The Meudon PDR code

Astrosim School

July 2017

Fortran code

- developed over 30 years
- several versions
- public access
  www.ism.obspm.fr
- services in progress

Programmers

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Franck Le Petit

Emeric Bron

Benjamin Godard

Goals

- chemical structure of interstellar clouds
- interactions with photons and cosmic rays
- treat detailed microphysical processes
- analyse their couplings
- interpret observations

Lecture description

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

1. Introduction on PDRs
2. Assumptions
3. User Guide - first steps
4. Examples

Lecture description

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1. Introduction on PDRs
2. Assumptions
3. User Guide - first steps
4. Examples
5. Physics & algorithms
6. Applications
7. Recent updates
8. Conclusions

Definition

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- introduction on PDRs
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PDR

- Photon Dominated Regions

or

- Photodissociation Regions

⇒ Interstellar environment where the FUV radiation impacts the chemical / thermal state and evolution of the gas and dust

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PDR

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☑ Photodissociation Regions

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Physical properties

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FUV photons

- 6 eV — 13.6 eV

impacts

- heating source
  dust - IR emission
  gas - photoelectric effect
- photodissociation / ionization
- excitation / pumping

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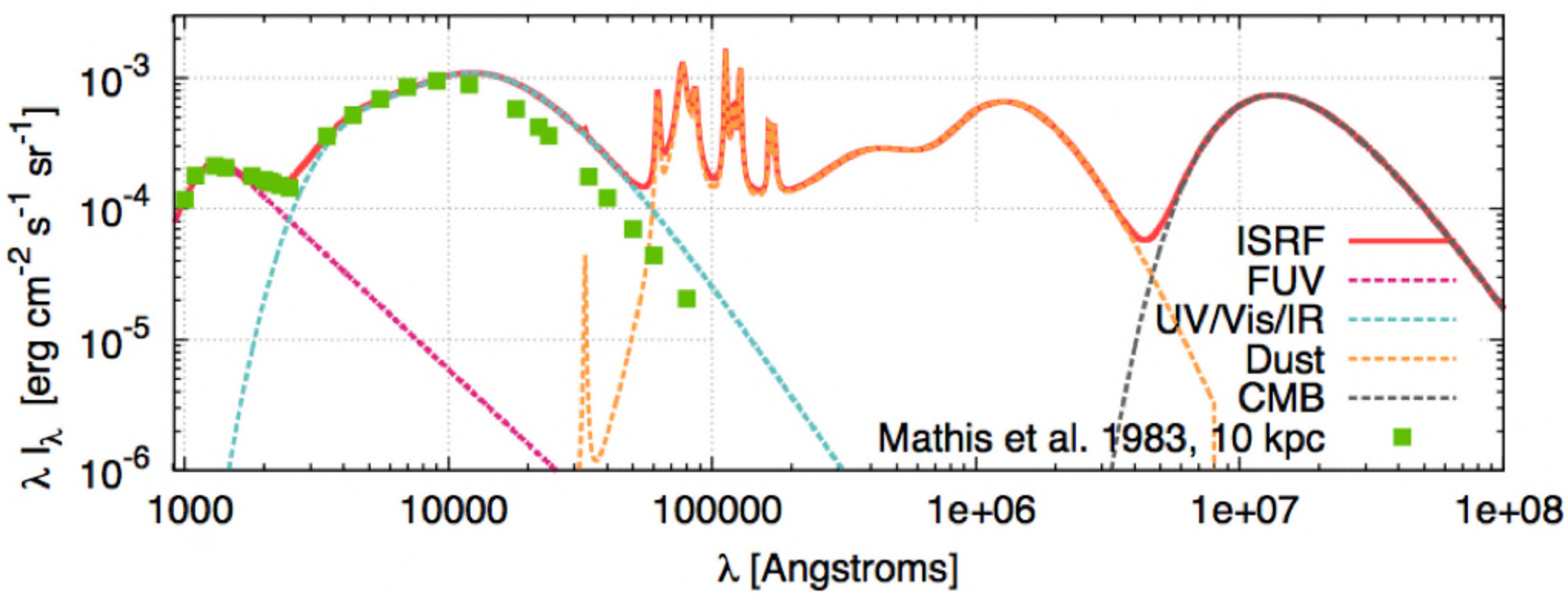

Physical properties

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FUV photons

- 6 eV — 13.6 eV
- ISRF - Mathis et al. (1983)
  flux: 1.6×10^{-3} erg cm^{-2} s^{-1}
- often parametrized with G_0

impacts

- heating source
  dust - IR emission
  gas - photoelectric effect
- photodissociation / ionization
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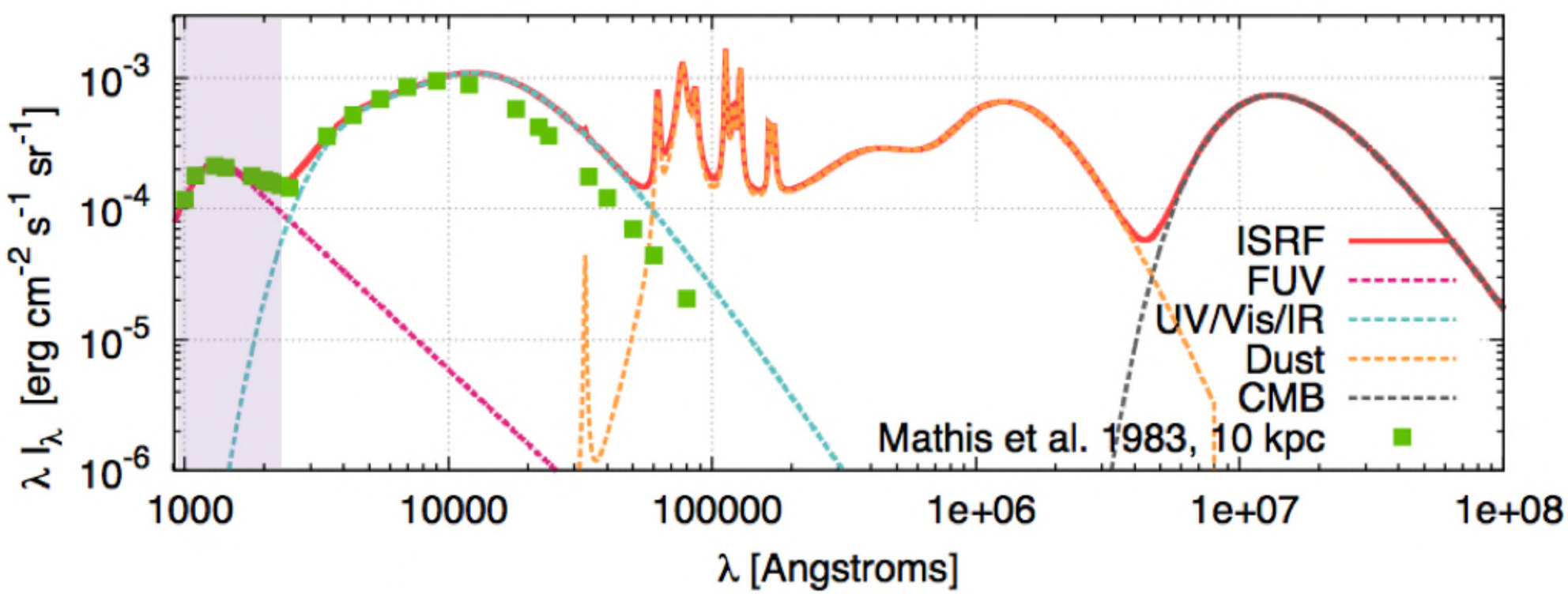

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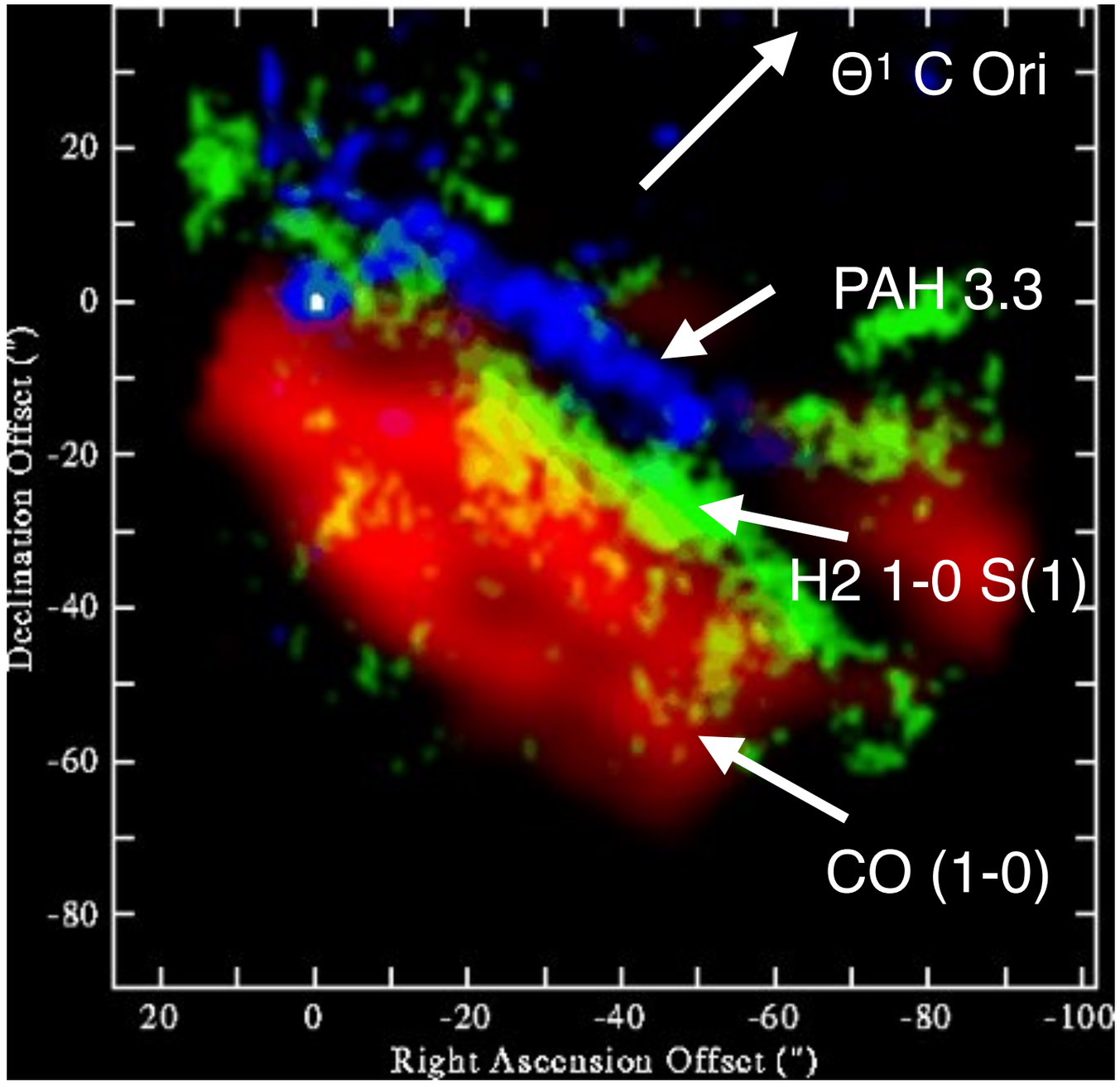

Tielens, Meixner, et al. (1993)

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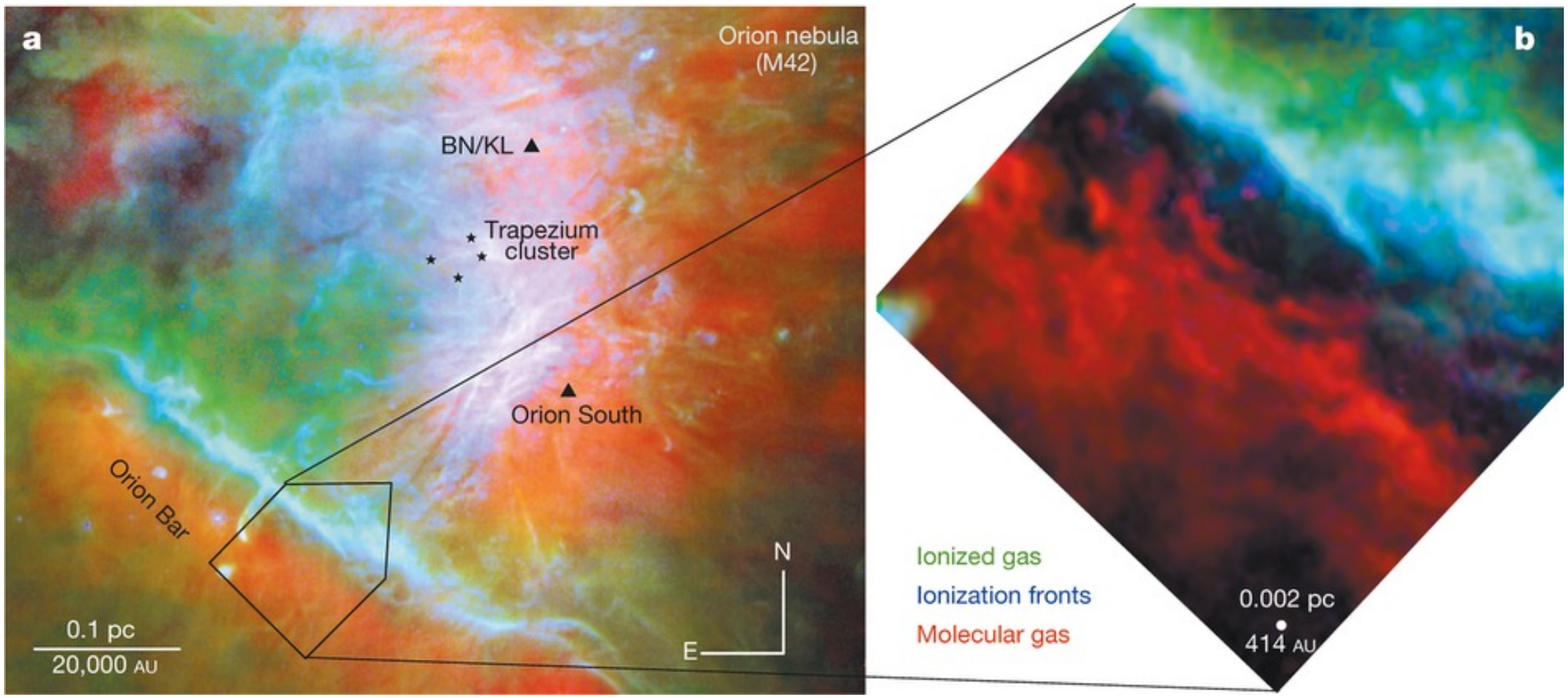

Goicoechea et al. (2016)

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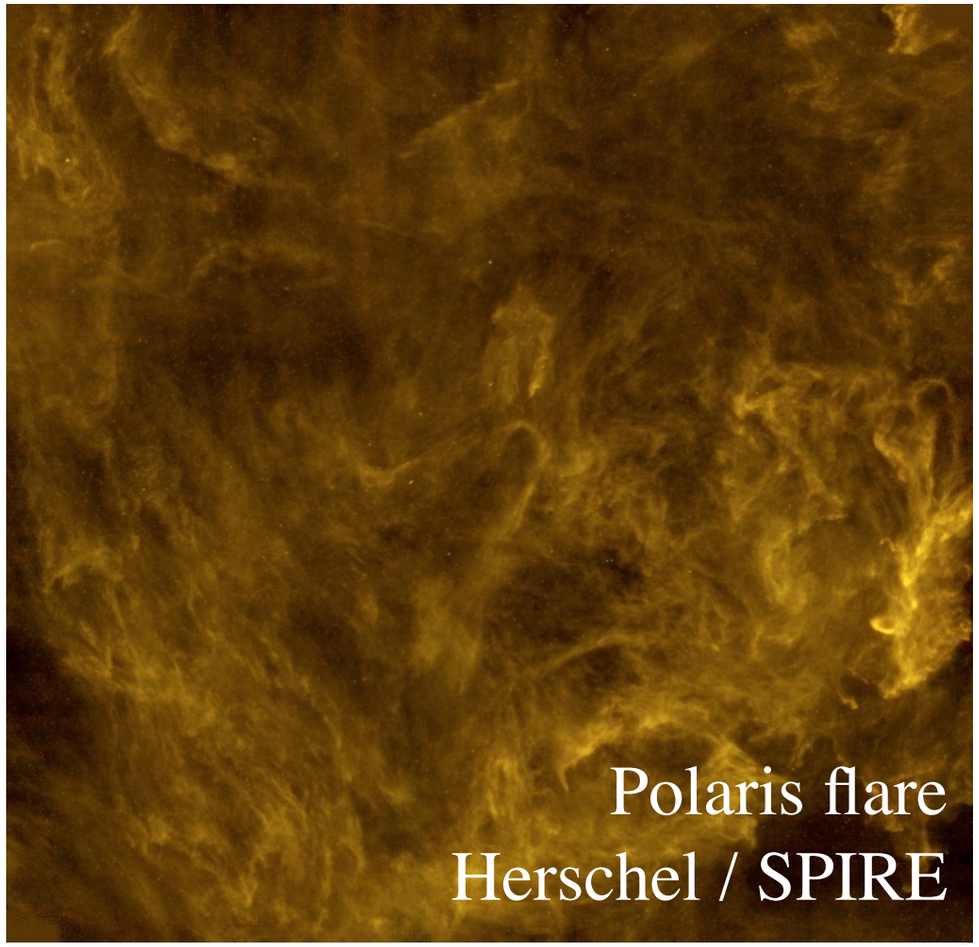
Examples

- Warm Neutral Medium
- Diffuse clouds
- star forming regions
- Reflection nebulae
- Neutral gas around PN
- Photodiss winds from red giants and AGB
- Protoplanetary disks



