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

Jacques Le Bourlot

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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

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4. Examples
5. Physics & algorithms
6. Applications
7. Recent updates
8. Conclusions

Definition

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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Physical properties

Outline

- introduction on PDRs
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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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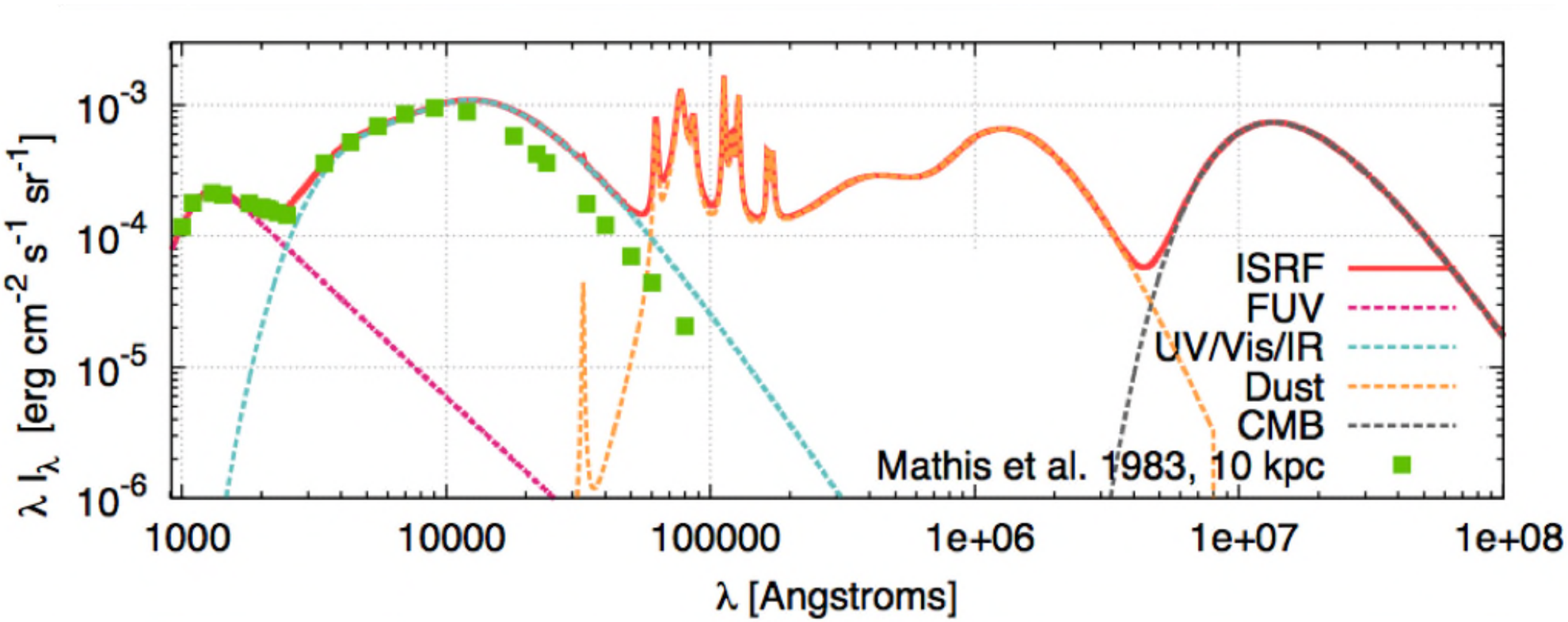

Physical properties

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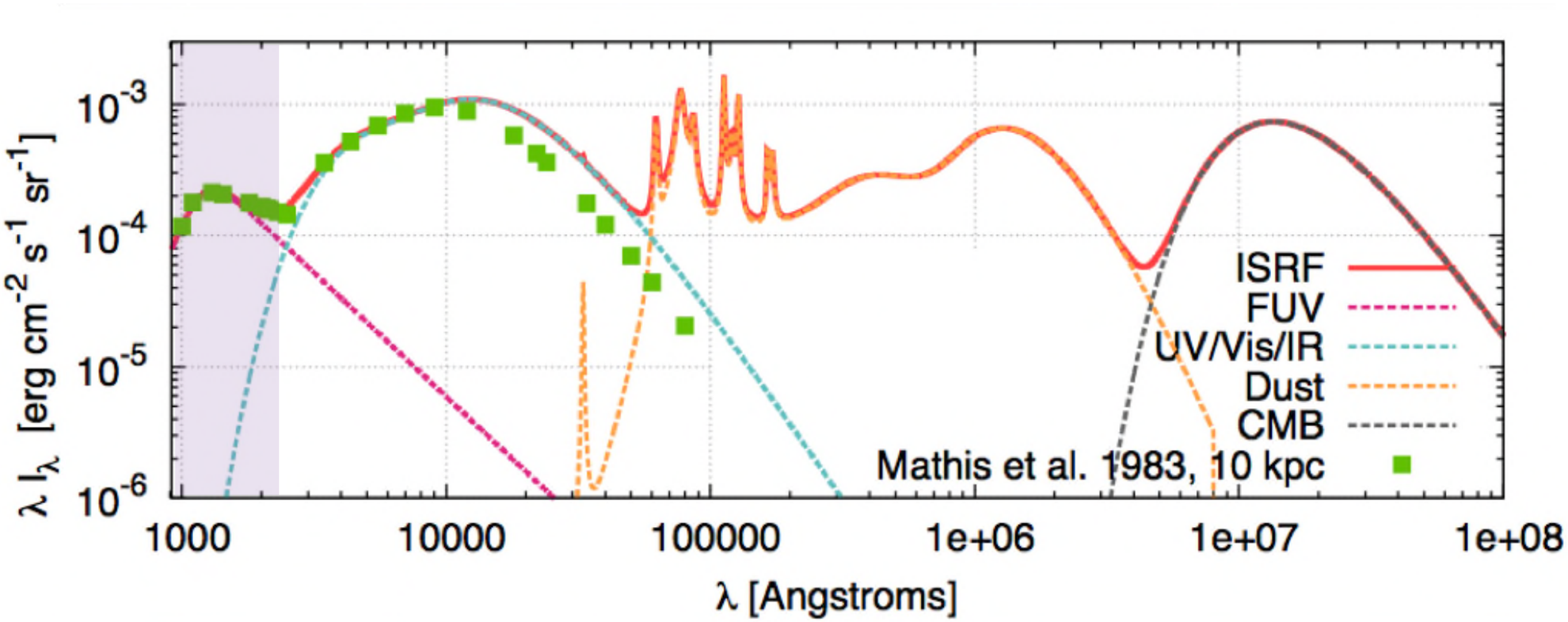
FUV photons

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

impacts

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



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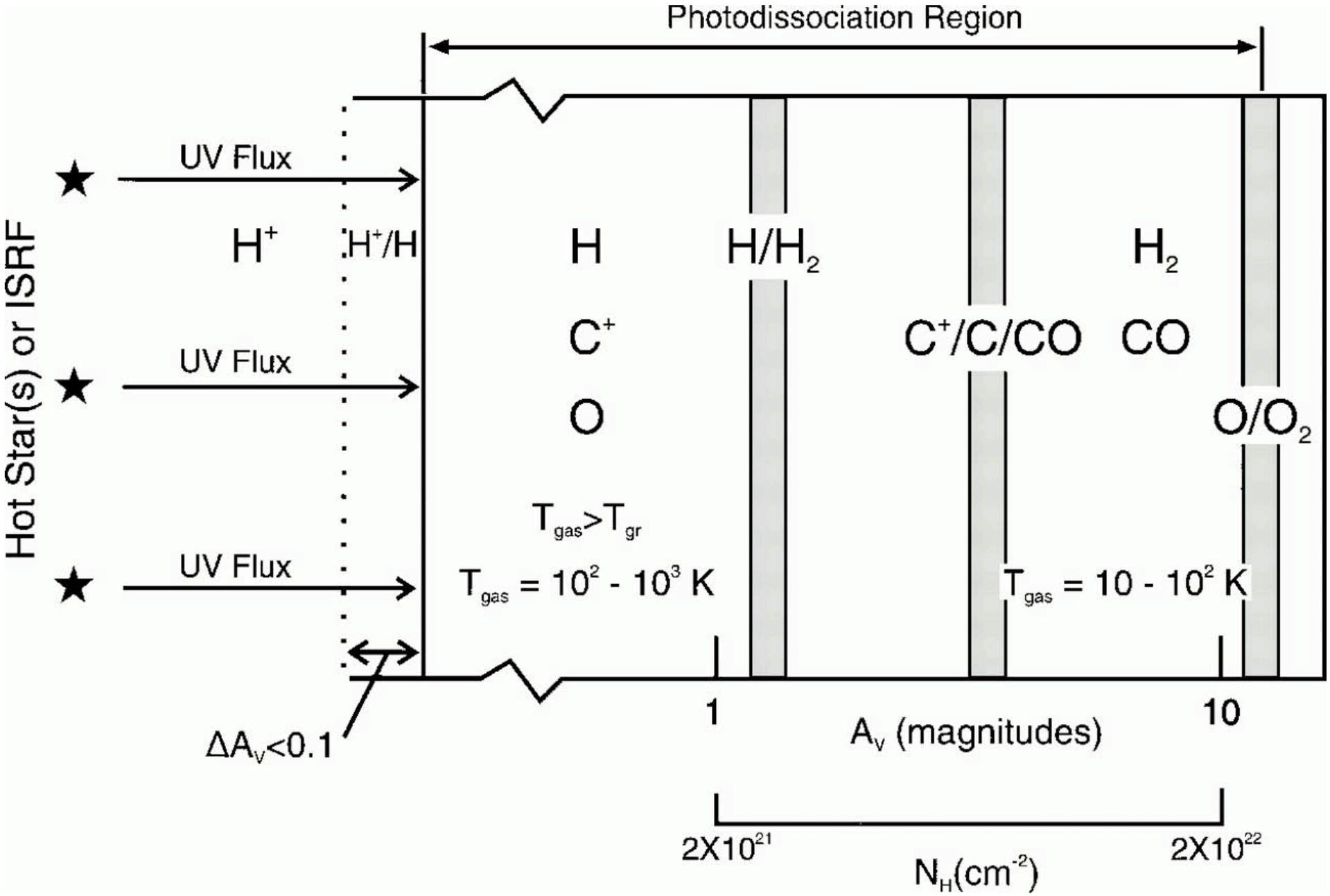
Structure of a PDR



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Example

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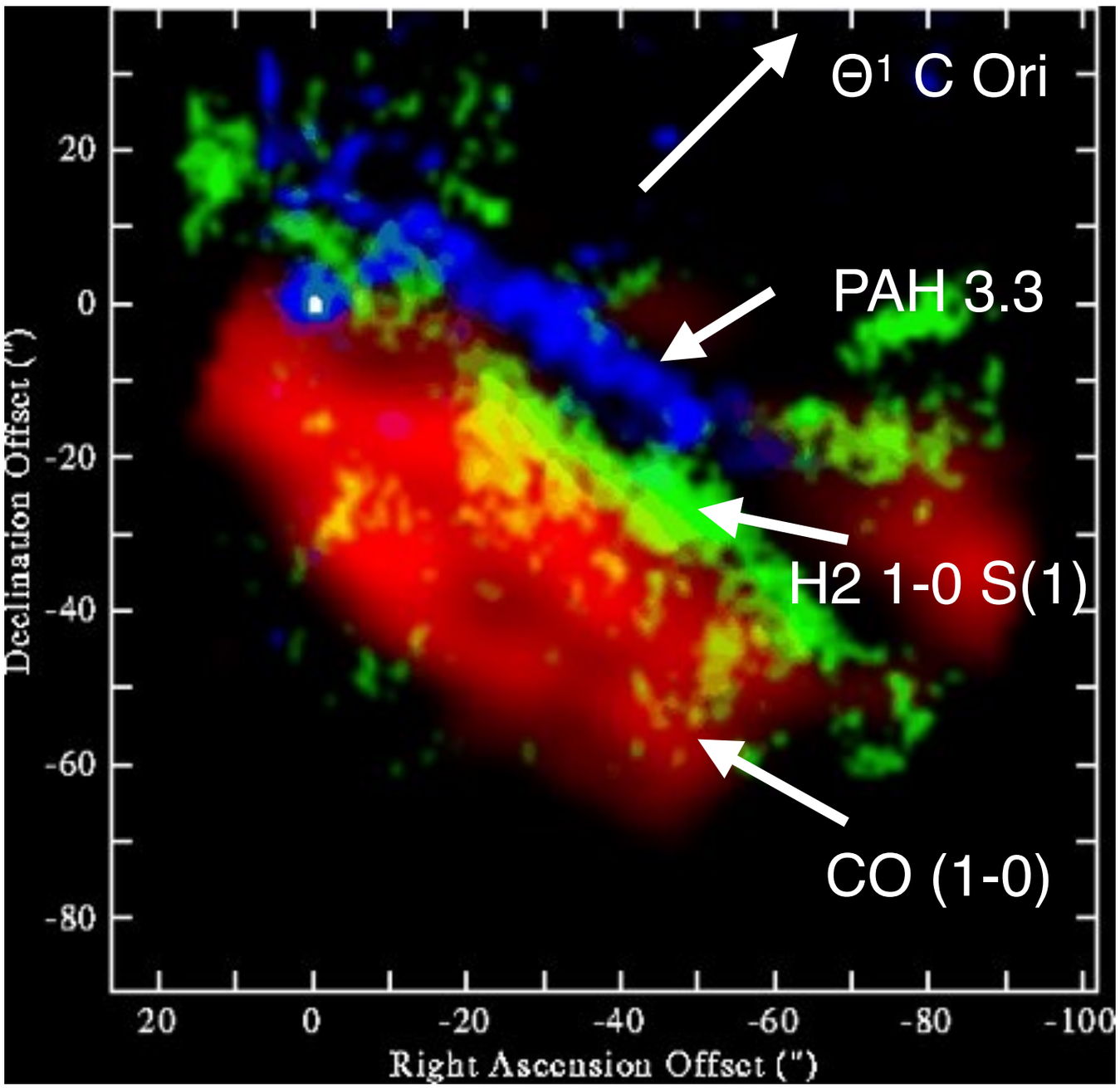

Tielens, Meixner, et al. (1993)

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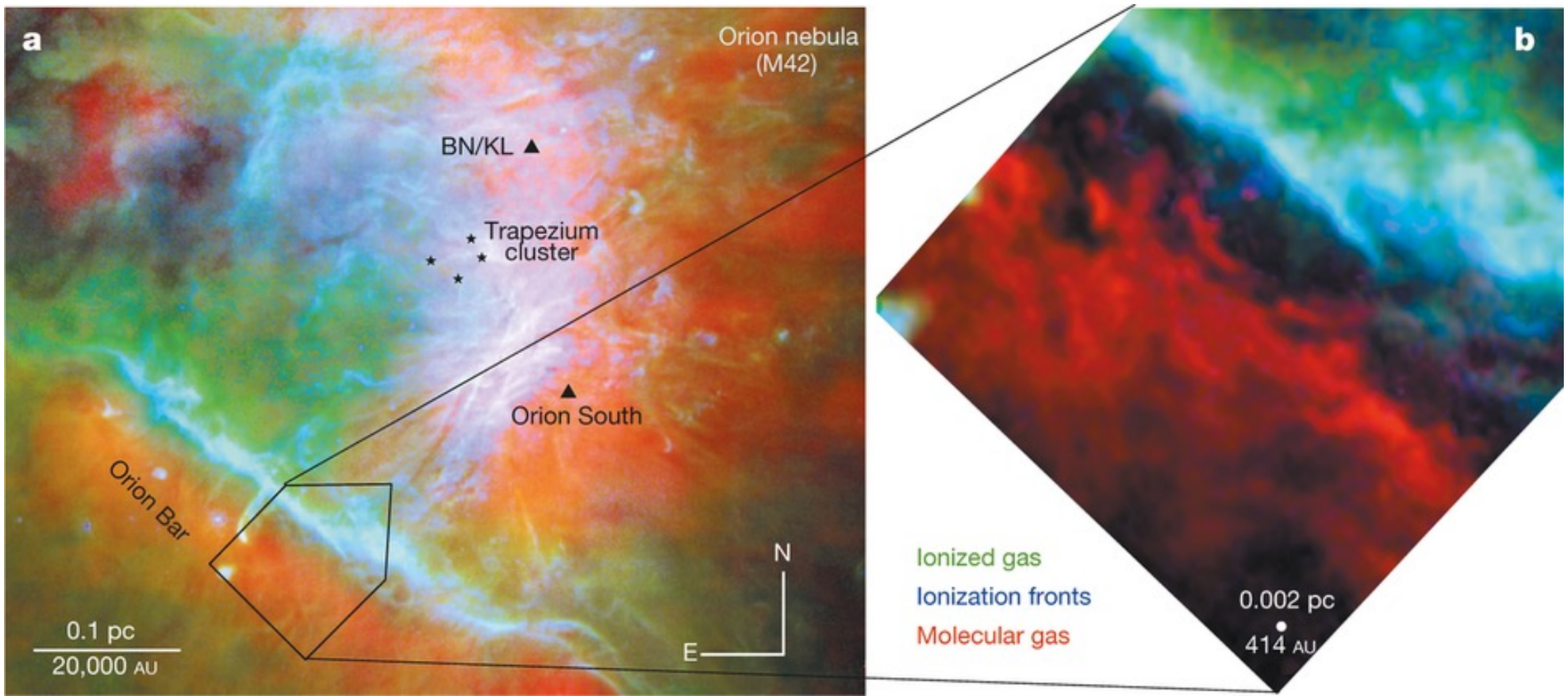

