

Microphysics and chemistry modelling with KROME

Tommaso Grassi
tgrassi@nbi.dk

University of Copenhagen
STARPLAN - Centre for Star and Planet Formation

November 2014



STARPLAN

**T. Haugbølle, Å. Nordlund, T. Frostholm, M. Küffmeier,
S. Friemann, S. Dib, J. Ramsey, ...**

Others involved in KROME

- **D.R.G.Schleicher, S.Bovino, M.Latif** (Göttingen University, ENZO)
- **J.Prieto** (Conception University, RAMSES)
- **D.Seifried** (Köln University, FLASH)
- **E.Simoncini** (INAF Arcetri, planetary atmospheres, biomarkers)
- **D.Galli** (INAF Arcetri, chemical networks)
- **E.Tognelli** (Pisa University, thermonuclear networks in stars)
- **M.Satta** (CNR, University of Rome, theoretical chemistry)
- **F.A.Gianturco, F.Carelli** (University of Innsbruck, theoretical chemistry)
- **S.Danielache** (Tokyo Inst. of Technology, primordial Earth chemistry)
- **K.Omukai** (Tohoku University, Early Universe)

Why chemistry?

“Chemistry has been termed by the physicist
as the messy part of physics”
(Frederick Soddy)

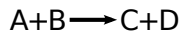
Why chemistry/microphysics? (in numerical simulations)

- 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 (see next slides)
- comparison with observations

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 (next slides)
- needs accurate rates for reaction rates
- network completeness (include all the necessary species)

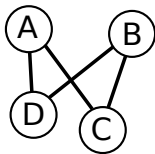
Chemistry, the full story (1/24)



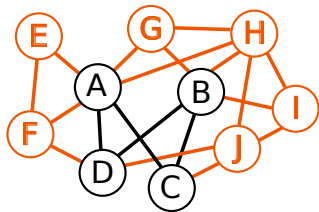
Chemistry, the full story (2/24)



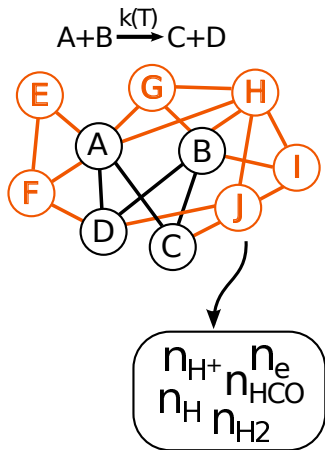
Chemistry, the full story (3/24)



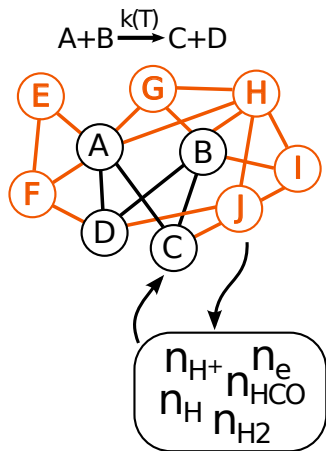
Chemistry, the full story (4/24)



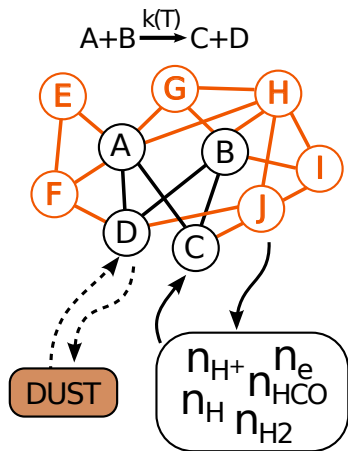
Chemistry, the full story (5/24)



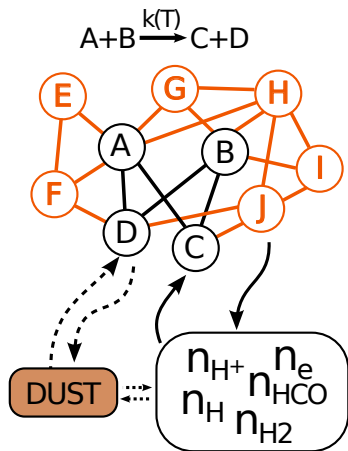
Chemistry, the full story (6/24)