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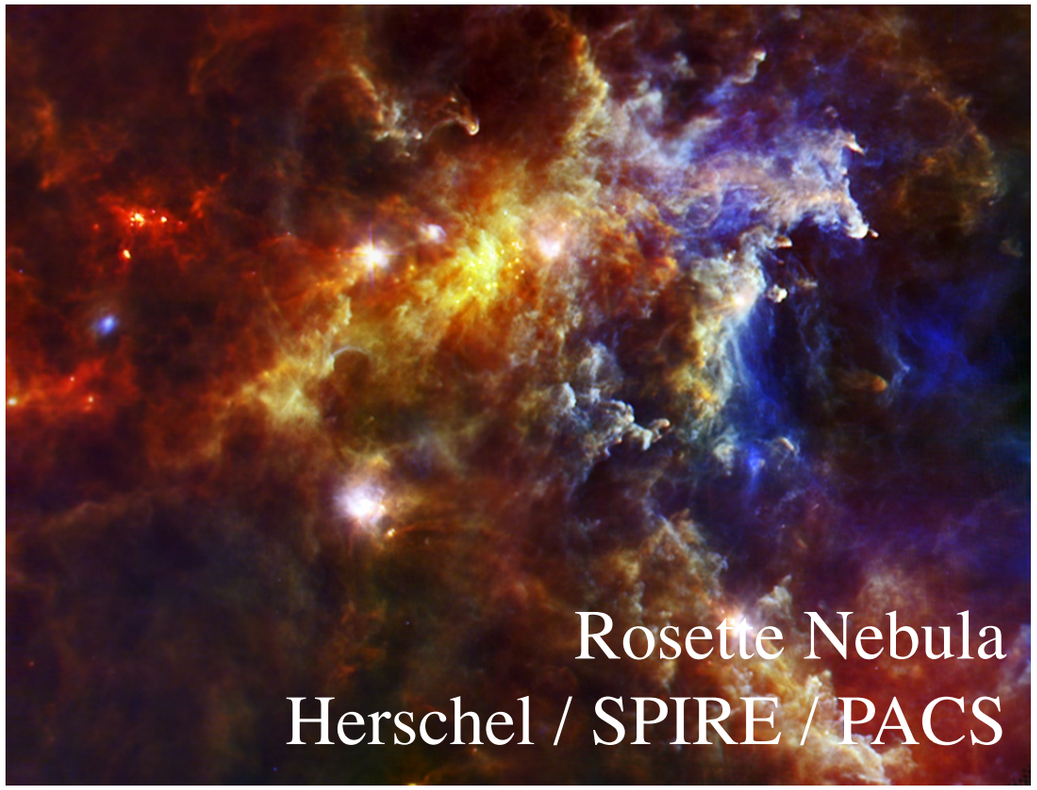

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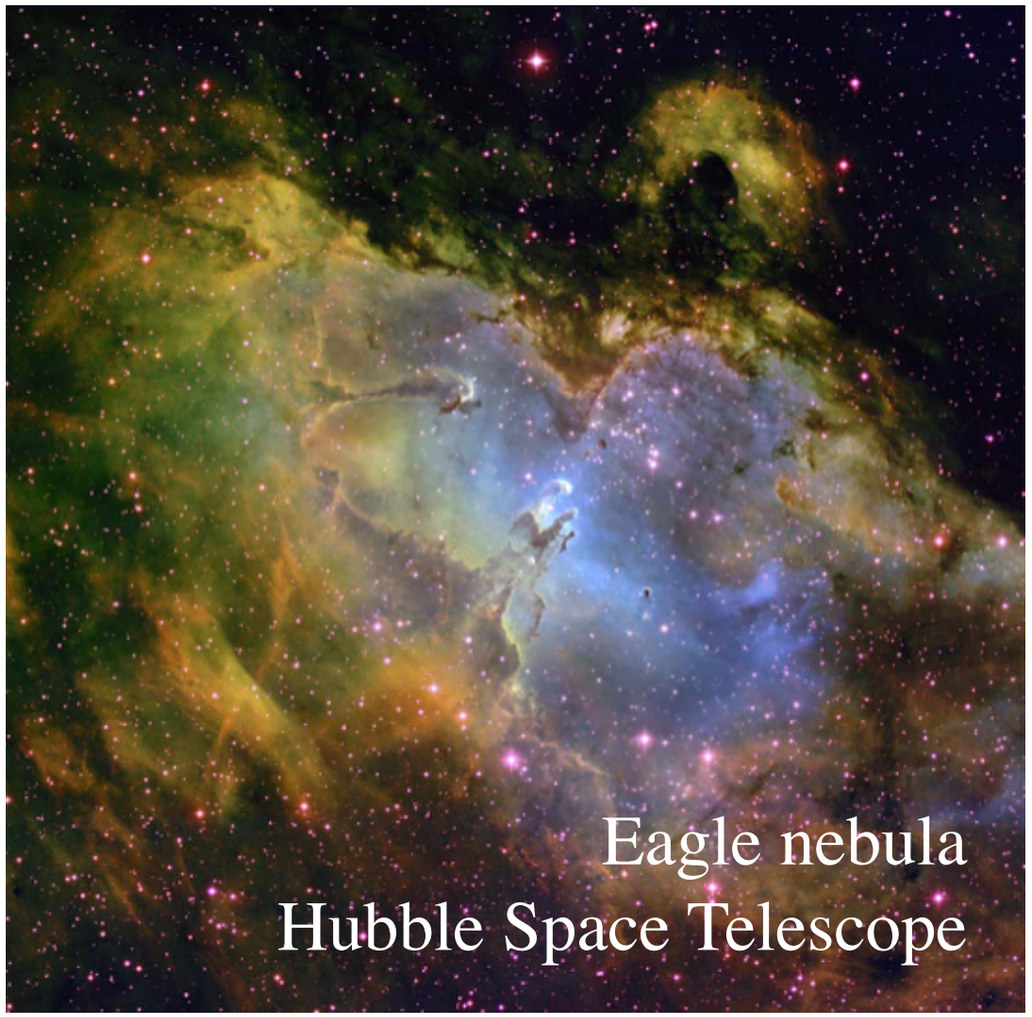

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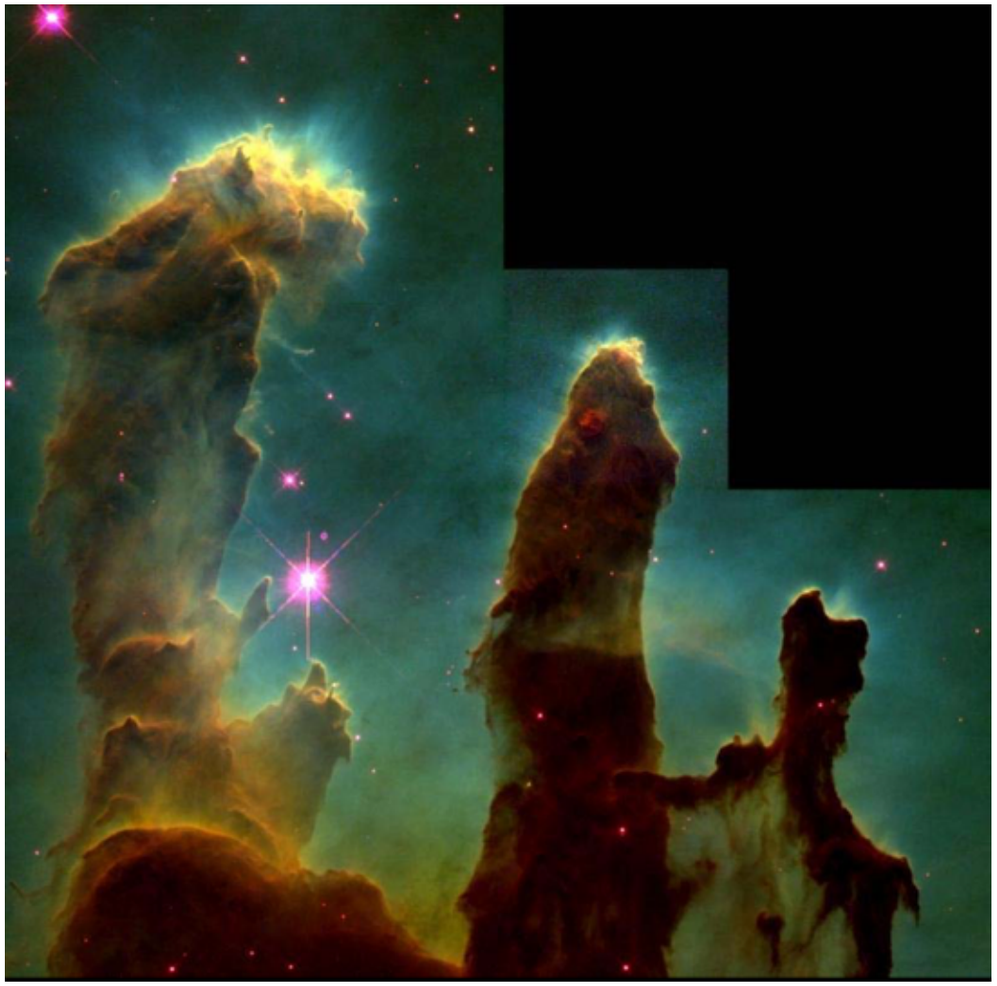

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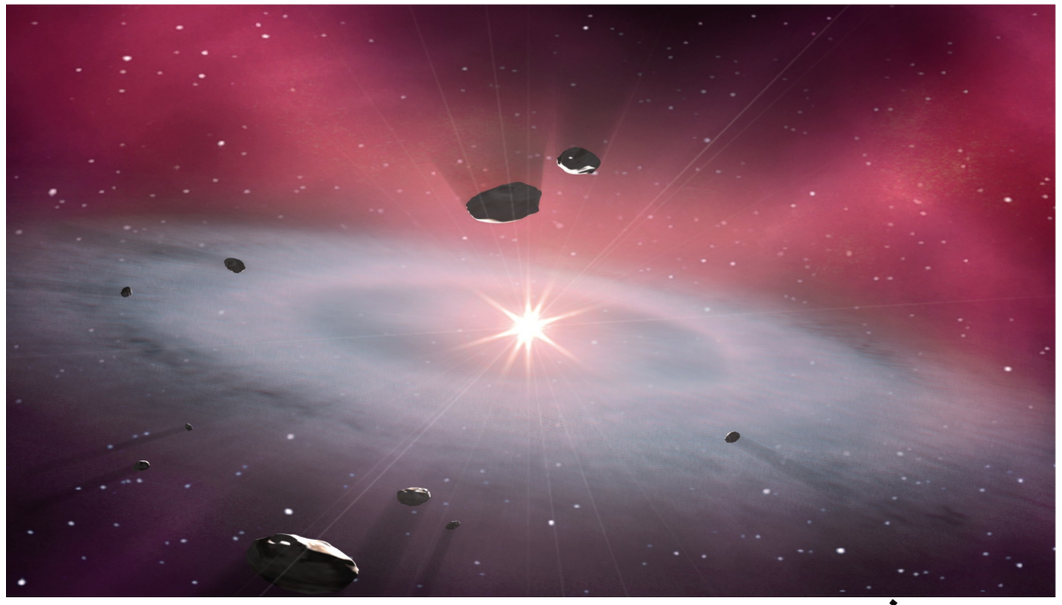

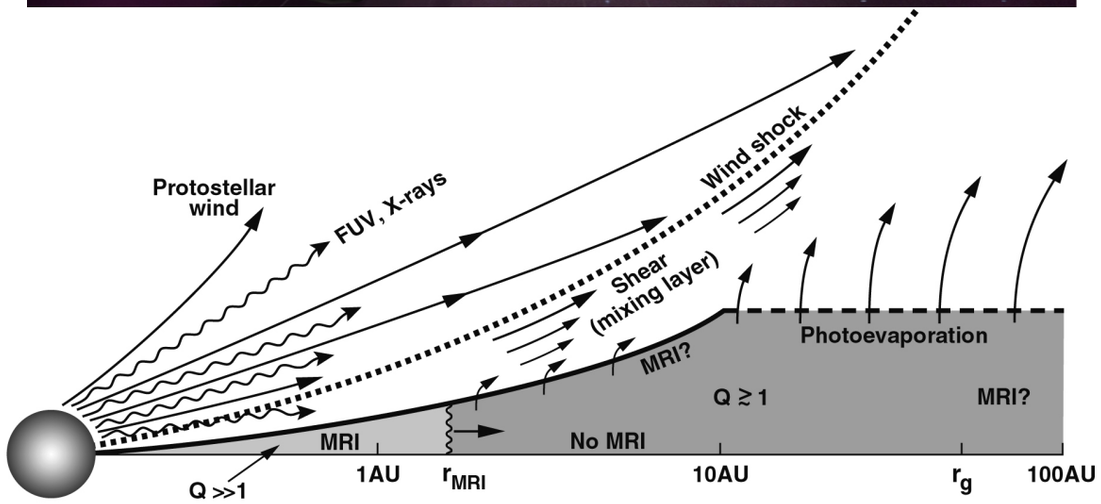

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Why studying PDRs ?

- most of interstellar matter in PDRs
- physics of PDRs
  - ✓ thermal instability → CNM / WNM
  - ✓ ionization → coupling with B
  - ✓ dust charge → dynamics
- emission of PDR
  - ✓ PAH & grain → large fraction of IR photons
  - ✓ C^+, O, H_2, CO, … → physical conditions
  - ✓ stratification → geometry of sources
- study of extragalactic environments

Fluid equations

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chemical mixture
mono fluid, no B

$$\frac{Dn_s}{Dt} = \frac{\partial n_s}{\partial t} + (\mathbf{u} \cdot \nabla)\, n_s = -n_s \nabla \cdot \mathbf{u} + F_s - D_s - \nabla \frac{1}{m_s} \mathbf{j_s}$$

$$\frac{D\mathbf{u}}{Dt} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\, \mathbf{u} = -\nabla V - \frac{1}{\rho} \nabla P + \frac{1}{\rho} \nabla \cdot \pi$$

$$\frac{D\varepsilon}{Dt} = \frac{\partial \varepsilon}{\partial t} + (\mathbf{u} \cdot \nabla)\, \varepsilon = -\frac{P}{\rho} \nabla \cdot \mathbf{u} + \frac{1}{\rho} \left(\Gamma_{\mathrm{vis}} + \Gamma - \Lambda\right) - \frac{1}{\rho} \nabla \cdot \mathbf{C}$$

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- - advection

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- - advection - - compression

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advection compression thermo-chemistry

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advection — compression — thermo-chemistry — diffusion

Simplifications

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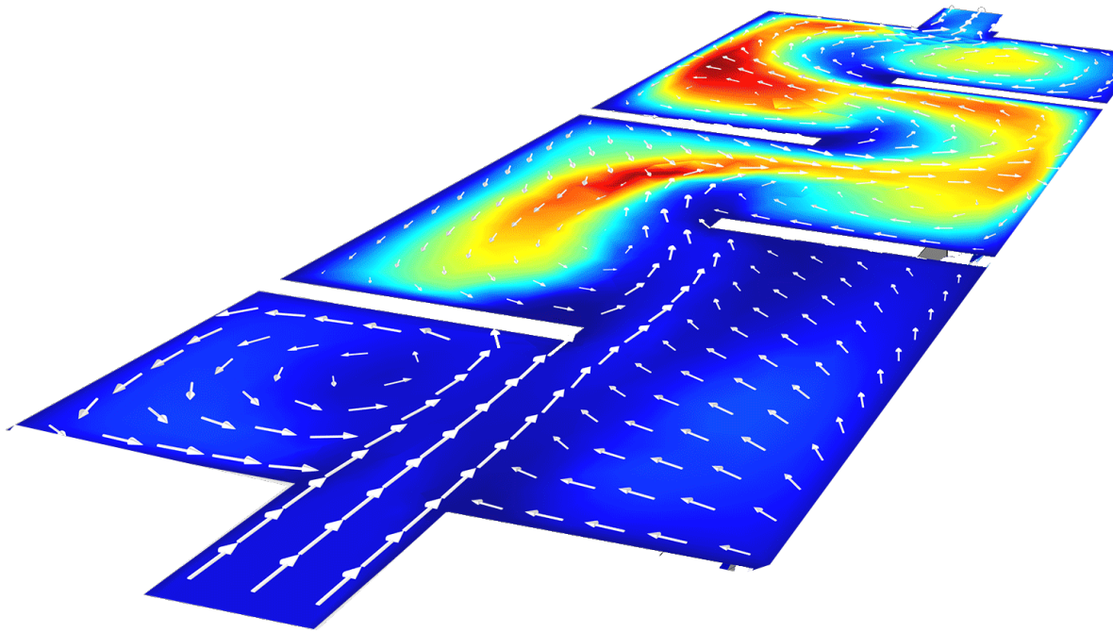
In a perfect world → 3D, diffusive, with radiative transfer

$$\frac{Dn_s}{Dt} = \frac{\partial n_s}{\partial t} + (\mathbf{u} \cdot \nabla)\, n_s = -n_s \nabla \cdot \mathbf{u} + F_s - D_s - \nabla \frac{1}{m_s} \mathbf{j_s}$$

Main simplifications



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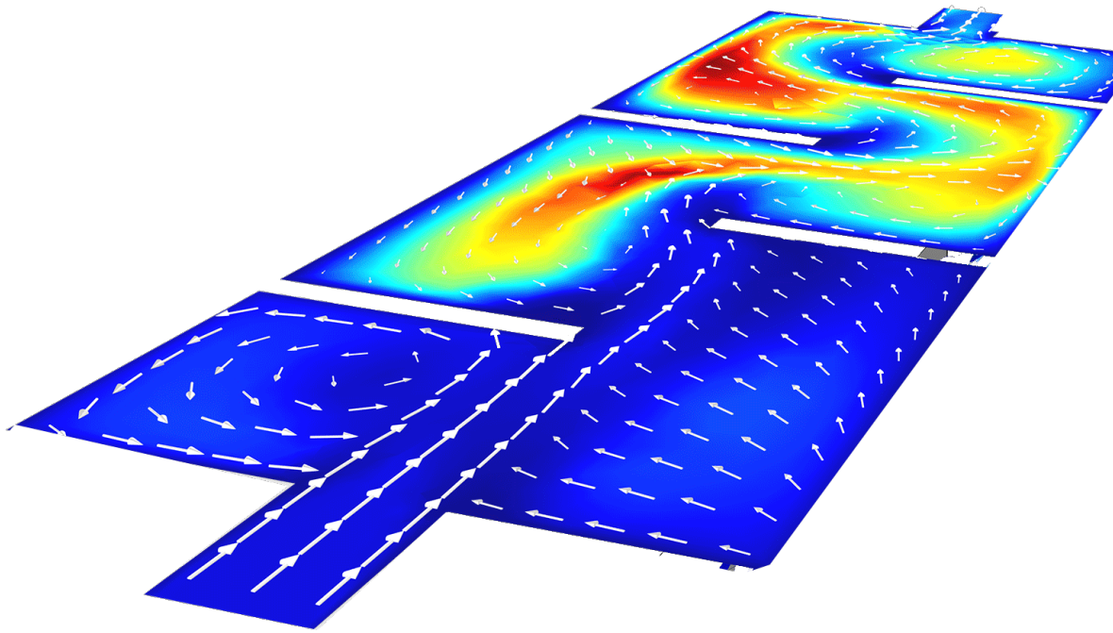
Main simplifications