Goicoechea et al. (2016)

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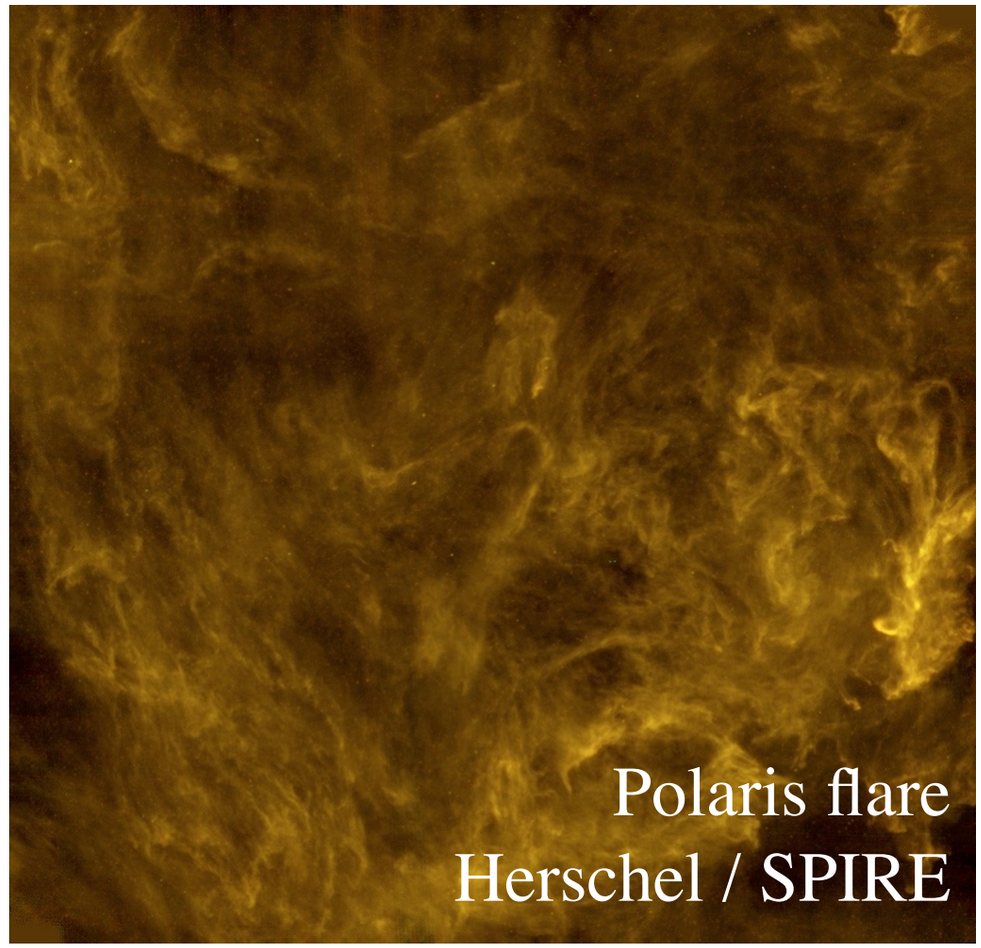
Examples

- 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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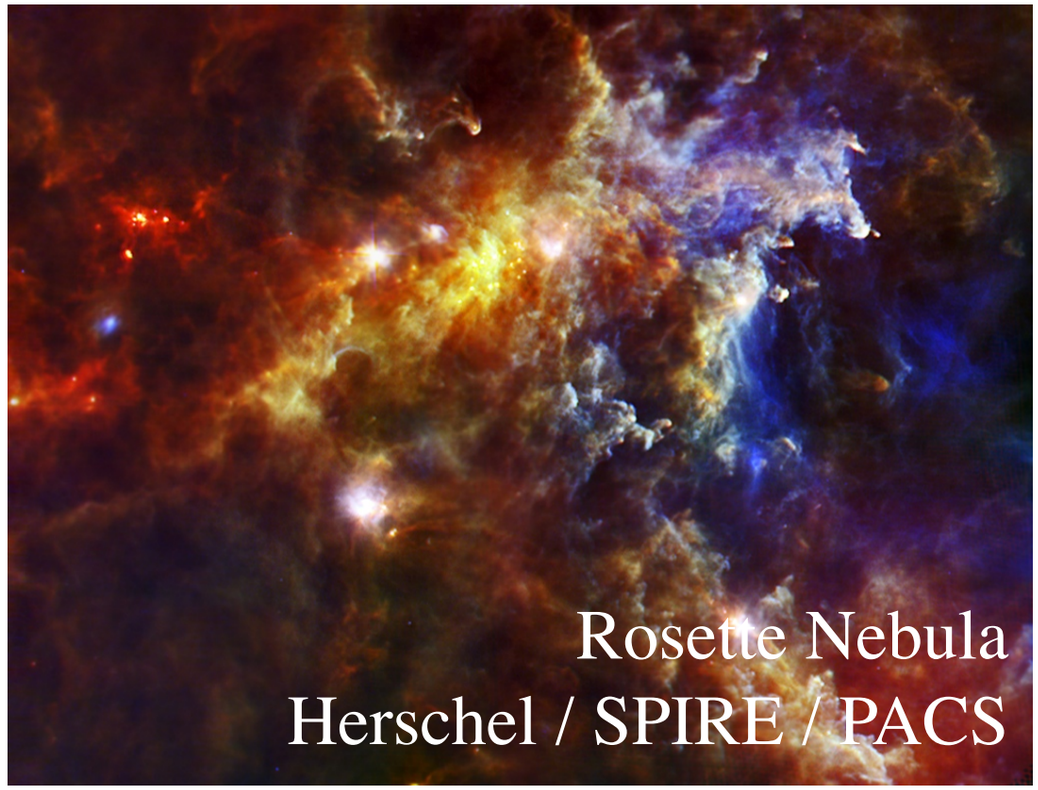

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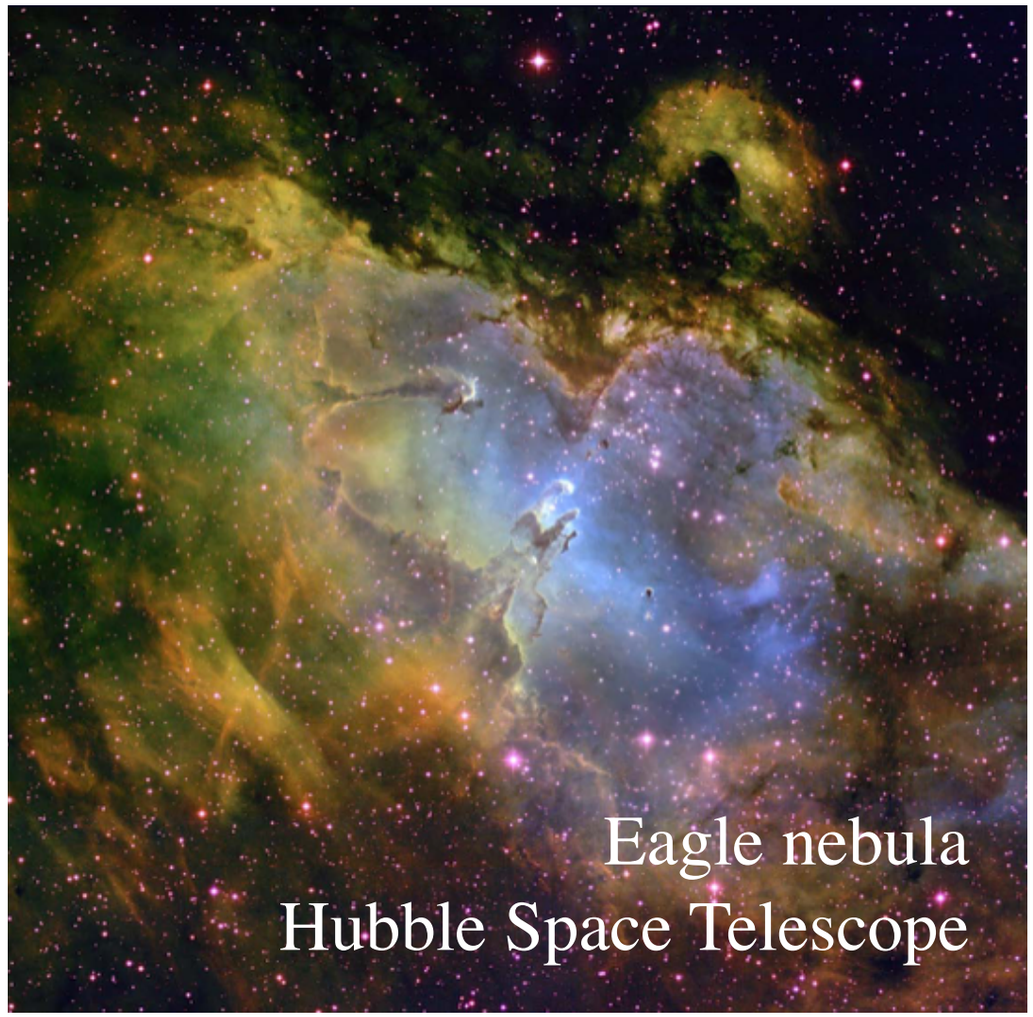

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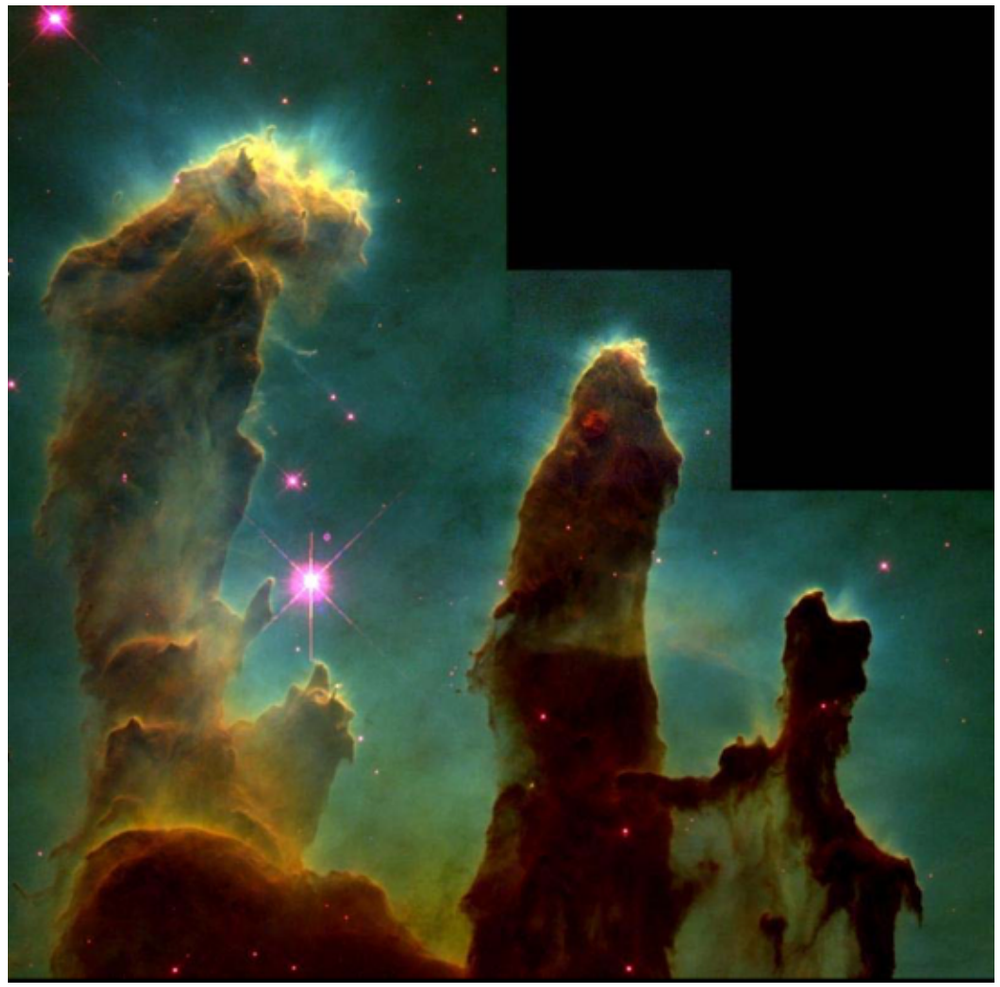

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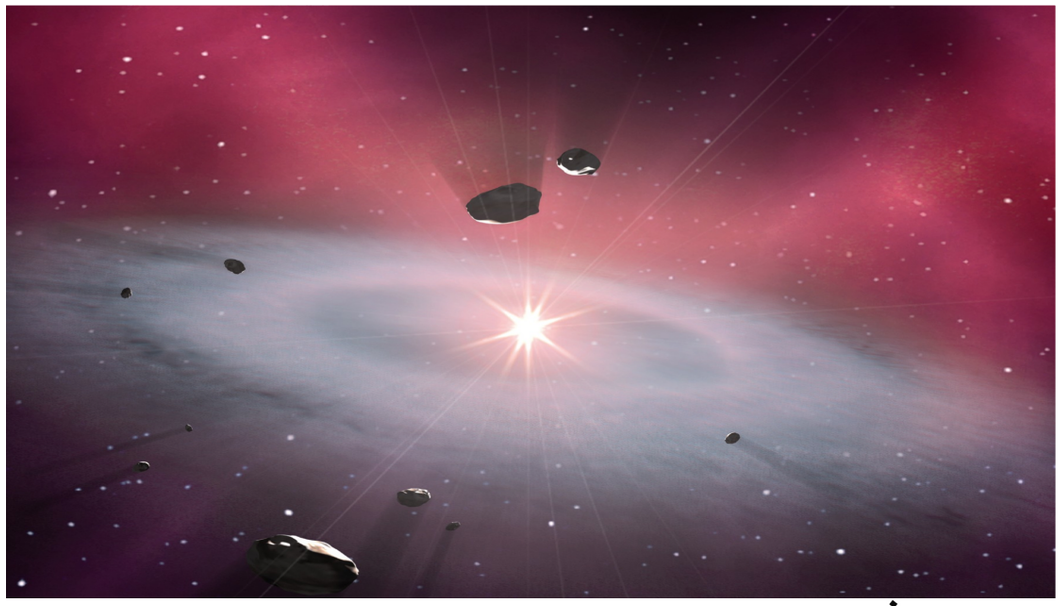

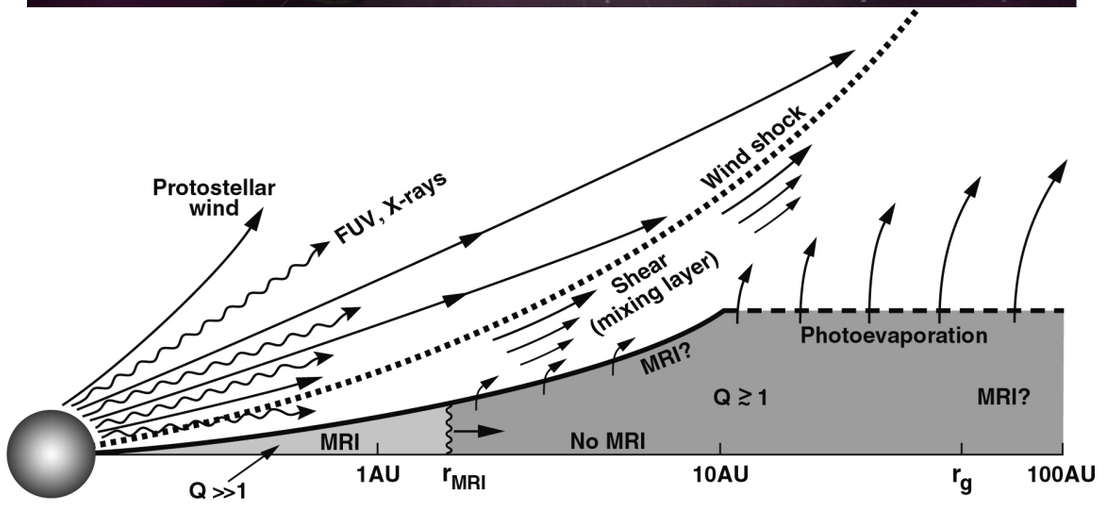

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Why studying PDRs ?

