Thermal processes in KROME: an overview

Tommaso Grassi
tgrassi@nbi.dk

Centre for Star and Planet Formation
University of Copenhagen
Museum of Natural History
Niels Bohr Institutet

September 2014

Aims of this talk

1. Understand that ~~microphysics~~ cooling functions are is a mess
2. Realize that KROME saves your day

- You know you'd better cool it down
(Lou Reed)

Chemical network = Cauchy's problem:

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \overbrace{\sum_{lm} k_{lm}(T) n_l(t) n_m(t)}^{formation} - \overbrace{n_i(t) \sum_j k_{ij} n_j(t)}^{destruction} \qquad [\times N_{\mathrm{gas}}]$$

$$J_{ij} = \frac{\partial^2 n_i}{\partial t \partial n_j} \qquad [N \times N]$$

- $n_i(t = 0) = \hat{n}_i$
- $\sum_i n_i(t) m_i = \mathrm{const}$

A simple chemical network

$$\mathrm{H^+ + e^-} \xrightarrow{k_1} \mathrm{H} + \gamma \tag{1}$$

$$\mathrm{H} + \gamma \xrightarrow{k_2} \mathrm{H^+ + e^-} \tag{2}$$

ODE and Jacobian (an excerpt)

$$\frac{\mathrm{d}n_\mathrm{H}}{\mathrm{d}t} = k_1 n_{\mathrm{H^+}} n_{\mathrm{e^-}} - k_2 n_\mathrm{H} \tag{3}$$

$$\frac{\partial^2 n_\mathrm{H}}{\partial t \partial n_\mathrm{H}} = k_2 \qquad \frac{\partial^2 n_\mathrm{H}}{\partial t \partial n_{\mathrm{H^+}}} = k_1 n_\mathrm{e} \tag{4}$$

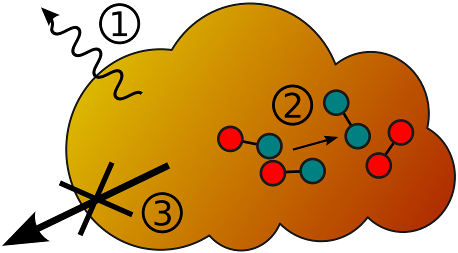
Expanding Cauchy

- $k_1(T)$ is a function of gas temperature!
- Hydro codes need temperature variation from chemistry/microphysics

$$\frac{\mathrm{d}T}{\mathrm{d}t} = f(?) \tag{5}$$

$$\frac{\partial^2 T}{\partial t \partial n_i} = ????? \tag{6}$$

- What is the coupling between $\mathrm{d}T/\mathrm{d}t$ and T?
- What is the coupling between $\mathrm{d}T/\mathrm{d}t$ and n_i?

