Problem 1: Chemical networks

Aims of this exercise

1. write a simple chemical network for water
2. play around with the parameters
3. tokens and user functions
4. use KIDA database

KROME Bootcamp 2015 - check the software

- ensure you have krome in your computer
- if not, clone the repository

  (`git clone https://stefanobovino@bitbucket.org/tgrassi/krome.git`)
- if you have KROME $\rightarrow$ `git pull origin`

The material for the exercises is provided on a bitbucket repository.

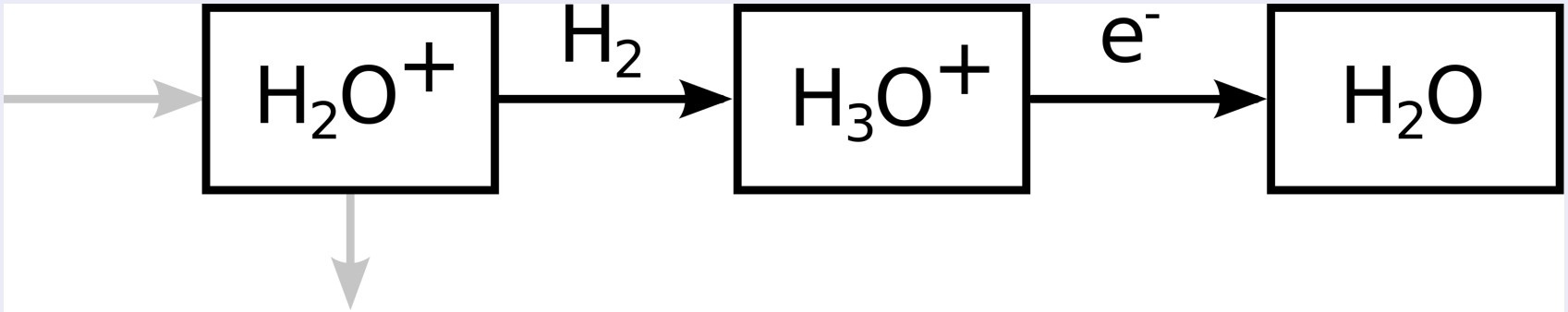
Basic commands for cloning the repository

- `http://bitbucket.org/tgrassi/krome-exercises-2015`
- select a folder that you use for all your repositories (e.g. `cd ~/repos/`)
- or create it (e.g. `mkdir ~/repos/`)
- clone the repository there

  (`git clone https://tgrassi@bitbucket.org/tgrassi/krome-exercises-2015.git`)

Core of part1

No coding: just write down a sketch of the chemical network



$$H_2O^+ + H_2 \rightarrow H_3O^+ + H$$
$$H_3O^+ + e^- \rightarrow H_2O + H$$

2 things worth knowing

1. provided file: `networkH2O.ntw`
2. cosmic ray reactions depend on the CR flux

Part2

- TODO: add the missing reactions
- TODO: define a common variable ξ_{cr} → `@common`
- REMINDER: the common variables name → `user_NAME`

Part 3: Run KROME pre-processor

- `-n networkH2O.ntw`
- WARNING!!! you're forming water but not destroying it (skip that)
- TODO: go into build/ and modify `test.f90`
- SUGGESTION: prepare a option file and run KROME with `-options=OPTION_FILE_NAME`
- do not forget `-noExample` option since now on!

Part 3 (cont'd): Initial conditions

1. $T_{gas} = 50$ K, constant
2. $t_{end} = 10^6$ yr (use the `spy` variable to convert in seconds)
3. $n_H = n_{tot} = 10^8$ cm^{-3}
4. $n_{H_2} = 0.1 n_{tot}$
5. oxygen?

the user module

- KROME provides a useful user module
- `python list_user_functions.py` to have a list
- `krome_scale_Z` used to obtain metal abundances based on $Z/Z_\odot$

provided in the exercises sheet

```
initialize species and temperature
intialize cosmic rays flux with the function in krome_user
t =0
dt  = 1e-2 yr
do
  dt = dt * 1.1
  t = t + dt
  call krome
  write output
  if(t>1e6 yr) break loop
end do
```

Make and run KROME

NOTE: if you use gnu compiler add the option
`-compiler = gfortran` or modify by hand the `Makefile`

Plot the H_2O time evolution and compare with Fig. 2 (left)!

Part 4: Key reaction rates

- each term of the RHS of the ODE system represent a reaction flux
- measures the "importance" of a reaction within a network, under given conditions.