- 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

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

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

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- - advection

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- - advection - - compression

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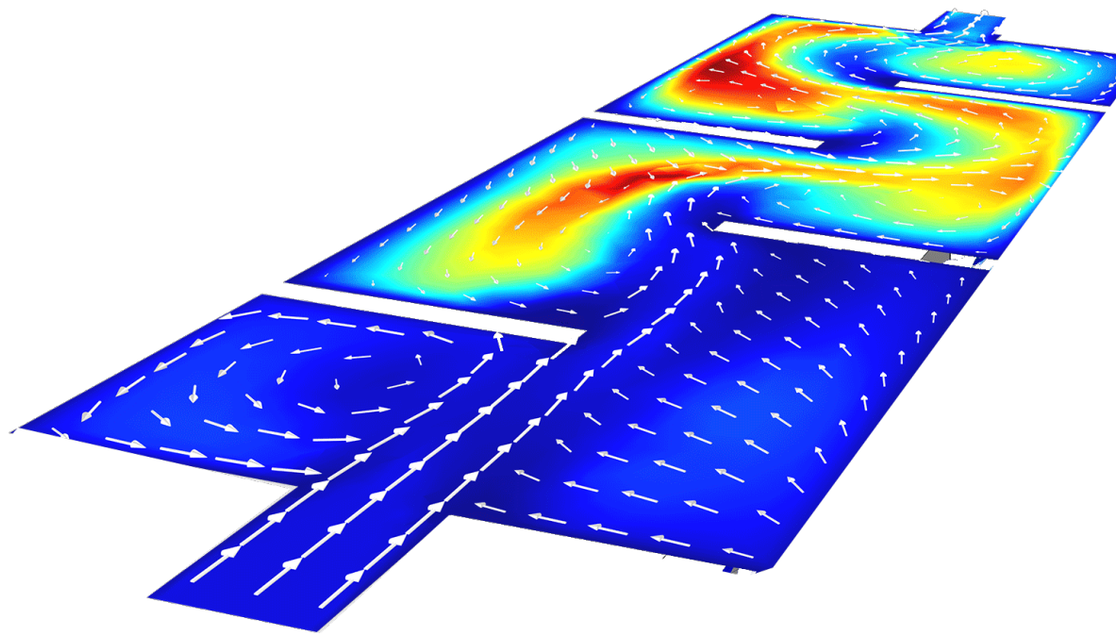
- - advection - - compression - - thermo-chemistry - - diffusion

Simplifications

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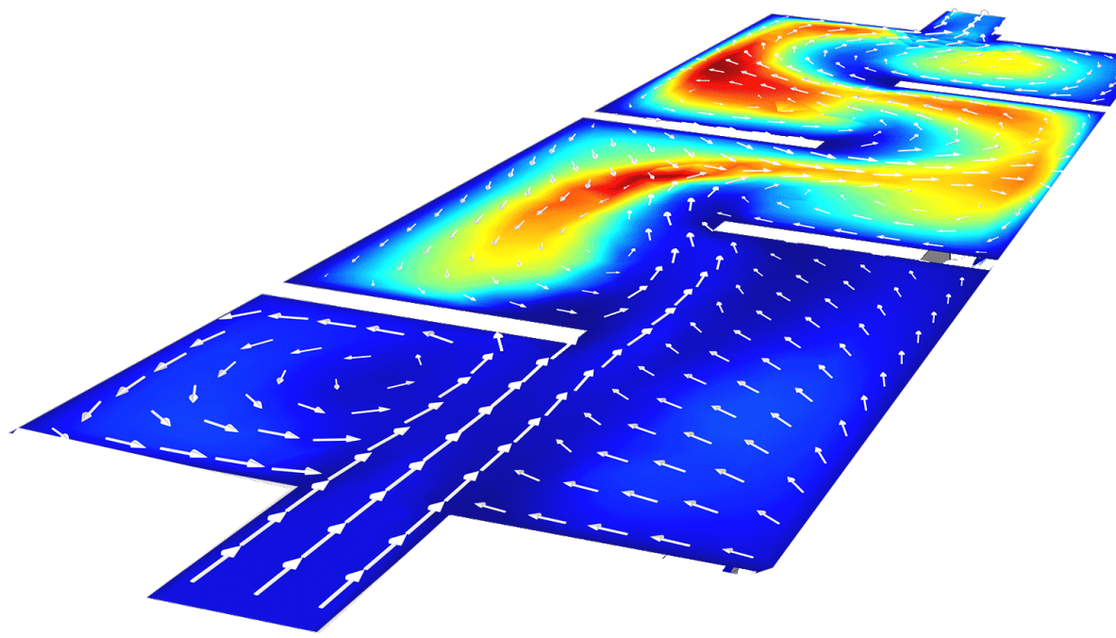
- number of spatial dimensions (2D, 1D, 0D)



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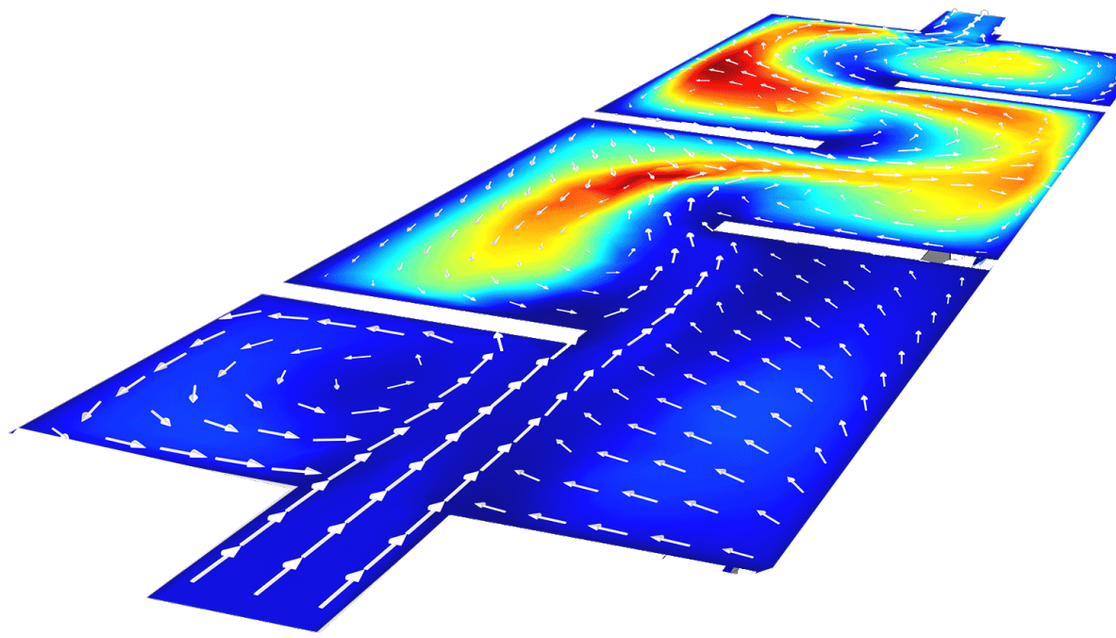

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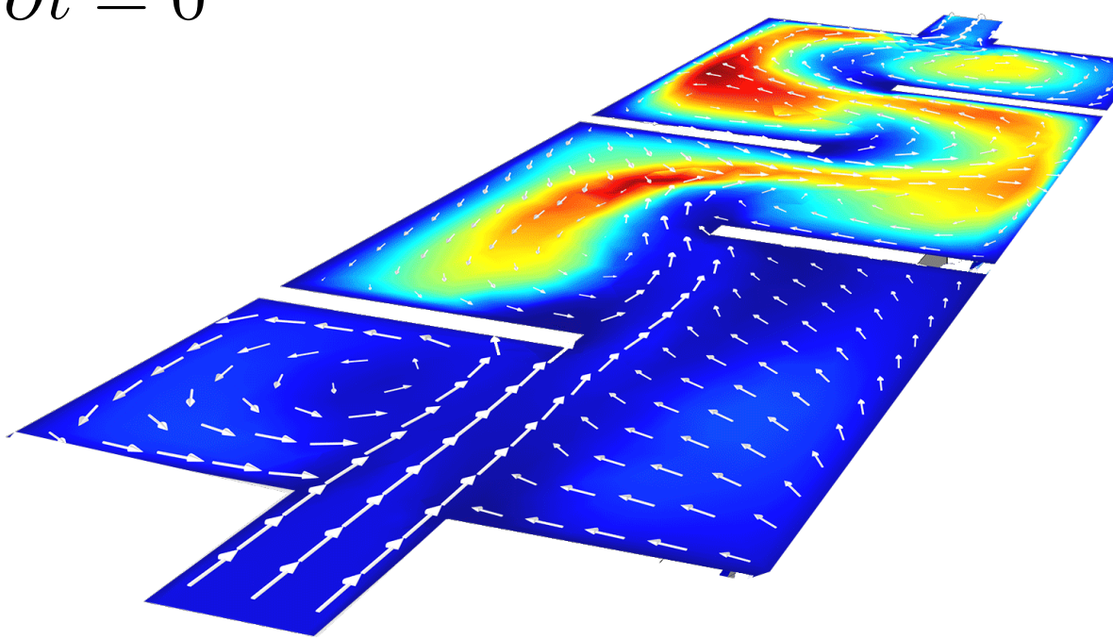
- steady-state (stationary) $\partial/\partial t = 0$



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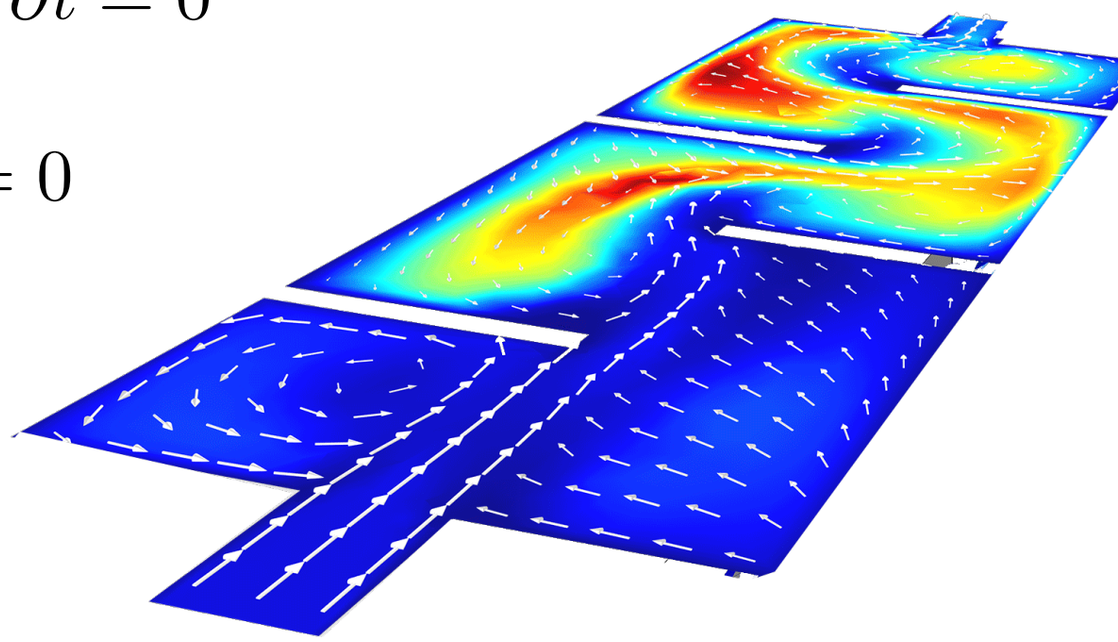
Main simplifications

- 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

Meudon PDR : method

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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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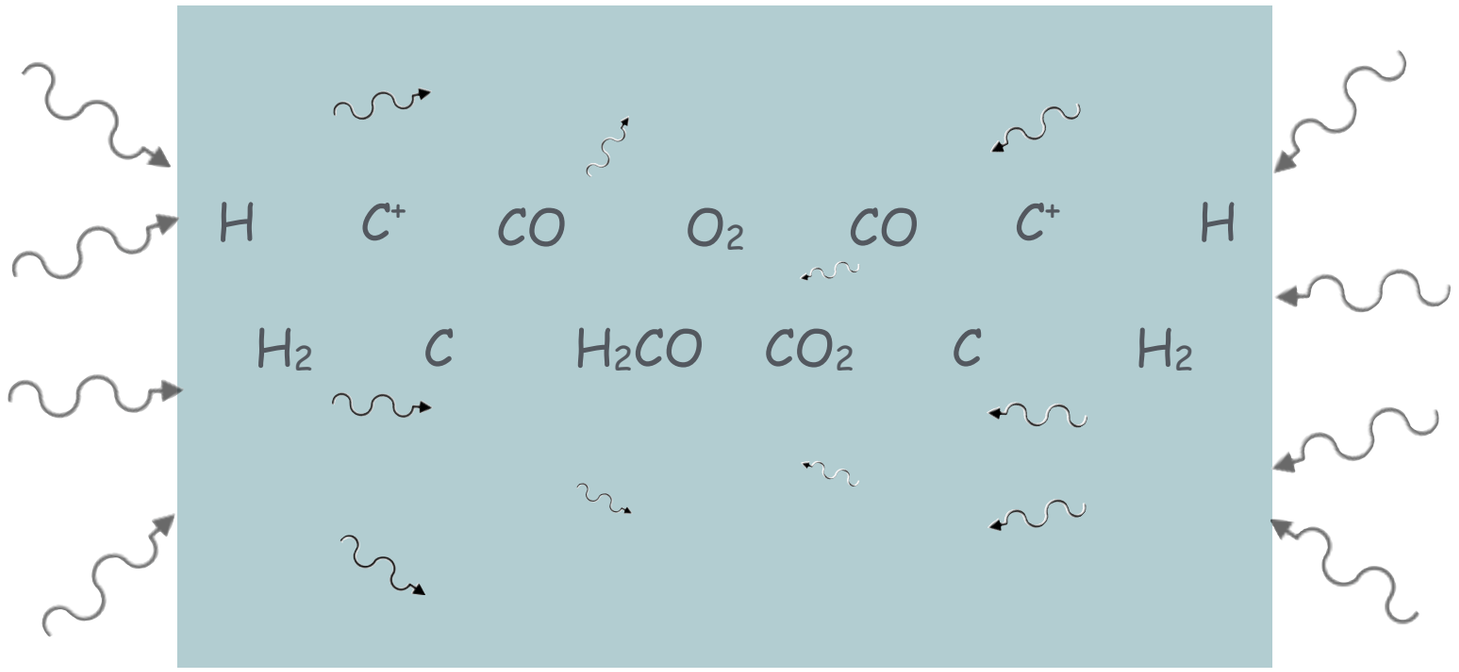

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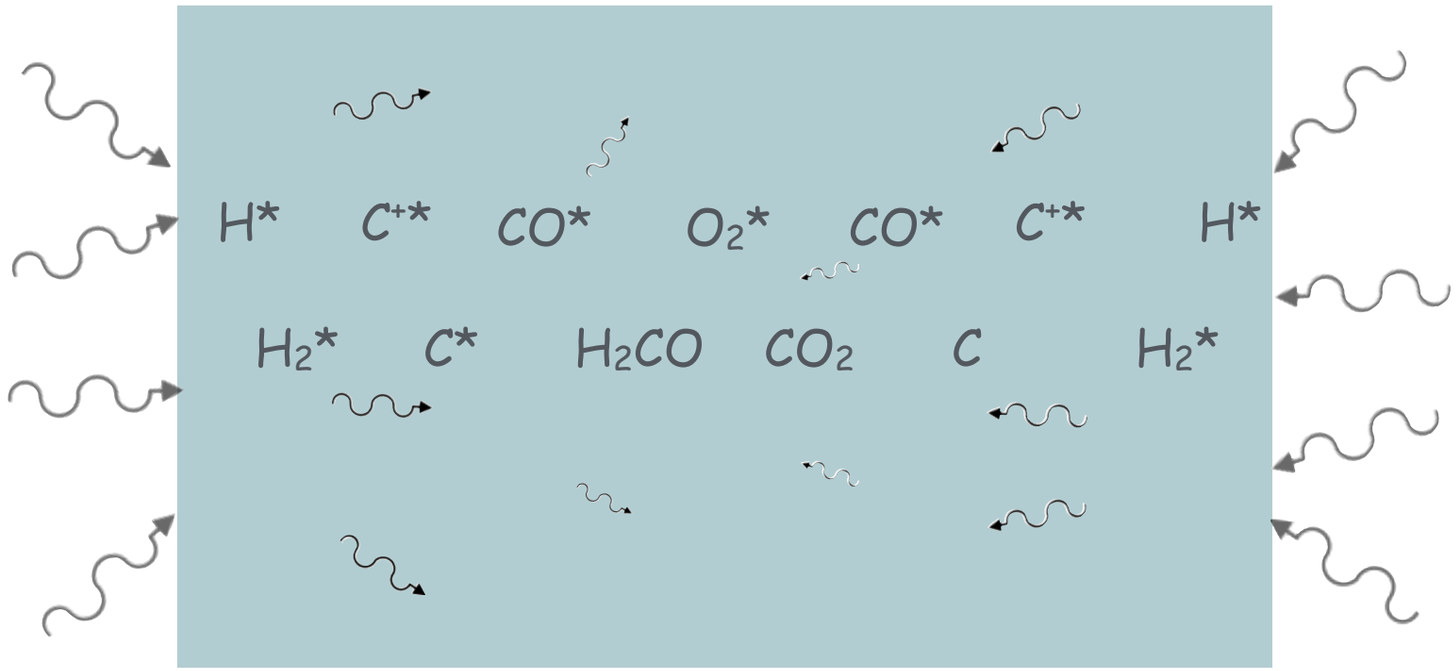

