

values of the parameters

names of variables in the code

short parameter descriptions

Outline

- introduction
- assumptions physics
- user guide first steps
- services

Inputs

Main input file : `input_mhd.in`

name of output directory
results are stored in
`output/example_preshock/`

```
input_mhd.in
1  !---- input files -----
2  example_preshock          ! modele   : output files radix
3  species_2022_05.in_depl  ! specfile : species file (species list)
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction rates)
5  none                     ! h2exfile : h2* file (if none, population)
6  none                     ! gridfile : file containing the grid coordinates
7  !---- shock parameters -----
8  S1                       ! shock_type : 'C' or 'J', Isoprotonic or 'J'
9  1                        ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                 ! Bbeta    : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                 ! Vs_km    : shock speed (km/s)-
12 1.00E+03                 ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                 ! nH_init  : initial nH = n(H) + 2.0 n(H)
14 1.00E+01                 ! Tn       : initial gas temperature (K)
15 3                        ! op_H2_in : initial H2 ortho/para ratio
16 !---- environment -----
17 5.00E-17                 ! Zeta     : cosmic ray ionization rate
18 1                        ! F_ISRF   : radiation field spectrum -
19 0.00E+00                 ! RAD      : radiation field intensity
20 1.00E-01                 ! Av0      : initial extinction (magnitudes)
21 0                        ! F_COUP_RAD : perform a full coupling with radiation
22 0                        ! F_AV     : integrate Av or not-
23 0                        ! F_invAv  : use grain coefficients to compute Av
24 5.34D-22                 ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                 ! N_H2_0   : column density of H2 buffer gas
26 1.00E+06                 ! N_CO_0   : column density of CO buffer gas
27 3.50E+00                 ! vturb    : turbulent velocity (km s-1)
28 !---- grain properties -----
29 0                        ! F_TGR    : compute grain temperature
30 15                       ! Tgrains  : initial grain temperature
31 1.00E-06                 ! amin_mrn : grain MRN minimum radius
32 3.00E-05                 ! amax_mrn : grain MRN maximum radius
33 3.50E+00                 ! alph_mrn : grain MRN index-
34 2.00E+00                 ! rho_grc  : grain core volumic mass (g cm-3)
35 1.00E+00                 ! rho_grm  : grain mantle volumic mass (g cm-3)
36 !---- excitation & cooling -----
37 1                        ! ieqth    : thermal Balance (1 : solve)
38 0                        ! Cool_KN  : Kaufman & Neufeld cooling
39 100                      ! NH2_lev  : number of H2 levels included
40 100                      ! NH2_lines_out : maximum number of H2 lines
41 BOTH                    ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                        ! iforH2   : formation on grain model
43 2                        ! ikinH2   : kinetic energy of H2 newly formed
44 0                        ! pumpH2   : H2 pumping by UV photons
45 50                       ! NCO_lev  : number of CO levels included
46 !---- numerical parameters -----
47 0                        ! integ_type : linear (0) or logarithmic
48 30000                   ! Nstep_max : maximum number of integration steps
49 9.99E+99                ! timeJ     : shock age (years)-
50 1.00E+06                ! duration_max : maximum shock duration
51 1.00E-07                ! Eps_V     : precision of computation-
52 1.00E+14                ! XLL      : characteristic viscous length
53 !---- output specifications -----
54 0                        ! F_W_HDF5_STD : write HDF5 standard output
```

Outline

- introduction
- assumptions physics
- user guide first steps
- services

Main input file : `input_mhd.in`

Outline

- introduction
- assumptions physics
- user guide first steps
- services

```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1  !---- input files -----
2  example_preshock          ! modele   : output files radix-
3  species_2022_05.in_depl  ! specfile : species file (species list)
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction rates)
5  none                      ! h2exfile : h2* file (if none, population)
6  none                      ! gridfile : file containing the grid coordinates
7  !---- shock parameters -----
8  S1                        ! shock_type : 'C' or 'J', Isoprotonic or 'J'
9  1                         ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                 ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                 ! Vs_km     : shock speed (km/s)-
12 1.00E+03                 ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                 ! nH_init   : initial nH = n(H) + 2.0 n(H2)
14 1.00E+01                 ! Tn        : initial gas temperature (K)
15 3                         ! op_H2_in  : initial H2 ortho/para ratio
16 !---- environment -----
17 5.00E-17                 ! Zeta      : cosmic ray ionization rate
18 1                         ! F_ISRF    : radiation field spectrum -
19 0.00E+00                 ! RAD       : radiation field intensity
20 1.00E-01                 ! Av0       : initial extinction (mag)
21 0                         ! F_COUP_RAD : perform a full coupling w/ radiation
22 0                         ! F_AV      : integrate Av or not-
23 0                         ! F_invAv   : use grain coefficients to compute Av
24 5.34D-22                 ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                 ! N_H2_0    : column density of H2 buffer gas
26 1.00E+06                 ! N_CO_0    : column density of CO buffer gas
27 3.50E+00                 ! vturb     : turbulent velocity (km s-1)
28 !---- grain properties -----
29 0                         ! F_TGR     : compute grain temperature
30 15                        ! Tgrains   : initial grain temperature (K)
31 1.00E-06                 ! amin_mrn  : grain MRN minimum radius (micrometers)
32 3.00E-05                 ! amax_mrn  : grain MRN maximum radius (micrometers)
33 3.50E+00                 ! alph_mrn  : grain MRN index-
34 2.00E+00                 ! rho_grc   : grain core volumic mass (g cm-3)
35 1.00E+00                 ! rho_grm   : grain mantle volumic mass (g cm-3)
36 !---- excitation & cooling -----
37 1                         ! ieqth     : thermal Balance (1 : solve)
38 0                         ! Cool_KN   : Kaufman & Neufeld cooling
39 100                       ! NH2_lev   : number of H2 levels included
40 100                       ! NH2_lines_out : maximum number of H2 lines
41 BOTH                     ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                         ! iforH2    : formation on grain model
43 2                         ! ikinH2    : kinetic energy of H2 newly formed
44 0                         ! pumpH2    : H2 pumping by UV photons
45 50                        ! NCO_lev   : number of CO levels included
46 !---- numerical parameters -----
47 0                         ! integ_type : linear (0) or logarithmic
48 30000                    ! Nstep_max : maximum number of integration steps
49 9.99E+99                 ! timeJ     : shock age (years)-
50 1.00E+06                 ! duration_max : maximum shock duration (years)
51 1.00E-07                 ! Eps_V     : precision of computation-
52 1.00E+14                 ! XLL       : characteristic viscous length
53 !---- output specifications -----
54 0                         ! F_W_HDF5_STD : write HDF5 standard output
```

file containing
the species list
their enthalpies
their initial abundances

↓
located in the `input/` directory

Main input file : `input_mhd.in`

```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1  !---- input files -----
2  example_preshock          ! modele   : output files radix-
3  species_2022_05.in depl   ! specfile : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5  none                      ! h2exfile : h2* file (if none, populat
6  none                      ! gridfile : file containing the grid
7  !---- shock parameters -----
8  S1                        ! shock_type : 'C' or 'J', Isoprotonic or
9  1                          ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                  ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                  ! Vs_km     : shock speed (km/s)-
12 1.00E+03                  ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                  ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                  ! Tn        : initial gas temperature (K)
15 3                          ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                  ! Zeta      : cosmic ray ionization rate
18 1                          ! F_ISRF    : radiation field spectrum -
19 0.00E+00                  ! RAD       : radiation field intensity
20 1.00E-01                  ! Av0       : initial extinction (magnit
21 0                          ! F_COUP_RAD : perform a full coupling w
22 0                          ! F_AV      : integrate Av or not-
23 0                          ! F_invAv   : use grain coefficients to
24 5.34D-22                  ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                  ! N_H2_0    : column density of H2 buffe
26 1.00E+06                  ! N_CO_0    : column density of CO buffe
27 3.50E+00                  ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                          ! F_TGR     : compute grain temperature
30 15                         ! Tgrains   : initial grain temperature
31 1.00E-06                  ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                  ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                  ! alph_mrn  : grain MRN index-
34 2.00E+00                  ! rho_grc   : grain core volumic mass (
35 1.00E+00                  ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                          ! ieqth     : thermal Balance (1 : solve
38 0                          ! Cool_KN   : Kaufman & Neufeld cooling
39 100                        ! NH2_lev   : number of H2 levels includ
40 100                        ! NH2_lines_out : maximum number of H2 l
41 BOTH                      ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                          ! iforH2    : formation on grain model
43 2                          ! ikinH2    : kinetic energy of H2 newly
44 0                          ! pumpH2    : H2 pumping by UV photons
45 50                          ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                          ! integ_type : linear (0) or logarithmic
48 30000                      ! Nstep_max : maximum number of integrat
49 9.99E+99                   ! timeJ     : shock age (years)-
50 1.00E+06                   ! duration_max : maximum shock duration
51 1.00E-07                   ! Eps_V     : precision of computation-
52 1.00E+14                   ! XLL       : characteristic viscous leng
53 !---- output specifications -----
54 0                          ! F_W_HDF5_STD : write HDF5 standard outp
L: 3 C: 28 (none) Unicode (UTF-8) Unix (LF) Saved: 18/05/2022 14:54:42 8 396 / 790 / 85
```