- number of spatial dimensions (2D, 1D, 0D)



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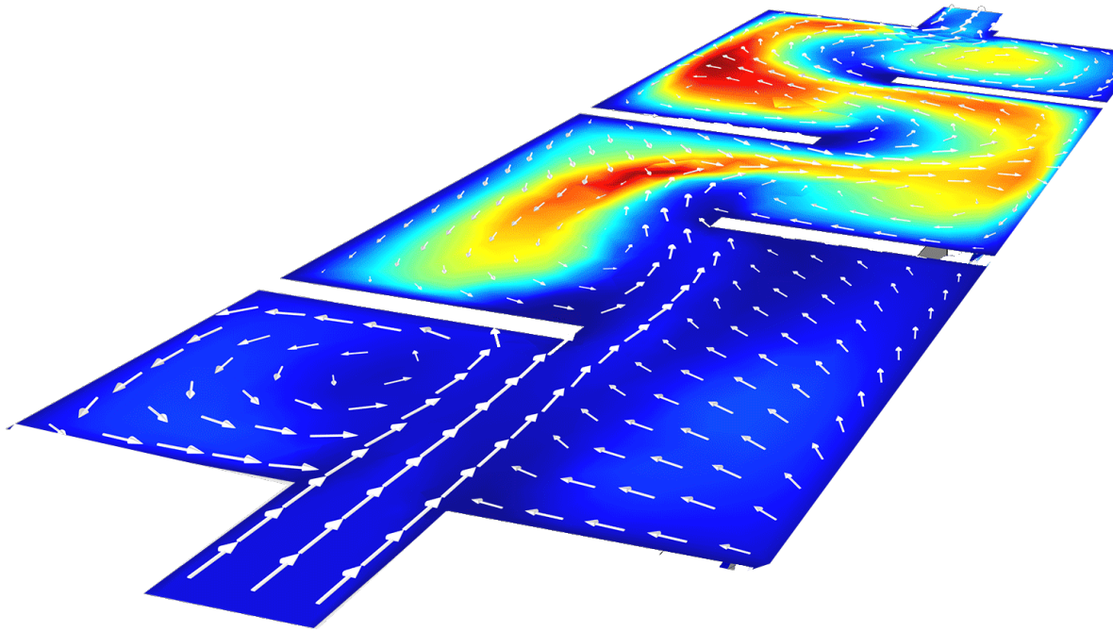
Main simplifications

- number of spatial dimensions (2D, 1D, 0D)
- neglect diffusion



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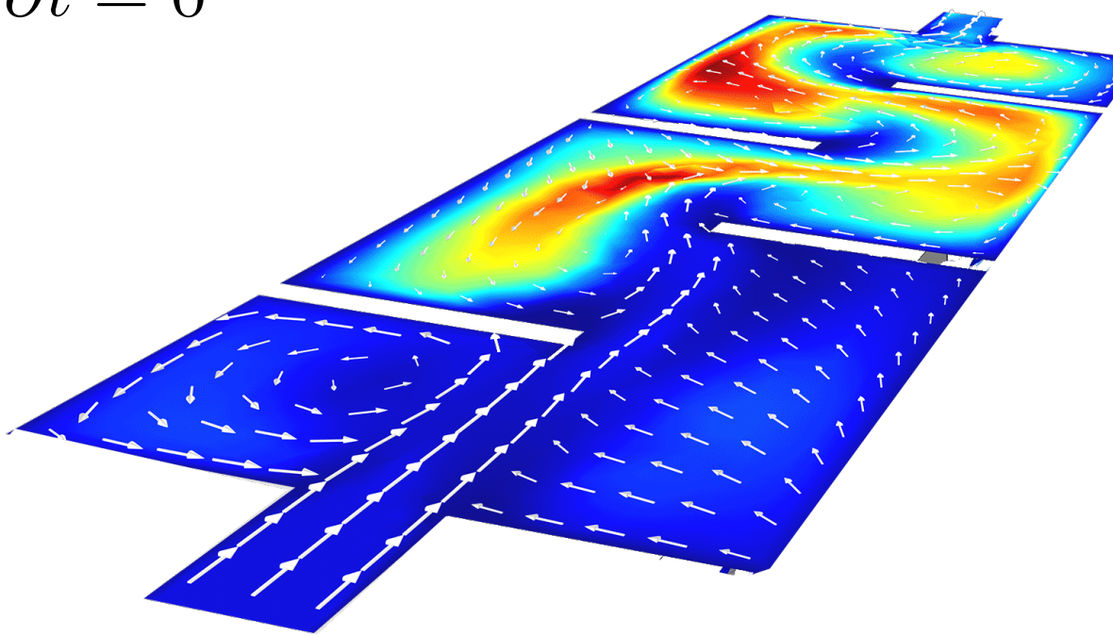
- neglect diffusion
- steady-state (stationary) $\partial/\partial t = 0$



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In a perfect world → 3D, diffusive, with radiative transfer

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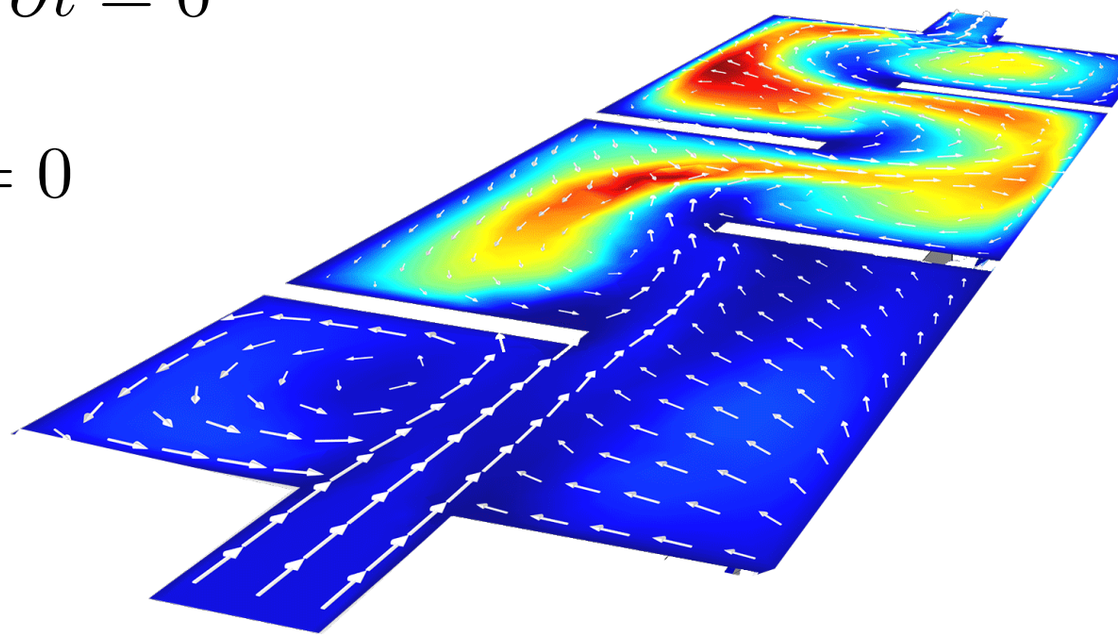
Main simplifications

- number of spatial dimensions (2D, 1D, 0D)
- neglect diffusion
- steady-state (stationary) $\partial/\partial t = 0$
- static (equilibrium) $D/Dt = 0$

⚠ $\frac{\partial}{\partial t} = 0 \neq \frac{D}{Dt} = 0$



Numerical codes

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	Nautilus	Meudon PXDR	CLOUDY	Paris-Durham shock	CHEMSES	RAMSES & KROME
dimension	0	1	1	1	3	3
dynamical				✓	✓	
thermal					✓	
chemical					✓	

static

steady

free

	NAHOON	TDR	MAPPING	ENZO	ZEUS	NIRVANA
dimension	0	1	1	3	3	3
dynamical		✓				✓
thermal				✓		✓
chemical						

✓ diffusion

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The Meudon PDR code

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The Meudon PDR code

- radiative transfer (UV to radio)
  gas and dust processes
- dust treatment
  charge, emissivities

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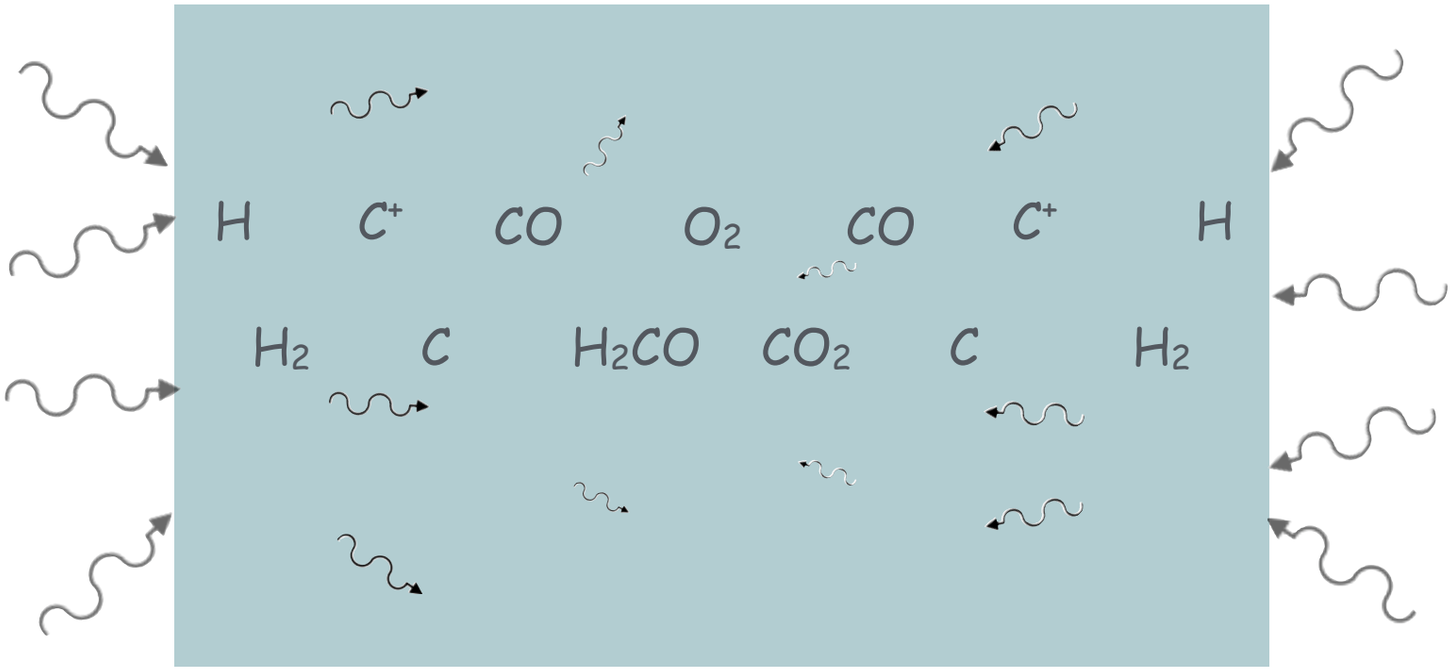

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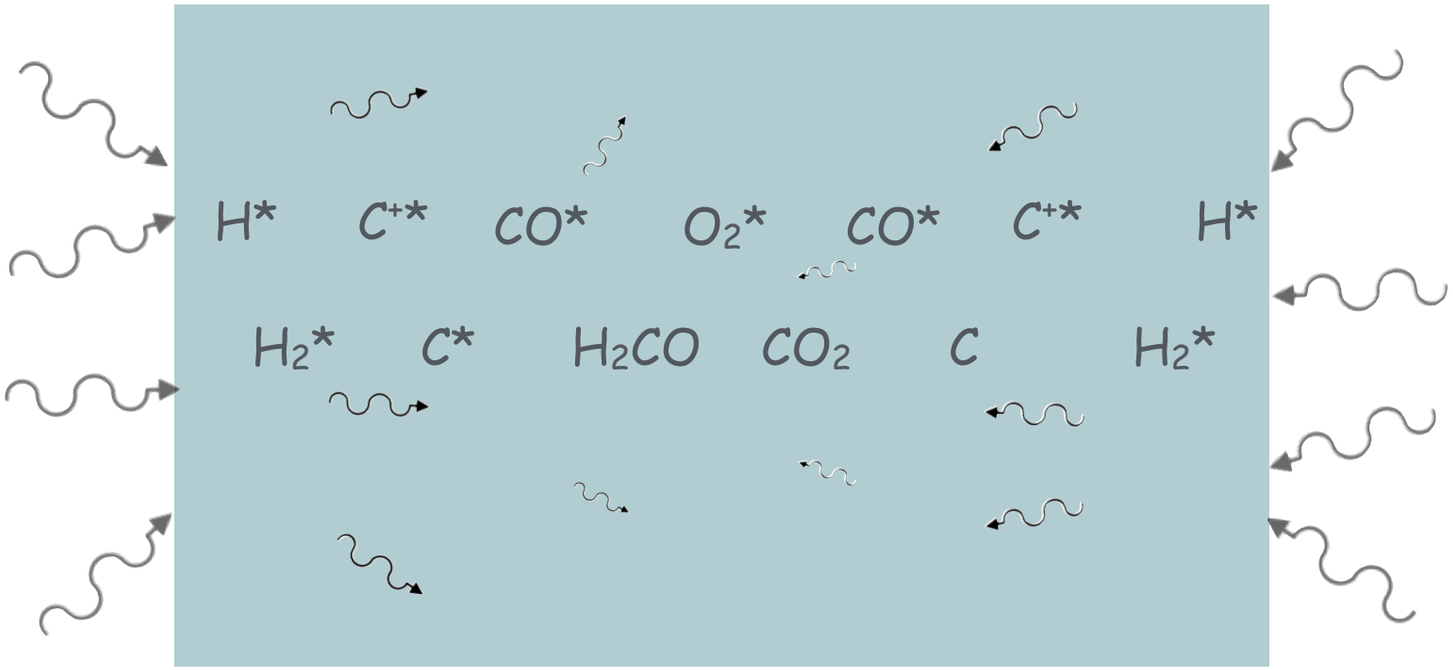

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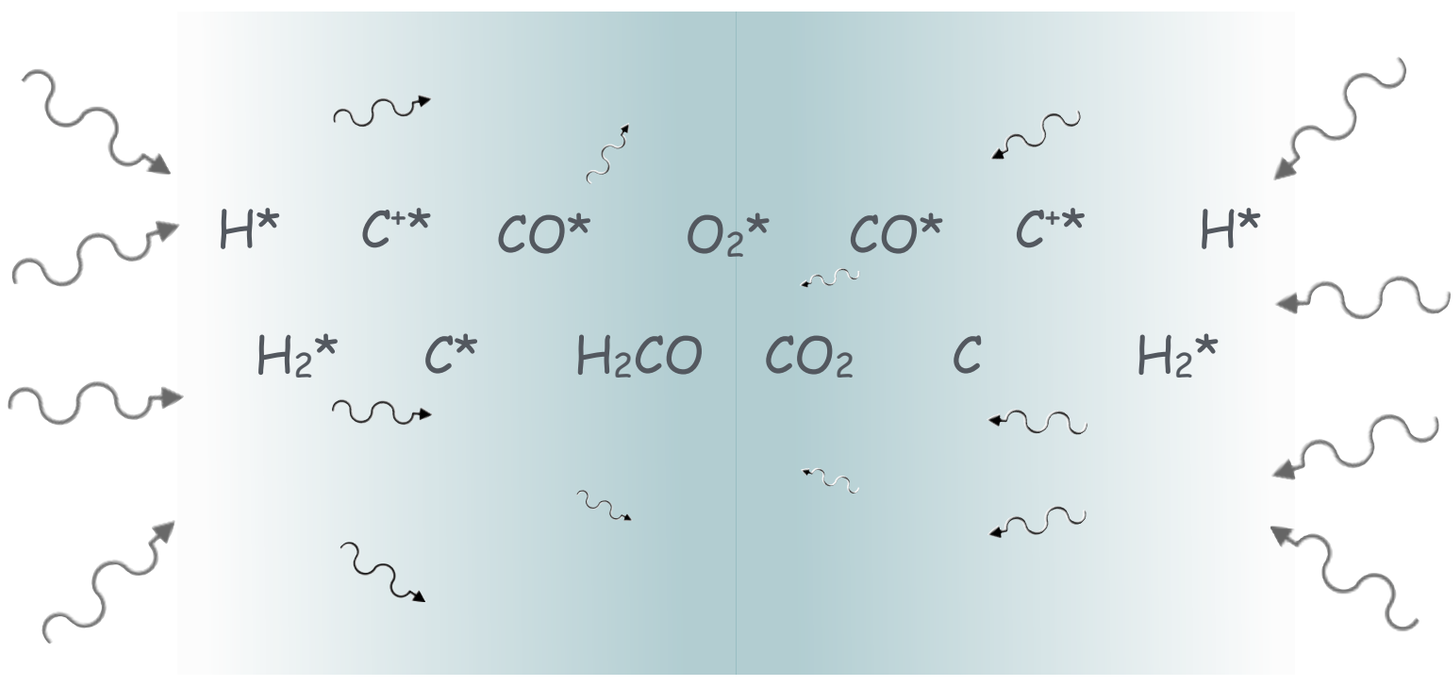