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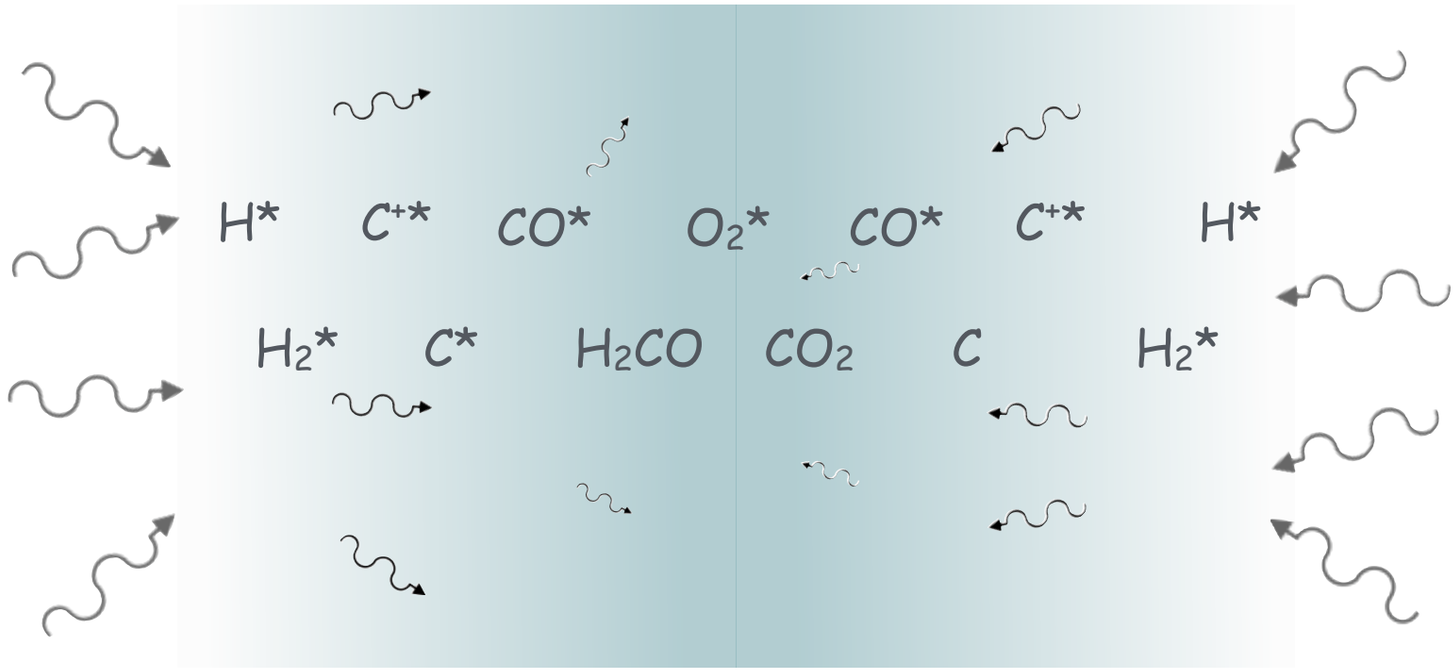

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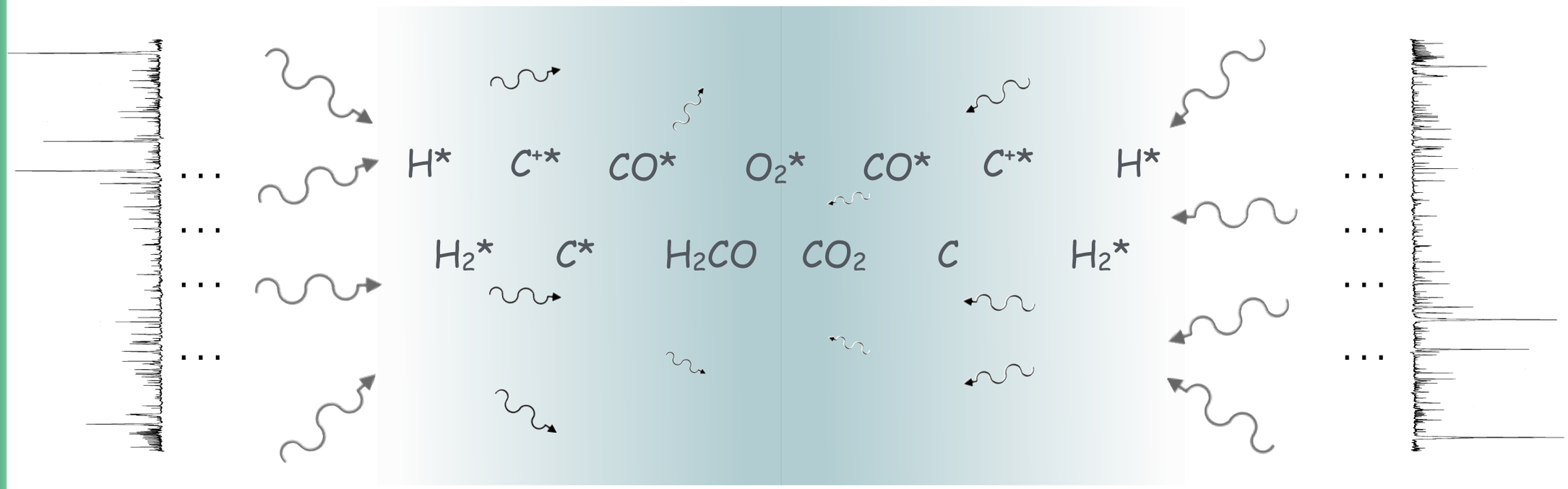
- dust treatment
  charge, emissivities
- excitation (thousands levels)
- tens thousands lines



Meudon PDR : advantages and limitations

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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 $t_{\rm if} \sim 3 \times 10^5 \left(\frac{10^3}{n_{\rm H}}\right) \left(\frac{N_0}{10^{21}}\right)\ {\rm yr}$

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

Meudon PDR : advantages and limitations

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

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

↓

initial conditions
chemical & temperature profiles, …

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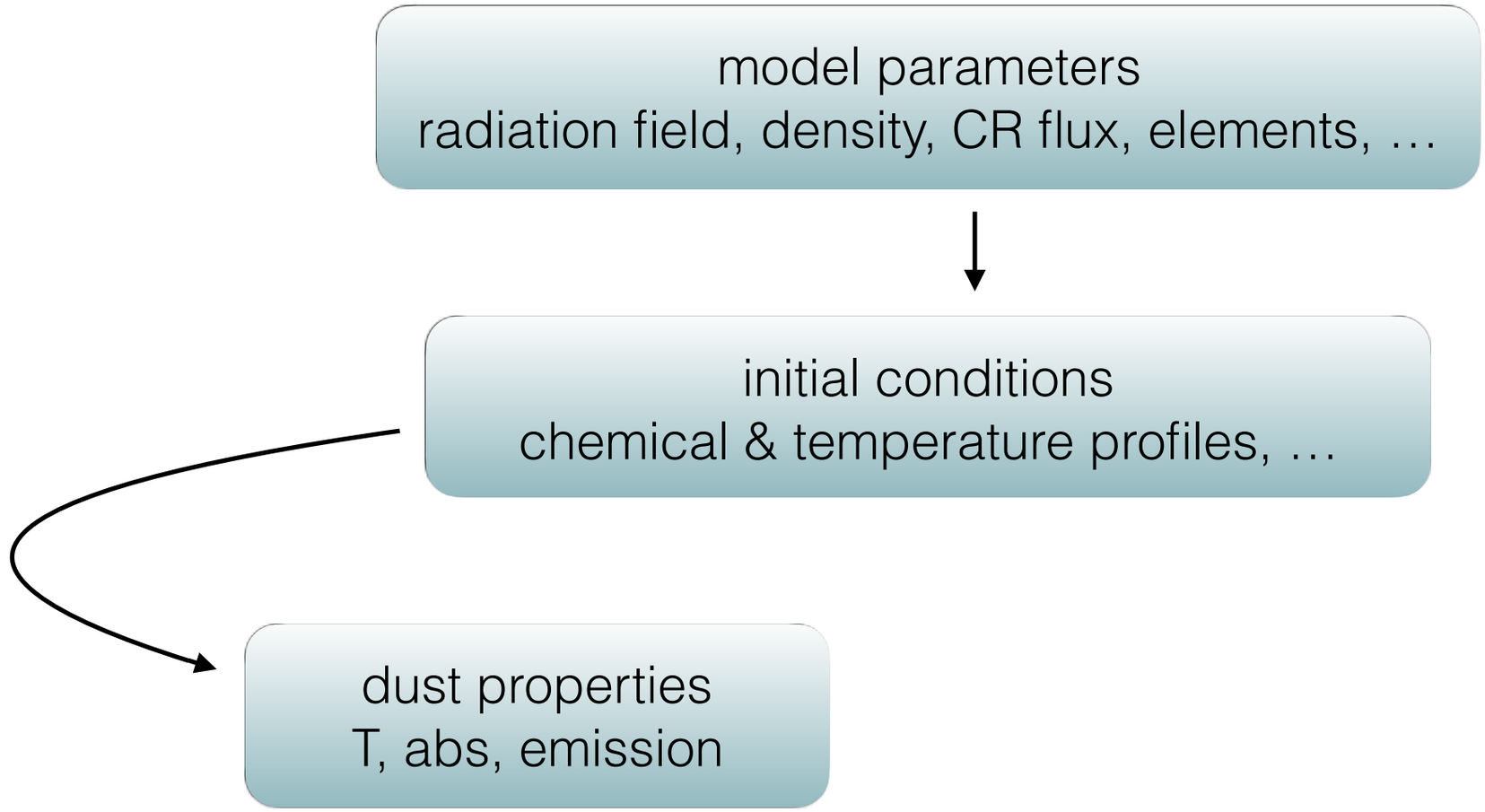
Iterative procedure



Iterative procedure

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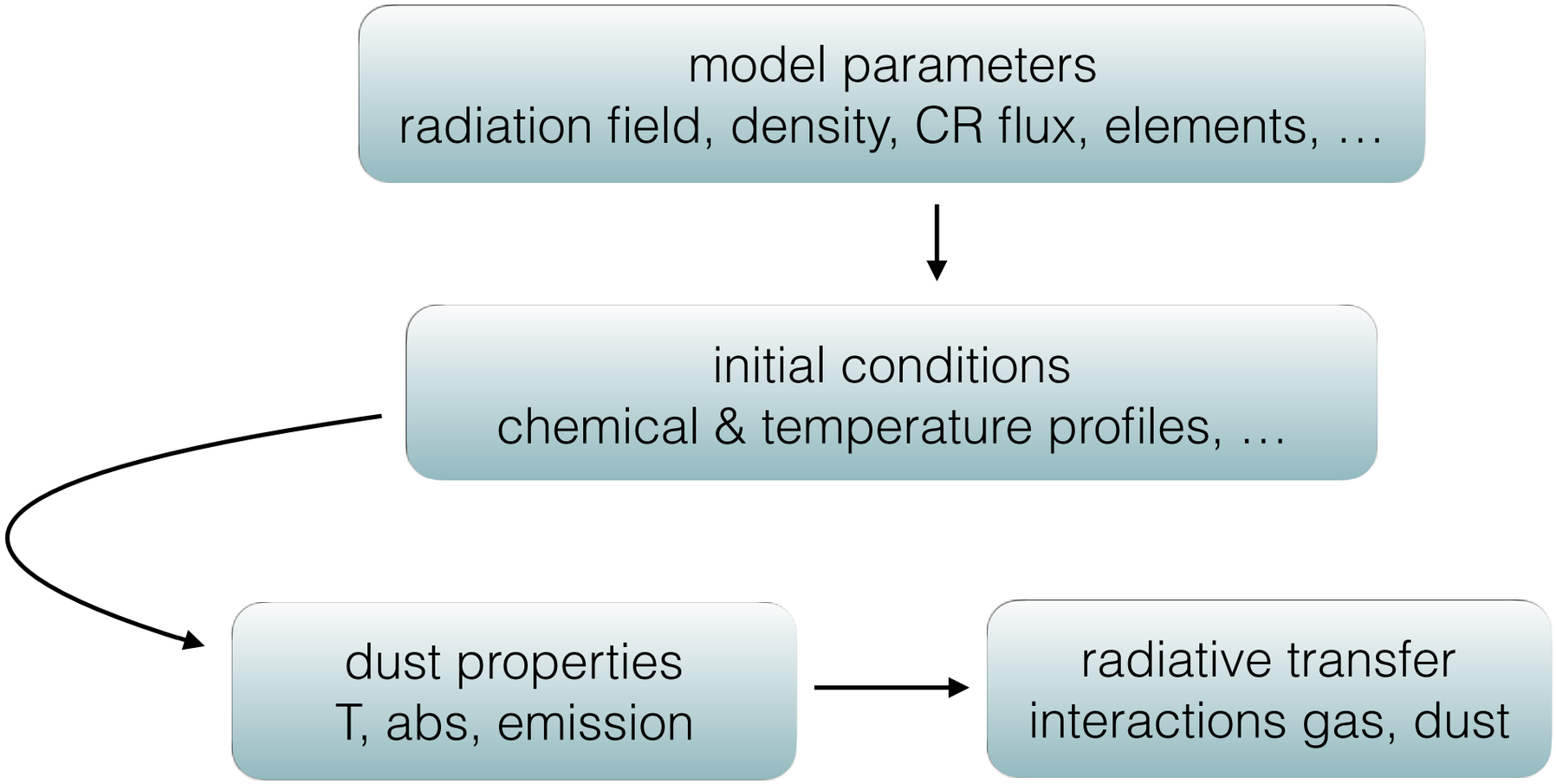
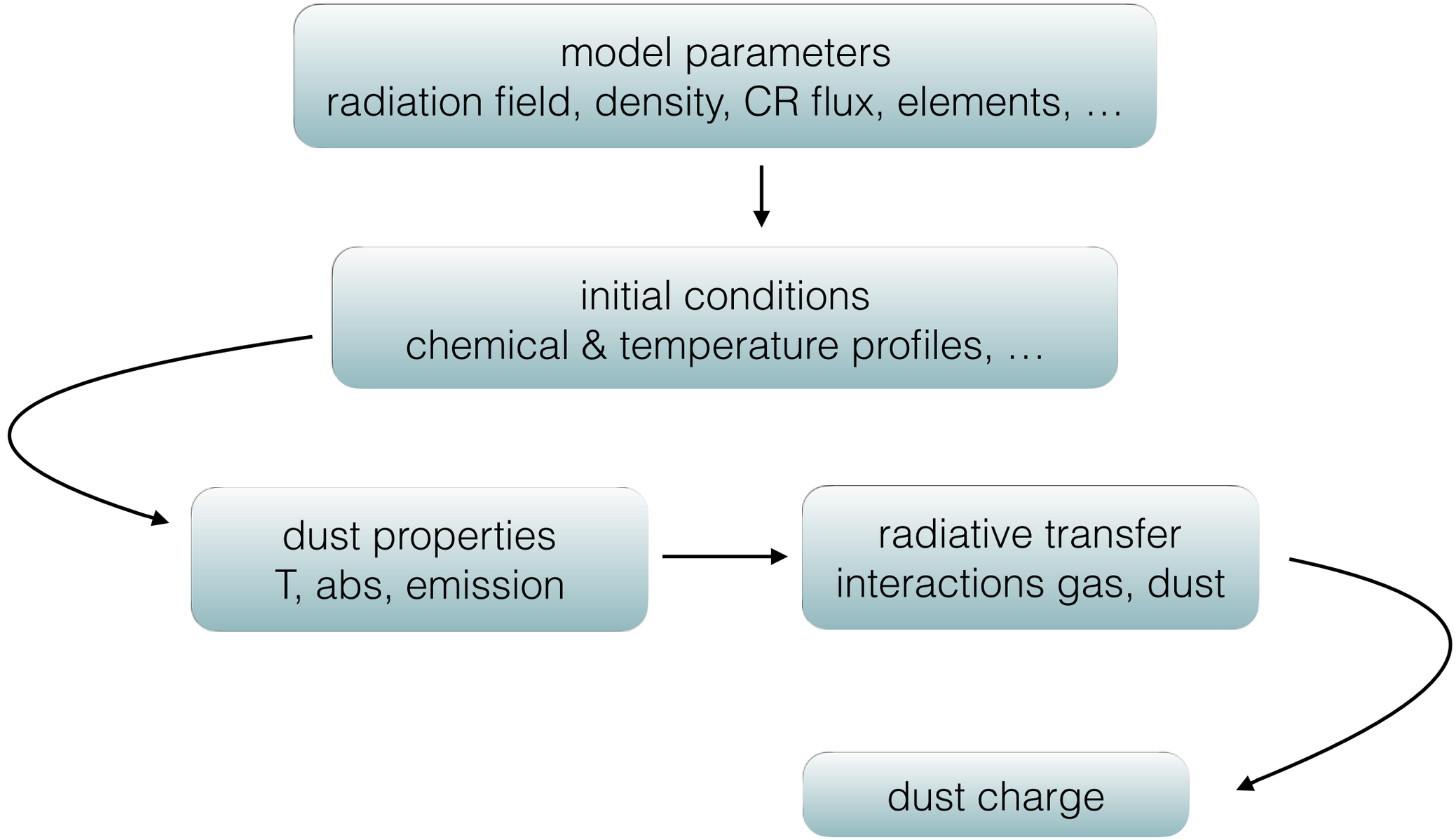