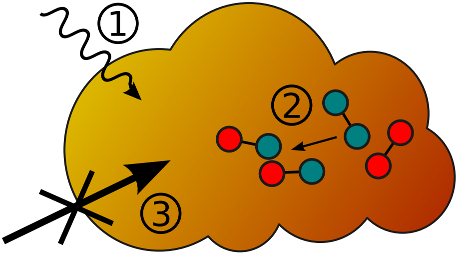


Template process

kinetic energy $\rightarrow$ something else

Trendy processes

1. radiative loss
2. endothermic reactions
3. ~~gas flows~~

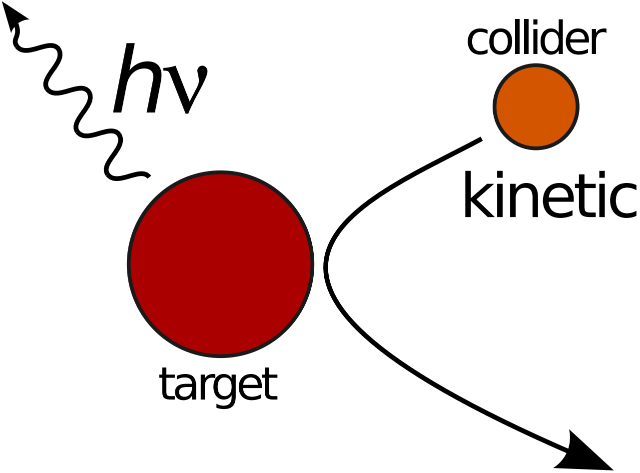


Template process

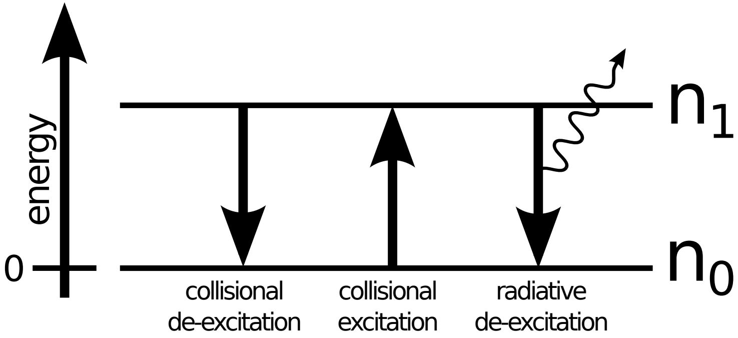
something else $\rightarrow$ kinetic energy

Trendy processes

1. photochemistry
2. exothermic reactions
3. ~~gas inflows~~



Prototype: metal atom (e.g. carbon) excited by gas particle collisions (e.g. H)



Two-levels ODE system

$$\begin{cases} \dot{n}_0 = -n_0 n_c C_{01} + n_1 \left(A_{10} + n_c C_{10}\right) \\ \dot{n}_1 = n_0 n_c C_{01} - n_1 \left(A_{10} + n_c C_{10}\right) \end{cases}$$

Looking for steady state

$$\begin{cases} 0 = -n_0 n_c C_{01} + n_1 \left(A_{10} + n_c C_{10}\right) \\ 0 = n_0 n_c C_{01} - n_1 \left(A_{10} + n_c C_{10}\right) \end{cases}$$

Looking for steady state

$$\begin{cases} 0 & = & -n_0 n_c C_{01} + n_1 \left(A_{10} + n_c C_{10}\right) \\ 0 & = & \cancel{n_0 n_c C_{01} - n_1 \left(A_{10} + n_c C_{10}\right)} \end{cases}$$

Looking for steady state

$$\begin{cases} 0 &= -n_0 n_c C_{01} + n_1 \left(A_{10} + n_c C_{10}\right) \\ n_{\mathrm{tot}} &= n_0 + n_1 \end{cases}$$

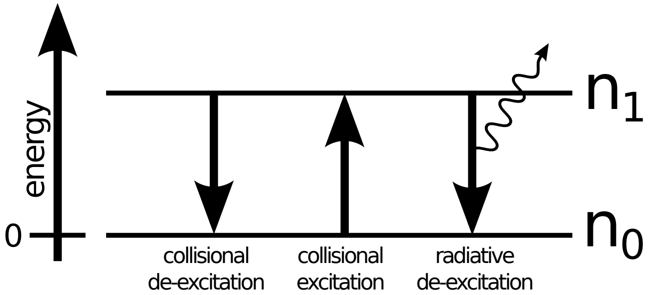
Looking for steady state

$$\begin{cases} 0 = -n_0 n_c C_{01} + n_1 \left(A_{10} + n_c C_{10}\right) \\ n_{\mathrm{tot}} = n_0 + n_1 \end{cases}$$