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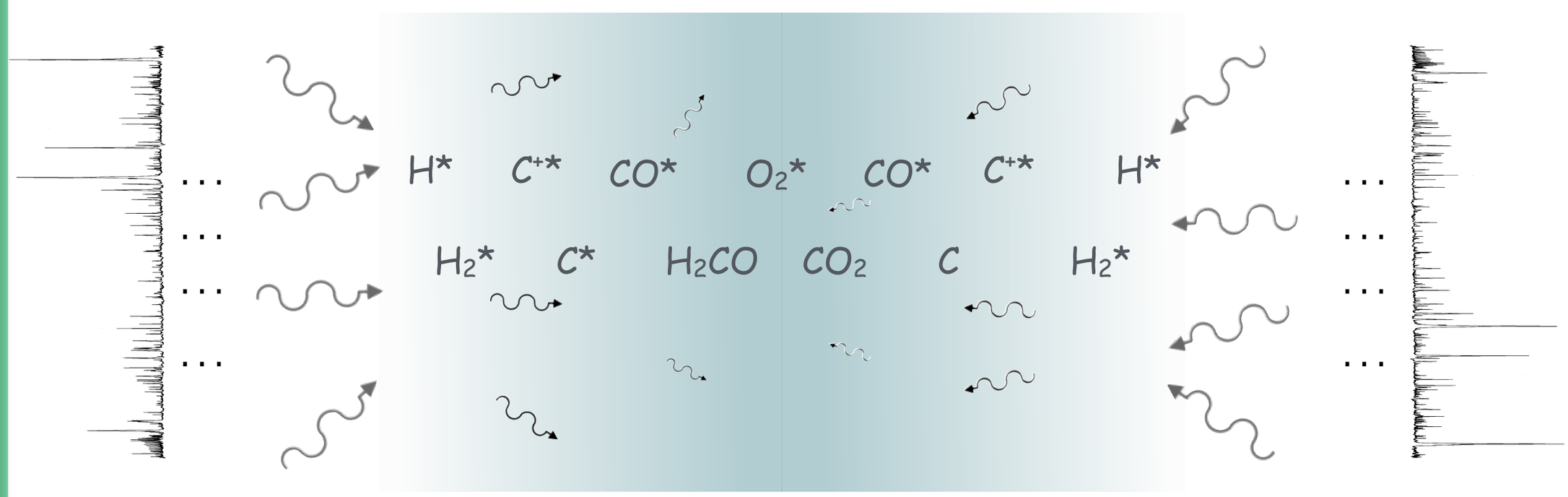
  charge, emissivities
- excitation (thousands levels)
- tens thousands lines



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Limitations : 1D static

- chemistry $\tau_{chem}^{i-n} \sim 3 \left(\frac{n_{\rm H}}{10^3\ {\rm cm}^{-3}}\right)^{-1}\ {\rm yr}$
- chemistry $\tau_{chem}^{n-n} \sim 300 \left(\frac{n_{\rm H}}{10^3\ {\rm cm}^{-3}}\right)^{-1}\ {\rm yr}$
- ionization $\tau_{\rm CR} \sim 0.03 - 3\ {\rm Gyr}$
- grains $\tau_{gr}^{\rm H_2} \sim 1 \left(\frac{n_{\rm H}}{10^3\ {\rm cm}^{-3}}\right)^{-1} \left(\frac{T}{50}\right)^{-1/2}\ {\rm Myr}$

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- free fall $\tau_{ff} \sim 0.14 \left(\frac{n_{\rm H}}{10^3\ {\rm cm}^{-3}}\right)^{-1/2}\ {\rm Myr}$
- turnover $\tau_{turn} \sim 3 \left(\frac{L}{3\ {\rm pc}}\right) \left(\frac{u}{3\ {\rm kms}^{-1}}\right)^{-1}\ {\rm Myr}$
- turb dissipation $\tau_{diss} \sim 10 \left(\frac{L}{3\ {\rm pc}}\right)^{1/2} \left(\frac{u}{3\ {\rm kms}^{-1}}\right)^{-3/2}\ {\rm yr}$
- Ionization front $t_{\rm if} \sim 3 \times 10^5 \left(\frac{10^3}{n_{\rm H}}\right) \left(\frac{N_0}{10^{21}}\right)\ {\rm yr}$

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Limitations : 1D static

- transient processes not described
- loosing influence of initial conditions
  - ✓ loose understanding of physical evolution
  - ✓ bistability not treated
- no 3D structure
  - ✓ lack of realistic geometry
  - ✓ no permeability to UV photons
  - ✓ miss opacity effects

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Advantages

- stress on microphysics
- asymptotic behavior
- avoid empirical laws
  ⇒ results from first principles
- exact transfer
  ⇒ non LTE, non LVG
- solve thousands couplings
- adaptative and versatile
- resolve chemical transitions
  H / H_2 $l_{\mathrm{H-H_2}} \sim 100$ AU
  C^+ / C $l_{\mathrm{C^+-C}} \sim 0.5$ pc
- use as virtual world
- large number of predictions
- exploration / grid of models
  - ✓ laws for simulations
  - ✓ efficient inversion tool

Iterative procedure

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model parameters
radiation field, density, CR flux, elements, …

↓

initial conditions
chemical & temperature profiles, …

Iterative procedure

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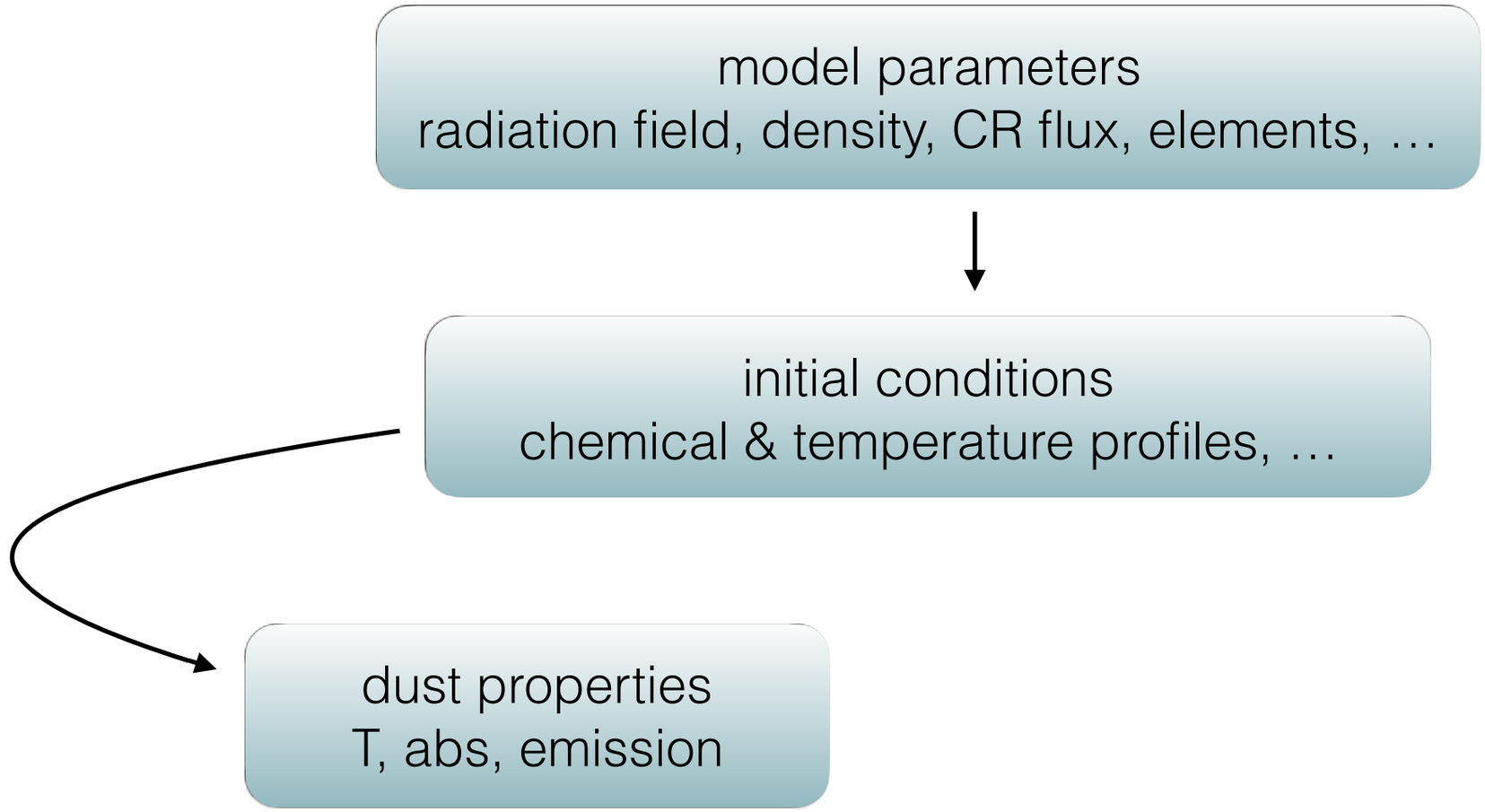
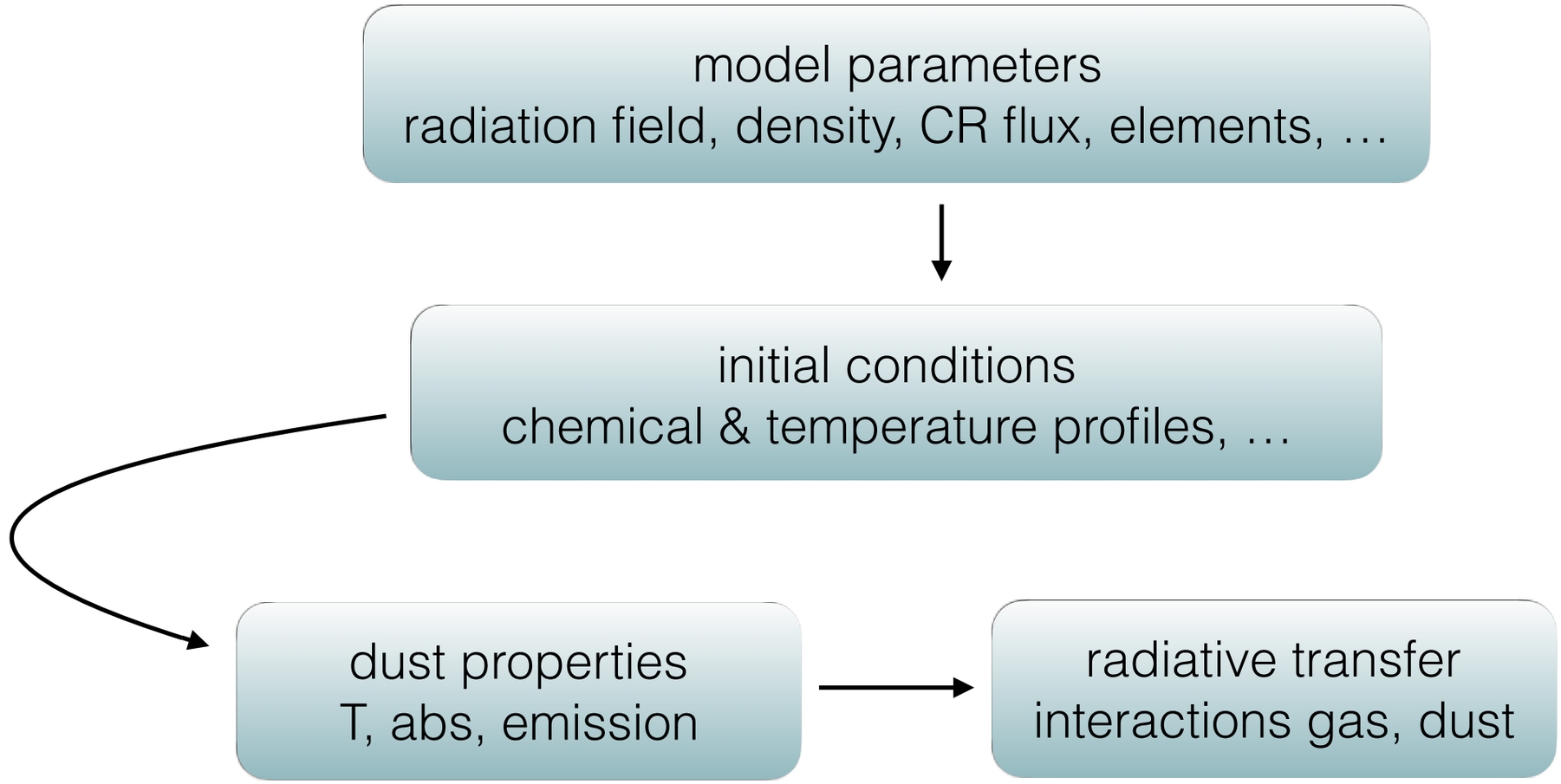


Iterative procedure

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples



Iterative procedure

Outline

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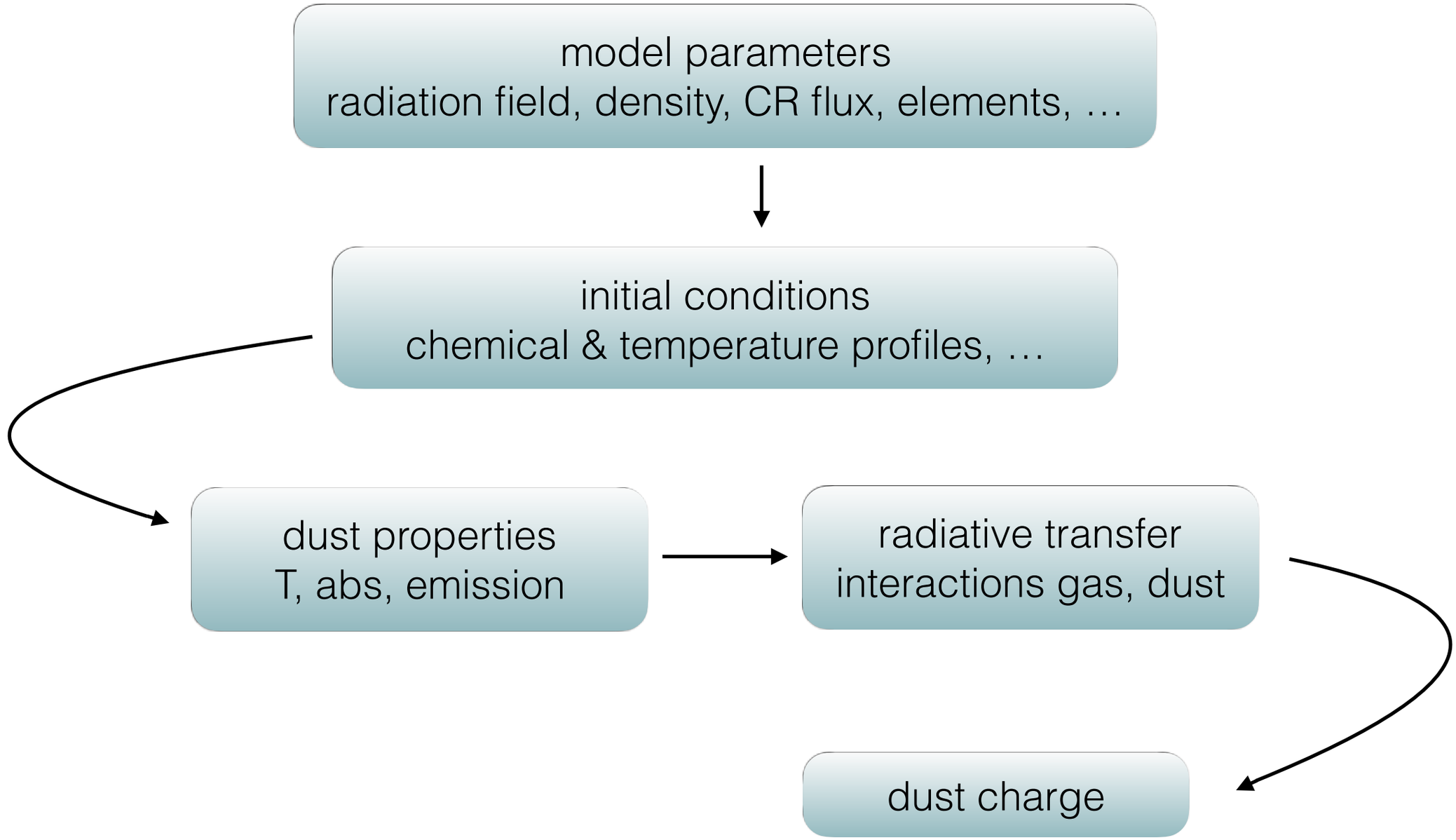

Iterative procedure

Outline

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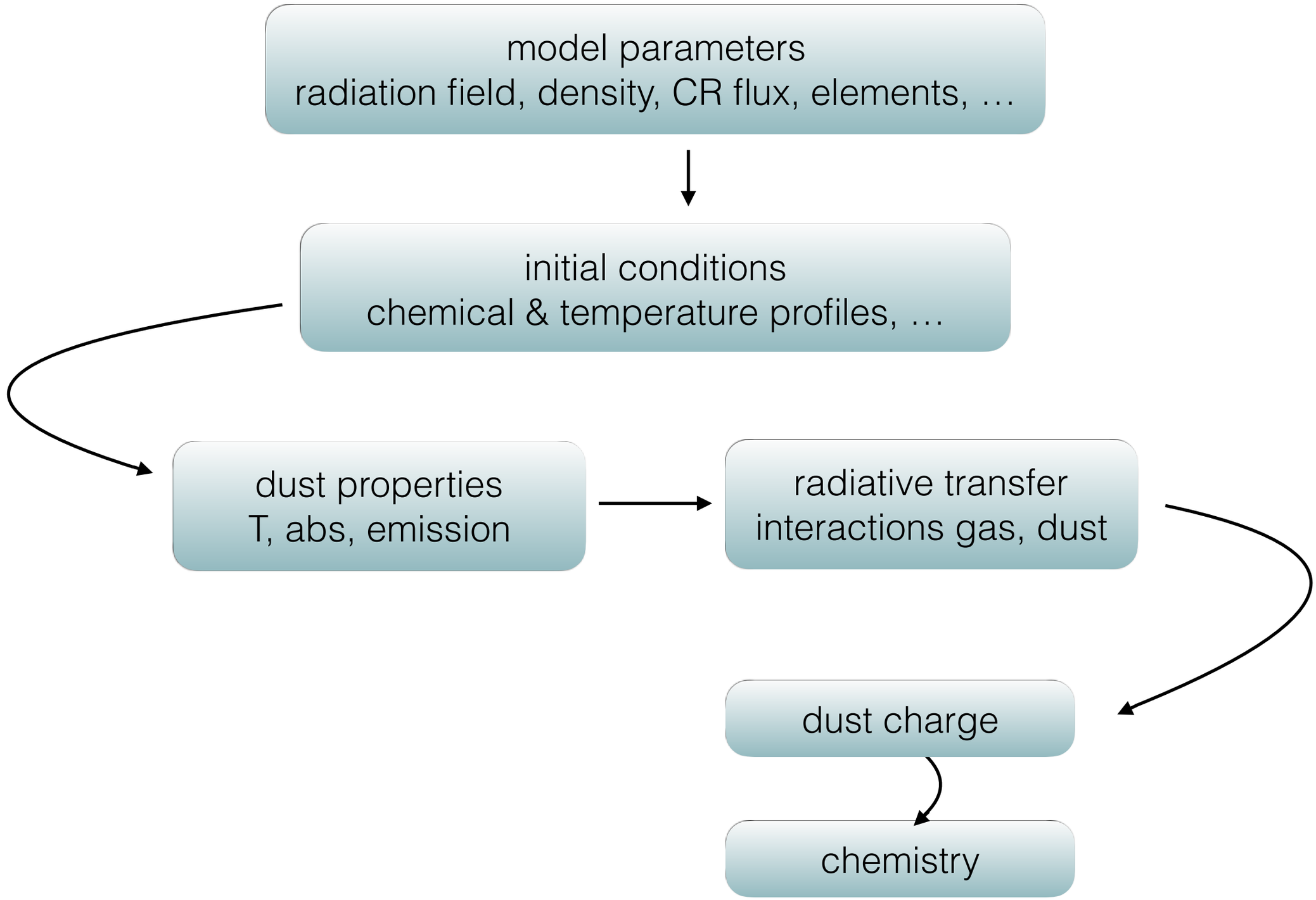