Iterative procedure

Outline

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



Iterative procedure

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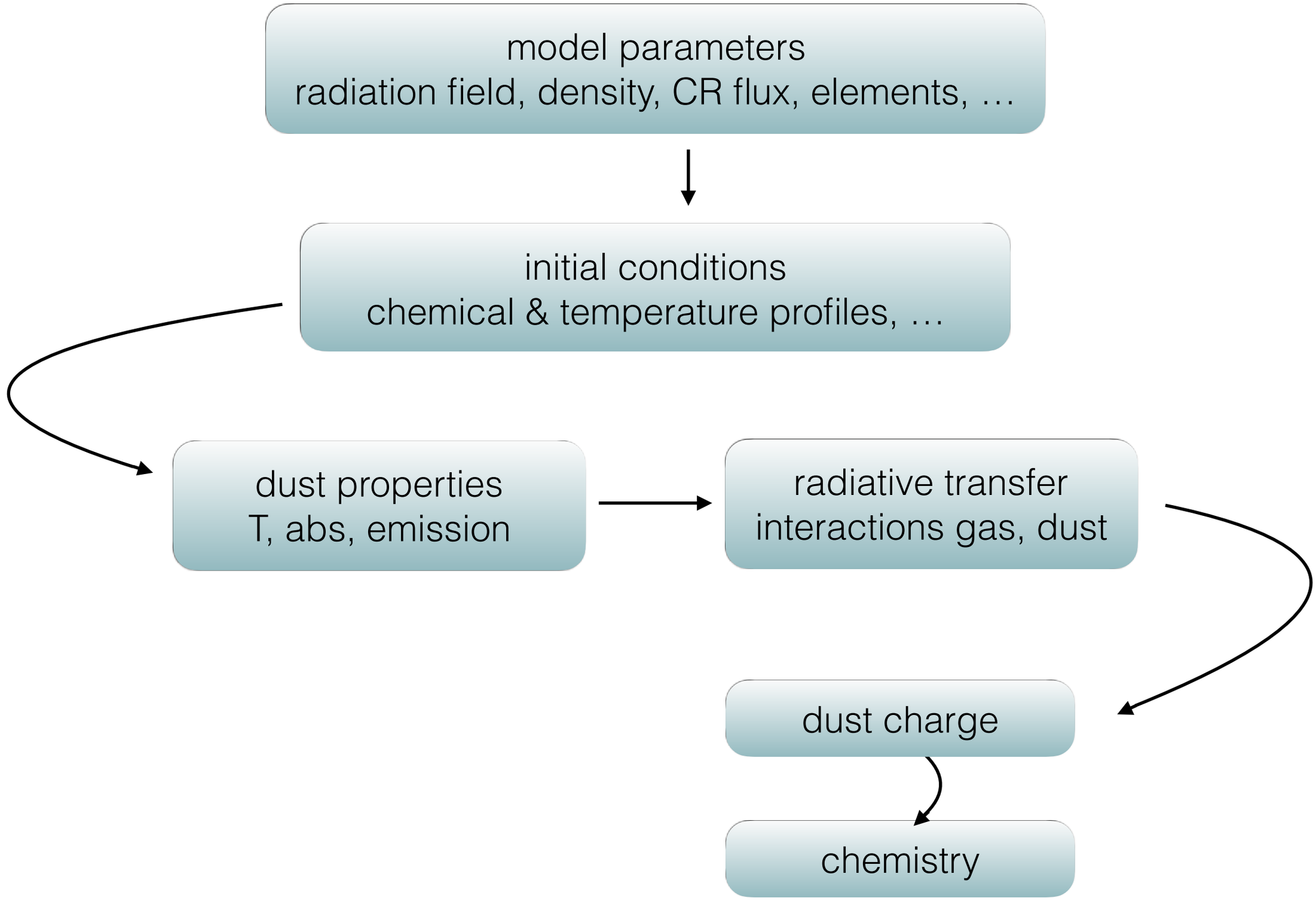

Iterative procedure

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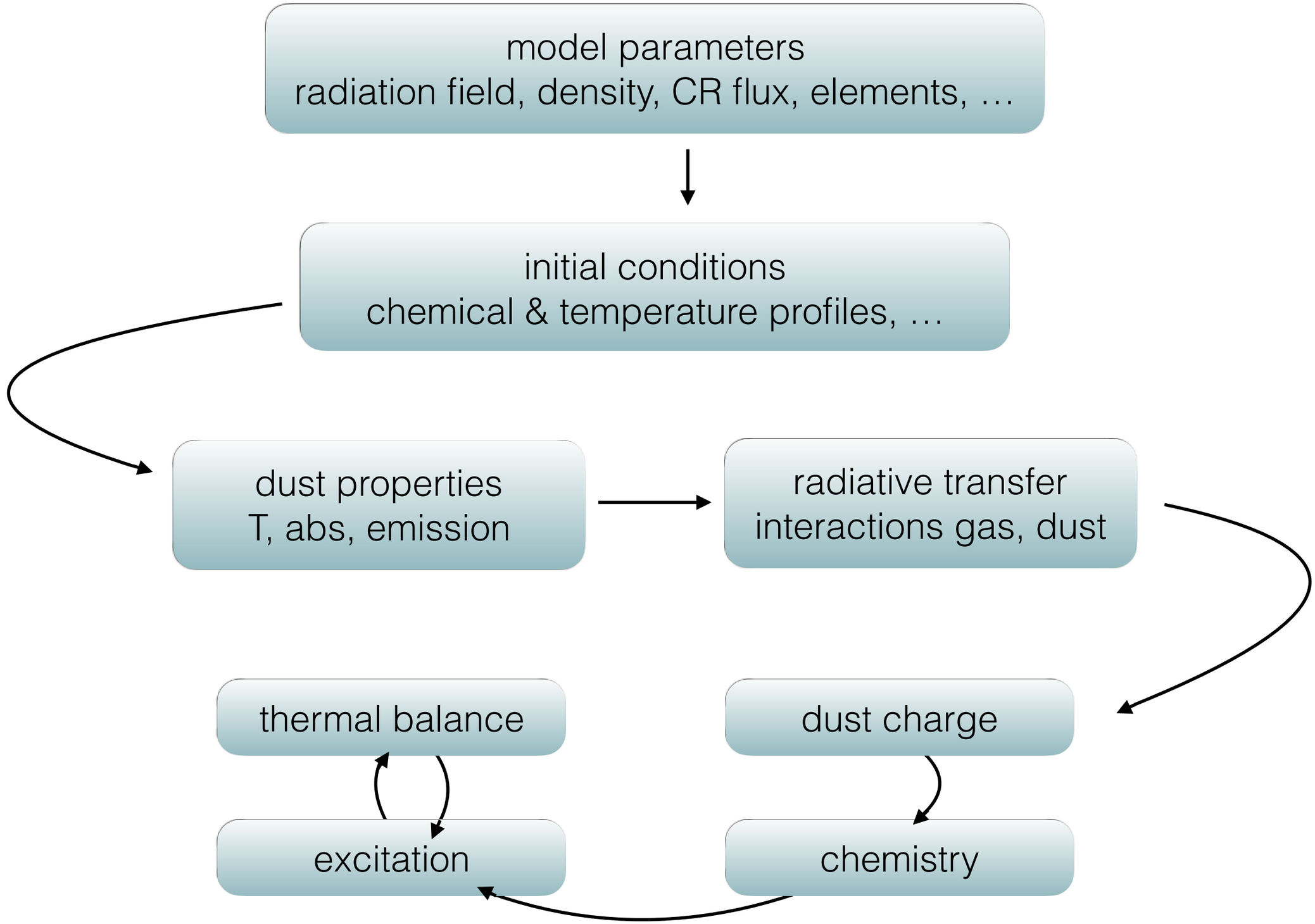

Iterative procedure

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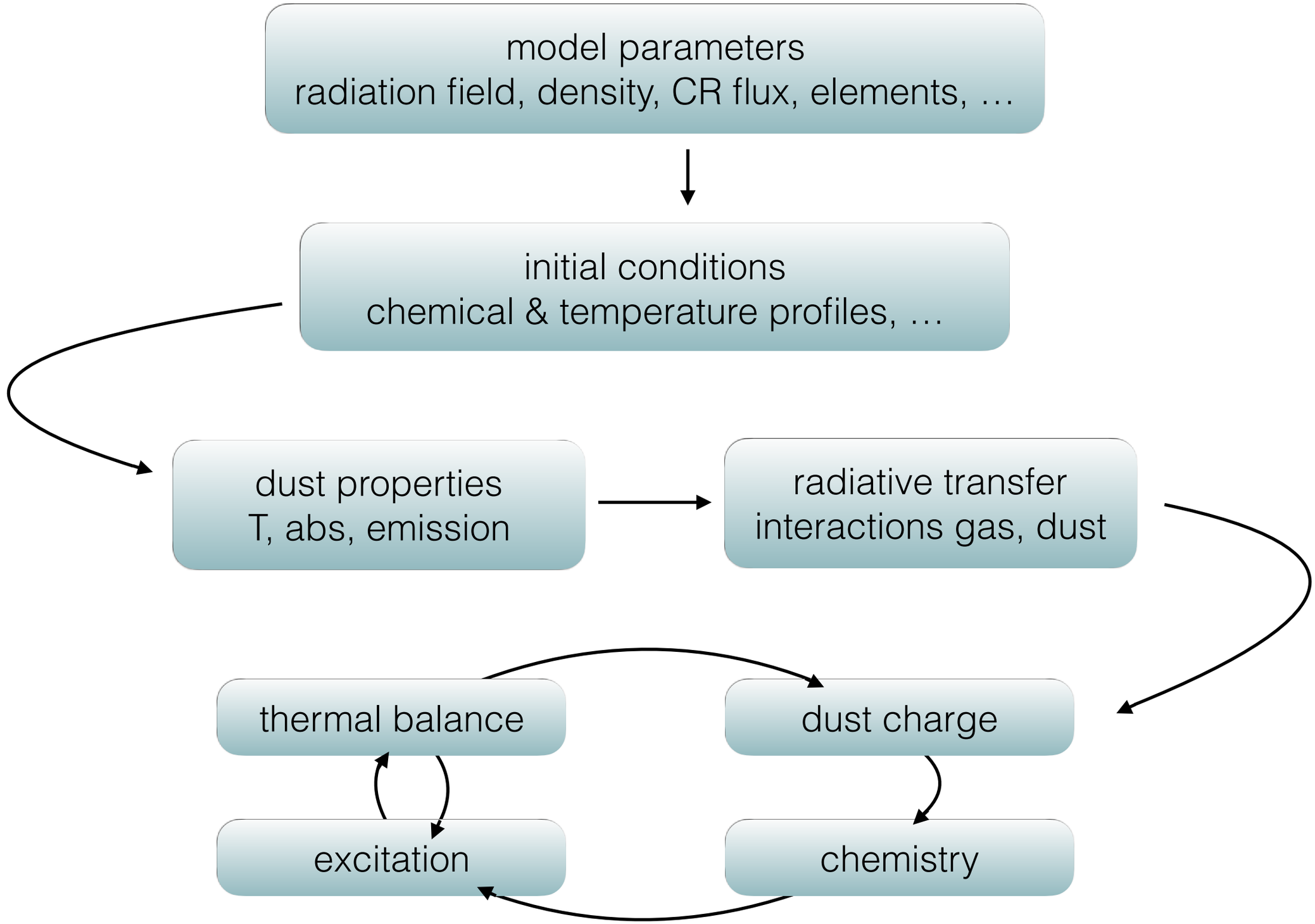

Iterative procedure

Outline

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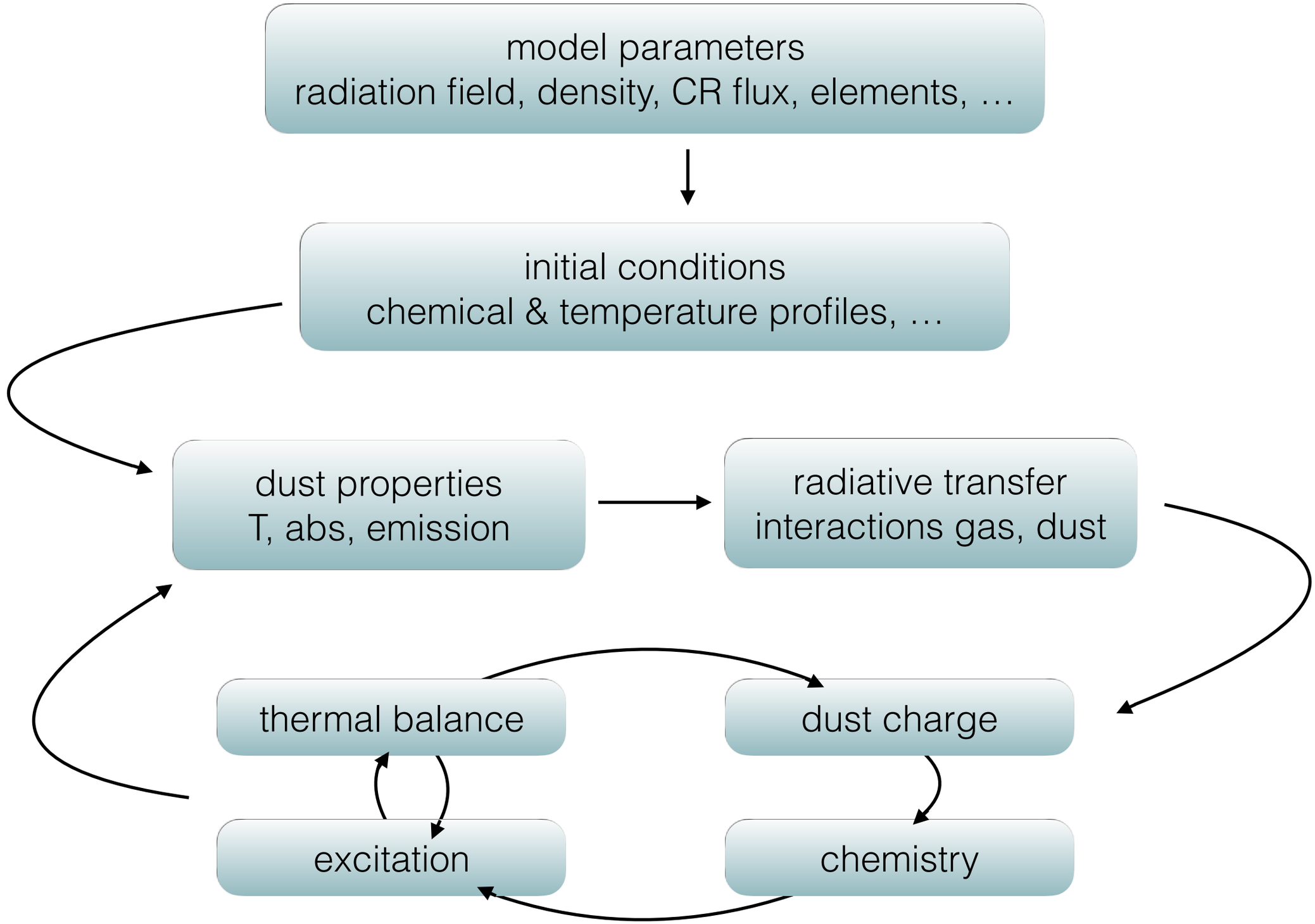