file containing
the chemical network
reactions types & rates

↓
*located in the input/
directory*

Outline

- introduction
- assumptions
physics
- user guide
first steps
- services

Main input file : `input_mhd.in`

```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1  !---- input files -----
2  example_preshock           ! modele   : output files radix-
3  species_2022_05.in_depl    ! specfile : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5  none                       ! h2exfile : h2+ file (if none, popula
6  none                       ! gridfile : file containing the grid
7  !---- shock parameters -----
8  S1                         ! shock_type : 'C' or 'J', Isoprotonic or
9  1                          ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                   ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                   ! Vs_km     : shock speed (km/s)-
12 1.00E+03                   ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                   ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                   ! Tn        : initial gas temperature (K)
15 3                          ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                   ! Zeta      : cosmic ray ionization rate
18 1                          ! F_ISRF    : radiation field spectrum-
19 0.00E+00                   ! RAD       : radiation field intensity
20 1.00E-01                   ! Av0       : initial extinction (magnit
21 0                          ! F_COUP_RAD : perform a full coupling w
22 0                          ! F_AV      : integrate Av or not-
23 0                          ! F_invAv   : use grain coefficients to
24 5.34D-22                   ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                   ! N_H2_0    : column density of H2 buffe
26 1.00E+06                   ! N_CO_0    : column density of CO buffe
27 3.50E+00                   ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                          ! F_TGR     : compute grain temperature
30 15                         ! Tgrains   : initial grain temperature
31 1.00E-06                   ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                   ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                   ! alph_mrn  : grain MRN index-
34 2.00E+00                   ! rho_grc   : grain core volumic mass (
35 1.00E+00                   ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                          ! ieqth     : thermal Balance (1 : solve
38 0                          ! Cool_KN   : Kaufman & Neufeld cooling
39 100                        ! NH2_lev   : number of H2 levels includ
40 100                        ! NH2_lines_out : maximum number of H2 l
41 BOTH                      ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                          ! iforH2    : formation on grain model
43 2                          ! ikinH2    : kinetic energy of H2 newl
44 0                          ! pumpH2    : H2 pumping by UV photons
45 50                         ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                          ! integ_type : linear (0) or logarithmic
48 30000                     ! Nstep_max  : maximum number of integrat
49 9.99E+99                   ! timeJ      : shock age (years)-
50 1.00E+06                   ! duration_max : maximum shock duration
51 1.00E-07                   ! Eps_V      : precision of computation-
52 1.00E+14                   ! XLL        : characteristic viscous leng
53 !---- output specifications -----
54 0                          ! F_W_HDF5_STD : write HDF5 standard outp
```

file containing
the initial abundances of
H₂ levels

↓
*located in the input/
directory*

if none - Boltzmann
distribution at T_n

Outline

- introduction
- assumptions physics
- user guide first steps
- services

Main input file : `input_mhd.in`

```

1  !---- input files -----
2  example_preshock           ! modele   : output files radix-
3  species_2022_05.in_depl    ! specfile  : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile  : chemistry file (reaction
5  none                       ! h2exfile  : h2* file (if none, populat
6  none                       ! gridfile  : file containing the grid
7  !---- shock parameters -----
8  S1                          ! shock_type : 'C' or 'J', Isochoric or
9  1                            ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                    ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                    ! Vs_km     : shock speed (km/s)-
12 1.00E+03                    ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                    ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                    ! Tn        : initial gas temperature (K)
15 3                            ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                    ! Zeta      : cosmic ray ionization rate
18 1                            ! F_ISRF    : radiation field spectrum-
19 0.00E+00                    ! RAD       : radiation field intensity
20 1.00E-01                    ! Av0       : initial extinction (magnit
21 0                            ! F_COUP_RAD : perform a full coupling w
22 0                            ! F_AV      : integrate Av or not-
23 0                            ! F_invAv   : use grain coefficients to
24 5.34D-22                    ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                    ! N_H2_0    : column density of H2 buffe
26 1.00E+06                    ! N_CO_0    : column density of CO buffe
27 3.50E+00                    ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                            ! F_TGR     : compute grain temperature
30 15                           ! Tgrains   : initial grain temperature
31 1.00E-06                    ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                    ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                    ! alph_mrn  : grain MRN index-
34 2.00E+00                    ! rho_grc   : grain core volumic mass (
35 1.00E+00                    ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                            ! ieqth     : thermal Balance (1 : solve
38 0                            ! Cool_KN   : Kaufman & Neufeld cooling
39 100                          ! NH2_lev   : number of H2 levels includ
40 100                          ! NH2_lines_out : maximum number of H2 l
41 BOTH                         ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                            ! iforH2    : formation on grain model
43 2                            ! ikinH2    : kinetic energy of H2 newly
44 0                            ! pumpH2    : H2 pumping by UV photons
45 50                            ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                            ! integ_type : linear (0) or logarithmic
48 30000                        ! Nstep_max : maximum number of integrat
49 9.99E+99                     ! timeJ     : shock age (years)-
50 1.00E+06                    ! duration_max : maximum shock duration
51 1.00E-07                    ! Eps_V     : precision of computation-
52 1.00E+14                    ! XLL       : characteristic viscous leng
53 !---- output specifications -----
54 0                            ! F_W_HDF5_STD : write HDF5 standard outp

```

shock type

examples

- S1 = Isochoric preshock

- J = J-type shock

- C = C-type shock

Outline

- introduction
- assumptions physics
- user guide first steps
- services

Main input file : `input_mhd.in`

```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1 !---- input files -----
2 example_preshock          ! modele   : output files radix-
3 species_2022_05.in_depl   ! specfile : species file (species list
4 chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5 none                      ! h2exfile : h2* file (if none, populat
6 none                      ! gridfile : file containing the grid
7 !---- shock parameters -----
8 S1                        ! shock_type : 'C' or 'J', Isoprotonic o
9 1                          ! Nfluids   : 1, 2 ou 3
10 1.00E-00                 ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                 ! Vs_km     : shock speed (km/s)-
12 1.00E+03                 ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                 ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                 ! Tn        : initial gas temperature (
15 3                          ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                 ! Zeta      : cosmic ray ionization rate
18 1                          ! F_ISRF    : radiation field spectrum -
19 0.00E+00                 ! RAD       : radiation field intensity
20 1.00E-01                 ! Av0       : initial extinction (magnit
21 0                          ! F_COUP_RAD : perform a full coupling w
22 0                          ! F_AV      : integrate Av or not-
23 0                          ! F_invAv   : use grain coefficients to
24 5.34D-22                 ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                 ! N_H2_0    : column density of H2 buffe
26 1.00E+06                 ! N_CO_0    : column density of CO buffe
27 3.50E+00                 ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                          ! F_TGR     : compute grain temperature
30 15                         ! Tgrains   : initial grain temperature
31 1.00E-06                 ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                 ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                 ! alph_mrn  : grain MRN index-
34 2.00E+00                 ! rho_grc   : grain core volumic mass (
35 1.00E+00                 ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                          ! ieqth     : thermal Balance (1 : solve
38 0                          ! Cool_KN   : Kaufman & Neufeld cooling
39 100                       ! NH2_lev   : number of H2 levels includ
40 100                       ! NH2_lines_out : maximum number of H2 l
41 BOTH                      ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                          ! iforH2    : formation on grain model
43 2                          ! ikinH2    : kinetic energy of H2 newly
44 0                          ! pumpH2    : H2 pumping by UV photons
45 50                         ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                          ! integ_type : linear (0) or logarithmic
48 30000                     ! Nstep_max : maximum number of integrat
49 9.99E+99                 ! timeJ     : shock age (years)-
50 1.00E+06                 ! duration_max : maximum shock duration
51 1.00E-07                 ! Eps_V     : precision of computation-
52 1.00E+14                 ! XLL       : characteristic viscous leng
53 !---- output specifications -----
54 0                          ! F_W_HDF5_STD : write HDF5 standard outp
L: 3 C: 28 (none) Unicode (UTF-8) Unix (LF) Saved: 18/05/2022 14:54:42 8 396 / 790 / 85
```

number of fluids

- 1 for preshock / J shock

- 3 for C shock

Outline

- introduction
- assumptions physics
- user guide first steps
- services

Main input file : `input_mhd.in`

```

1  !---- input files -----
2  example_preshock           ! modele   : output files radix-
3  species_2022_05.in_depl   ! specfile : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5  none                       ! h2exfile : h2* file (if none, populat
6  none                       ! gridfile : file containing the grid
7  !---- shock parameters -----
8  S1                          ! shock_type : 'C' or 'J', Isoprotonic or
9  1                            ! Nfluids   : 1, 2 ou 3-
10  1.00E-00                    ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11  1.00E+01                    ! Vs_km     : shock speed (km/s)-
12  1.00E+03                    ! DeltaVmin : initial Vn - Vi (cm s-1)-
13  1.00E+04                    ! nH_init   : initial nH = n(H) + 2.0 n
14  1.00E+01                    ! Tn        : initial gas temperature (K)
15  3                            ! op_H2_in  : initial H2 ortho/para rat
16  !---- environment -----
17  5.00E-17                    ! Zeta      : cosmic ray ionization rate
18  1                            ! F_ISRF    : radiation field spectrum-
19  0.00E+00                    ! RAD       : radiation field intensity
20  1.00E-01                    ! Av0       : initial extinction (magnit
21  0                            ! F_COUP_RAD : perform a full coupling w
22  0                            ! F_AV      : integrate Av or not-
23  0                            ! F_invAv   : use grain coefficients to
24  5.34D-22                    ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25  1.00E+06                    ! N_H2_0    : column density of H2 buffe
26  1.00E+06                    ! N_CO_0    : column density of CO buffe
27  3.50E+00                    ! vturb     : turbulent velocity (km s-
28  !---- grain properties -----
29  0                            ! F_TGR     : compute grain temperature
30  15                           ! Tgrains   : initial grain temperature
31  1.00E-06                    ! amin_mrn  : grain MRN minimum radius
32  3.00E-05                    ! amax_mrn  : grain MRN maximum radius
33  3.50E+00                    ! alph_mrn  : grain MRN index-
34  2.00E+00                    ! rho_grc   : grain core volumic mass (
35  1.00E+00                    ! rho_grm   : grain mantle volumic mass
36  !---- excitation & cooling -----
37  1                            ! ieqth     : thermal Balance (1 : solve
38  0                            ! Cool_KN   : Kaufman & Neufeld cooling
39  100                          ! NH2_lev   : number of H2 levels includ
40  100                          ! NH2_lines_out : maximum number of H2 l
41  BOTH                         ! H_H2_flag : H-H2 collisions : DRF, MM
42  1                            ! iforH2    : formation on grain model
43  2                            ! ikinH2    : kinetic energy of H2 newly
44  0                            ! pumpH2    : H2 pumping by UV photons
45  50                           ! NCO_lev   : number of CO levels includ
46  !---- numerical parameters -----
47  0                            ! integ_type : linear (0) or logarithmic
48  30000                        ! Nstep_max : maximum number of integrat
49  9.99E+99                    ! timeJ     : shock age (years)-
50  1.00E+06                    ! duration_max : maximum shock duration
51  1.00E-07                    ! Eps_V     : precision of computation-
52  1.00E+14                    ! XLL       : characteristic viscous leng
53  !---- output specifications -----
54  0                            ! F_W_HDF5_STD : write HDF5 standard outp

