Exercise # 1

simple chemical network and heating function

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Before to start
we would like to know you

Please introduce yourself

- name, institution, topic
- why you want to employ KROME
- what you expect from the school

The exercises preparation
acknowledgment

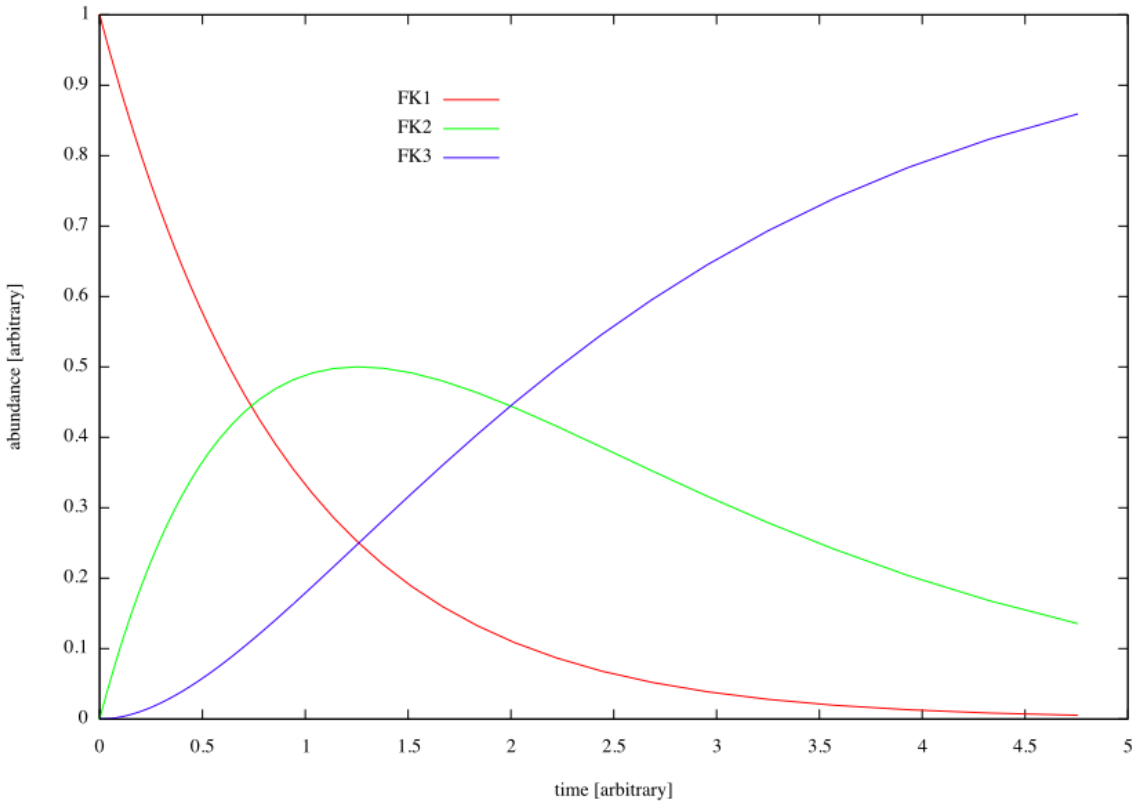
Thanks to:

- Troels Haugboelle
- Dominik Schleicher
- Daniel Seifried

Sanity check

Before to start:

- having KROME installed
- prepare the "hello" test `./krome -test=hello`
- compile and run the test and check the results



Exercise
Part 1

- it is a pure kinetic exercise
- how to use the KROME tokens
- reaction flux "usefulness"

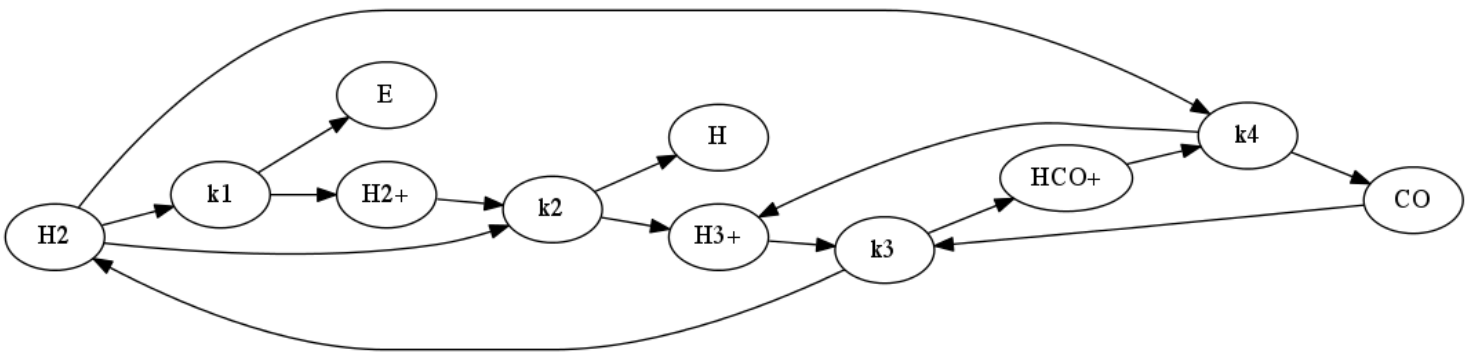
- init: full H_2
- a small amount of CO
- evolve to the steady-state

the basic chemical network

1. $H_2 + CR \rightarrow H_2^+ + e^-$
2. $H_2 + H_2^+ \rightarrow H_3^+ + H$
3. $H_3^+ + CO \rightarrow HCO^+ + H_2$
4. $HCO^+ + H_2 \rightarrow H_3^+ + CO$ (to add in the 2nd part)

tokens to be used

- @format
- @common (for the user_crate)
- @CR_begin, @CR_end



Reaction flux

Each term of the RHS of the ODE represent a reaction flux, it measures the "importance" of a reaction within a network, under given conditions.

1. $\mathrm{H} + \mathrm{e}^- \rightarrow \mathrm{H}^+ + 2\mathrm{e}^-$
2. $\mathrm{H}^+ + \mathrm{e}^- \rightarrow \mathrm{H} + \gamma$

$$\frac{dH}{dt} = -k_1(T) n_{\mathrm{H}} n_{\mathrm{e}} + k_2(T) n_{\mathrm{H}^+} n_{\mathrm{e}} \quad (1)$$

In KROME there are utilities to print the fluxes, e.g. the subroutine krome_print_best_flux which provide the most important reaction fluxes.

New tokens
part 2 of the exercise

Part 2: add cosmic rays heating

- CR processes release 30 eV into the gas (tomorrow's talk)
- in this test there is no cooling
- we expect a large increase of the temperature

Token to be used

@CR_begin, @CR_end, simple usage

```
@CR_begin
#REACTION
idx,R,P,P, rate
@CR_end
```

then enable the option `-heating=CR`

For gnuplot users
the species.gps file

Useful tool to plot the abundances

- define the offset `nkrome`
- load the gps file `load 'species.gps'`
- plot following the instructions

```
gnuplot> nkrome =2
gnuplot> load 'species.gps'
All variables set as e.g. krome_idx_H2
plot 'your_file' u 1:(column(krome_idx_H2))
 the offset is nkrome=2
```

Let's start

To start the exercise download the needed files at

`http://kromepackage.org/bootcamp/exercises/day1_1.tar.gz`

- the test.f90 template
- benchmark plots!

Do not hesitate to ask questions during the exercises!

Good Work!

Thank you for your attention!