Iterative procedure

Outline

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Computational time

⇒ Radiative transfer and statistical treatments are time consuming

⇒ Chemistry and thermal balance are fast

Iterative procedure

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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

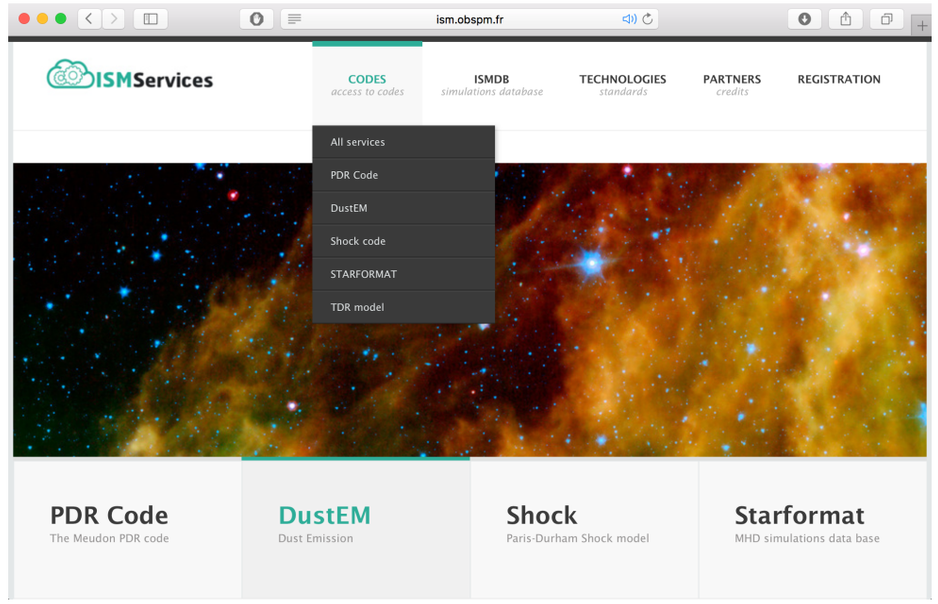
Outline

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

- download from the platform

  ism.obspm.fr

  code & documentation



ISM plateform

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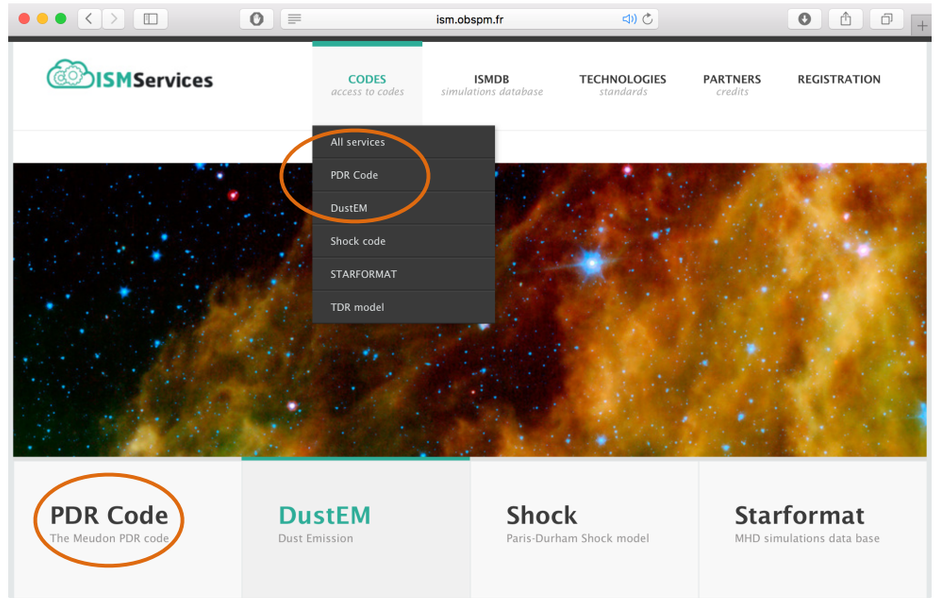

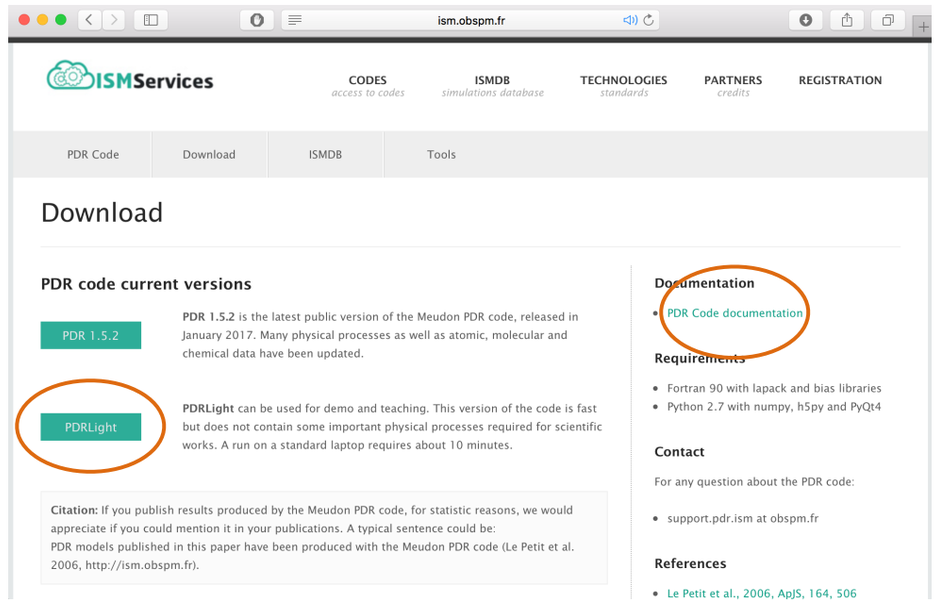

ISM plateform

Outline

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- assumptions
- user guide first steps
- examples

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  ism.obspm.fr

  code & documentation

- untar and compile

  fortran compiler / librairies

  python2.7 / librairies

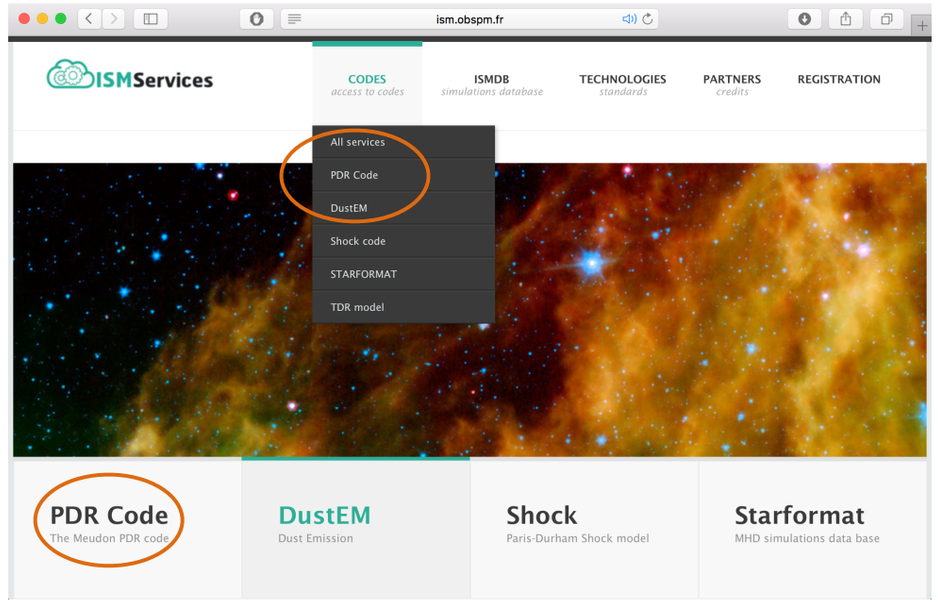
  web browser

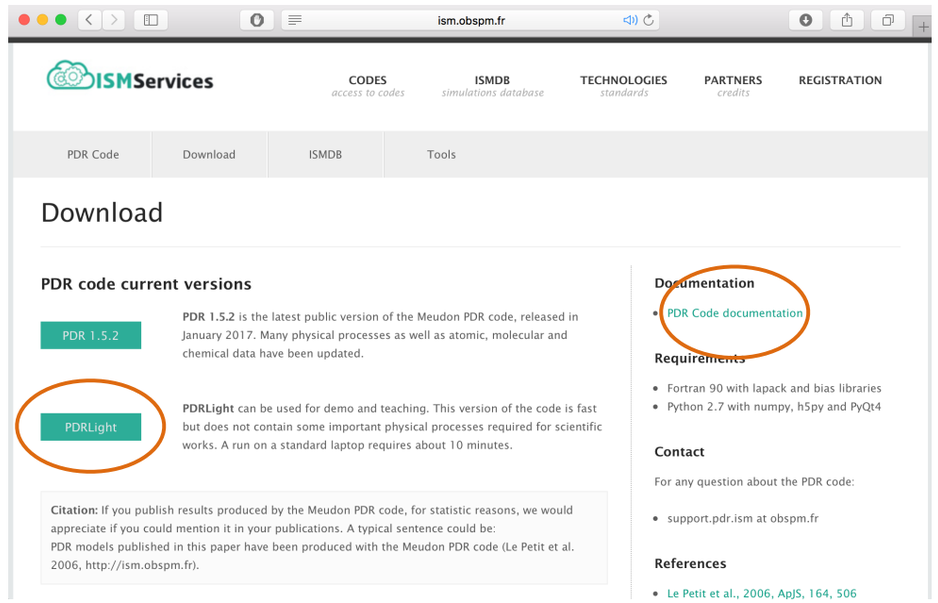
- prepare the input files

  end criterion

  output options

- run the model
- extract & analyse the results

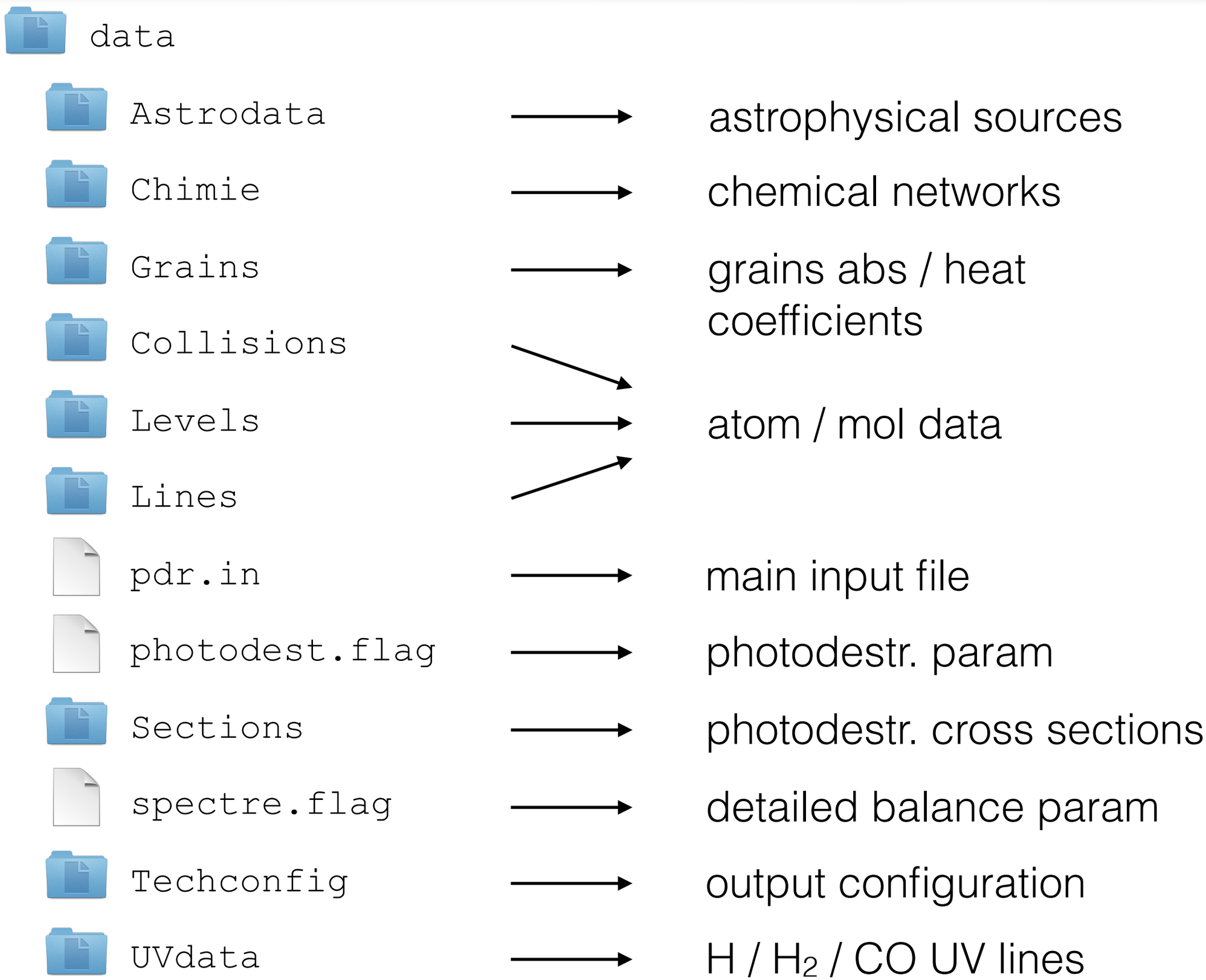




Inputs

`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



Inputs

Outline

- introduction on PDRs
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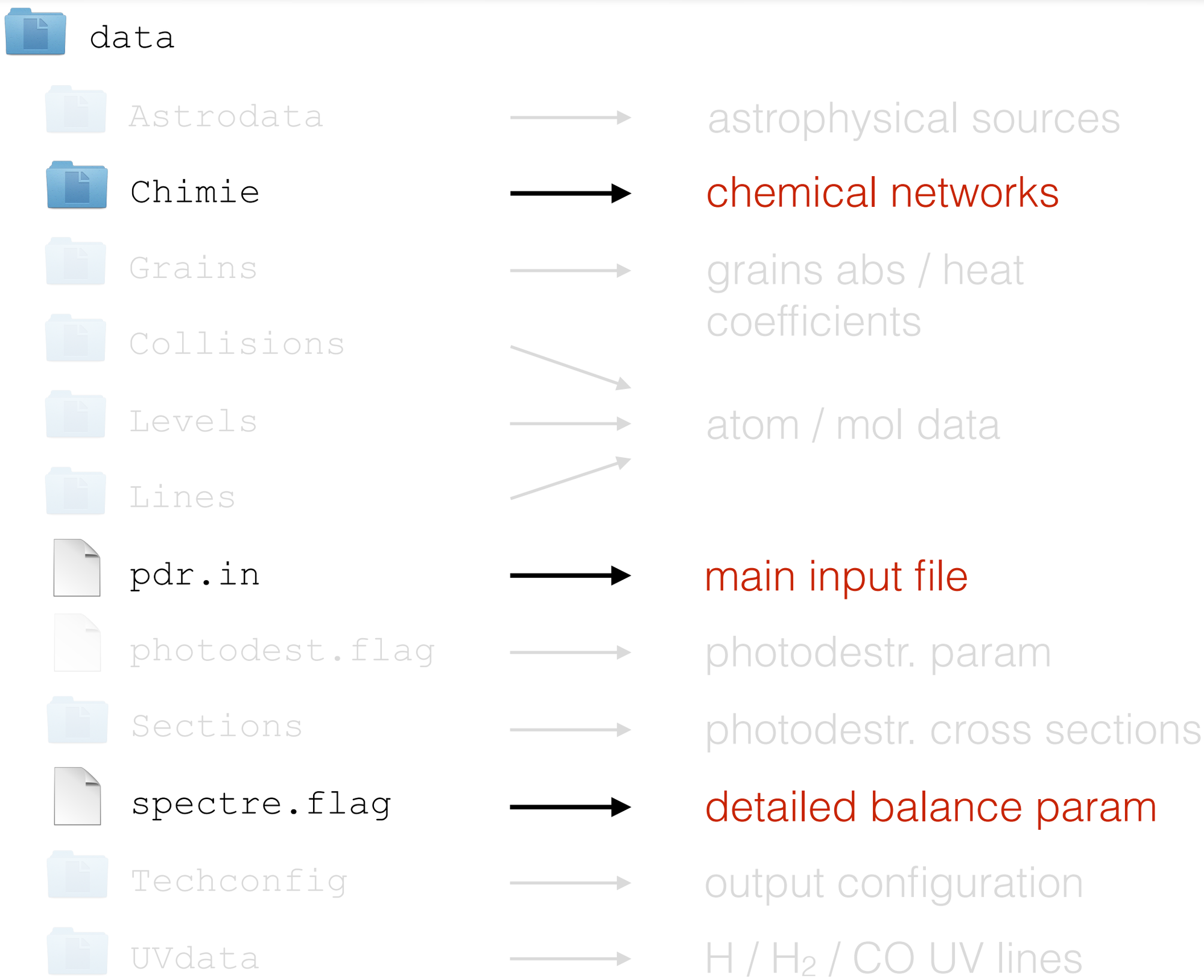