Iterative procedure

Outline

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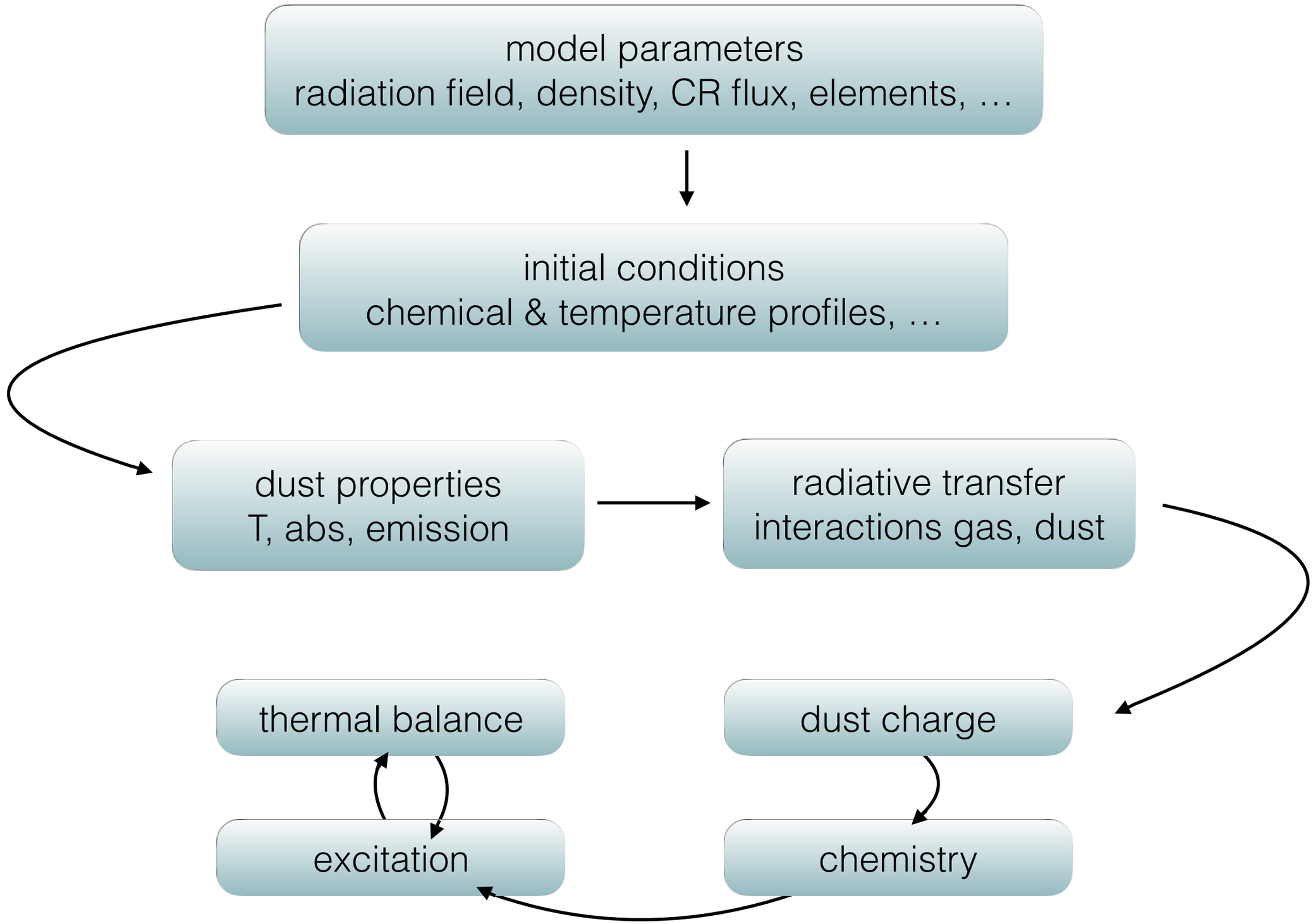

Iterative procedure

Outline

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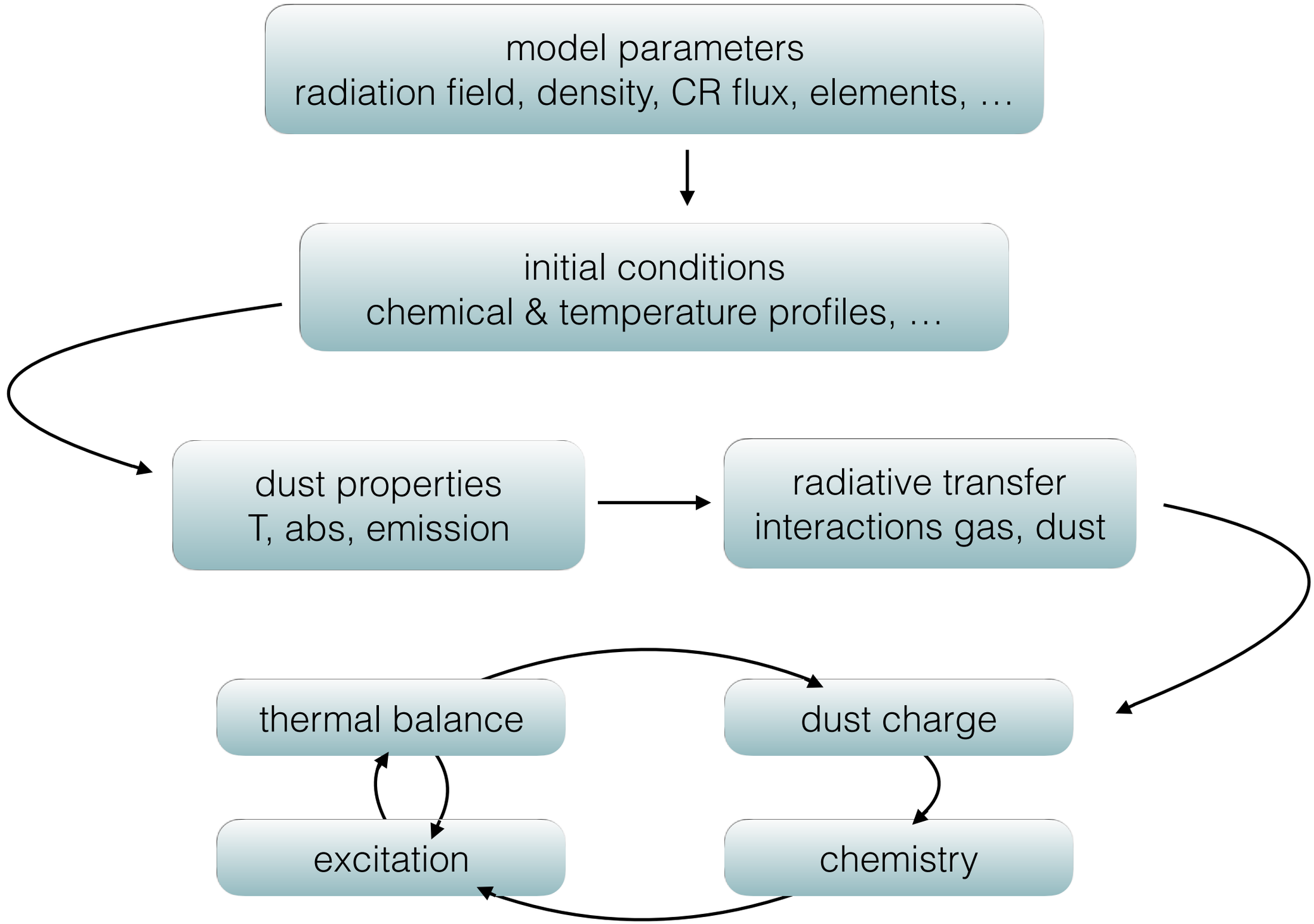
- examples



Iterative procedure

Outline

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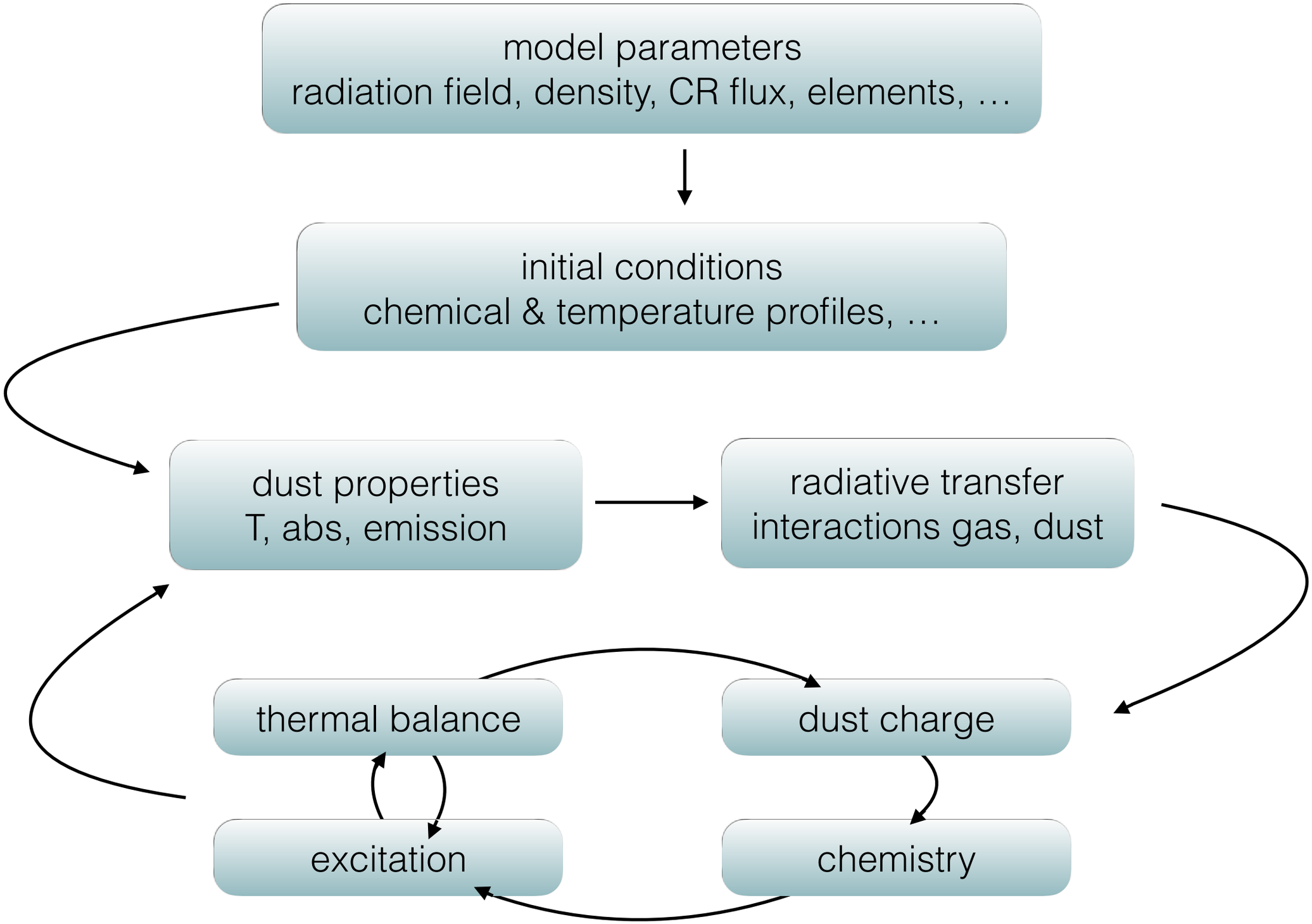
- examples



Iterative procedure

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

Computational time

⇒ Radiative transfer and statistical treatments are time consuming

⇒ Chemistry and thermal balance are fast

Iterative procedure

Outline

- introduction on PDRs
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- examples

Computational time

⇒ Radiative transfer and statistical treatments are time consuming

⇒ Chemistry and thermal balance are fast

version	Method	point in grid	time
PDRLight	dust absorption / emission	7 000	1/2 h
PDR 1.5.2	+ gas continuum absorption	13 000	4 h
PDR 1.5.2	+ H2 mutual lines shielding	27 000	9 h
PDR 1.5.2	+ CO mutual lines shielding	59 000	17 h
PDR 1.5.2	+ isotopes	77 000	26 h

ISM plateform

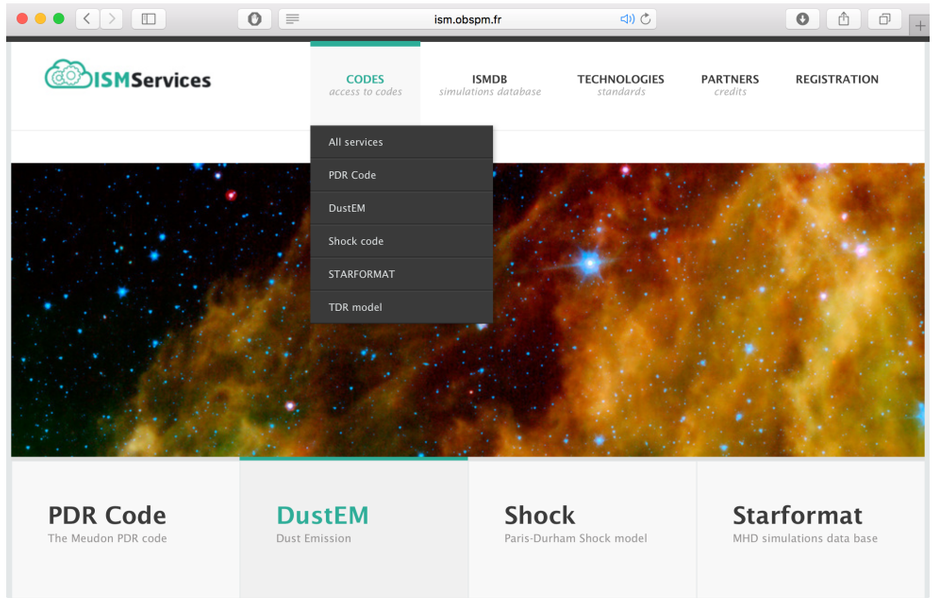
Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

- download from the platform

  ism.obspm.fr

  code & documentation



ISM plateform

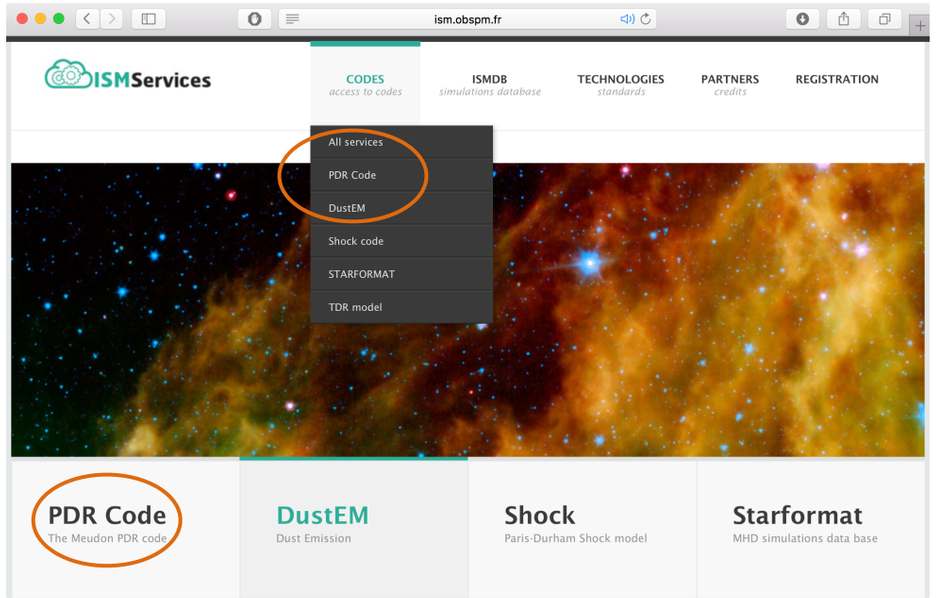
Outline

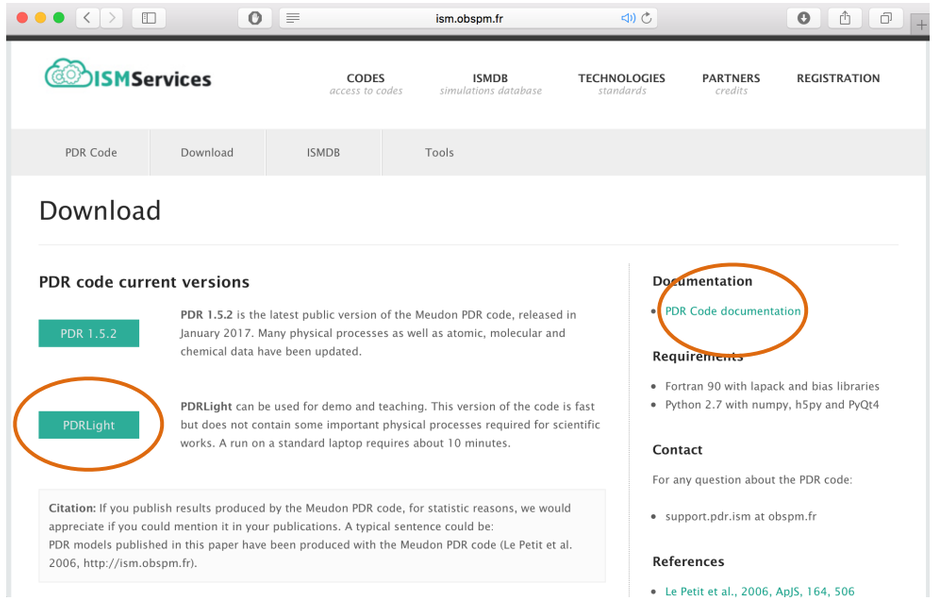
- introduction on PDRs
- assumptions
- user guide first steps
- examples