```

magnetic field strength

$$\frac{B}{1 \mu\text{G}} = b \sqrt{\frac{n_{\text{H}}}{1 \text{ cm}^{-3}}}$$

Outline

- introduction
- assumptions physics
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- services

Main input file : `input_mhd.in`

```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1  !---- input files -----
2  example_preshock          ! modele   : output files radix-
3  species_2022_05.in_depl  ! specfile : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5  none                      ! h2exfile : h2* file (if none, populat
6  none                      ! gridfile : file containing the grid
7  !---- shock parameters -----
8  S1                        ! shock_type : 'C' or 'J', Isoprotonic or
9  1                          ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                   ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                   ! Vs_km     : shock speed (km/s)
12 1.00E+03                   ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                   ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                   ! Tn        : initial gas temperature (K)
15 3                           ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                   ! Zeta      : cosmic ray ionization rate
18 1                           ! F_ISRF    : radiation field spectrum -
19 0.00E+00                   ! RAD       : radiation field intensity
20 1.00E-01                   ! Av0       : initial extinction (magnit
21 0                           ! F_COUP_RAD : perform a full coupling w
22 0                           ! F_AV      : integrate Av or not-
23 0                           ! F_invAv   : use grain coefficients to
24 5.34D-22                   ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                   ! N_H2_0    : column density of H2 buffe
26 1.00E+06                   ! N_CO_0    : column density of CO buffe
27 3.50E+00                   ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                           ! F_TGR     : compute grain temperature
30 15                          ! Tgrains   : initial grain temperature
31 1.00E-06                   ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                   ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                   ! alph_mrn  : grain MRN index-
34 2.00E+00                   ! rho_grc   : grain core volumic mass (
35 1.00E+00                   ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                           ! ieqth     : thermal Balance (1 : solve
38 0                           ! Cool_KN   : Kaufman & Neufeld cooling
39 100                         ! NH2_lev   : number of H2 levels includ
40 100                         ! NH2_lines_out : maximum number of H2 l
41 BOTH                       ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                           ! iforH2    : formation on grain model
43 2                           ! ikinH2    : kinetic energy of H2 newly
44 0                           ! pumpH2    : H2 pumping by UV photons
45 50                          ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                           ! integ_type : linear (0) or logarithmic
48 30000                       ! Nstep_max : maximum number of integrat
49 9.99E+99                    ! timeJ     : shock age (years)-
50 1.00E+06                   ! duration_max : maximum shock duration
51 1.00E-07                   ! Eps_V     : precision of computation-
52 1.00E+14                   ! XLL       : characteristic viscous leng
53 !---- output specifications -----
54 0                           ! F_W_HDF5_STD : write HDF5 standard outp
```

shock velocity (km s⁻¹)

Outline

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Main input file : `input_mhd.in`

```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1  !---- input files -----
2  example_preshock          ! modele   : output files radix-
3  species_2022_05.in_depl   ! specfile : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5  none                      ! h2exfile : h2* file (if none, populat
6  none                      ! gridfile : file containing the grid
7  !---- shock parameters -----
8  S1                        ! shock_type : 'C' or 'J', Isoprotonic o
9  1                          ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                  ! Bbeta     : Bfield = Bbeta * sqrt(nH)
111.00E+01                  ! Vs_km     : shock speed (km/s)-
121.00E+03                  ! DeltaVmin : initial Vn - Vi (cm s-1)-
131.00E+04                  ! nH_init   : initial nH = n(H) : 2.0 n
141.00E+01                  ! Tn        : initial gas temperature (K)
153                          ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                  ! Zeta      : cosmic ray ionization rate
181                          ! F_ISRF    : radiation field spectrum -
190.00E+00                  ! RAD       : radiation field intensity
201.00E-01                  ! Av0       : initial extinction (magnit
210                          ! F_COUP_RAD : perform a full coupling w
220                          ! F_AV      : integrate Av or not-
230                          ! F_invAv   : use grain coefficients to
245.34D-22                  ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
251.00E+06                  ! N_H2_0    : column density of H2 buffe
261.00E+06                  ! N_CO_0    : column density of CO buffe
273.50E+00                  ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
290                          ! F_TGR     : compute grain temperature
3015                         ! Tgrains   : initial grain temperature
311.00E-06                  ! amin_mrn  : grain MRN minimum radius
323.00E-05                  ! amax_mrn  : grain MRN maximum radius
333.50E+00                  ! alph_mrn  : grain MRN index-
342.00E+00                  ! rho_grc   : grain core volumic mass (
351.00E+00                  ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
371                          ! ieqth     : thermal Balance (1 : solve
380                          ! Cool_KN   : Kaufman & Neufeld cooling
39100                        ! NH2_lev   : number of H2 levels includ
40100                        ! NH2_lines_out : maximum number of H2 l
41BOTH                       ! H_H2_flag : H-H2 collisions : DRF, MM
421                          ! iforH2    : formation on grain model
432                          ! ikinH2    : kinetic energy of H2 newly
440                          ! pumpH2    : H2 pumping by UV photons
4550                         ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
470                          ! integ_type : linear (0) or logarithmic
4830000                     ! Nstep_max : maximum number of integrat
499.99E+99                  ! timeJ     : shock age (years)-
501.00E+06                  ! duration_max : maximum shock duration
511.00E-07                  ! Eps_V     : precision of computation-
521.00E+14                  ! XLL       : characteristic viscous leng
53 !---- output specifications -----
540                          ! F_W_HDF5_STD : write HDF5 standard outp
L: 3 C: 28 (none) Unicode (UTF-8) Unix (LF) Saved: 18/05/2022 14:54:42 8 396 / 790 / 85
```

initial proton density (cm^{-3})

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Main input file : `input_mhd.in`

```

1  !---- input files -----
2  example_preshock           ! modele   : output files radix-
3  species_2022_05.in_depl    ! specfile  : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile  : chemistry file (reaction
5  none                       ! h2exfile  : h2* file (if none, populat
6  none                       ! gridfile  : file containing the grid
7  !---- shock parameters -----
8  S1                          ! shock_type : 'C' or 'J', Isoprotonic o
9  1                           ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                    ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                    ! Vs_km     : shock speed (km/s)-
12 1.00E+03                    ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                    ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                    ! Tn       : initial gas temperature (
15 3                            ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                    ! Zeta      : cosmic ray ionization rate
18 1                            ! F_ISRF    : radiation field spectrum -
19 0.00E+00                    ! RAD       : radiation field intensity
20 1.00E-01                    ! Av0       : initial extinction (magnit
21 0                            ! F_COUP_RAD : perform a full coupling w
22 0                            ! F_AV      : integrate Av or not-
23 0                            ! F_invAv   : use grain coefficients to
24 5.34D-22                    ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                    ! N_H2_0    : column density of H2 buffe
26 1.00E+06                    ! N_CO_0    : column density of CO buffe
27 3.50E+00                    ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                            ! F_TGR     : compute grain temperature
30 15                          ! Tgrains   : initial grain temperature
31 1.00E-06                    ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                    ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                    ! alph_mrn  : grain MRN index-
34 2.00E+00                    ! rho_grc   : grain core volumic mass (
35 1.00E+00                    ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                            ! ieqth     : thermal Balance (1 : solve
38 0                            ! Cool_KN   : Kaufman & Neufeld cooling
39 100                         ! NH2_lev   : number of H2 levels includ
40 100                         ! NH2_lines_out : maximum number of H2 l
41 BOTH                       ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                            ! iforH2    : formation on grain model
43 2                            ! ikinH2    : kinetic energy of H2 newly
44 0                            ! pumpH2    : H2 pumping by UV photons
45 50                          ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                            ! integ_type : linear (0) or logarithmic
48 30000                       ! Nstep_max  : maximum number of integrat
49 9.99E+99                    ! timeJ     : shock age (years)-
50 1.00E+06                    ! duration_max : maximum shock duration
51 1.00E-07                    ! Eps_V     : precision of computation-
52 1.00E+14                    ! XLL       : characteristic viscous leng
53 !---- output specifications -----
54 0                            ! F_W_HDF5_STD : write HDF5 standard outp

```

specification of CO, ¹³CO, and H₂O cooling

- 0 = analytical (preshock)

- 1 = LVG cooling tables from NK1993 (shock)