Inputs

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)
  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%

Outline

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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
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31     0                    ! F_W_ALL_IFAF : 1 = Write output f
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```

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parameters descrip

Outline

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parameters descrip

in & out files

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31     0                          ! F_W_ALL_IFAF : 1 = Write output f
32
```

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parameters descrip

in & out files

main parameters

Outline

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

Inputs

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
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```

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

parameters descrip

in & out files

main parameters

extinction curve

Outline

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Inputs

Main input file : `pdr.in`

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```
1   ExampleDiffuse                ! modele   : Output files radix
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3   1                             ! ifafm    : Number of global itera
4   3.00e+00                      ! Avmax    : Integration limit (Av)
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12     1                          ! ieqth    : thermal Balance (1 : s
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16  1.00e+06                      ! presse   : Initial Pressure (cm-3
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28     0                          ! F_DUST_P : 0 - Without DUSTEM, F&
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31     0                          ! F_W_ALL_IFAF : 1 = Write output f
32
```

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parameters descrip

in & out files

main parameters

extinction curve

dust model

Inputs

Outline

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Chemistry file

`ch1612_iso_Mathis.chi`

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

(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
 11 ¬
343  -                  -¬
344  -                  - cosmic-ray direct processes¬
345  -                  -¬
346 jan11 h2      crp     h       h                     1.00E-01   .00      .00   1
347 jan11 h       crp     h+      electr                4.60E-01   .00      .00   1
348 jan11 h2      crp     h+      h       electr        4.00E-02   .00      .00   1
349 jan11 h2      crp     h2+     electr                9.60E-01   .00      .00   1
350 ¬
535  -                  -¬
536  -                  - neutral-neutral reactions¬
537  -                  -¬
538 jan11 h       n2      nh      n                     8.63E-11   .50 71457.00   4
539 jan11 h       nh      n       h2                    8.19E-11   .68   950.00   4
540 jan11 h       no      n       oh                    3.60E-10   .00 24912.00   4
541 ¬
2958 -                  -¬
2959 -                  - photoprocesses (ISRF of Mathis et al 1983)¬
2960 -                  -¬
2961 jan11 ch     photon  c       h                     6.60E-10   .00     1.15   5
2962 jan11 ch2    photon  ch      h                     4.90E-10   .00     1.67   5
2963 jan11 ch3    photon  ch2     h                     3.20E-10   .00     1.88   5
2964 jan11 ch3    photon  ch      h2                    3.20E-10   .00     1.88   5
2965 ¬
3194 -                  -¬
3195 -                  - Ions and electrons / Grains¬
3196 -                  -¬
3197 NEUTR h+     grain   h                             1.00E+00  0.00     0.00  14
3198 NEUTR he+    grain   he                            1.00E+00  0.00     0.00  14
3199 NEUTR c+     grain   c                             1.00E+00  0.00     0.00  14
3200 NEUTR o+     grain   o                             1.00E+00  0.00     0.00  14
3201 NEUTR n+     grain   n                             1.00E+00  0.00     0.00  14
3202 NEUTR s+     grain   s                             1.00E+00  0.00     0.00  14
3203 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
 11  ...
343  -                   -
344  -                   - cosmic-ray direct processes
345  -                   -
346  jan11 h2      crp     h       h                      1.00E-01   .00      .00   1
347  jan11 h       crp     h+      electr                 4.60E-01   .00      .00   1
348  jan11 h2      crp     h+      h       electr         4.00E-02   .00      .00   1
349  jan11 h2      crp     h2+     electr                 9.60E-01   .00      .00   1
350  ...
535  -                   -
536  -                   - neutral-neutral reactions
537  -                   -
538  jan11 h       n2      nh      n                      8.63E-11   .50 71457.00   4
539  jan11 h       nh      n       h2                     8.19E-11   .68   950.00   4
540  jan11 h       no      n       oh                     3.60E-10   .00 24912.00   4
541  ...
2958 -                   -
2959 -                   - photoprocesses (ISRF of Mathis et al 1983)
2960 -                   -
2961 jan11 ch      photon  c       h                      6.60E-10   .00     1.15   5
2962 jan11 ch2     photon  ch      h                      4.90E-10   .00     1.67   5
2963 jan11 ch3     photon  ch2     h                      3.20E-10   .00     1.88   5
2964 jan11 ch3     photon  ch      h2                     3.20E-10   .00     1.88   5
2965 ...
3194 -                   -
3195 -                   - Ions and electrons / Grains
3196 -                   -
3197 NEUTR h+      grain   h                              1.00E+00  0.00     0.00  14
3198 NEUTR he+     grain   he                             1.00E+00  0.00     0.00  14
3199 NEUTR c+      grain   c                              1.00E+00  0.00     0.00  14
3200 NEUTR o+      grain   o                              1.00E+00  0.00     0.00  14
3201 NEUTR n+      grain   n                              1.00E+00  0.00     0.00  14
3202 NEUTR s+      grain   s                              1.00E+00  0.00     0.00  14
3203 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

`ch1612_iso_Mathis.chi`

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

(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
 11  ...
343  -                   -
344  -                   - cosmic-ray direct processes
345  -                   -
346 jan11 h2      crp     h       h                     1.00E-01   .00      .00   1
347 jan11 h       crp     h+      electr                4.60E-01   .00      .00   1
348 jan11 h2      crp     h+      h       electr        4.00E-02   .00      .00   1
349 jan11 h2      crp     h2+     electr                9.60E-01   .00      .00   1
350  ...
535  -                   -
536  -                   - neutral-neutral reactions
537  -                   -
538 jan11 h       n2      nh      n                     8.63E-11   .50 71457.00   4
539 jan11 h       nh      n       h2                    8.19E-11   .68   950.00   4
540 jan11 h       no      n       oh                    3.60E-10   .00 24912.00   4
541  ...
2958 -                   -
2959 -                   - photoprocesses (ISRF of Mathis et al 1983)
2960 -                   -
2961 jan11 ch     photon  c       h                     6.60E-10   .00     1.15   5
2962 jan11 ch2    photon  ch      h                     4.90E-10   .00     1.67   5
2963 jan11 ch3    photon  ch2     h                     3.20E-10   .00     1.88   5
2964 jan11 ch3    photon  ch      h2                    3.20E-10   .00     1.88   5
2965 ...
3194 -                   -
3195 -                   - Ions and electrons / Grains
3196 -                   -
3197 NEUTR h+     grain   h                             1.00E+00  0.00     0.00  14
3198 NEUTR he+    grain   he                            1.00E+00  0.00     0.00  14
3199 NEUTR c+     grain   c                             1.00E+00  0.00     0.00  14
3200 NEUTR o+     grain   o                             1.00E+00  0.00     0.00  14
3201 NEUTR n+     grain   n                             1.00E+00  0.00     0.00  14
3202 NEUTR s+     grain   s                             1.00E+00  0.00     0.00  14
3203 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

`ch1612_iso_Mathis.chi`

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

(New Document)

```
1    #INCHI num  espece    hcnohe isot metos  metos  - abinit-rel enthalpf  INCHIKeyis
2    #---------1---------2---------3---------4---------5---------6---------7----------
3      1  h         1 0000 0000 00000 000000  0   .800E+00   51.634  YZCKVEUIGOORGS-UH
4      2  d         0 0000 1000 00000 000000  0   .000E+00   52.520  NOINCHIFOUND
5      3  h2        2 0000 0000 00000 000000  0   .100E+00     .000  UFHFLCQGNIYNRP-UH
6      4  hd        1 0000 1000 00000 000000  0  1.500E-05    0.079  NOINCHIFOUND
7      5  he        0 0001 0000 00000 000000  0   .100E+00     .000  SWQJXJOGLNCZEY-UH
8      6  c         0 1000 0000 00000 000000  0   .000E+00  169.978  OKTJSMMVPCPJKN-UH
9      7  c*        0 0000 0100 00000 000000  0   .000E+00  169.978  NOINCHIFOUND
10     8  ch        1 1000 0000 00000 000000  0   .000E+00  141.177  VRLIPUYDFBXWCH-UH
11   ...
343    -                  -
344    -                  - cosmic-ray direct processes
345    -                  -
346  jan11 h2      crp     h       h                      1.00E-01   .00      .00   1
347  jan11 h       crp     h+      electr                 4.60E-01   .00      .00   1
348  jan11 h2      crp     h+      h       electr         4.00E-02   .00      .00   1
349  jan11 h2      crp     h2+     electr                 9.60E-01   .00      .00   1
350  ...
535    -                  -
536    -                  - neutral-neutral reactions
537    -                  -
538  jan11 h       n2      nh      n                      8.63E-11   .50 71457.00   4
539  jan11 h       nh      n       h2                     8.19E-11   .68   950.00   4
540  jan11 h       no      n       oh                     3.60E-10   .00 24912.00   4
541  ...
2958   -                  -
2959   -                  - photoprocesses (ISRF of Mathis et al 1983)
2960   -                  -
2961 jan11 ch      photon  c       h                      6.60E-10   .00     1.15   5
2962 jan11 ch2     photon  ch      h                      4.90E-10   .00     1.67   5
2963 jan11 ch3     photon  ch2     h                      3.20E-10   .00     1.88   5
2964 jan11 ch3     photon  ch      h2                     3.20E-10   .00     1.88   5
2965 ...
3194   -                  -
3195   -                  - Ions and electrons / Grains
3196   -                  -
3197 NEUTR h+      grain   h                              1.00E+00  0.00     0.00  14
3198 NEUTR he+     grain   he                             1.00E+00  0.00     0.00  14
3199 NEUTR c+      grain   c                              1.00E+00  0.00     0.00  14
3200 NEUTR o+      grain   o                              1.00E+00  0.00     0.00  14
3201 NEUTR n+      grain   n                              1.00E+00  0.00     0.00  14
3202 NEUTR s+      grain   s                              1.00E+00  0.00     0.00  14
3203 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

`ch1612_iso_Mathis.chi`

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

(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
 11 ...
343  -                   -
344  -                   - cosmic-ray direct processes
345  -                   -
346 jan11 h2      crp     h       h                      1.00E-01   .00      .00   1
347 jan11 h       crp     h+      electr                 4.60E-01   .00      .00   1
348 jan11 h2      crp     h+      h       electr         4.00E-02   .00      .00   1
349 jan11 h2      crp     h2+     electr                 9.60E-01   .00      .00   1
350 ...
535  -                   -
536  -                   - neutral-neutral reactions
537  -                   -
538 jan11 h       n2      nh      n                      8.63E-11   .50 71457.00   4
539 jan11 h       nh      n       h2                     8.19E-11   .68   950.00   4
540 jan11 h       no      n       oh                     3.60E-10   .00 24912.00   4
541 ...
2958 -                   -
2959 -                   - photoprocesses (ISRF of Mathis et al 1983)
2960 -                   -
2961 jan11 ch     photon  c       h                      6.60E-10   .00     1.15   5
2962 jan11 ch2    photon  ch      h                      4.90E-10   .00     1.67   5
2963 jan11 ch3    photon  ch2     h                      3.20E-10   .00     1.88   5
2964 jan11 ch3    photon  ch      h2                     3.20E-10   .00     1.88   5
2965 ...
3194 -                   -
3195 -                   - Ions and electrons / Grains
3196 -                   -
3197 NEUTR h+     grain   h                              1.00E+00  0.00     0.00  14
3198 NEUTR he+    grain   he                             1.00E+00  0.00     0.00  14
3199 NEUTR c+     grain   c                              1.00E+00  0.00     0.00  14
3200 NEUTR o+     grain   o                              1.00E+00  0.00     0.00  14
3201 NEUTR n+     grain   n                              1.00E+00  0.00     0.00  14
3202 NEUTR s+     grain   s                              1.00E+00  0.00     0.00  14
3203 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

`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

Outline

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

`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

use or drop species

Inputs

`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

use or drop species

use at least 10 lev of CO

use at most 64 lev of CO

Inputs

Outline

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

`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

use or drop species

use at least 10 lev of CO

use at most 64 lev of CO

use all levels of C^+

Run

Outline

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

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 -traceba
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
- user guide first steps
- examples

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)

```
#=======================================================================#
#                              IFORT (Intel)                            #
#=======================================================================#
#  FC = ifort
#
#- Version 14.0
#  FFLAGS = -g -O2 -parallel -mkl -xSSSE3 -axSSSE3 -m64
#  FFLAGS = -g3 -O0 -mkl -check all -warn all -check:noarg_temp_created -traceba
#
#  LIBS1 = -lpthread
#
#=======================================================================#
#                              GFORTRAN                                 #
#=======================================================================#
  FC = gfortran
#
# Options and Path
# FFLAGS = -g3 -O0 -fno-second-underscore -Wall -Wextra -Wno-compare-reals -fchec
# FFLAGS = -g -Ofast -fno-second-underscore -falign-loops=16 -march=corei7 -ffast
# FFLAGS = -g -O2    -fno-second-underscore -falign-loops=16 -march=corei7 -ffast
  FFLAGS = -g -O2    -fno-second-underscore -falign-loops=16 -ffast-math -fassoci
#
  LIBS1 = -llapack -lblas
#
#=======================================================================#
#                              G95                                      #
#=======================================================================#
# FC = g95
#
# Options and Path
# FFLAGS = -O2 -fno-second-underscore
# FFLAGS = -g3 -fno-second-underscore -Wall -Wextra -fbounds-check -ftrace=full -
# FFLAGS = -g3 -gdwarf-2 -fno-second-underscore -Wall -Wextra -fbounds-check -ftr
#
# LIBS1 = -llapack -lblas
#
```

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

Run (in the `src/` directory)

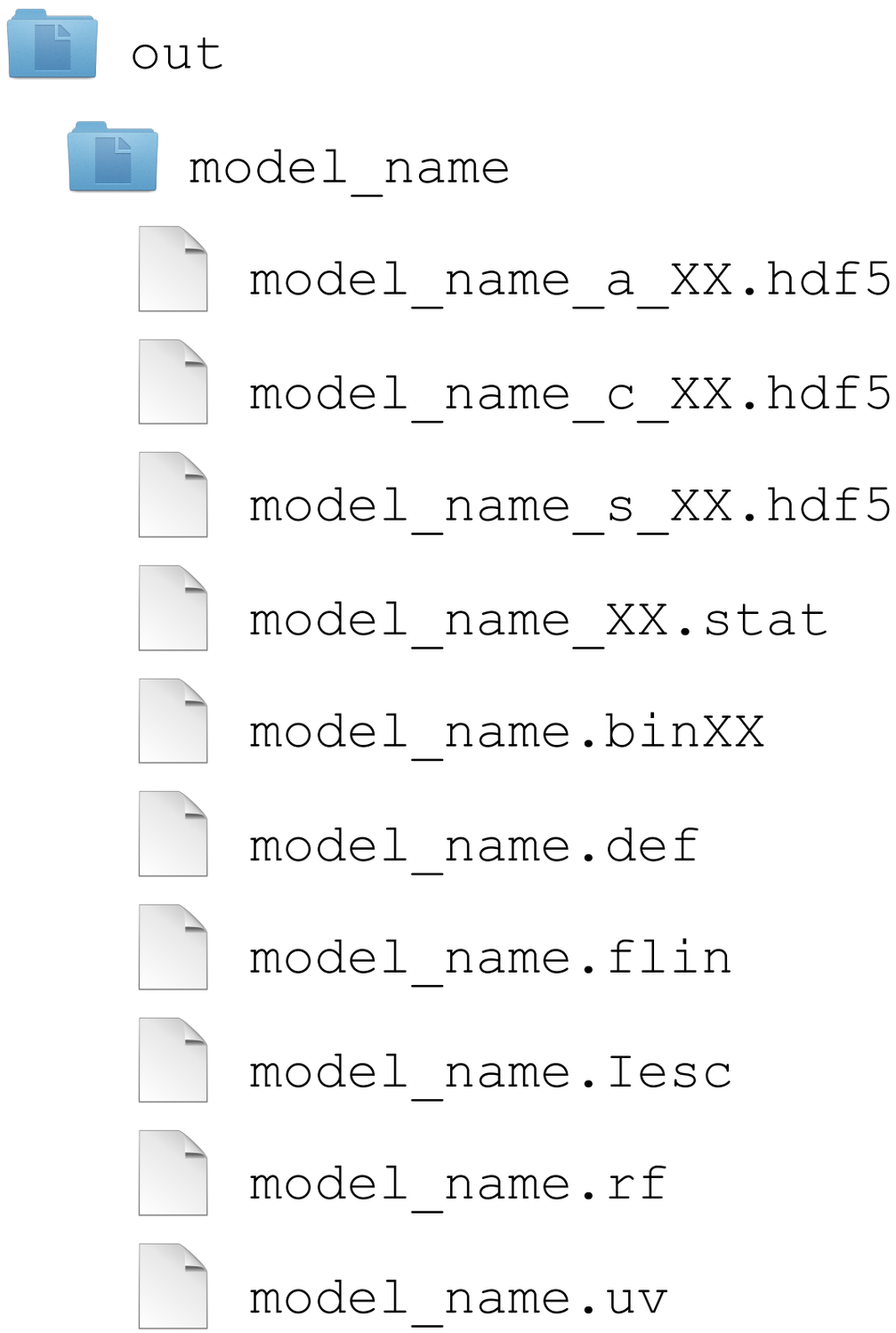
- with default input file (`pdr.in`)

