Microphysics modelling with KROME

Tommaso Grassi
T.Haugbølle (NBI), S.Bovino (UniHam), D.Schleicher (UniCon)

Centre for Star and Planet Formation
Niels Bohr Institute

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Note: actual sunny day in Copenhagen, no photoshop!
ISM chemistry/microphysics

Why chemistry/microphysics? (in numerical simulations)

• chemistry (and microphysics) is everywhere and plays a crucial role
• PDR, HII, disks, stars, planet atmospheres, ISM, WIM, CNM, HIM, MCs, …
• controls gas thermal evolution
• controls opacity
• comparison with observations
ISM chemistry/microphysics

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Why chemistry/microphysics is troublesome (in numerical simulations)

- very CPU demanding (solving stiff ODEs)
- has a non-linear/complex behaviour (e.g. MC)
- connected with (and influenced by) many physical processes
- many atomic, molecular, thermochemical, ... data required
- needs accurate rates for reaction rates (and xsecs)
- network completeness (include all species/reactions)
A + B → C + D
A + B \xrightarrow{k(T)} C + D
A + B $\rightarrow$ C + D

$\text{k(T)}$

T. Grassi (STARPLAN)
Chemistry, the full story (4/25)

\[ A + B \xrightarrow{k(T)} C + D \]
A + B \rightarrow^{k(T)} C + D

\nH_n + nH^+ + n_e + n_{HCO} + n_H + n_{H_2}
A + B \xrightarrow{k(T)} C + D

\begin{align*}
  n_{H^+} & n_e \\
  n_H & n_{HCO} \\
  n_{H} & n_{H2}
\end{align*}
A + B \xrightarrow{k(T)} C + D

\begin{align*}
E & \quad G \\
A & \quad B \\
F & \quad D \\
C & \quad I \\
J &
\end{align*}

\begin{align*}
n_{H^+} & \quad n_e \\
n_H & \quad n_{HCO} \\
n_{H_2} & \\
\end{align*}

COOLING
A + B \xrightarrow{k(T)} C + D

\[ n_{H^+} n_e n_{\text{HCO}} \]
\[ n_H n_{\text{H}_2} \]

RAD + CR

HEATING

COOLING
\[ A + B \rightleftharpoons C + D \]

\[ \text{RAD} + \text{CR} \]

\[ n_{H^+} \quad n_e \quad n_{\text{HCO}} \]

\[ n_H \quad n_{\text{H}_2} \]

\[ \text{HEATING} \]

\[ \text{COOLING} \]
A+B → C+D

\[ k(T) \]

Rad + CR → Heating

Opacity

Cooling

\[ n_{H^+}, n_e, n_{HCO}, n_H, n_{H_2} \]
A + B → C + D

A

COOLING

E

F

J

I

HG

RAD + CR

HEATING

COOLING

T

n_{H^+} n_e n_{HCO} n_H n_{H_2}

T. Grassi (STARPLAN)
A + B \rightarrow C + D

k(T)

T. Grassi (STARPLAN)
Chemistry, the full story (24/25)

$$A + B \rightarrow C + D$$

$$k(T)$$

HYDRO

RAD+CR

HEATING

COOLING

DUST

$$n_{H^+}, n_e, n_{HCO}, n_H, n_{H2}$$

T. Grassi (STARPLAN)

TDE 2015 - Nice

October 2015
What is KROME?

- Python pre-processor creates \textit{ad hoc} F90 modules
- Chemistry, dust-related physics, cooling, heating, photoionization, …
- Open source, \texttt{kromepackage.org}, Grassi+2014 (MNRAS)
- Highly optimized, “fast” solver (DLSODES)
- Can be coupled to hydrocodes, RAMSES, Enzo, FLASH, Gasoline, …
- Growing community, 19 papers, 2 schools (\texttt{kromepackage.org/bootcamp})
KROME - Basic design

preprocessor stage

- your network
- Pyton pre-processing
- your options

compilation/run stage

- your code
- library-like fortran
  - (photo) chemistry
  - cooling/heating
  - dust
  - ...