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Main input file : `input_mhd.in`

```
input_mhd.in
~/Desktop/Shock_1.1_rev122/input/input_mhd.in
1  !---- input files -----
2  example_preshock          ! modele   : output files radix-
3  species_2022_05.in_depl   ! specfile : species file (species list
4  chemistry_2022_05_all.in_noadso ! chemfile : chemistry file (reaction
5  none                      ! h2exfile : h2* file (if none, populat
6  none                      ! gridfile : file containing the grid
7  !---- shock parameters -----
8  S1                        ! shock_type : 'C' or 'J', Isoprotonic or
9  1                          ! Nfluids   : 1, 2 ou 3-
10 1.00E-00                  ! Bbeta     : Bfield = Bbeta * sqrt(nH)
11 1.00E+01                  ! Vs_km     : shock speed (km/s)-
12 1.00E+03                  ! DeltaVmin : initial Vn - Vi (cm s-1)-
13 1.00E+04                  ! nH_init   : initial nH = n(H) + 2.0 n
14 1.00E+01                  ! Tn        : initial gas temperature (K)
15 3                          ! op_H2_in  : initial H2 ortho/para rat
16 !---- environment -----
17 5.00E-17                  ! Zeta      : cosmic ray ionization rate
18 1                          ! F_ISRF    : radiation field spectrum -
19 0.00E+00                  ! RAD       : radiation field intensity
20 1.00E-01                  ! Av0       : initial extinction (magnit
21 0                          ! F_COUP_RAD : perform a full coupling w
22 0                          ! F_AV      : integrate Av or not-
23 0                          ! F_invAv   : use grain coefficients to
24 5.34D-22                  ! inv_Av_fac : AV/NH (Galaxy : 5.34D-22)
25 1.00E+06                  ! N_H2_0    : column density of H2 buffe
26 1.00E+06                  ! N_CO_0    : column density of CO buffe
27 3.50E+00                  ! vturb     : turbulent velocity (km s-
28 !---- grain properties -----
29 0                          ! F_TGR     : compute grain temperature
30 15                         ! Tgrains   : initial grain temperature
31 1.00E-06                  ! amin_mrn  : grain MRN minimum radius
32 3.00E-05                  ! amax_mrn  : grain MRN maximum radius
33 3.50E+00                  ! alph_mrn  : grain MRN index-
34 2.00E+00                  ! rho_grc   : grain core volumic mass (
35 1.00E+00                  ! rho_grm   : grain mantle volumic mass
36 !---- excitation & cooling -----
37 1                          ! ieqth     : thermal Balance (1 : solve
38 0                          ! Cool_KN   : Kaufman & Neufeld cooling
39 100                        ! NH2_lev   : number of H2 levels includ
40 100                        ! NH2_lines_out : maximum number of H2 l
41 BOTH                       ! H_H2_flag : H-H2 collisions : DRF, MM
42 1                          ! iforH2    : formation on grain model
43 2                          ! ikinH2    : kinetic energy of H2 newly
44 0                          ! pumpH2    : H2 pumping by UV photons
45 50                          ! NCO_lev   : number of CO levels includ
46 !---- numerical parameters -----
47 0                          ! integ_type : linear (0) or logarithmic
48 30000                      ! Nstep_max : maximum number of integrat
49 9.99F+99                   ! timeJ     : shock age (years)-
50 1.00E+06                   ! duration_max : maximum shock duration
51 1.00E-07                   ! Eps_V     : precision of computation-
52 1.00E+14                   ! XLL       : characteristic viscous leng
53 !---- output specifications -----
54 0                          ! F_W_HDF5_STD : write HDF5 standard outp
L: 3 C: 28 (none) Unicode (UTF-8) Unix (LF) Saved: 18/05/2022 14:54:42 8 396 / 790 / 85
```

maximum duration of the model

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chemical files : species_...in

Outline

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```

species_2022_05.in
~/Desktop/Shock_1.1_rev122/input/species_2022_05.in
1  !---- list of chemical species --- Steady state at T = 19.24 K -----
2  !---- nH = 30.00 cm-3 -----
3  !---- Av = 3.00 mag -----
4  !---- RAD = 1.00 -----
5  !---- N_H2_0 = 3.000E+21 cm-2 -----
6  !---- N_CO_0 = 0.000E+00 cm-2 -----
7  !---- WARNING : order = neutrals, species on mantles, ions >0, ions <0 -----
8  !---- name, compo, initial density (n/nH), form enthalpy & err (kCal/mol), notes ---
9  !-----
10 1 H      01000000000000 4.000D-01  51.633  0.000      ! ΔHf(0K): Active Th
11 2 H2     02000000000000 3.000D-01   0.000  0.000      ! ΔHf(0K): reference
12 3 He     00000010000000 1.000D-01   0.000  0.000      ! ΔHf(0K): reference
13 4 C      00010000000000 1.000D-20 170.028  0.011  --> [C] = 8.27(-05) ! ΔHf(0K): Active Th
14 5 CH     01010000000000 1.000D-20 141.687  0.024  A&G ... 3.55(-04) ! ΔHf(0K): Active Th
15 6 CH2    02010000000000 1.000D-20  93.466  0.023      ! ΔHf(0K): Active Th
16 7 CH3    03010000000000 1.000D-20  35.819  0.014      ! ΔHf(0K): Active Th
17 8 CH4    04010000000000 1.000D-20 -15.908  0.016      ! ΔHf(0K): Active Th
18 9 C2     00020000000000 1.000D-20 196.052  0.062      ! ΔHf(0K): Active Th
19 10 C2H   01020000000000 1.000D-20 134.768  0.033      ! ΔHf(0K): Active Th
20 11 C2H2  02020000000000 1.000D-20  54.689  0.031      ! ΔHf(0K): Active Th
21 12 C3    00030000000000 1.000D-20 214.842  0.382      ! ΔHf(0K): Active Th
22 13 C3H   01030000000000 1.000D-20 169.909  0.263      ! ΔHf(0K): Active Th
23 14 C3H2  02030000000000 1.000D-20 118.798  0.110      ! ΔHf(0K): Active Th
24 15 O      00000100000000 3.020D-04  58.997  0.001  --> [O] = 3.02(-04) ! ΔHf(0K): Active Th
25 16 OH    01000100000000 1.000D-20  8.902  0.006  A&G ... 7.41(-04) ! ΔHf(0K): Active Th
26 17 H2O   02000100000000 1.000D-20 -57.106  0.006      ! ΔHf(0K): Active Th
27 18 O2    00000200000000 1.000D-20   0.000  0.000      ! ΔHf(0K): reference
28 19 CO     00010100000000 1.000D-20 -27.200  0.006      ! ΔHf(0K): Active Th
29 20 HCO   01010100000000 1.000D-20  9.893  0.023      ! ΔHf(0K): Active Th
30 21 H2CO  02010100000000 1.000D-20 -25.186  0.023      ! ΔHf(0K): Active Th
31 22 CH3OH 04010100000000 1.000D-20 -45.421  0.036      ! ΔHf(0K): Active Th
32 23 CO2   00010200000000 1.000D-20 -93.955  0.004      ! ΔHf(0K): Active Th
33 24 HCO2H 02010200000000 1.000D-20 -88.697  0.053      ! ΔHf(0K): Active Th
34 25 N      00001000000000 7.940D-05 112.471  0.006  --> [N] = 7.94(-05) ! ΔHf(0K): Active Th
35 26 NH     01001000000000 1.000D-20  85.741  0.041  A&G ... 9.33(-05) ! ΔHf(0K): Active Th
36 27 NH2    02001000000000 1.000D-20  45.151  0.026      ! ΔHf(0K): Active Th
37 28 NH3    03001000000000 1.000D-20  -9.217  0.007      ! ΔHf(0K): Active Th
38 29 N2     00002000000000 1.000D-20   0.000  0.000      ! ΔHf(0K): reference
39 30 CN     00011000000000 1.000D-20 104.386  0.033      ! ΔHf(0K): Active Th
40 31 HCN    01011000000000 1.000D-20  30.990  0.022      ! ΔHf(0K): Active Th
41 32 HNC    01011000000000 1.000D-20  45.860  0.086      ! ΔHf(0K): Active Th
42 33 NO     00001100000000 1.000D-20  21.658  0.016      ! ΔHf(0K): Active Th
43 34 S      00000000010000 1.000D-20  65.710  0.036  A&G ... 1.86(-05) ! ΔHf(0K): NIST sear
44 35 SH     01000000010000 1.000D-20  33.450  unkwn      ! ΔHf(0K): NIST sear
45 36 H2S    02000000010000 1.000D-20  -4.220  0.120      ! ΔHf(0K): NIST sear
46 37 CS     00010000010000 1.000D-20  65.300  unkwn      ! ΔHf(0K): NIST sear
47 38 SO     00000100010000 1.000D-20   1.200  unkwn      ! ΔHf(0K): NIST sear
48 39 SO2    00000200010000 1.000D-20 -70.340  unkwn      ! ΔHf(0K): NIST sear
49 40 OCS    00010100010000 1.000D-20 -33.900  unkwn      ! ΔHf(0K): NIST sear
50 41 Si     00000000001000 1.000D-20 106.520  unkwn  A&G ... 3.55(-05) ! ΔHf(0K): NIST sear
51 42 SiH    01000000001000 1.000D-20  87.700  unkwn      ! ΔHf(0K): NIST sear
52 43 SiH2   02000000001000 1.000D-20  65.730  unkwn      ! ΔHf(0K): NIST sear
53 44 SiH3   03000000001000 1.000D-20  49.240  unkwn      ! ΔHf(0K): NIST sear
54 45 SiH4   04000000001000 1.000D-20  10.500  unkwn      ! ΔHf(0K): NIST sear

```

chemical files : species_...in

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```

species_2022_05.in
~/Desktop/Shock_1.1_rev122/input/species_2022_05.in
1  !---- list of chemical species --- Steady state at T = 19.24 K -----
2  !---- nH = 30.00 cm-3 -----
3  !---- Av = 3.00 mag -----
4  !---- RAD = 1.00 -----
5  !---- N_H2_0 = 3.000E+21 cm-2 -----
6  !---- N_CO_0 = 0.000E+00 cm-2 -----
7  !---- WARNING : order = neutrals, species on mantles, ions >0, ions <0 -----
8  !---- name, compo, initial density (n/nH), form enthalpy & err (kCal/mol), notes ---
9  !-----
10 1 H 01000000000000 4.000D-01 51.633 0.000 ! ΔHf(0K): Active Th
11 2 H2 02000000000000 3.000D-01 0.000 0.000 ! ΔHf(0K): reference
12 3 He 00000010000000 1.000D-01 0.000 0.000 ! ΔHf(0K): reference
13 4 C 00010000000000 1.000D-20 170.028 0.011 --> [C] = 8.27(-05) ! ΔHf(0K): Active Th
14 5 CH 01010000000000 1.000D-20 141.687 0.024 A&G ... 3.55(-04) ! ΔHf(0K): Active Th
15 6 CH2 02010000000000 1.000D-20 93.466 0.023 ! ΔHf(0K): Active Th
16 7 CH3 03010000000000 1.000D-20 35.819 0.014 ! ΔHf(0K): Active Th
17 8 CH4 04010000000000 1.000D-20 -15.908 0.016 ! ΔHf(0K): Active Th
18 9 C2 00020000000000 1.000D-20 196.052 0.062 ! ΔHf(0K): Active Th
19 10 C2H 01020000000000 1.000D-20 134.768 0.033 ! ΔHf(0K): Active Th
20 11 C2H2 02020000000000 1.000D-20 54.689 0.031 ! ΔHf(0K): Active Th
21 12 C3 00030000000000 1.000D-20 214.842 0.382 ! ΔHf(0K): Active Th
22 13 C3H 01030000000000 1.000D-20 169.909 0.263 ! ΔHf(0K): Active Th
23 14 C3H2 02030000000000 1.000D-20 118.798 0.110 ! ΔHf(0K): Active Th
24 15 O 00000100000000 3.020D-04 58.997 0.001 --> [O] = 3.02(-04) ! ΔHf(0K): Active Th
25 16 OH 01000100000000 1.000D-20 8.902 0.006 A&G ... 7.41(-04) ! ΔHf(0K): Active Th
26 17 H2O 02000100000000 1.000D-20 -57.106 0.006 ! ΔHf(0K): Active Th
27 18 O2 00000200000000 1.000D-20 0.000 0.000 ! ΔHf(0K): reference
28 19 CO 00010100000000 1.000D-20 -27.200 0.006 ! ΔHf(0K): Active Th
29 20 HCO 01010100000000 1.000D-20 9.893 0.023 ! ΔHf(0K): Active Th
30 21 H2CO 02010100000000 1.000D-20 -25.186 0.023 ! ΔHf(0K): Active Th
31 22 CH3OH 04010100000000 1.000D-20 -45.421 0.036 ! ΔHf(0K): Active Th
32 23 CO2 00010200000000 1.000D-20 -93.955 0.004 ! ΔHf(0K): Active Th
33 24 HCO2H 02010200000000 1.000D-20 -88.697 0.053 ! ΔHf(0K): Active Th
34 25 N 00001000000000 7.940D-05 112.471 0.006 --> [N] = 7.94(-05) ! ΔHf(0K): Active Th
35 26 NH 01001000000000 1.000D-20 85.741 0.041 A&G ... 9.33(-05) ! ΔHf(0K): Active Th
36 27 NH2 02001000000000 1.000D-20 45.151 0.026 ! ΔHf(0K): Active Th
37 28 NH3 03001000000000 1.000D-20 -9.217 0.007 ! ΔHf(0K): Active Th
38 29 N2 00002000000000 1.000D-20 0.000 0.000 ! ΔHf(0K): reference
39 30 CN 00011000000000 1.000D-20 104.386 0.033 ! ΔHf(0K): Active Th
40 31 HCN 01011000000000 1.000D-20 30.990 0.022 ! ΔHf(0K): Active Th
41 32 HNC 01011000000000 1.000D-20 45.860 0.086 ! ΔHf(0K): Active Th
42 33 NO 00001100000000 1.000D-20 21.658 0.016 ! ΔHf(0K): Active Th
43 34 S 00000000010000 1.000D-20 65.710 0.036 A&G ... 1.86(-05) ! ΔHf(0K): NIST sear
44 35 SH 01000000010000 1.000D-20 33.450 unkwn ! ΔHf(0K): NIST sear
45 36 H2S 02000000010000 1.000D-20 -4.220 0.120 ! ΔHf(0K): NIST sear
46 37 CS 00010000010000 1.000D-20 65.300 unkwn ! ΔHf(0K): NIST sear
47 38 SO 00000100010000 1.000D-20 1.200 unkwn ! ΔHf(0K): NIST sear
48 39 SO2 00000200010000 1.000D-20 -70.340 unkwn ! ΔHf(0K): NIST sear
49 40 OCS 00010100010000 1.000D-20 -33.900 unkwn ! ΔHf(0K): NIST sear
50 41 Si 00000000001000 1.000D-20 106.520 unkwn A&G ... 3.55(-05) ! ΔHf(0K): NIST sear
51 42 SiH 01000000001000 1.000D-20 87.700 unkwn ! ΔHf(0K): NIST sear
52 43 SiH2 02000000001000 1.000D-20 65.730 unkwn ! ΔHf(0K): NIST sear
53 44 SiH3 03000000001000 1.000D-20 49.240 unkwn ! ΔHf(0K): NIST sear
54 45 SiH4 04000000001000 1.000D-20 10.500 unkwn ! ΔHf(0K): NIST sear