- download from the platform

  ism.obspm.fr

  code & documentation





ISM plateform

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

- download from the platform

  ism.obspm.fr

  code & documentation

- untar and compile

  fortran compiler / librairies

  python2.7 / librairies

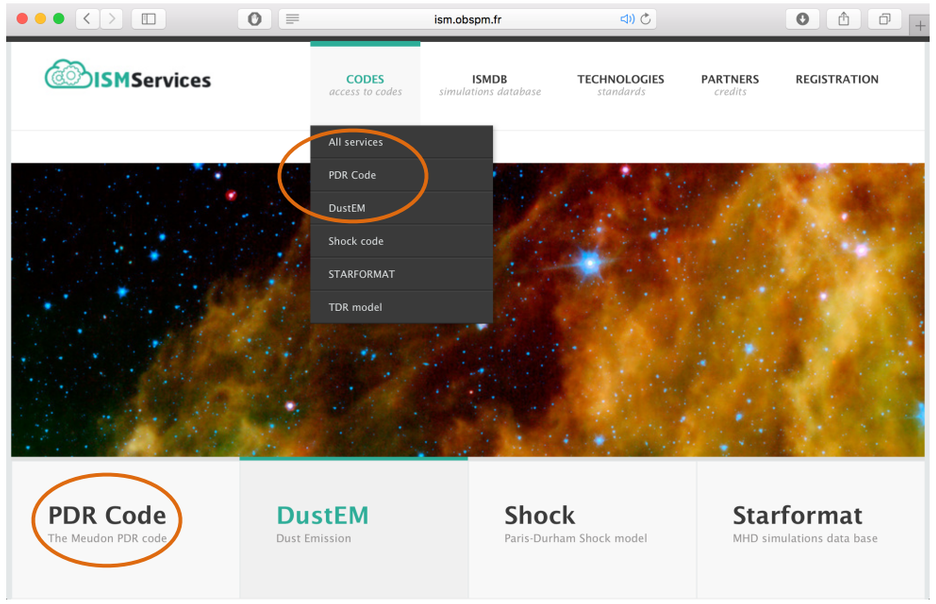
  web browser

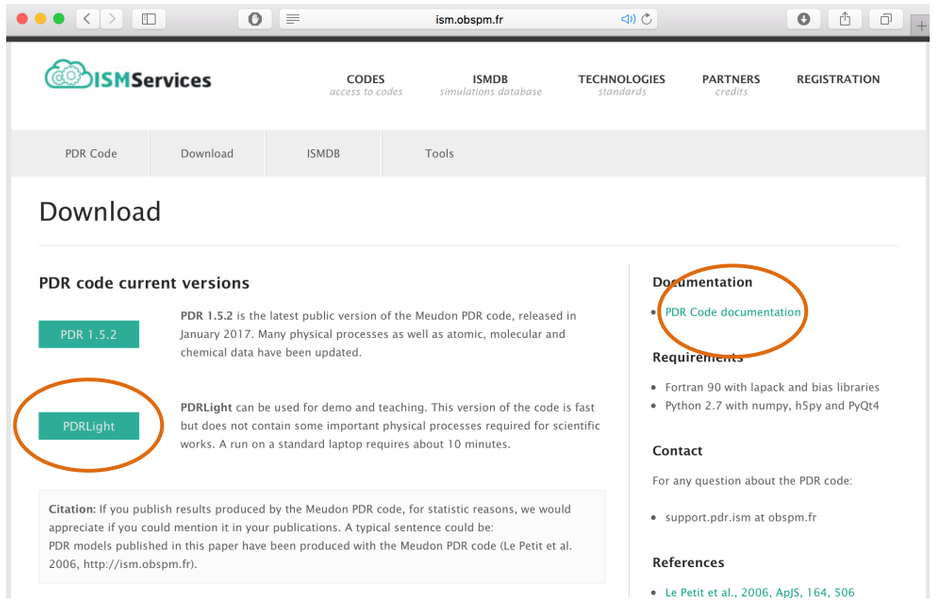
- prepare the input files

  end criterion

  output options

- run the model
- extract & analyse the results





Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

`AnalysisTools`	→	extraction / analysis tools
`data`	→	input files
`out`	→	output files
`PDRDoc.html`	→	link to online doc
`PDRLight_1.0_svn`	→	xcode project
`README`	→	short help
`src`	→	source code - compilation - run

Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

`data`	
`Astrodata`	astrophysical sources
`Chimie`	chemical networks
`Grains`	grains abs / heat coefficients
`Collisions`	
`Levels`	atom / mol data
`Lines`	
`pdr.in`	main input file
`photodest.flag`	photodestr. param
`Sections`	photodestr. cross sections
`spectre.flag`	detailed balance param
`Techconfig`	output configuration
`UVdata`	H / H_2 / CO UV lines

Inputs

Outline

- introduction on PDRs
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- examples

data	
Astrodata	astrophysical sources
Chimie	chemical networks
Grains	grains abs / heat coefficients
Collisions	
Levels	atom / mol data
Lines	
pdr.in	main input file
photodest.flag	photodestr. param
Sections	photodestr. cross sections
spectre.flag	detailed balance param
Techconfig	output configuration
UVdata	H / H_2 / CO UV lines

Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

Main input file : `pdr.in`

~/Travail/Codes-Chimie/PDR_svn/1.5.2_light_svn/data/pdr.in

```
ExampleDiffuse          ! modele   : Output files radix
ch1612_iso_Mathis.chi   ! chimie   : Chemistry file (ex: ch
1                       ! ifafm    : Number of global itera
3.00e+00                ! Avmax    : Integration limit (Av)
1.00e+02                ! densh    : Initial density (nH =
   1                    ! F_ISRF   : 1 = Mathis, 2 = Draine
1.00e+00                ! radm     : Radiation field intens
1.00e+00                ! radp     : Radiation field intens
none.txt                ! srcpp    : Additional plan parall
-0.000e+00              ! d_sour   : Star distance (pc) (<0
5.00e+00                ! fmrc     : Cosmic rays ionisation
   1                    ! ieqth    : thermal Balance (1 : s
7.00e+01                ! tgaz     : Initial temperature (K
   0                    ! ifisob   : State equation (0: nH
none.pfl                ! fprofil  : Temperature-density pr
1.00e+06                ! presse   : Initial Pressure (cm-3
2.00e+00                ! vturb    : turbulent velocity (Do
   2                    ! ichh2    : H + H2 collision rate
Galaxy                  ! los_ext  : Line of sight extincti
3.10                    ! rrr      : Rv = Av / E(B-V)  (Typ
1.00e-00                ! metal    : metallicity Z (automat
5.80e+21                ! cdunit_0 : NH / E(B-V) for Z = 1,
1.00e-02                ! gratio_0 : Mass grains / mass gas
4.60e-02                ! q_pah    : PAH mass fraction (def
3.50e+00                ! alpgr    : grains distribution in
1.00e-07                ! rgrmin   : Grains minimum radius
3.00e-05                ! rgrmax   : Grains maximum radius
   0                    ! F_DUST_P : 0 - Without DUSTEM, F&
   0                    ! iforh2   : H2 formation on grains
   4                    ! istic    : H2 sticking on grain m
   0                    ! F_W_ALL_IFAF : 1 = Write output f
```

L: 32 C: 1 (none) Unicode (UTF-8) Unix (LF) 2 692 / 316 / 32 100%

Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

Main input file : `pdr.in`

~/Travail/Codes-Chimie/PDR_svn/1.5.2_light_svn/data/pdr.in

```
ExampleDiffuse            ! modele   : Output files radix
ch1612_iso_Mathis.chi     ! chimie   : Chemistry file (ex: ch
1                         ! ifafm    : Number of global itera
3.00e+00                  ! Avmax    : Integration limit (Av)
1.00e+02                  ! densh    : Initial density (nH =
   1                      ! F_ISRF   : 1 = Mathis, 2 = Draine
1.00e+00                  ! radm     : Radiation field intens
1.00e+00                  ! radp     : Radiation field intens
none.txt                  ! srcpp    : Additional plan parall
-0.000e+00                ! d_sour   : Star distance (pc) (<0
5.00e+00                  ! fmrc     : Cosmic rays ionisation
   1                      ! ieqth    : thermal Balance (1 : s
7.00e+01                  ! tgaz     : Initial temperature (K
   0                      ! ifisob   : State equation (0: nH
none.pfl                  ! fprofil  : Temperature-density pr
1.00e+06                  ! presse   : Initial Pressure (cm-3
2.00e+00                  ! vturb    : turbulent velocity (Do
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Galaxy                    ! los_ext  : Line of sight extincti
3.10                      ! rrr      : Rv = Av / E(B-V)  (Typ
1.00e-00                  ! metal    : metallicity Z (automat
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   0                      ! F_W_ALL_IFAF : 1 = Write output f
```

L: 32 C: 1 (none) Unicode (UTF-8) Unix (LF) 2 692 / 316 / 32 100%

parameters descrip

Outline

- introduction on PDRs
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- examples

Main input file : `pdr.in`

~/Travail/Codes-Chimie/PDR_svn/1.5.2_light_svn/data/pdr.in

```
ExampleDiffuse          ! modele   : Output files radix
ch1612_iso_Mathis.chi   ! chimie   : Chemistry file (ex: ch
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   1                    ! F_ISRF   : 1 = Mathis, 2 = Draine
1.00e+00                ! radm     : Radiation field intens
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none.txt                ! srcpp    : Additional plan parall
-0.000e+00              ! d_sour   : Star distance (pc) (<0
5.00e+00                ! fmrc     : Cosmic rays ionisation
   1                    ! ieqth    : thermal Balance (1 : s
7.00e+01                ! tgaz     : Initial temperature (K
   0                    ! ifisob   : State equation (0: nH
none.pfl                ! fprofil  : Temperature-density pr
1.00e+06                ! presse   : Initial Pressure (cm-3
2.00e+00                ! vturb    : turbulent velocity (Do
   2                    ! ichh2    : H + H2 collision rate
Galaxy                  ! los_ext  : Line of sight extincti
3.10                    ! rrr      : Rv = Av / E(B-V)  (Typ
1.00e-00                ! metal    : metallicity Z (automat
5.80e+21                ! cdunit_0 : NH / E(B-V) for Z = 1,
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4.60e-02                ! q_pah    : PAH mass fraction (def
3.50e+00                ! alpgr    : grains distribution in
1.00e-07                ! rgrmin   : Grains minimum radius
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   0                    ! F_DUST_P : 0 - Without DUSTEM, F&
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   0                    ! F_W_ALL_IFAF : 1 = Write output f
```

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parameters descrip

in & out files

Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

Main input file : `pdr.in`

~/Travail/Codes-Chimie/PDR_svn/1.5.2_light_svn/data/pdr.in

```
 1   ExampleDiffuse          ! modele   : Output files radix
 2   ch1612_iso_Mathis.chi   ! chimie   : Chemistry file (ex: ch
 3   1                       ! ifafm    : Number of global itera
 4   3.00e+00                ! Avmax    : Integration limit (Av)
 5   1.00e+02                ! densh    : Initial density (nH =
 6      1                    ! F_ISRF   : 1 = Mathis, 2 = Draine
 7   1.00e+00                ! radm     : Radiation field intens
 8   1.00e+00                ! radp     : Radiation field intens
 9   none.txt                ! srcpp    : Additional plan parall
10  -0.000e+00               ! d_sour   : Star distance (pc) (<0
11   5.00e+00                ! fmrc     : Cosmic rays ionisation
12      1                    ! ieqth    : thermal Balance (1 : s
13   7.00e+01                ! tgaz     : Initial temperature (K
14      0                    ! ifisob   : State equation (0: nH
15   none.pfl                ! fprofil  : Temperature-density pr
16   1.00e+06                ! presse   : Initial Pressure (cm-3
17   2.00e+00                ! vturb    : turbulent velocity (Do
18      2                    ! ichh2    : H + H2 collision rate
19   Galaxy                  ! los_ext  : Line of sight extincti
20   3.10                    ! rrr      : Rv = Av / E(B-V)  (Typ
21   1.00e-00                ! metal    : metallicity Z (automat
22   5.80e+21                ! cdunit_0 : NH / E(B-V) for Z = 1,
23   1.00e-02                ! gratio_0 : Mass grains / mass gas
24   4.60e-02                ! q_pah    : PAH mass fraction (def
25   3.50e+00                ! alpgr    : grains distribution in
26   1.00e-07                ! rgrmin   : Grains minimum radius
27   3.00e-05                ! rgrmax   : Grains maximum radius
28      0                    ! F_DUST_P : 0 - Without DUSTEM, F&
29      0                    ! iforh2   : H2 formation on grains
30      4                    ! istic    : H2 sticking on grain m
31      0                    ! F_W_ALL_IFAF : 1 = Write output f
32
```

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parameters descrip

in & out files

main parameters

Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

Main input file : `pdr.in`

~/Travail/Codes-Chimie/PDR_svn/1.5.2_light_svn/data/pdr.in

```
 1   ExampleDiffuse          ! modele   : Output files radix
 2   ch1612_iso_Mathis.chi   ! chimie   : Chemistry file (ex: ch
 3   1                       ! ifafm    : Number of global itera
 4   3.00e+00                ! Avmax    : Integration limit (Av)
 5   1.00e+02                ! densh    : Initial density (nH =
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 7   1.00e+00                ! radm     : Radiation field intens
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13   7.00e+01                ! tgaz     : Initial temperature (K
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15   none.pfl                ! fprofil  : Temperature-density pr
16   1.00e+06                ! presse   : Initial Pressure (cm-3
17   2.00e+00                ! vturb    : turbulent velocity (Do
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24   4.60e-02                ! q_pah    : PAH mass fraction (def
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27   3.00e-05                ! rgrmax   : Grains maximum radius
28      0                    ! F_DUST_P : 0 - Without DUSTEM, F&
29      0                    ! iforh2   : H2 formation on grains
30      4                    ! istic    : H2 sticking on grain m
31      0                    ! F_W_ALL_IFAF : 1 = Write output f
32
```

L: 32 C: 1 (none) Unicode (UTF-8) Unix (LF) 2 692 / 316 / 32 100%

parameters descrip

in & out files

main parameters

extinction curve

Inputs

Main input file : `pdr.in`

~/Travail/Codes-Chimie/PDR_svn/1.5.2_light_svn/data/pdr.in

```
ExampleDiffuse              ! modele    : Output files radix
ch1612_iso_Mathis.chi       ! chimie    : Chemistry file (ex: ch
1                           ! ifafm     : Number of global itera
3.00e+00                    ! Avmax     : Integration limit (Av)
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   1                        ! ieqth     : thermal Balance (1 : s
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   0                        ! ifisob    : State equation (0: nH
none.pfl                    ! fprofil   : Temperature-density pr
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2.00e+00                    ! vturb     : turbulent velocity (Do
   2                        ! ichh2     : H + H2 collision rate
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3.10                        ! rrr       : Rv = Av / E(B-V)  (Typ
1.00e-00                    ! metal     : metallicity Z (automat
5.80e+21                    ! cdunit_0  : NH / E(B-V) for Z = 1,
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4.60e-02                    ! q_pah     : PAH mass fraction (def
3.50e+00                    ! alpgr     : grains distribution in
1.00e-07                    ! rgrmin    : Grains minimum radius
3.00e-05                    ! rgrmax    : Grains maximum radius
   0                        ! F_DUST_P  : 0 - Without DUSTEM, F&
   0                        ! iforh2    : H2 formation on grains
   4                        ! istic     : H2 sticking on grain m
   0                        ! F_W_ALL_IFAF : 1 = Write output f
```

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parameters descrip

in & out files

main parameters

extinction curve

dust model

Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

Chemistry file

- sets species
  - ✓ composition
  - ✓ initial abundances
- sets reactions
  - ✓ reactants / products
  - ✓ type & rate
- consistency
  - ✓ for all species at least
    1 formation
    1 destruction
  - ✓ set elem abundance

ch1612_iso_Mathis.chi

(New Document)

```
#INCHI num  espece    hcnohe isot metos  metos  - abinit-rel enthalpf  INCHIKeyis
#---------1---------2---------3---------4---------5---------6---------7----------
  1  h         1 0000 0000 00000 000000  0   .800E+00   51.634  YZCKVEUIGOORGS-UH
  2  d         0 0000 1000 00000 000000  0   .000E+00   52.520  NOINCHIFOUND
  3  h2        2 0000 0000 00000 000000  0   .100E+00     .000  UFHFLCQGNIYNRP-UH
  4  hd        1 0000 1000 00000 000000  0  1.500E-05    0.079  NOINCHIFOUND
  5  he        0 0001 0000 00000 000000  0   .100E+00     .000  SWQJXJOGLNCZEY-UH
  6  c         0 1000 0000 00000 000000  0   .000E+00  169.978  OKTJSMMVPCPJKN-UH
  7  c*        0 0000 0100 00000 000000  0   .000E+00  169.978  NOINCHIFOUND
  8  ch        1 1000 0000 00000 000000  0   .000E+00  141.177  VRLIPUYDFBXWCH-UH
 ...
  -                   -
  -                   - cosmic-ray direct processes
  -                   -
jan11 h2      crp     h       h                     1.00E-01   .00      .00   1
jan11 h       crp     h+      electr                4.60E-01   .00      .00   1
jan11 h2      crp     h+      h       electr        4.00E-02   .00      .00   1
jan11 h2      crp     h2+     electr                9.60E-01   .00      .00   1
 ...
  -                   -
  -                   - neutral-neutral reactions
  -                   -
jan11 h       n2      nh      n                     8.63E-11   .50 71457.00   4
jan11 h       nh      n       h2                    8.19E-11   .68   950.00   4
jan11 h       no      n       oh                    3.60E-10   .00 24912.00   4
 ...
  -                   -
  -                   - photoprocesses (ISRF of Mathis et al 1983)
  -                   -
jan11 ch      photon  c       h                     6.60E-10   .00     1.15   5
jan11 ch2     photon  ch      h                     4.90E-10   .00     1.67   5
jan11 ch3     photon  ch2     h                     3.20E-10   .00     1.88   5
jan11 ch3     photon  ch      h2                    3.20E-10   .00     1.88   5
 ...
  -                   -
  -                   - Ions and electrons / Grains
  -                   -
NEUTR h+      grain   h                             1.00E+00  0.00     0.00  14
NEUTR he+     grain   he                            1.00E+00  0.00     0.00  14
NEUTR c+      grain   c                             1.00E+00  0.00     0.00  14
NEUTR o+      grain   o                             1.00E+00  0.00     0.00  14
NEUTR n+      grain   n                             1.00E+00  0.00     0.00  14
NEUTR s+      grain   s                             1.00E+00  0.00     0.00  14
NEUTR si+     grain   si                            1.00E+00  0.00     0.00  14
```