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TDE 2015 - Nice
October 2015
Minimum example

!init krome (once for all)
call krome_init()

!init species (1/cm3)
x(:) = 0d0
x(krome_idx_H2) = 1d4
x(krome_idx_O) = 1d0
x(krome_idx_C) = 0.5d0

!set Tgas (K)
Tgas = 5d1

!set time-step (s)
dt = 1d6*seconds_per_year

!call KROME
call krome(x(:), Tgas, dt)

!print results
print *,x(:)
print *,Tgas
Simple chemical network (example)

\[
\begin{align*}
H^+ + e^- & \rightarrow H + \gamma \quad \text{recombination} \\
H + e^- & \rightarrow H^- + \gamma \quad \text{radiative attachment} \\
H^+ + H^- & \rightarrow H + H \quad \text{mutual recombination} \\
H + e^- & \rightarrow H^+ + 2e^- \quad \text{collisional ionization} \\
H^- + H & \rightarrow 2H + e^- \quad \text{collisional detachment}
\end{align*}
\]

### Example Rate Expressions

1. \(H^+, E, H, 3.5d-12 \times (T_{\text{gas}}/3d2)^{-0.7}\)
2. \(H, E, H-, \text{myLovelyFunction}(T_{\text{gas}})\)
3. \(H^+, H^-, H, H, \text{auto}\)
4. \(H, E, H^+, E, E, \text{auto}\)
5. \(H^-, H, H, H, E, \text{auto}\)
```
./krome -n network.ntw -usePhotoBins=2

13.6 14.3 15.6

E
1 2
15.4

real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 15.4d0/) !eV
arrayR(:) = (/14.3d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
mid(:) = krome_get_photoBinE_mid()
print *,mid(:)
```

13.95000000000000 15.50000000000000
External cross section (network), e.g. $\text{H}^- + \gamma \rightarrow \text{H}^+ + \text{e}^-$

```plaintext
@photo_start
1,H-,H,E,@xsecFile=SWRI
@photo_end
```

data/database/swri_xsecs/H-.dat

**External cross section (data file)**

<table>
<thead>
<tr>
<th>Lambda</th>
<th>Total</th>
<th>H+/2e</th>
<th>H/e</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>2.00E-27</td>
<td>0.00E+00</td>
<td>2.00E-27</td>
</tr>
<tr>
<td>5.2</td>
<td>6.11E-25</td>
<td>4.58E-28</td>
<td>6.11E-25</td>
</tr>
<tr>
<td>10.0</td>
<td>5.60E-24</td>
<td>9.00E-27</td>
<td>5.59E-24</td>
</tr>
<tr>
<td>15.5</td>
<td>2.40E-23</td>
<td>6.22E-26</td>
<td>2.39E-23</td>
</tr>
<tr>
<td>20.0</td>
<td>5.53E-23</td>
<td>1.87E-25</td>
<td>5.51E-23</td>
</tr>
</tbody>
</table>

...
bitbucket.org/tgrassi/krome

Just google: kromeuser google groups
sourceforge.org/gitstats
Prototypical problem

Context

**Turbulent Molecular Clouds** (w T.Haugbølle)

- Star-forming regions
- Complex structures at all scales
- Molecular richness (mainly H-C-O, but also F-S)
- Large CO variability
- \( \text{CH}^+ \) and \( \text{SH}^+ \) unexpected abundances
- CO-to-H\(_2\) conversion factor still under investigation

Caveats and bottlenecks (computational)

- Multi-scale interaction
- Chemistry/microphysics at different scales ("hierarchical chemical legacy")
- Non-trivial coupling between "pure" chemistry, microphysics, and dynamics
- Radiative-transfer and other amenities
Prototypical problem/2

**RAMSES-CPH (+KROME, w T.Haugbølle)**

- **Non-equilibrium** H-C-O chemistry (+CRs, +photo, \(\sim\)Glover+2009)
- **Fully coupled thermochemistry** (on-the-fly fine-structure +tables, \(\sim\)Maio+2007)
- **Consistent adiabatic index** (partition functions, Boyle+2007)
- **Dust chemistry** (H\(_2\), Cazaux+2009), dust cooling/photoheating (Dopcke+2011)
- Workaround: local density-based photochemistry, i.e. \(A_v = f(n_{\text{tot}})\)
- Optional: access to photochemistry-based opacity (RT-ready)
- Testing: more dust chemistry (Hocuk+2015) + dust tables (Grassi+2015 in prep.)