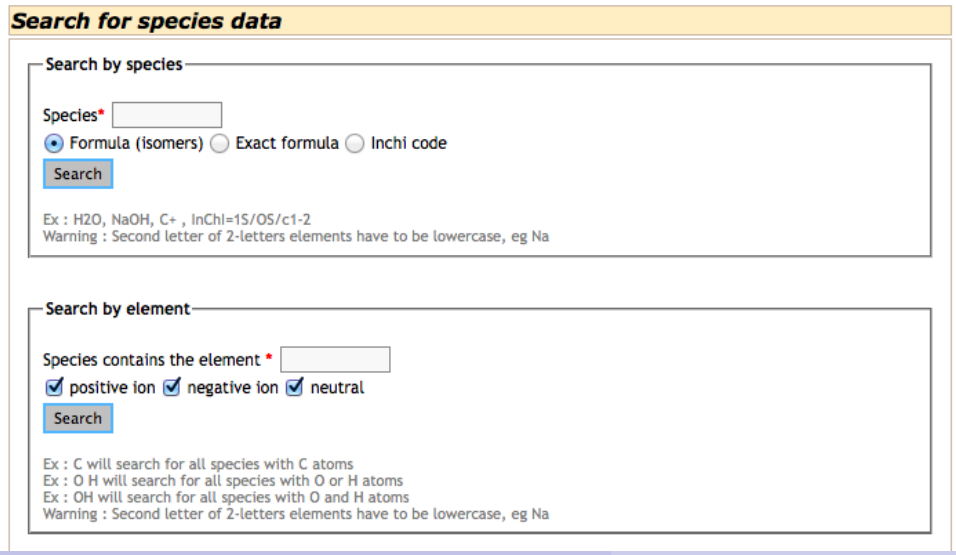
$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C}$ regulated by $k_1(T)$

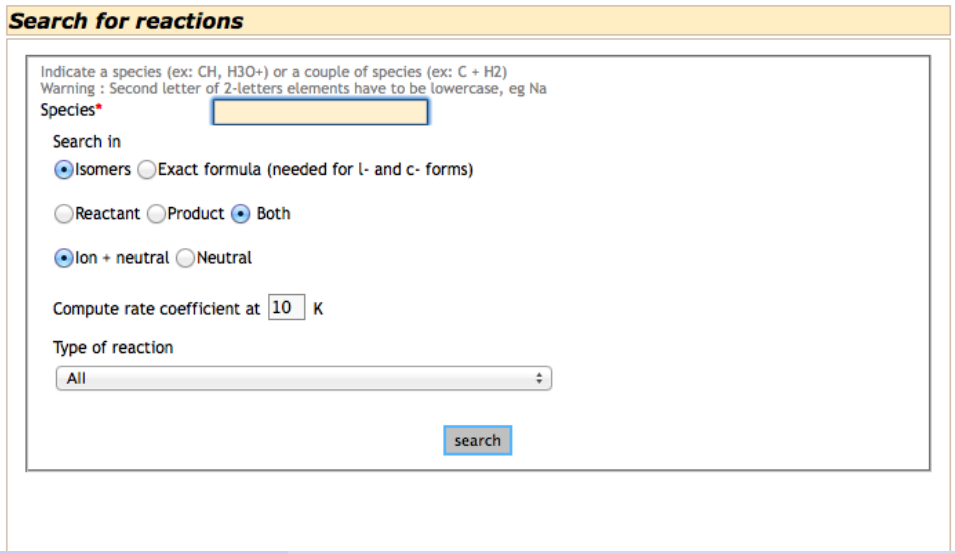
$$k_1(T) n_A n_B \tag{1}$$

In KROME $\rightarrow$ subroutine `krome_print_best_flux` ranks the most important reaction fluxes.

Part 5: add a reaction

- use KIDA database (http://kida.obs.u-bordeaux1.fr)
- TODO: look for $H_2O + CRP \rightarrow H + OH$
- $k_i = \alpha_i \xi_{cr}$
- TODO: add the rate to your network file
- TODO: plot the OH abundance with and without this reaction





Part 6a: simple sensitivity analysis

- REMINDER: use `-noExample` option to avoid to overwrite your test.f90 file
- TODO: change by an order of magnitude the cosmic rays flux
- TODO: compare the results

Part 6b: massive sensitivity analysis

- TODO: change the first three *auto* reactions
- new rates: $k_i = c_i \varphi_i$
- as for ξ_{cr} use `@common` token and the corresponding user function to define and initialize the new three variables φ_i
- $\varphi_i = dex(2 \times rand() - 1)$

GOOD WORK!