System solution

$$\begin{cases} n_1 = n_{\mathrm{tot}} \frac{C_{01} n_c}{(C_{01}+C_{10}) n_c + A_{10}} \\ n_0 = n_{\mathrm{tot}} - n_1 \end{cases}$$

good news: $\propto n_{\mathrm{tot}}$
bad news: $\propto \phi(n_c)$



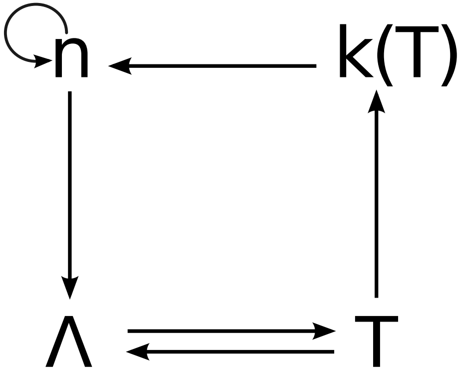
Total cooling

$$\Lambda_{\rm 2level} = n_1 \Delta E_{10} A_{10} \text{ erg/cm}^3\text{/ s}$$

$$\Lambda_{\rm 2level} = n_{\rm tot} f(n_c, T)$$

wait a moment... T?

Collisional rate coefficients are functions of T! $\rightarrow C_{ij}(T)$



$\dot{n}_i$ and $\dot{T}$ must be solved together!
DLSODES: *"and a splendid time(step) is guaranteed for all"*

e.g. collisions with H and e$^-$

$$\begin{aligned} \dot{n}_0 &= -n_0\left[n_\mathrm{H}C^\mathrm{H}_{01} + n_\mathrm{e}C^\mathrm{e}_{01}\right] + n_1\left[A_{10} + (n_\mathrm{H}C^\mathrm{H}_{10} + n_\mathrm{e}C^\mathrm{e}_{10})\right] \\ n_\mathrm{tot} &= n_0 + n_1 \end{aligned}$$

General expression

$$\begin{cases} \dot{n}_0 = -n_0 \sum_k n_{ck} C^{(k)}_{01} + n_1 \left(A_{10} + \sum_k n_{ck} C^{(k)}_{10}\right) \\ n_1 = n_\mathrm{tot} \dfrac{\sum_k C^{(k)}_{01} n_{ck}}{\sum_k n_{ck}\left(C^{(k)}_{01} + C^{(k)}_{10}\right) + A_{10}} \end{cases}$$

$$\Lambda = n_\mathrm{tot} f(\{n_{ck}\}, T)$$

A_{ij} - Einstein's coefficients

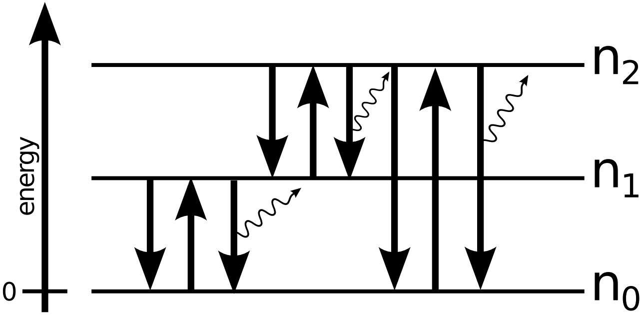
- Probability of spontaneous radiative de-excitations (1/s)
- Easy to retrieve (e.g. NIST), accurate
- Constants

E_i - Energy of the ith level

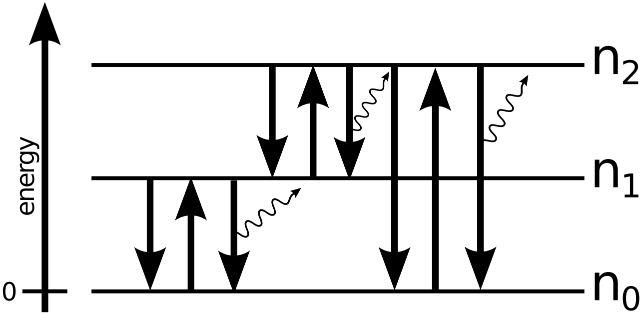
- Needed to get $\Delta E_{ij} = E_i - E_j$ (erg or K)
- Easy to retrieve (e.g. NIST), accurate
- Constants