```
$ ./PDR
```

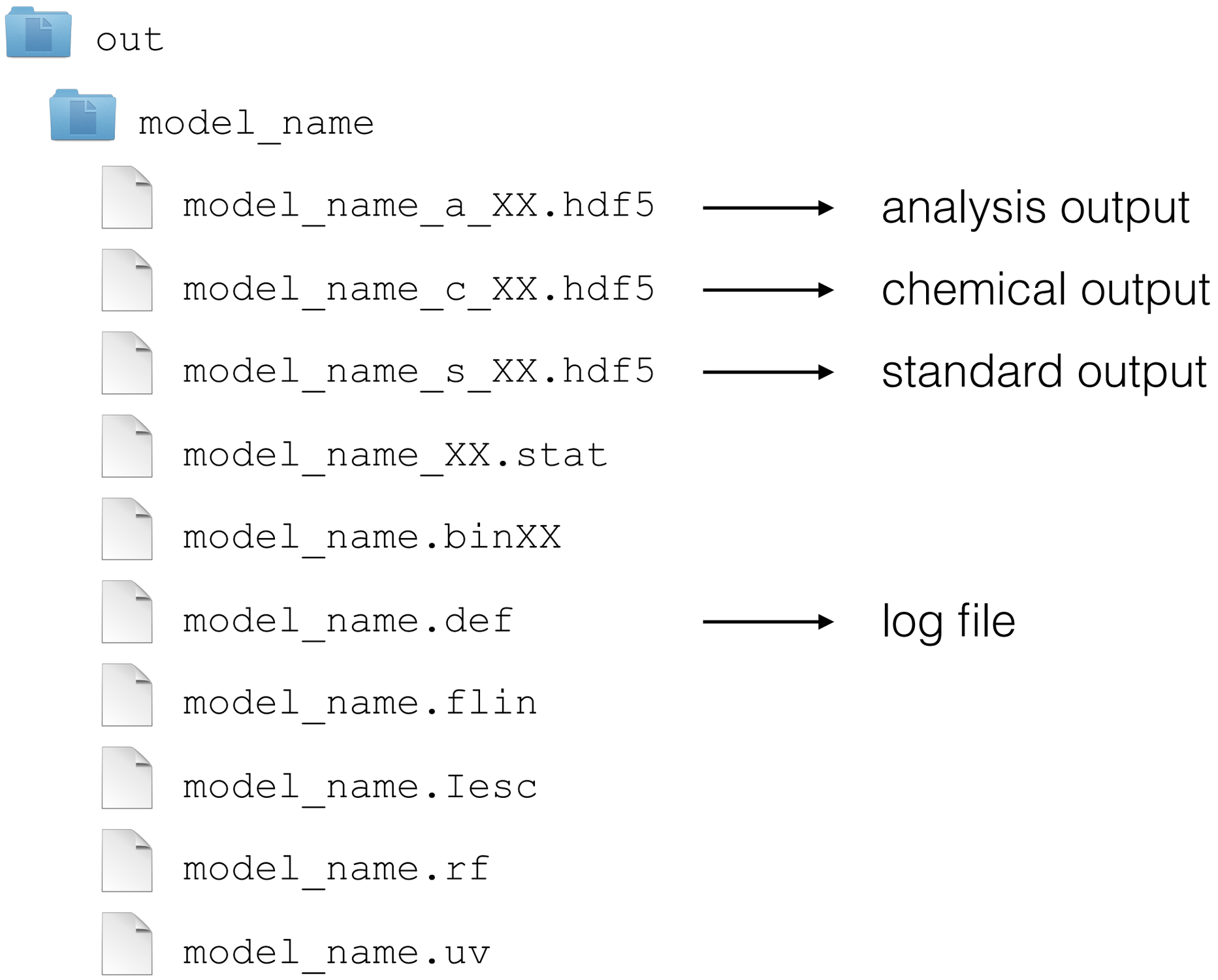
- with another input file other_input.in

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

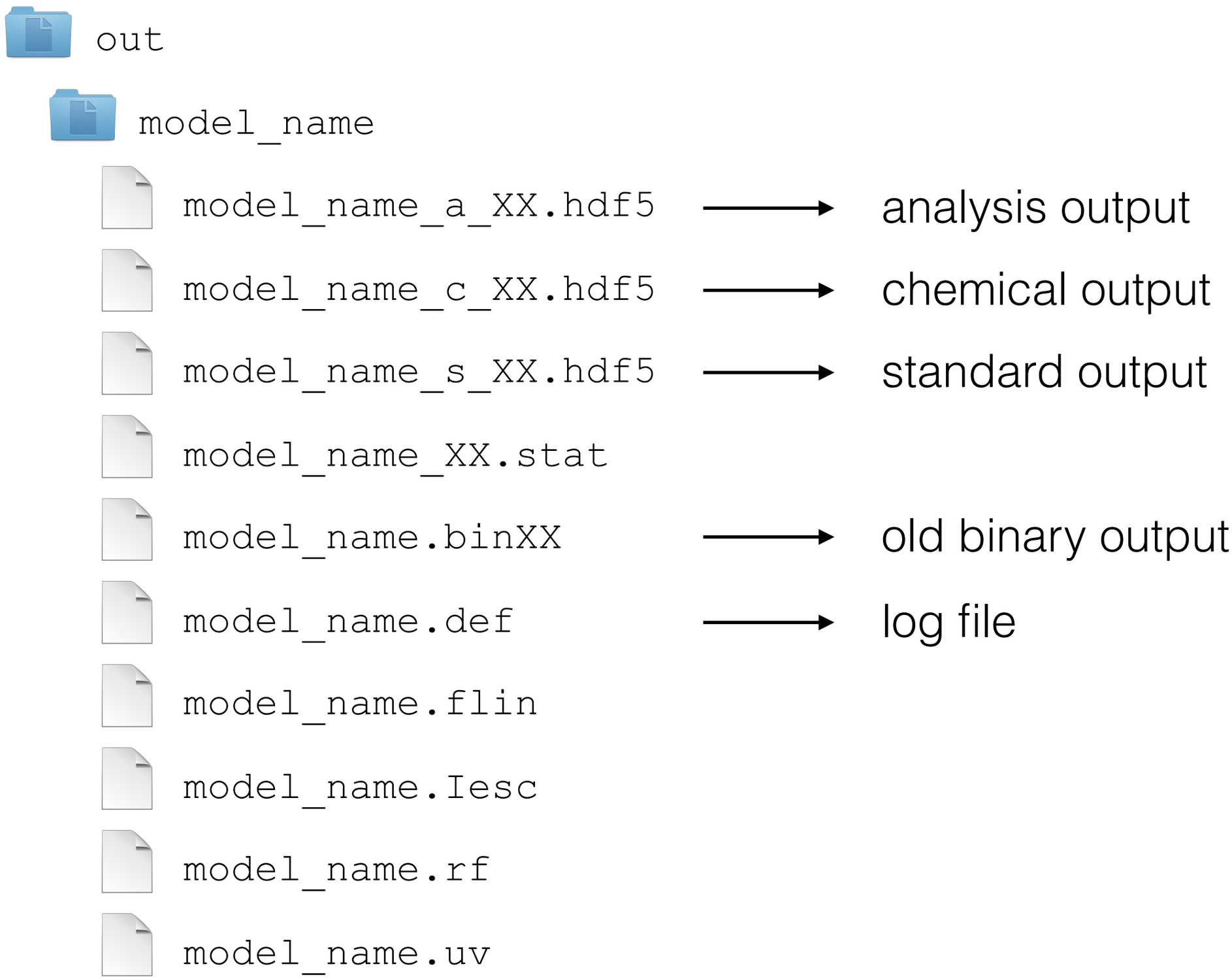
Outputs



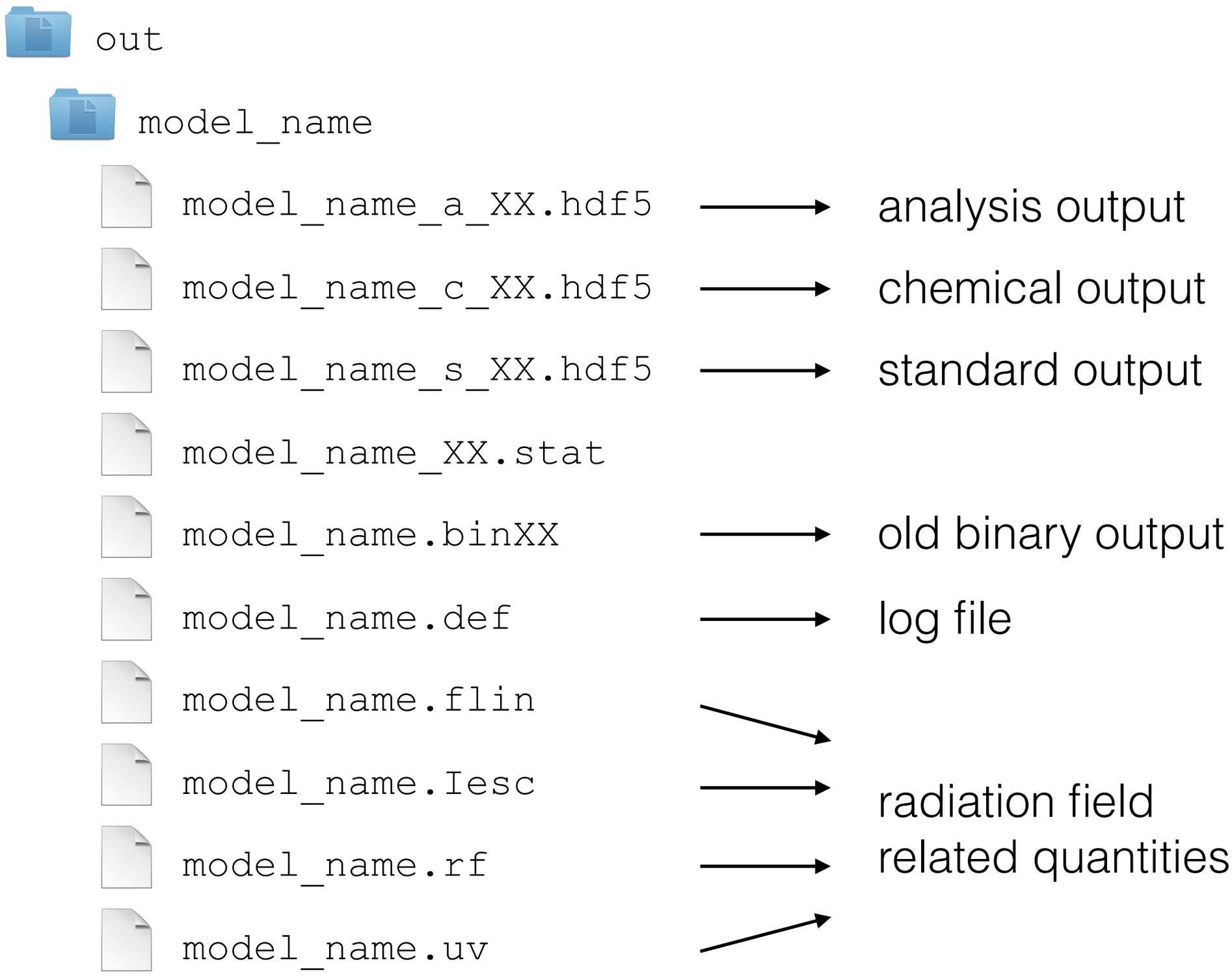
Outputs



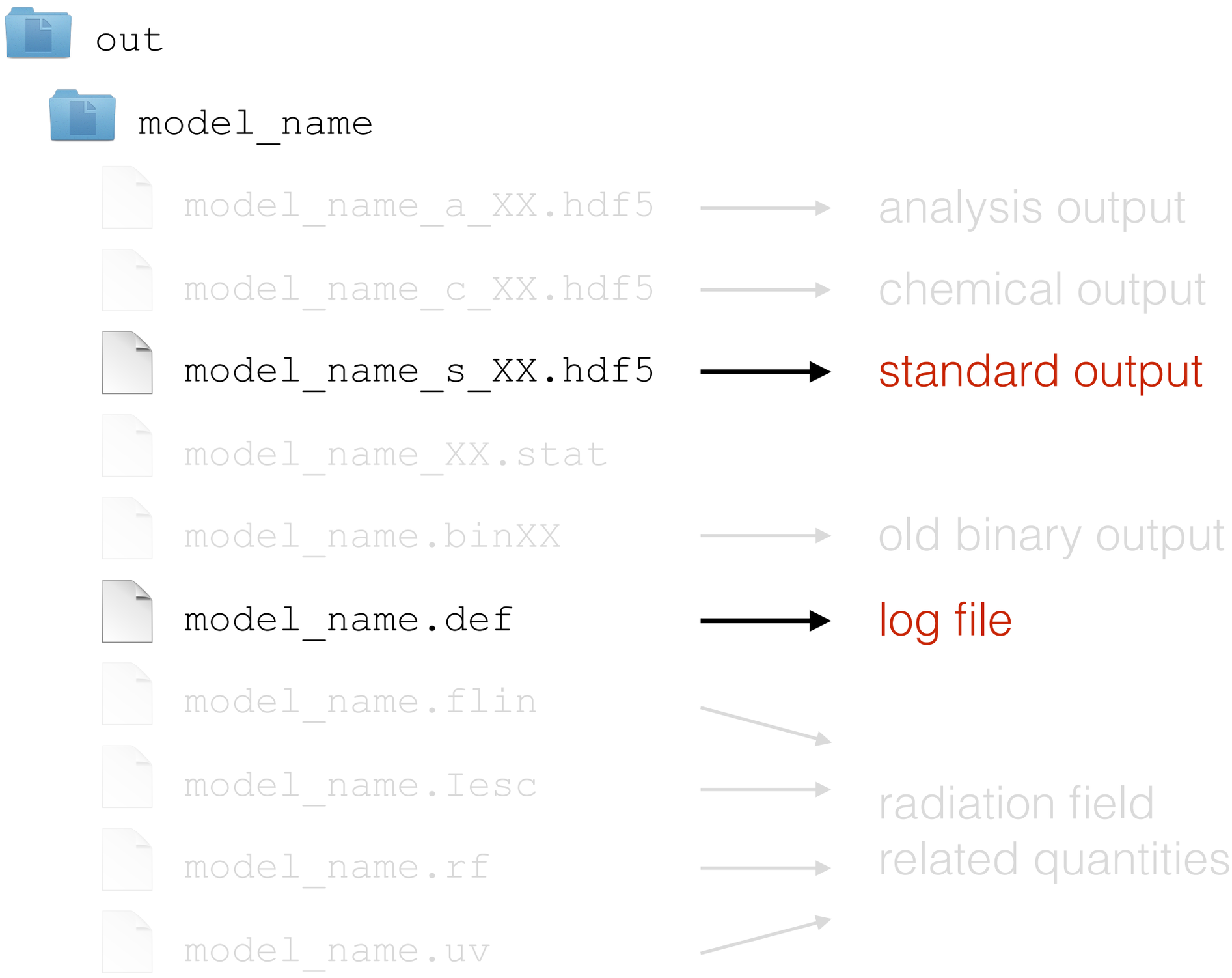
Outputs



Outputs



Outputs



Results analysis

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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Method

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

Visible extinction

Outline

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

Natural variables for radiative transfer

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

Visible extinction

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Natural variables for radiative transfer

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absorption & scattering coefficients

Visible extinction

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 $N_{\rm H} = C_D / R_V \times A_V$

Visible extinction

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extinction curve

Visible extinction

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A_V / E_{B-V}

Visible extinction

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N_H / E_{B-V}

Results

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