```

header

list of species

elemental compositions

initial abundances

enthalpies / errors

comments & references

chemical files : chemistry_...all.in

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```

chemistry_2022_05_all.in_noadso
~/Desktop/Shock_1.1_rev122/input/chemistry_2022_05_all.in_noadso
102 ! =====
103 !date R1      R2      P1      P2      P3      P4      gamma  alpha  beta  type  file  ! commen
104 ! =====
105 -
106 =====
107 ===== direct cosmic ray ionizations and dissociations =====
108 =====
109 -
110 <2013 H      CRP      H+      ELECTR      4.60E-01  0.00    0.0    30      ! Prasad
111 <2013 H2     CRP      H+      H      ELECTR      4.00E-02  0.00    0.0    30      ! Prasad
112 21-05 H2     CRP      H      H      ELECTR      1.00E-01  0.00    0.0    30      ! KIDA (
113 <2013 H2     CRP      H2+     ELECTR      9.60E-01  0.00    0.0    30      ! Prasad
114 <2013 He     CRP      He+     ELECTR      5.00E-01  0.00    0.0    30      ! Prasad
115 <2013 C      CRP      C+      ELECTR      1.80E+00  0.00    0.0    30      ! Prasad
116 <2013 O      CRP      O+      ELECTR      2.80E+00  0.00    0.0    30      ! Prasad
117 21-05 CO     CRP      CO+     ELECTR      3.00E+00  0.00    0.0    30      ! KIDA (
118 21-05 CO     CRP      C      O      ELECTR      5.00E+00  0.00    0.0    30      ! KIDA (
119 <2013 N      CRP      N+      ELECTR      2.10E+00  0.00    0.0    30      ! Prasad
120 21-05 S      CRP      S+      ELECTR      2.80E+00  0.00    0.0    30      ! same a
121 21-05 Si     CRP      Si+     ELECTR      1.80E+00  0.00    0.0    30      ! same a
122 21-05 Mg     CRP      Mg+     ELECTR      1.00E+00  0.00    0.0    30      ! arbitr
123 21-05 Fe     CRP      Fe+     ELECTR      1.00E+00  0.00    0.0    30      ! arbitr
124 -
125 =====
126 ===== secondary photon ionizations =====
127 =====
128 -
129 21-05 H      SECPHO  H+      ELECTR      0.00E-00  0.00    0.0    30      ! Heays
130 21-05 H2     SECPHO  H2+     ELECTR      0.00E-00  0.00    0.0    30      ! Heays
131 21-05 He     SECPHO  He+     ELECTR      0.00E-00  0.00    0.0    30      ! not fo
132 19-03 C      SECPHO  C+      ELECTR      2.60E+02  0.00    0.0    30      ! Heays
133 19-03 CH     SECPHO  CH+     ELECTR      5.80E+02  0.00    0.0    30      ! Heays
134 21-05 CH2    SECPHO  CH2+    ELECTR      0.00E-00  0.00    0.0    30      ! Heays
135 19-03 CH3    SECPHO  CH3+    ELECTR      3.80E+02  0.00    0.0    30      ! Heays
136 19-03 CH4    SECPHO  CH4+    ELECTR      2.20E+01  0.00    0.0    30      ! Heays
137 19-03 C2     SECPHO  C2+     ELECTR      2.50E+02  0.00    0.0    30      ! Heays
138 21-05 C2H    SECPHO  C2H+    ELECTR      0.00E-00  0.00    0.0    30      ! Heays
139 19-03 C2H2   SECPHO  C2H2+   ELECTR      3.80E+02  0.00    0.0    30      ! Heays
140 21-05 C3     SECPHO  C3+     ELECTR      8.90E+01  0.00    0.0    30      ! Heays
141 21-05 C3H    SECPHO  C3H+    ELECTR      0.00E-00  0.00    0.0    30      ! Heays
142 21-05 C3H2   SECPHO  C3H2+   ELECTR      0.00E-00  0.00    0.0    30      ! Heays
143 21-05 O      SECPHO  O+      ELECTR      2.70E+00  0.00    0.0    30      ! Heays
144 21-05 OH     SECPHO  OH+     ELECTR      0.00E-00  0.00    0.0    30      ! Heays
145 19-03 H2O    SECPHO  H2O+    ELECTR      2.30E+01  0.00    0.0    30      ! Heays
146 19-03 O2     SECPHO  O2+     ELECTR      2.80E+01  0.00    0.0    30      ! Heays
147 19-03 CO     SECPHO  CO+     ELECTR      1.40E+01  0.00    0.0    30      ! Heays
148 21-05 HCO    SECPHO  HCO+    ELECTR      0.00E-00  0.00    0.0    30      ! Heays
149 19-03 H2CO   SECPHO  H2CO+   ELECTR      2.90E+02  0.00    0.0    30      ! Heays
150 19-03 CH3OH  SECPHO  CH3OH+  ELECTR      2.40E+02  0.00    0.0    30      ! Heays
151 21-05 N      SECPHO  N+      ELECTR      0.00E-00  0.00    0.0    30      ! Heays
152 19-03 NH     SECPHO  NH+     ELECTR      7.10E+00  0.00    0.0    30      ! Heays
153 19-03 NH2    SECPHO  NH2+    ELECTR      1.40E+02  0.00    0.0    30      ! Heays
154 19-03 NH3    SECPHO  NH3+    ELECTR      2.20E+02  0.00    0.0    30      ! Heays
155 21-05 N2     SECPHO  N2+     ELECTR      0.00E-00  0.00    0.0    30      ! Heays
L: 1 C: 1 (none) Unicode (UTF-8) Unix (LF) Saved: 05/05/2022 11:42:06 541 452 / 69 733 / 2 883 100%

```

chemical files : chemistry_...all.in

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```

chemistry_2022_05_all.in_noadso
~/Desktop/Shock_1.1_rev122/input/chemistry_2022_05_all.in_noadso
=====
!date R1 R2 P1 P2 P3 P4 gamma alpha beta type file ! commen
=====
===== direct cosmic ray ionizations and dissociations =====
-----
<2013 H CRP H+ ELECTR 4.60E-01 0.00 0.0 30 ! Prasad
<2013 H2 CRP H+ H ELECTR 4.00E-02 0.00 0.0 30 ! Prasad
21-05 H2 CRP H H 1.00E-01 0.00 0.0 30 ! KIDA (
<2013 H2 CRP H2+ ELECTR 9.60E-01 0.00 0.0 30 ! Prasad
<2013 He CRP He+ ELECTR 5.00E-01 0.00 0.0 30 ! Prasad
<2013 C CRP C+ ELECTR 1.80E+00 0.00 0.0 30 ! Prasad
<2013 O CRP O+ ELECTR 2.80E+00 0.00 0.0 30 ! Prasad
21-05 CO CRP CO+ ELECTR 3.00E+00 0.00 0.0 30 ! KIDA (
21-05 CO CRP C O 5.00E+00 0.00 0.0 30 ! KIDA (
<2013 N CRP N+ ELECTR 2.10E+00 0.00 0.0 30 ! Prasad
21-05 S CRP S+ ELECTR 2.80E+00 0.00 0.0 30 ! same a
21-05 Si CRP Si+ ELECTR 1.80E+00 0.00 0.0 30 ! same a
21-05 Mg CRP Mg+ ELECTR 1.00E+00 0.00 0.0 30 ! arbitr
21-05 Fe CRP Fe+ ELECTR 1.00E+00 0.00 0.0 30 ! arbitr
-----
===== secondary photon ionizations =====
-----
21-05 H SECPHO H+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
21-05 H2 SECPHO H2+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
21-05 He SECPHO He+ ELECTR 0.00E-00 0.00 0.0 30 ! not fo
19-03 C SECPHO C+ ELECTR 2.60E+02 0.00 0.0 30 ! Heays
19-03 CH SECPHO CH+ ELECTR 5.80E+02 0.00 0.0 30 ! Heays
21-05 CH2 SECPHO CH2+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
19-03 CH3 SECPHO CH3+ ELECTR 3.80E+02 0.00 0.0 30 ! Heays
19-03 CH4 SECPHO CH4+ ELECTR 2.20E+01 0.00 0.0 30 ! Heays
19-03 C2 SECPHO C2+ ELECTR 2.50E+02 0.00 0.0 30 ! Heays
21-05 C2H SECPHO C2H+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
19-03 C2H2 SECPHO C2H2+ ELECTR 3.80E+02 0.00 0.0 30 ! Heays
21-05 C3 SECPHO C3+ ELECTR 8.90E+01 0.00 0.0 30 ! Heays
21-05 C3H SECPHO C3H+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
21-05 C3H2 SECPHO C3H2+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
21-05 O SECPHO O+ ELECTR 2.70E+00 0.00 0.0 30 ! Heays
21-05 OH SECPHO OH+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
19-03 H2O SECPHO H2O+ ELECTR 2.30E+01 0.00 0.0 30 ! Heays
19-03 O2 SECPHO O2+ ELECTR 2.80E+01 0.00 0.0 30 ! Heays
19-03 CO SECPHO CO+ ELECTR 1.40E+01 0.00 0.0 30 ! Heays
21-05 HCO SECPHO HCO+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
19-03 H2CO SECPHO H2CO+ ELECTR 2.90E+02 0.00 0.0 30 ! Heays
19-03 CH3OH SECPHO CH3OH+ ELECTR 2.40E+02 0.00 0.0 30 ! Heays
21-05 N SECPHO N+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays
19-03 NH SECPHO NH+ ELECTR 7.10E+00 0.00 0.0 30 ! Heays
19-03 NH2 SECPHO NH2+ ELECTR 1.40E+02 0.00 0.0 30 ! Heays
19-03 NH3 SECPHO NH3+ ELECTR 2.20E+02 0.00 0.0 30 ! Heays
21-05 N2 SECPHO N2+ ELECTR 0.00E-00 0.00 0.0 30 ! Heays