L: 3204 C: 1 (none) Unicode (UTF-8) Unix (LF) (never saved) 83 / 9 / 1 100%

Inputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

Chemistry file

- sets species
  - ✓ **composition**
  - ✓ initial abundances
- sets reactions
  - ✓ reactants / products
  - ✓ type & rate
- consistency
  - ✓ for all species at least
    1 formation
    1 destruction
  - ✓ set elem abundance

ch1612_iso_Mathis.chi

(New Document)

```
#INCHI num  espece    hcnobe isot metos  metos  - abinit-rel enthalpf  INCHIKeyis
#---------1---------2---------3---------4---------5---------6---------7----------
  1  h         1 0000 0000 00000 000000  0   .800E+00   51.634  YZCKVEUIGOORGS-UH
  2  d         0 0000 1000 00000 000000  0   .000E+00   52.520  NOINCHIFOUND
  3  h2        2 0000 0000 00000 000000  0   .100E+00     .000  UFHFLCQGNIYNRP-UH
  4  hd        1 0000 1000 00000 000000  0  1.500E-05    0.079  NOINCHIFOUND
  5  he        0 0001 0000 00000 000000  0   .100E+00     .000  SWQJXJOGLNCZEY-UH
  6  c         0 1000 0000 00000 000000  0   .000E+00  169.978  OKTJSMMVPCPJKN-UH
  7  c*        0 0000 0100 00000 000000  0   .000E+00  169.978  NOINCHIFOUND
  8  ch        1 1000 0000 00000 000000  0   .000E+00  141.177  VRLIPUYDFBXWCH-UH
  -                   -
  -                   - cosmic-ray direct processes
  -                   -
jan11 h2      crp     h       h                     1.00E-01   .00      .00   1
jan11 h       crp     h+      electr                4.60E-01   .00      .00   1
jan11 h2      crp     h+      h       electr        4.00E-02   .00      .00   1
jan11 h2      crp     h2+     electr                9.60E-01   .00      .00   1
  -                   -
  -                   - neutral-neutral reactions
  -                   -
jan11 h       n2      nh      n                     8.63E-11   .50 71457.00   4
jan11 h       nh      n       h2                    8.19E-11   .68   950.00   4
jan11 h       no      n       oh                    3.60E-10   .00 24912.00   4
  -                   -
  -                   - photoprocesses (ISRF of Mathis et al 1983)
  -                   -
jan11 ch      photon  c       h                     6.60E-10   .00     1.15   5
jan11 ch2     photon  ch      h                     4.90E-10   .00     1.67   5
jan11 ch3     photon  ch2     h                     3.20E-10   .00     1.88   5
jan11 ch3     photon  ch      h2                    3.20E-10   .00     1.88   5
  -                   -
  -                   - Ions and electrons / Grains
  -                   -
NEUTR h+      grain   h                             1.00E+00  0.00     0.00  14
NEUTR he+     grain   he                            1.00E+00  0.00     0.00  14
NEUTR c+      grain   c                             1.00E+00  0.00     0.00  14
NEUTR o+      grain   o                             1.00E+00  0.00     0.00  14
NEUTR n+      grain   n                             1.00E+00  0.00     0.00  14
NEUTR s+      grain   s                             1.00E+00  0.00     0.00  14
NEUTR si+     grain   si                            1.00E+00  0.00     0.00  14
```

L: 3204 C: 1 (none) Unicode (UTF-8) Unix (LF) (never saved) 83 / 9 / 1 100%

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Chemistry file

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- sets reactions
  - ✓ reactants / products
  - ✓ type & rate
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  - ✓ for all species at least
    1 formation
    1 destruction
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ch1612_iso_Mathis.chi

(New Document)

```
#INCHI num  espece    hcnohe isot metos  metos  - abinit-rel enthalpf  INCHIKeyis
#---------1---------2---------3---------4---------5---------6---------7----------
  1  h         1 0000 0000 00000 000000  0   .800E+00   51.634  YZCKVEUIGOORGS-UH
  2  d         0 0000 1000 00000 000000  0   .000E+00   52.520  NOINCHIFOUND
  3  h2        2 0000 0000 00000 000000  0   .100E+00     .000  UFHFLCQGNIYNRP-UH
  4  hd        1 0000 1000 00000 000000  0  1.500E-05    0.079  NOINCHIFOUND
  5  he        0 0001 0000 00000 000000  0   .100E+00     .000  SWQJXJOGLNCZEY-UH
  6  c         0 1000 0000 00000 000000  0   .000E+00  169.978  OKTJSMMVPCPJKN-UH
  7  c*        0 0000 0100 00000 000000  0   .000E+00  169.978  NOINCHIFOUND
  8  ch        1 1000 0000 00000 000000  0   .000E+00  141.177  VRLIPUYDFBXWCH-UH
 ...
  -                   -
  -                   - cosmic-ray direct processes
  -                   -
jan11 h2      crp     h       h                     1.00E-01   .00      .00   1
jan11 h       crp     h+      electr                4.60E-01   .00      .00   1
jan11 h2      crp     h+      h       electr        4.00E-02   .00      .00   1
jan11 h2      crp     h2+     electr                9.60E-01   .00      .00   1
 ...
  -                   -
  -                   - neutral-neutral reactions
  -                   -
jan11 h       n2      nh      n                     8.63E-11   .50 71457.00   4
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jan11 h       no      n       oh                    3.60E-10   .00 24912.00   4
 ...
  -                   -
  -                   - photoprocesses (ISRF of Mathis et al 1983)
  -                   -
jan11 ch      photon  c       h                     6.60E-10   .00     1.15   5
jan11 ch2     photon  ch      h                     4.90E-10   .00     1.67   5
jan11 ch3     photon  ch2     h                     3.20E-10   .00     1.88   5
jan11 ch3     photon  ch      h2                    3.20E-10   .00     1.88   5
 ...
  -                   -
  -                   - Ions and electrons / Grains
  -                   -
NEUTR h+      grain   h                             1.00E+00  0.00     0.00  14
NEUTR he+     grain   he                            1.00E+00  0.00     0.00  14
NEUTR c+      grain   c                             1.00E+00  0.00     0.00  14
NEUTR o+      grain   o                             1.00E+00  0.00     0.00  14
NEUTR n+      grain   n                             1.00E+00  0.00     0.00  14
NEUTR s+      grain   s                             1.00E+00  0.00     0.00  14
NEUTR si+     grain   si                            1.00E+00  0.00     0.00  14
```

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  2  d         0 0000 1000 00000 000000  0   .000E+00   52.520  NOINCHIFOUND
  3  h2        2 0000 0000 00000 000000  0   .100E+00     .000  UFHFLCQGNIYNRP-UH
  4  hd        1 0000 1000 00000 000000  0  1.500E-05    0.079  NOINCHIFOUND
  5  he        0 0001 0000 00000 000000  0   .100E+00     .000  SWQJXJOGLNCZEY-UH
  6  c         0 1000 0000 00000 000000  0   .000E+00  169.978  OKTJSMMVPCPJKN-UH
  7  c*        0 0000 0100 00000 000000  0   .000E+00  169.978  NOINCHIFOUND
  8  ch        1 1000 0000 00000 000000  0   .000E+00  141.177  VRLIPUYDFBXWCH-UH
  ...
  -                   -
  -                   - cosmic-ray direct processes
  -                   -
jan11 h2      crp     h       h                     1.00E-01   .00      .00   1
jan11 h       crp     h+      electr                4.60E-01   .00      .00   1
jan11 h2      crp     h+      h       electr        4.00E-02   .00      .00   1
jan11 h2      crp     h2+     electr                9.60E-01   .00      .00   1
  ...
  -                   -
  -                   - neutral-neutral reactions
  -                   -
jan11 h       n2      nh      n                     8.63E-11   .50 71457.00   4
jan11 h       nh      n       h2                    8.19E-11   .68   950.00   4
jan11 h       no      n       oh                    3.60E-10   .00 24912.00   4
  ...
  -                   -
  -                   - photoprocesses (ISRF of Mathis et al 1983)
  -                   -
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jan11 ch3     photon  ch2     h                     3.20E-10   .00     1.88   5
jan11 ch3     photon  ch      h2                    3.20E-10   .00     1.88   5
  ...
  -                   -
  -                   - Ions and electrons / Grains
  -                   -
NEUTR h+      grain   h                             1.00E+00  0.00     0.00  14
NEUTR he+     grain   he                            1.00E+00  0.00     0.00  14
NEUTR c+      grain   c                             1.00E+00  0.00     0.00  14
NEUTR o+      grain   o                             1.00E+00  0.00     0.00  14
NEUTR n+      grain   n                             1.00E+00  0.00     0.00  14
NEUTR s+      grain   s                             1.00E+00  0.00     0.00  14
NEUTR si+     grain   si                            1.00E+00  0.00     0.00  14
```

L: 3204 C: 1 (none) Unicode (UTF-8) Unix (LF) (never saved) 83 / 9 / 1 100%

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  2  d         0 0000 1000 00000 000000  0   .000E+00   52.520  NOINCHIFOUND
  3  h2        2 0000 0000 00000 000000  0   .100E+00     .000  UFHFLCQGNIYNRP-UH
  4  hd        1 0000 1000 00000 000000  0  1.500E-05    0.079  NOINCHIFOUND
  5  he        0 0001 0000 00000 000000  0   .100E+00     .000  SWQJXJOGLNCZEY-UH
  6  c         0 1000 0000 00000 000000  0   .000E+00  169.978  OKTJSMMVPCPJKN-UH
  7  c*        0 0000 0100 00000 000000  0   .000E+00  169.978  NOINCHIFOUND
  8  ch        1 1000 0000 00000 000000  0   .000E+00  141.177  VRLIPUYDFBXWCH-UH
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  -                   -
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jan11 h2      crp     h+      h       electr         4.00E-02   .00      .00   1
jan11 h2      crp     h2+     electr                 9.60E-01   .00      .00   1
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jan11 ch3     photon  ch2     h                      3.20E-10   .00     1.88   5
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  ...
  -                   -
  -                   - Ions and electrons / Grains
  -                   -
NEUTR h+      grain   h                              1.00E+00  0.00     0.00  14
NEUTR he+     grain   he                             1.00E+00  0.00     0.00  14
NEUTR c+      grain   c                              1.00E+00  0.00     0.00  14
NEUTR o+      grain   o                              1.00E+00  0.00     0.00  14
NEUTR n+      grain   n                              1.00E+00  0.00     0.00  14
NEUTR s+      grain   s                              1.00E+00  0.00     0.00  14
NEUTR si+     grain   si                             1.00E+00  0.00     0.00  14
```

L: 3204 C: 1 (none) Unicode (UTF-8) Unix (LF) (never saved) 83 / 9 / 1 100%

Inputs

Outline

- introduction on PDRs
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spectre.flag

~/Travail/Codes-Chimie/P.../.../data/spectre.flag

```
#Activation(1: yes,0:no)  Species nused nus
1 h          -1   1  1.0 !
1 h2        250  50  2.0 !
1 hd          9   9  3.0 !
1 co         64  10 28.0 !  12C 160
1 c*o        32  10 29.0 !  13C 160
1 co*        32  10 30.0 !  12C 180
1 c*o*       31  10 31.0 !  13C 180
1 c          -1   3 12.0 !
1 n          -1   1 14.0 !
1 o          -1   3 16.0 ! Set 5,5 to conside
1 o2         -1  24 32.0 !
1 s          -1   3 32.0 !
1 si         -1   3 28.0 !
1 cs         -1  10 44.0 !
1 hcn        -1  10 27.0 !
1 oh         -1  20 17.0 !
1 h2o        -1  15 18.0 !
1 c+         -1   2 12.0 !
0 c++        -1   1 12.0 !
0 n+         -1   1 14.0 !
0 n++        -1   2 14.0 !
0 o+         -1   1 16.0 !
0 o++        -1   3 16.0 !
0 s+         -1   1 32.0 !
0 s++        -1   3 32.0 !
1 si+        -1   2 28.0 !
```

L: 1 C: 1 (none) Unicode (UTF-8) Unix (LF)

Detailed balance parameters

↕

- thermal balance
- atom / mol level excitation
- adaptative method

Inputs

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- introduction on PDRs
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`spectre.flag`

~/Travail/Codes-Chimie/P.../.../data/spectre.flag

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1 c*o        32  10 29.0 !  13C 160
1 co*        32  10 30.0 !  12C 180
1 c*o*       31  10 31.0 !  13C 180
1 c          -1   3 12.0 !
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1 o2         -1  24 32.0 !
1 s          -1   3 32.0 !
1 si         -1   3 28.0 !
1 cs         -1  10 44.0 !
1 hcn        -1  10 27.0 !
1 oh         -1  20 17.0 !
1 h2o        -1  15 18.0 !
1 c+         -1   2 12.0 !
0 c++        -1   1 12.0 !
0 n+         -1   1 14.0 !
0 n++        -1   2 14.0 !
0 o+         -1   1 16.0 !
0 o++        -1   3 16.0 !
0 s+         -1   1 32.0 !
0 s++        -1   3 32.0 !
1 si+        -1   2 28.0 !
```

L: 1 C: 1 (none) Unicode (UTF-8) Unix (LF)

Detailed balance parameters

↕

- thermal balance
- atom / mol level excitation
- adaptative method

use or drop species

Inputs

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spectre.flag

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1 h        -1   1  1.0 !
1 h2      250  50  2.0 !
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1 co       64  10 28.0 !  12C 160
1 c*o      32  10 29.0 !  13C 160
1 co*      32  10 30.0 !  12C 180
1 c*o*     31  10 31.0 !  13C 180
1 c        -1   3 12.0 !
1 n        -1   1 14.0 !
1 o        -1   3 16.0 ! Set 5,5 to conside
1 o2       -1  24 32.0 !
1 s        -1   3 32.0 !
1 si       -1   3 28.0 !
1 cs       -1  10 44.0 !
1 hcn      -1  10 27.0 !
1 oh       -1  20 17.0 !
1 h2o      -1  15 18.0 !
1 c+       -1   2 12.0 !
0 c++      -1   1 12.0 !
0 n+       -1   1 14.0 !
0 n++      -1   2 14.0 !
0 o+       -1   1 16.0 !
0 o++      -1   3 16.0 !
0 s+       -1   1 32.0 !
0 s++      -1   3 32.0 !
1 si+      -1   2 28.0 !
```

L: 1 C: 1 (none) Unicode (UTF-8) Unix (LF)

Detailed balance parameters

↕

- thermal balance
- atom / mol level excitation
- adaptative method

use or drop species

use at least 10 lev of CO

use at most 64 lev of CO

Inputs

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1 h2      250  50  2.0 !
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1 co       64  10 28.0 !  12C 160
1 c*o      32  10 29.0 !  13C 160
1 co*      32  10 30.0 !  12C 180
1 c*o*     31  10 31.0 !  13C 180
1 c        -1   3 12.0 !
1 n        -1   1 14.0 !
1 o        -1   3 16.0 ! Set 5,5 to conside
1 o2       -1  24 32.0 !
1 s        -1   3 32.0 !
1 si       -1   3 28.0 !
1 cs       -1  10 44.0 !
1 hcn      -1  10 27.0 !
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1 c+       -1   2 12.0 !
0 c++      -1   1 12.0 !
0 n+       -1   1 14.0 !
0 n++      -1   2 14.0 !
0 o+       -1   1 16.0 !
0 o++      -1   3 16.0 !
0 s+       -1   1 32.0 !
0 s++      -1   3 32.0 !
1 si+      -1   2 28.0 !
```

L: 1 C: 1 (none) Unicode (UTF-8) Unix (LF)

Detailed balance parameters

↕

- thermal balance
- atom / mol level excitation
- adaptative method

use or drop species

use at least 10 lev of CO

use at most 64 lev of CO

use all levels of C^+

Run

Makefile (in the `src/` directory)

- set the compiler name
- set compiler's options
- set libraries' paths
- compile

  `$ make`

  → `PDR`

~/Travail/Codes-Chimie/PDR_svn/1.5.2_light_svn/src/Makefile (no function selected)