**Molecular cloud model details**

- MHD
- \(\sim 3.3 \times 3.3 \times 3.3\) pc
- Turbulence: Mach 11 @ 10 K
- \(\langle n_{\text{tot}}\rangle \sim 10^3\) cm\(^{-3}\)
- \(\langle B \rangle \sim 7\) \(\mu\)G
- > 18 Mcells
- 4.7 Myr \(\sim 3.5\) \(\tau_d\) \(\sim 4.5\) \(\tau_{ff}\)
- \(\sim 300\) rates, \(\sim 40\) species
A set of one-zone models: one for each cell (this case $\geq 18M$).
RAMSES+KROME results

Log$_{10}$ Column Density [cm$^{-2}$]

Log$_{10}$ OH Column Density [cm$^{-2}$]
Problem 1 - nodes (species)

- atoms (H, He, C, N, O, Si, Ne, S, P, F, Al, ...)?
- species (H, H2, CO, CH, ...)?
- cations and anions (H−, H+, C3+, CH− ...)?
- isomers (HOC⁺, HCO⁺, ...)?
- isotopes (¹²C¹⁶O, ¹³C¹⁶O, ...)?
- “fancy” stuff (dust, PAH, ...)?

Problem 2 - edges (reactions)

- bimolecular (OH⁺ + e⁻ → O + H)?
- photochemistry (H⁻ + γ → H + e⁻)
- cosmic rays (CO + CR → C + O)
- cosmic rays secondary (CO + CRP → C + O)
- 3-body (H + H + H₂ → H₂ + H₂)

You can always expand a chemical network.
Problem 3 - rate coefficients

\[ A + B \xrightarrow{k} C + D \]
\[ \dot{n}_A(t) = -k(T) n_A(t) n_B(t) \]

Methods to determine \( k(T) \)

- Experimental (lucky, often single \( T \))
- Langevin (estimate, constant \( T \), could be completely off!)
- Physical considerations (e.g. HD==H\(_2\), extremely dangerous!)
- \textit{ab initio} calculations (not always available, small systems only)

How to retrieve \( k(T) \)?

- Databases (KIDA, UMIST, …)
- Literature search (best, but time-consuming)
- Do it yourself! (strongly discouraged)
- Educated guess (also strongly discouraged)
- Ask a (theoretical) chemist!
Modelling: getting started/3

Problem 4 - initial conditions
- metallicity
- individual metallicity ratios (e.g. C/O is critical)
- ionization level
- temperature(s)
- dust content
- ...

Problem 5 - ambient
- density range
- temperature range
- radiation flux (mainly UV, X)
- extinction (opacity, self-shielding)
- cosmic ray ionization flux
- dust type, size, distribution, ...
- ...

Think first, code later
Summary/Outlook

• KROME is a state-of-the-art and growing code
• note: KROME takes care of chemistry/microphysics
• fully-consistent non-equilibrium microphyiscs/chemistry
• KROME is flexible
• KROME successfully coupled with 3D simulations (but not only)

The eternal struggle (aka: cheap, fast, accurate. pick two)

ACCURACY ←→ EFFICIENCY

Perspective

• go beyond computational bottlenecks (solver: GPU, vectorization, Xeon-Phi)
• improve dust model (see also above)
• release environment-tailored recipes (Bovino+2015, submitted)
• improve user interface and network format (coming soon)
• test! test! test!
Thank you for your attention!

“A git pull a day, keeps the doctor away.”
(github.com/AntJanus)

T.Haugbølle (NBI), S.Bovino (UniHam), D.Schleicher (UniCon)
J.Ramsey (NBI), D.Seifried (UniKöln)
D.Galli (INAF), M.Satta (CNR), E.Simoncini (INAF)

kromepackage.org/
kromepackage.org/bootcamp
bitbucket.org/tgrassi/krome