```

headers

modification date

list of reactions

rate parameters

comments & references

Advices to run models













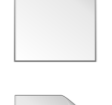



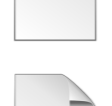

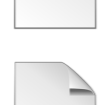



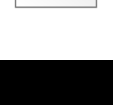

1. never modify the file `input_mhd.in`
create a new input file with understandable name
e.g. `input_pshk_n1p3_r1p0_z5m17.in`
`./mhd_vode input/input_pshk_n1p3_r1p0_z1m17.in`
2. use the same terminology for output directory
e.g. `pshk_n1p3_r1p0_z5m17`

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outputs and plot routines

pshk_n1p3_r1p0_z5m17

	<code>energetics.out</code>		local energy fluxes
	<code>pshk_..._c.hdf5</code>		for chemistry analyser tool
	<code>pshk_..._s.hdf5</code>		for IDAT tool
	<code>H2_lev.out</code>		local abundances of H ₂ lev
	<code>h2levels.out</code>		final abundances of H ₂ lev
	<code>info_mhd.out</code>		information on the run
	<code>intensity.out</code>		lines intensities
	<code>mhd_coldens.out</code>		column density profiles
	<code>mhd_phys.out</code>		local physical variables
	<code>mhd_speci.out</code>		local species abundances
	<code>species.out</code>		final species abundances
	<code>thermal_balance.out</code>		heating / cooling rates

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 *output/*

 *python_plot*

 *mono_panel*



single panel plot routines

 *mult_panel*



multi panels plot routines

 *README.txt*



notice to use the routines

- go in the results directory and run a script

the scripts use the output files found in the current directory

```
python ../python_plots/mono_panel/script_plot_temp.py
```

- simple routines for beginners

33 scripts available

interactive plot or pdf files

change main axis and range

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Advices to run models

1. never modify the file `input_mhd.in`
create a new input file with understandable name
e.g. input_pshk_n1p3_r1p0_z5m17.in
`./mhd_vode input/input_pshk_n1p3_r1p0_z1m17.in`
2. use the same terminology for output directory
e.g. pshk_n1p3_r1p0_z5m17
3. when running a shock, copy outputs of the preshock run
species.out and *h2levels.out*
in the `input/` directory and use them as input files for the run
`cp output/pshk_n1p3_r1p0_z5m17/species.out`
`input/species_pshk_n1p3_r1p0_z5m17.in`

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SERVICES

Grid of models

- o accessible online through the ISM database **ISMDB**
- o contains 4538 models (~14000 models « soon »)

$$10^2 \text{ cm}^{-3} \leq n_{\text{H}} \leq 10^8 \text{ cm}^{-3}$$

$$0.1 \leq b \leq 10$$

$$10^{-17} \text{ s}^{-1} \leq \zeta_{\text{H}_2} \leq 10^{-15} \text{ s}^{-1}$$

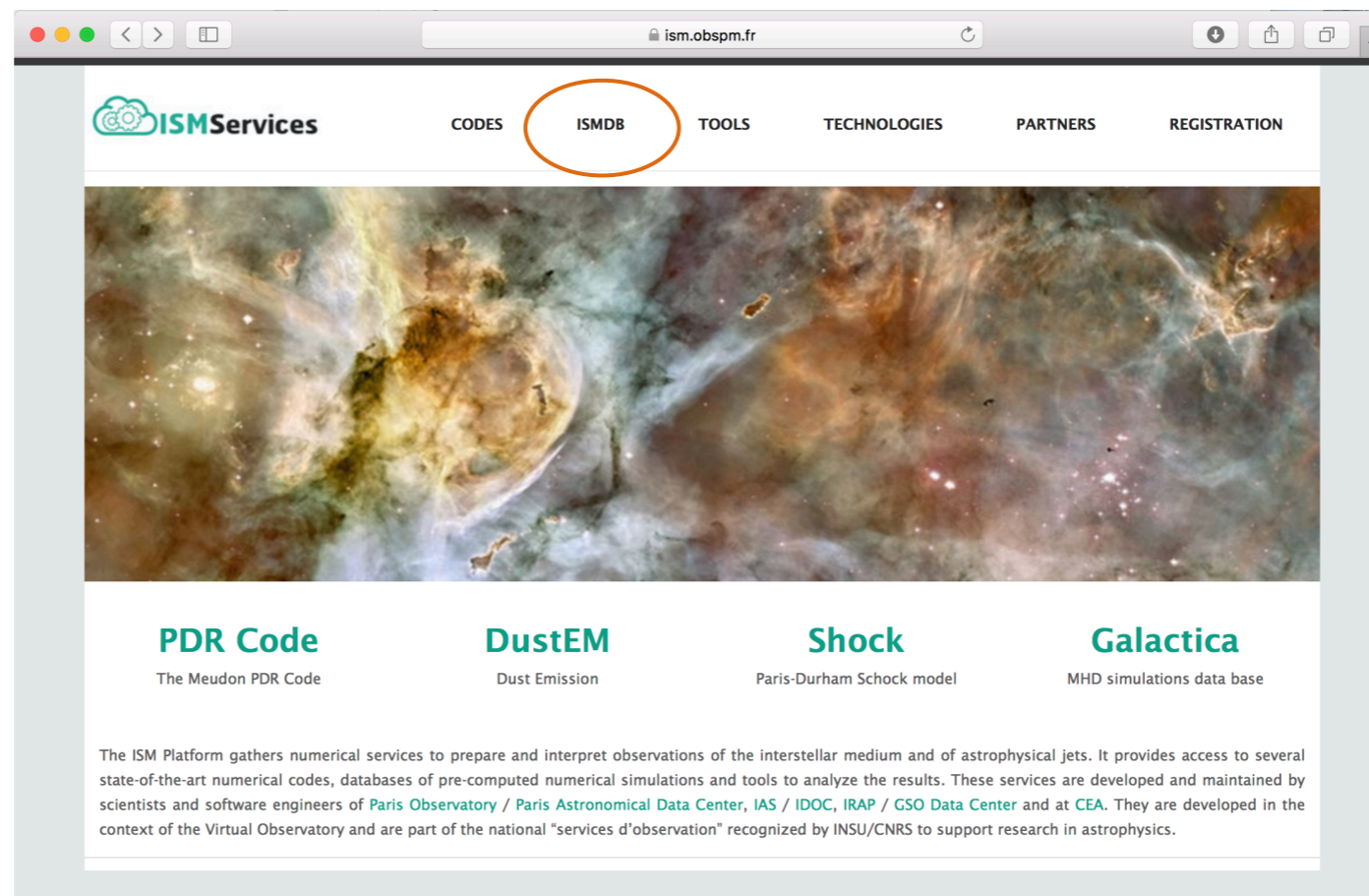
$$2 \text{ km s}^{-1} \leq V_{\text{s}} \leq 90 \text{ km s}^{-1}$$

$$0 \leq G_0 \leq 10^3$$

$$x(\text{PAH}) = 10^{-8}$$

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The screenshot shows a web browser window with the URL ism.obspm.fr. The website header includes the logo for ISMServices and a navigation menu with the following items: CODES, ISMDB (circled in orange), TOOLS, TECHNOLOGIES, PARTNERS, and REGISTRATION. Below the navigation menu is a large image of a colorful interstellar nebula. Underneath the image, there are four service cards: PDR Code (The Meudon PDR Code), DustEM (Dust Emission), Shock (Paris-Durham Shock model), and Galactica (MHD simulations data base). At the bottom of the page, there is a paragraph of text describing the ISM Platform's mission and the institutions involved in its development.