$C_{ij}^{(k)}(T)$ - collisional (de)excitation rate coefficient

- Not-so-easy to retrieve (e.g. database and literature search), accuracy?
- Temperature dependence ($\rightarrow$ functions, $\rightarrow$ limits)
- Collider dependent $^{(k)}$



$$\dot{n}_0 = -n_0 \sum_k n_{ck} \left(C_{01}^{(k)} + C_{02}^{(k)} \right) + n_1 \left(A_{10} + \sum_k n_{ck} C_{10}^{(k)} \right) + n_2 \left(A_{20} + \sum_k n_{ck} C_{20}^{(k)} \right) \quad (7)$$



$$\dot{n}_1 = n_0 \sum_k n_{ck} C_{01}^{(k)} - n_1 \left[A_{10} + \sum_k n_{ck} \left(C_{10}^{(k)} + C_{12}^{(k)} \right) \right] + n_2 \left[A_{21} + \sum_k n_{ck} \left(C_{21}^{(k)} + C_{20}^{(k)} \right) \right] \quad (8)$$

Complete system

$$\begin{cases} 0 &= \dot{n}_0 = -n_0 \sum_k n_{ck} \left(C_{01}^{(k)} + C_{02}^{(k)} \right) + n_1 \left(A_{10} + \sum_k n_{ck} C_{10}^{(k)} \right) \\ &+ n_2 \left(A_{20} + \sum_k n_{ck} C_{20}^{(k)} \right) \\ 0 &= \dot{n}_1 = n_0 \sum_k n_{ck} C_{01}^{(k)} - n_1 \left[A_{10} + \sum_k n_{ck} \left(C_{10}^{(k)} + C_{12}^{(k)} \right) \right] \\ &+ n_2 \left[A_{21} + \sum_k n_{ck} \left(C_{21}^{(k)} + C_{20}^{(k)} \right) \right] \\ n_{\mathrm{tot}} &= n_0 + n_1 + n_2 \end{cases}$$

$$\Lambda = n_1 \Delta E_{10} A_{10} + n_2 \left(\Delta E_{20} A_{20} + \Delta E_{21} A_{21} \right)$$

Full Matrix

$$\begin{pmatrix} 1 & \cdots & 1 \\ M_{1,1} & \cdots & M_{1,N-1} \\ \vdots & \ddots & \vdots \\ M_{N-1,1} & \cdots & M_{N-1,N-1} \end{pmatrix} \times \begin{pmatrix} n_1 & \cdots & n_{N-1} \end{pmatrix} = \begin{pmatrix} n_{\mathrm{tot}} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

where

$$M_{l,m} = g_{l,m}(A_{ij}, C_{ij}, \{n_k\})$$

Linear solver in KROME

- 2 levels: analytic (fast)
- 3 levels: analytic (fast)
- $>$ 3 levels: LAPACK (fast for $N \gg 3$)

General expression (N levels)

$$\dot{n}_i = -n_i\left(\sum_{j<i} A_{ij} + \sum_{i\neq j}\sum_k n_{ck} C_{ij}^{(k)}\right) + \left(\sum_{j>i} n_j A_{ji} + \sum_{i\neq j} n_j \sum_k n_{ck} C_{ji}^{(k)}\right) \quad (9)$$

$$\Lambda = \sum_i n_i \sum_{j<i} \Delta E_{ij} A_{ij} \quad (10)$$

OK, this is a mess...

Recap on problems

- Search for atomic data
- How to solve linear systems? (many caveats not shown here)
- Convert messy equations into efficient code (e.g. tables for $C_{ij}^{(k)}$)
- Avoid typos in atomic data (less trivial than expected)
- Adding a collider later could be troublesome

KROME saves your day(s)!

Fitting cooling functions

- usually functions of T and of the chemical composition
- OK when parameters are independent
- PRO: very fast (depends)
- CON: less accurate (depends)
- CON: difficult to update with new atomic data (re-build machinery)
- Example: H_2 from Simon Glover (colliders H,H^+,e^-,H_2,He)

Live demo!

"No matter how slick the demo is in rehearsal, when you do it in front of a live audience, the probability of a flawless presentation is inversely proportional to the number of people watching, raised to the power of the amount of money involved."

(Mark Gibbs)

Thank you for your attention!

"The only legitimate use of a computer is to play games"
(Eugene Jarvis)

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KROME
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