```
43  #==============================================================================#
44  #                                IFORT (Intel)                                 #
45  #==============================================================================#
46  #  FC = ifort
47
48  #- Version 14.0
49  #  FFLAGS = -g -O2 -parallel -mkl -xSSSE3 -axSSSE3 -m64
50  #  FFLAGS = -g3 -O0 -mkl -check all -warn all -check:noarg_temp_created -tracebac
51
52  #  LIBS1 = -lpthread
53
54  #==============================================================================#
55  #                                 GFORTRAN                                     #
56  #==============================================================================#
57    FC = gfortran
58
59  # Options and Path
60  # FFLAGS = -g3 -O0 -fno-second-underscore -Wall -Wextra -Wno-compare-reals -fchec
61  # FFLAGS = -g -Ofast -fno-second-underscore -falign-loops=16 -march=corei7 -ffast
62  # FFLAGS = -g -O2    -fno-second-underscore -falign-loops=16 -march=corei7 -ffast
63    FFLAGS = -g -O2    -fno-second-underscore -falign-loops=16 -ffast-math -fassoci
64
65    LIBS1 = -llapack -lblas
66
67  #==============================================================================#
68  #                                    G95                                       #
69  #==============================================================================#
70  # FC = g95
71
72  # Options and Path
73  # FFLAGS = -O2 -fno-second-underscore
74  # FFLAGS = -g3 -fno-second-underscore -Wall -Wextra -fbounds-check -ftrace=full -
75  # FFLAGS = -g3 -gdwarf-2 -fno-second-underscore -Wall -Wextra -fbounds-check -ftr
76
77  # LIBS1 = -llapack -lblas
78
```

L: 1 C: 1 Make Unicode (UTF-8) Unix (LF) Saved: 13/06/2017 10:55:28 8 374 / 665 / 166

Run

Outline

- introduction on PDRs
- assumptions
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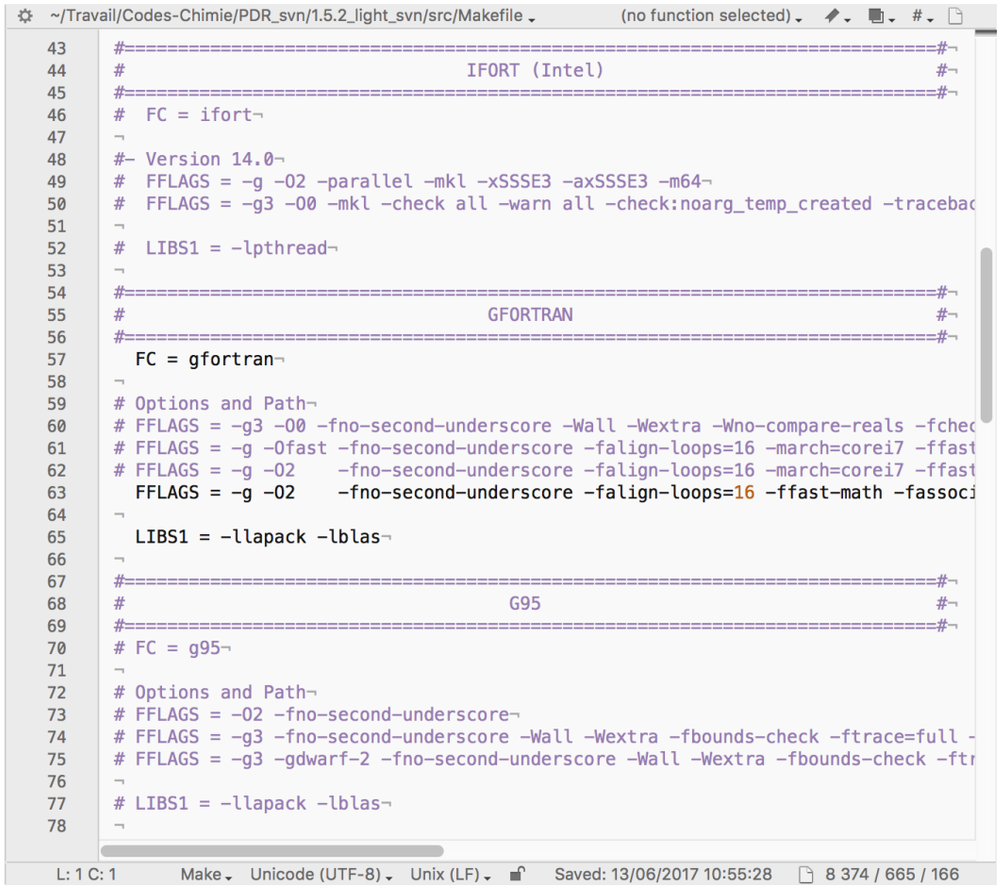
- examples

Makefile (in the `src/` directory)

- set the compiler name
- set compiler's options
- set libraries' paths
- compile

```
$ make
→ PDR
```



Run (in the `src/` directory)

- with default input file (`pdr.in`)

```
$ ./PDR
```

- with another input file other_input.in

```
$ ./PDR ../data/other_input.in
```

Outputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
- examples

```
out
    model_name
        model_name_a_XX.hdf5
        model_name_c_XX.hdf5
        model_name_s_XX.hdf5
        model_name_XX.stat
        model_name.binXX
        model_name.def
        model_name.flin
        model_name.Iesc
        model_name.rf
        model_name.uv
```

Outputs

Outline

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- assumptions
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```
out
    model_name
        model_name_a_XX.hdf5   ──→  analysis output
        model_name_c_XX.hdf5   ──→  chemical output
        model_name_s_XX.hdf5   ──→  standard output
        model_name_XX.stat
        model_name.binXX
        model_name.def         ──→  log file
        model_name.flin
        model_name.Iesc
        model_name.rf
        model_name.uv
```

Outputs

Outline

- introduction on PDRs
- assumptions
- user guide first steps
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```
out
    model_name
        model_name_a_XX.hdf5      ──→  analysis output
        model_name_c_XX.hdf5      ──→  chemical output
        model_name_s_XX.hdf5      ──→  standard output
        model_name_XX.stat
        model_name.binXX          ──→  old binary output
        model_name.def            ──→  log file
        model_name.flin
        model_name.Iesc
        model_name.rf
        model_name.uv
```

Outputs

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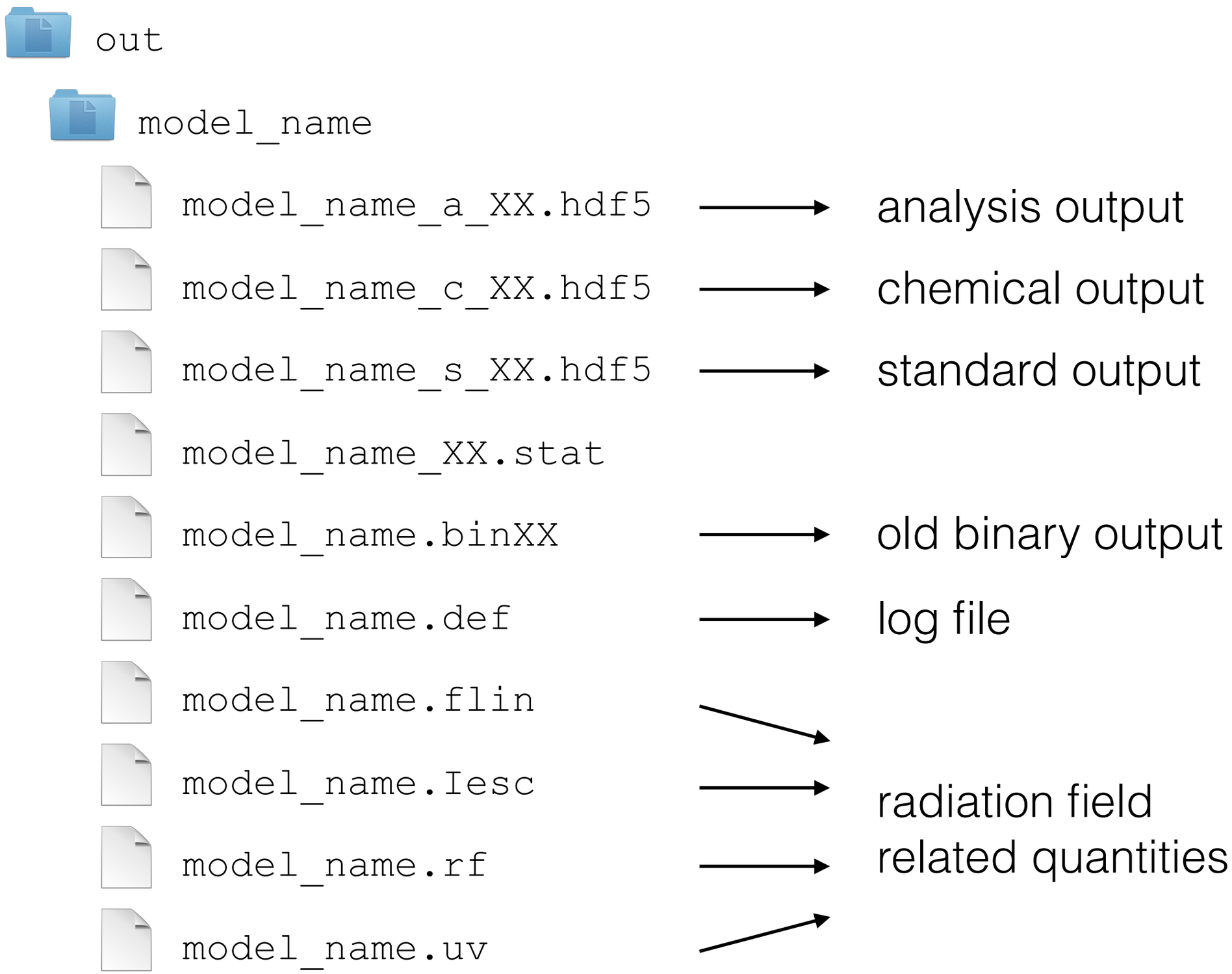

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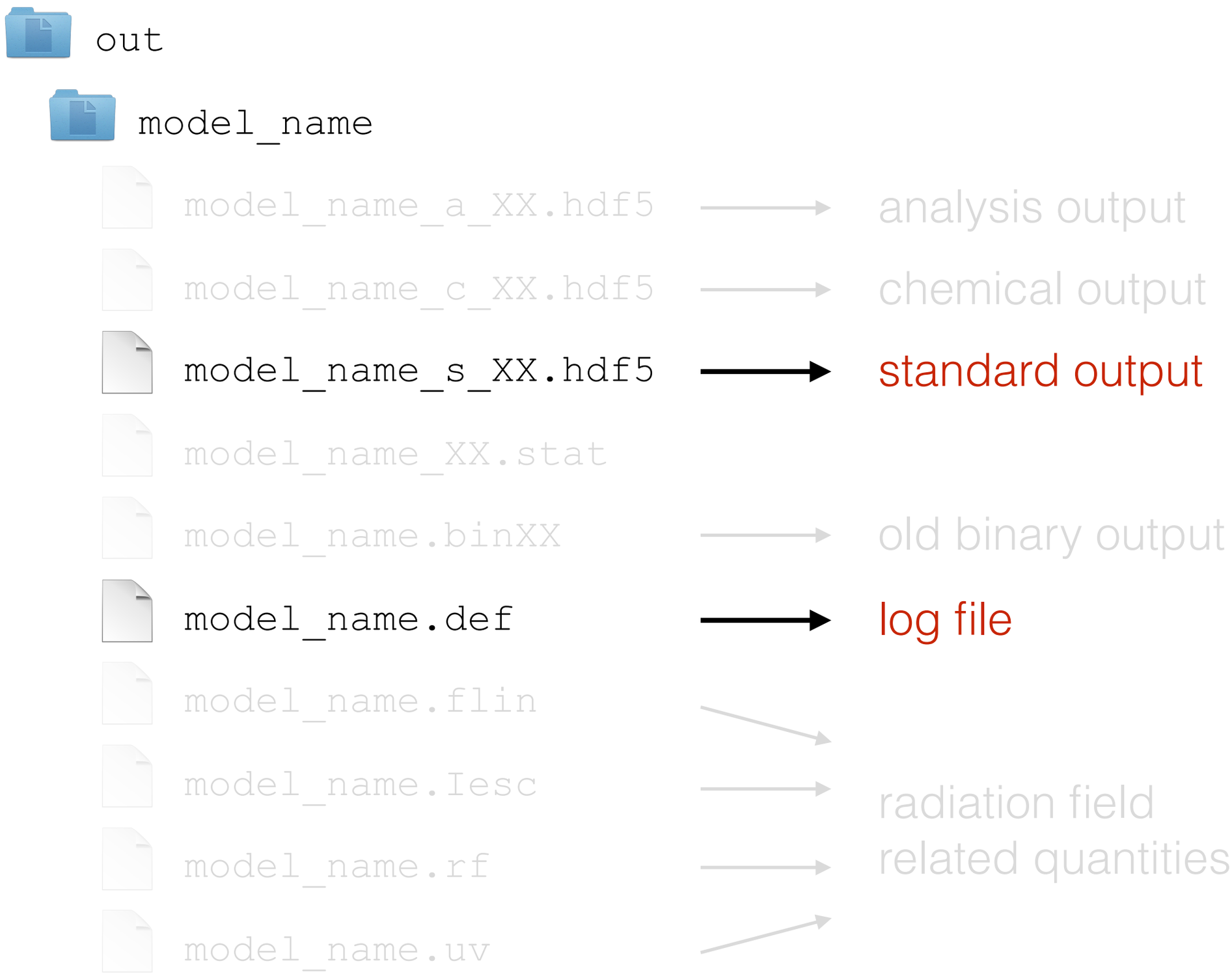

Results analysis

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Tools (in `AnalysisTools/` directory)

- read HDF5 files (in `extractor/`)

```
$ python2.7 extractor.py
```

- analyse chemistry (in `ChemistryAnalyser/`)

```
$ python2.7 server/server.py
```

launch `visualizer/index.html` with a web browser

Results analysis

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launch `visualizer/index.html` with a web browser

Method

- always check
  - ✓ convergence
  - ✓ temperature, density & ionization profiles
  - ✓ H / H_2 & C^+ / C / CO transitions
- understand local before integrated quantities

Visible extinction

Natural variables for radiative transfer

$$\frac{\partial I_\lambda}{\partial s} = -(\kappa_\lambda + \sigma_\lambda) I_\lambda + \text{scattering} + \text{emission}$$

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Visible extinction

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Natural variables for radiative transfer

$$\frac{\partial I_\lambda}{\partial s} = -(\kappa_\lambda + \sigma_\lambda) I_\lambda + \text{scattering} + \text{emission}$$

absorption & scattering coefficients

Visible extinction

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Natural variables for radiative transfer

$$\frac{\partial I_\lambda}{\partial s} = -(\kappa_\lambda + \sigma_\lambda) I_\lambda + \text{scattering} + \text{emission}$$

- optical depth $d\tau_\lambda = (\kappa_\lambda + \sigma_\lambda) ds$
- extinction $A_\lambda = 2.5 \log_{10}(e)\, \tau_\lambda$
- visible extinction $A_\lambda = A_V \left(1 + \frac{k(\lambda - V)}{R_V}\right)$
- H column density $N_{\mathrm{H}} = C_D / R_V \times A_V$

Visible extinction

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Natural variables for radiative transfer

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extinction curve

- optical depth $d\tau_\lambda = (\kappa_\lambda + \sigma_\lambda) ds$
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Visible extinction

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A_V / E_{B-V}

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N_H / E_{B-V}

Results

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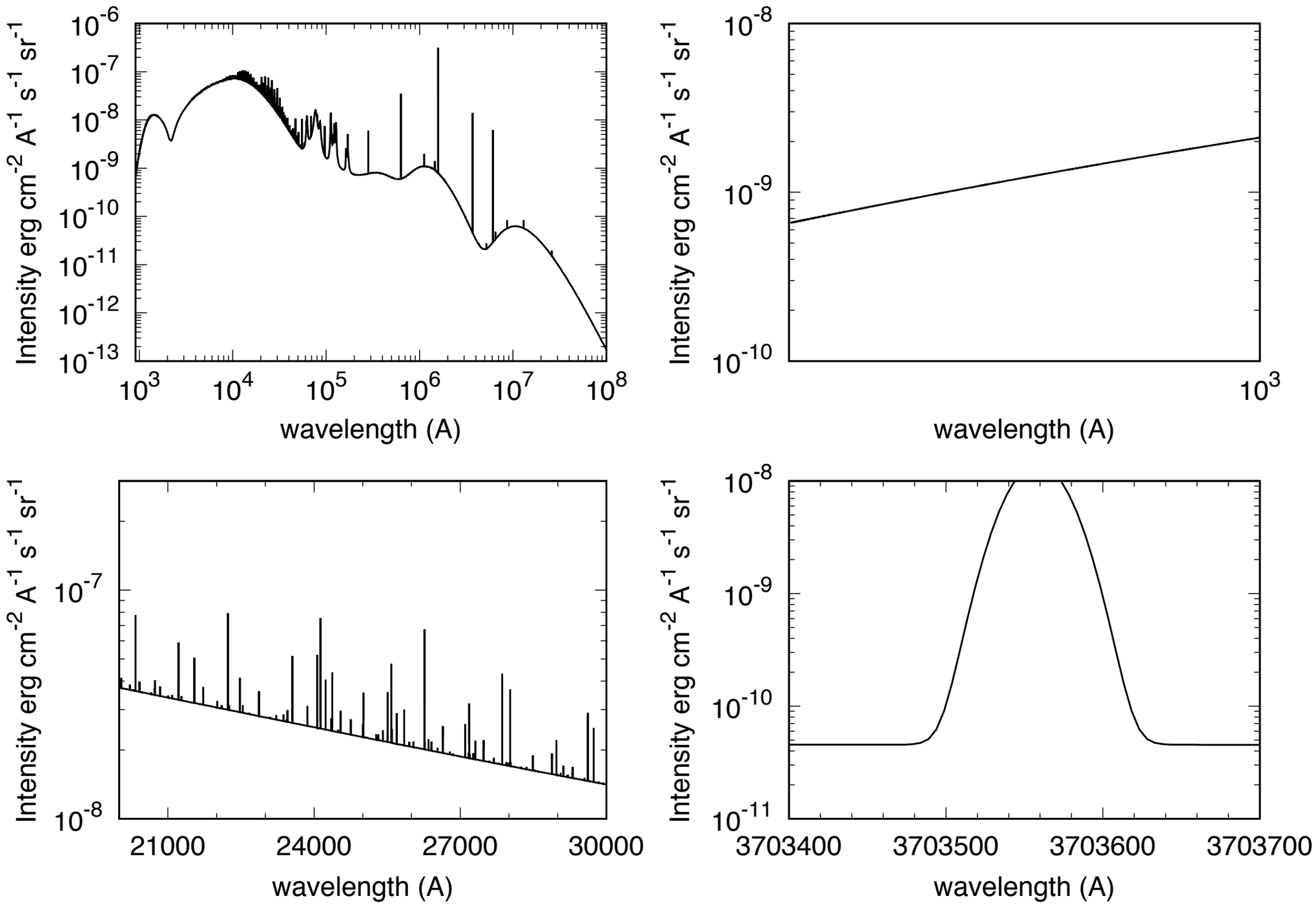
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