Extraction and analysis tools

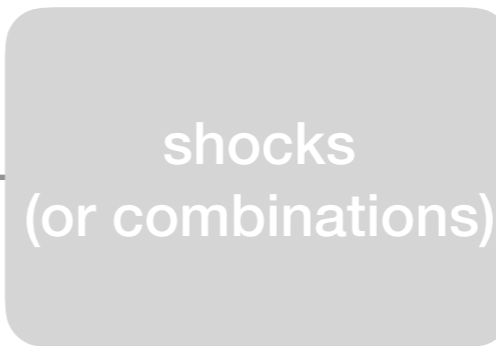
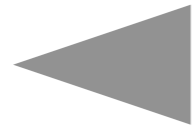
- IDAT (works with the ..._s.hdf5 files)
 - build for all the models of the ISM platform
 - can be used in interactive mode or in command line
 - allows to build your own ascii files
 - allows to make interactive plots
 - works within **ISMDB**
- chemistry analyser (works with the ..._c.hdf5 files)
 - build for all the models of the ISM platform
 - find the main chemical formation & destruction routes of any species
 - provide the local chemical rates
 - follow up versions in progress
 - not implemented in **ISMDB** yet

Outline

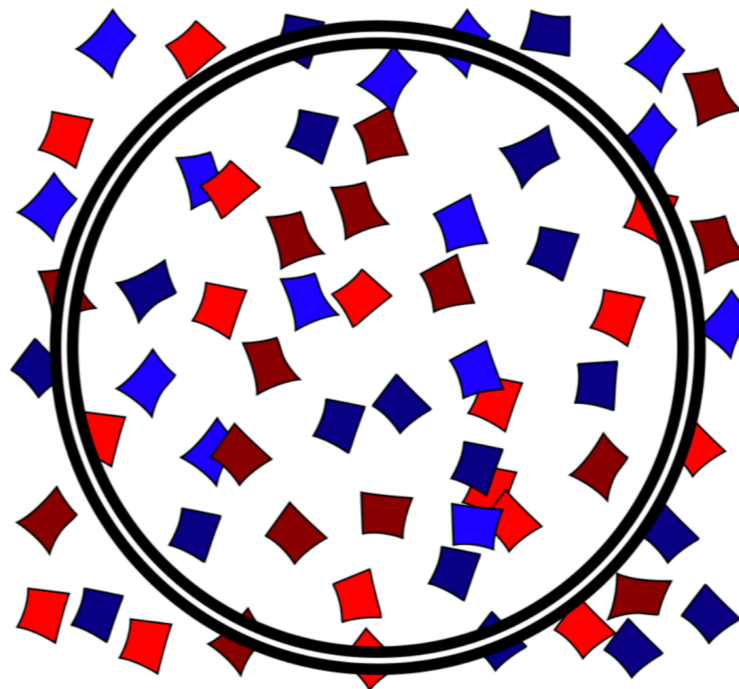
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LVG postprocessing tool
(not available yet)

observer



background or not
(extended or not)

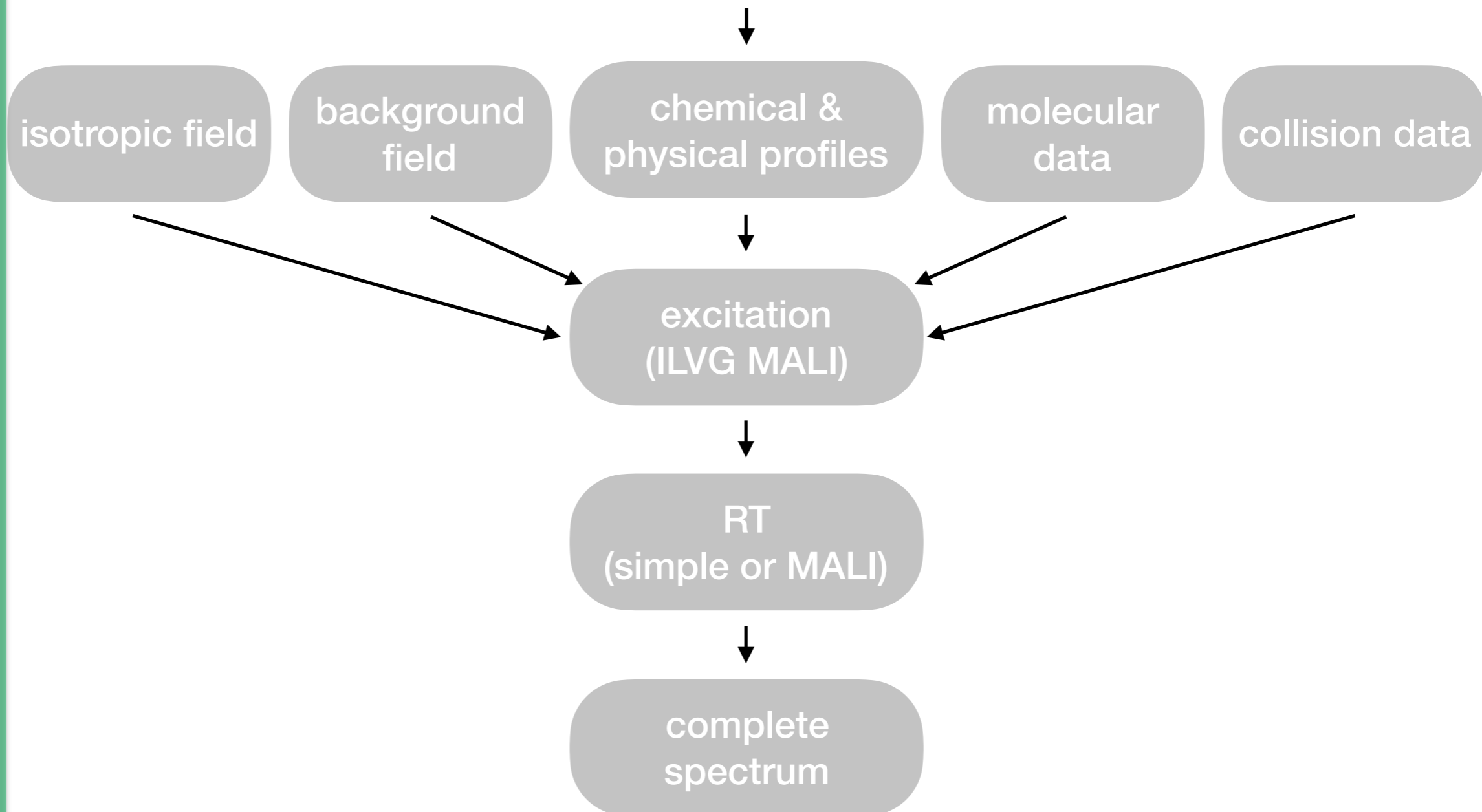


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Postprocessing

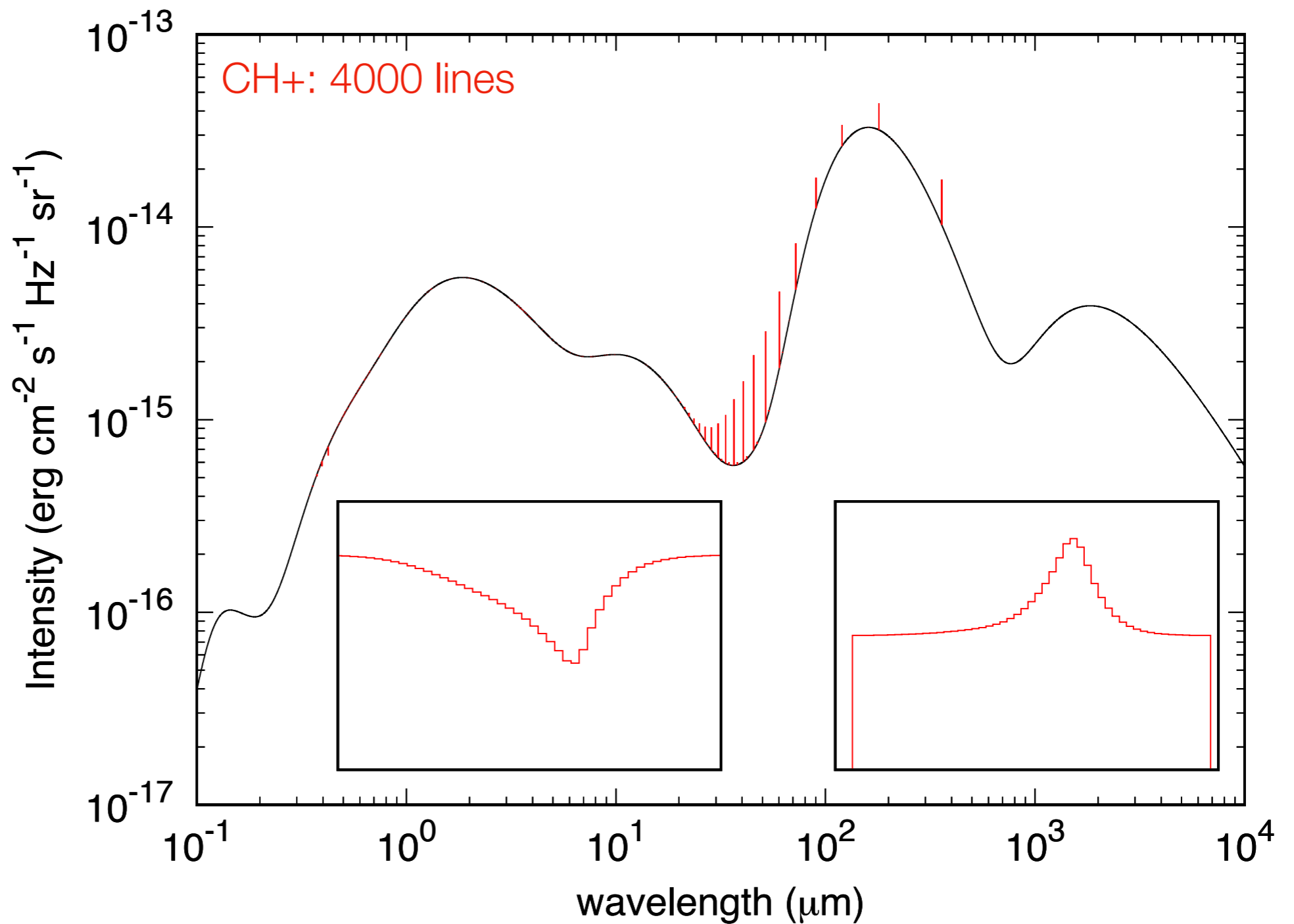
```
postprocess.in
Not registered
slab%pop
Done
~/Travail/Codes-Chimie/Shock_svn/LVG_postprocess/postprocess.in
1 /Users/godard/Travail/Codes-Chimie/Shock_svn/1.1/AnalysisTools/extractor/ ! pat
2 /Users/godard/Travail/Codes-Chimie/Shock_svn/grid_results_paper2020/shock/hdf5/ ! pat
3 mhd_n1p4r1p3z1p1q1m6v1p0p1b1p0_pump1_s ! hdf
4 H2 ! spe
5 50 ! num
6 2.00E-00 ! tur
7 0.0 ! ang
8
```



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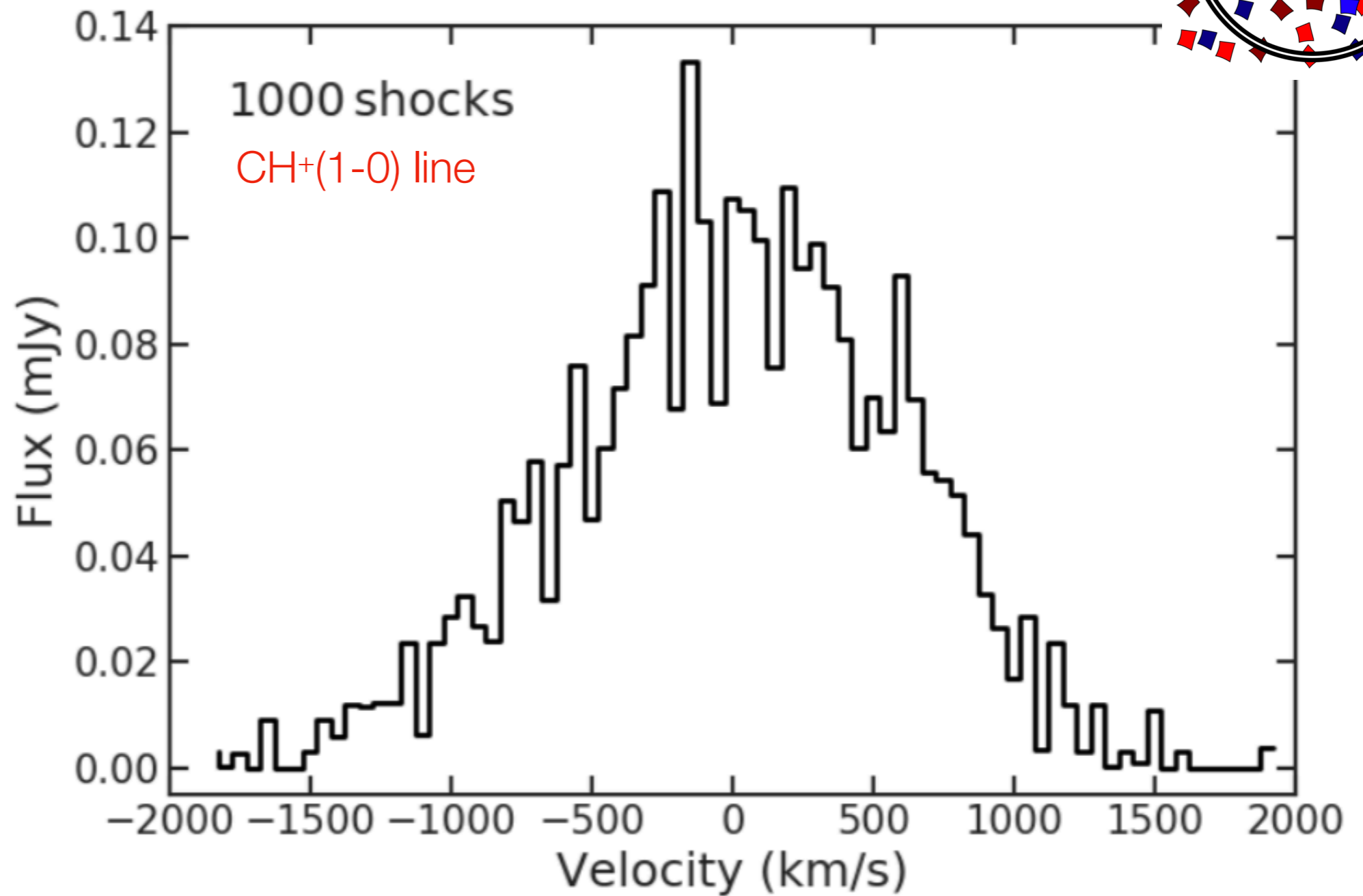
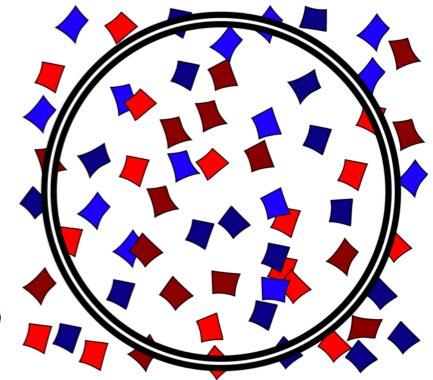
signature of a single shock



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signature of a combination of shocks



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Postprocessing

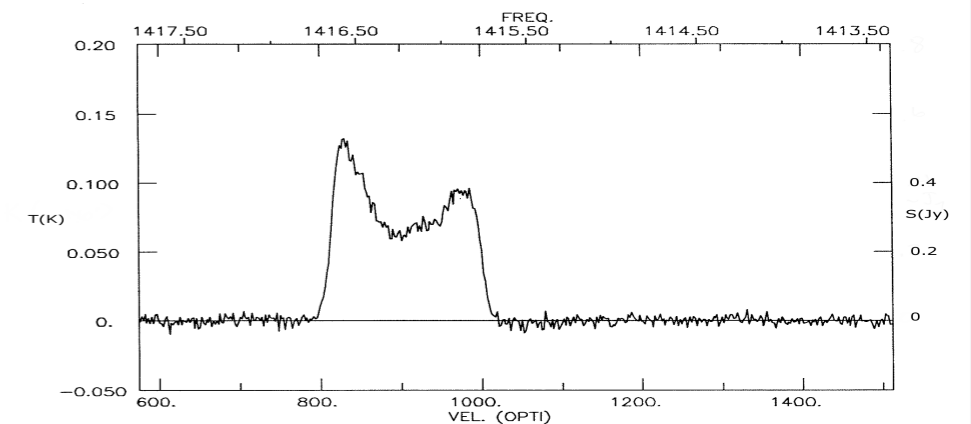
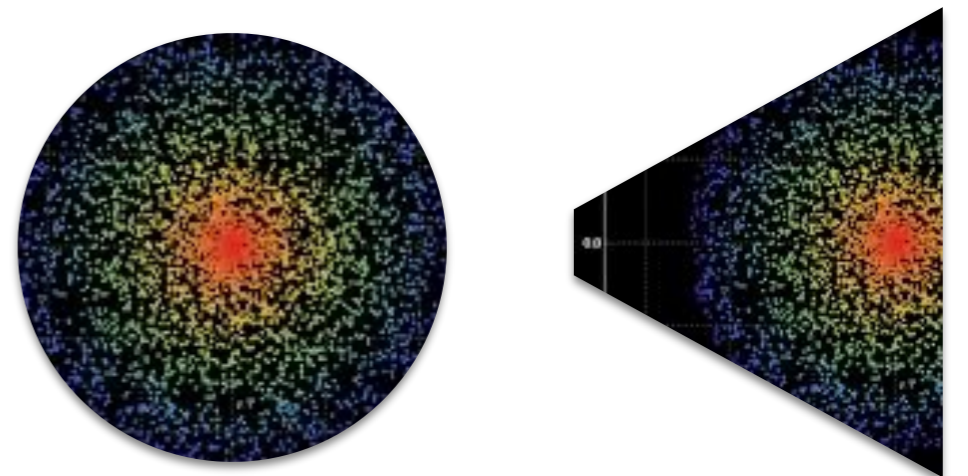
In progress

- test known scenarios
- distribution of structures
- implement MALI RT
- increase database
done: H, H₂, CO, CH⁺, SiO

Pending

- include instrument properties
- build an interactive tool

beam panel



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CONCLUSIONS

In a nutshell

- public code
- thermochemical structures of plane parallel shock at steady state
- variety of environments
 - diffuse / dense gas
 - irradiated or not by an external UV field
- living code developed by generations
 - v1.2 soon available
 - online services (plot & analysis tools, grid of models)
 - services in development (LVG postprocessing)

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