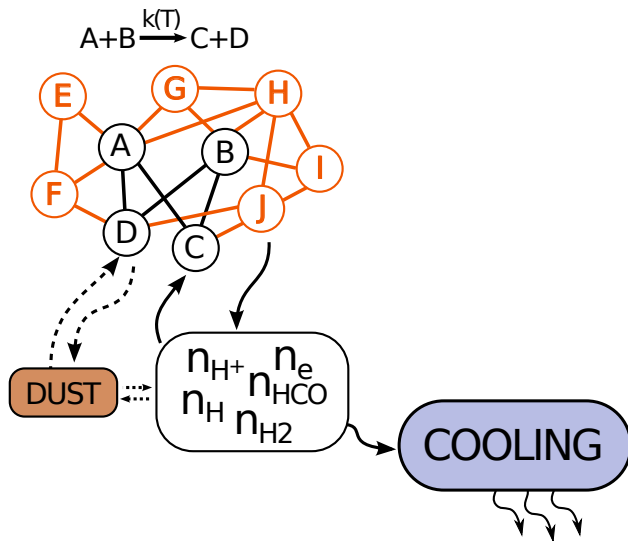
Chemistry, the full story (7/24)



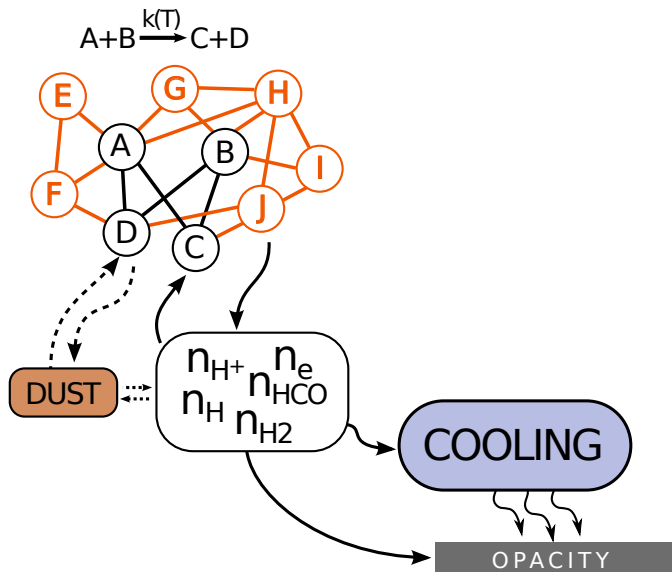
Chemistry, the full story (8/24)



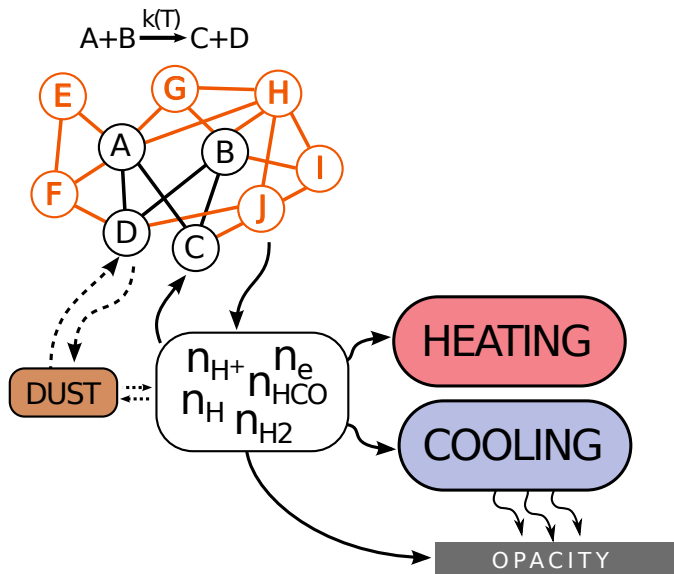
Chemistry, the full story (9/24)



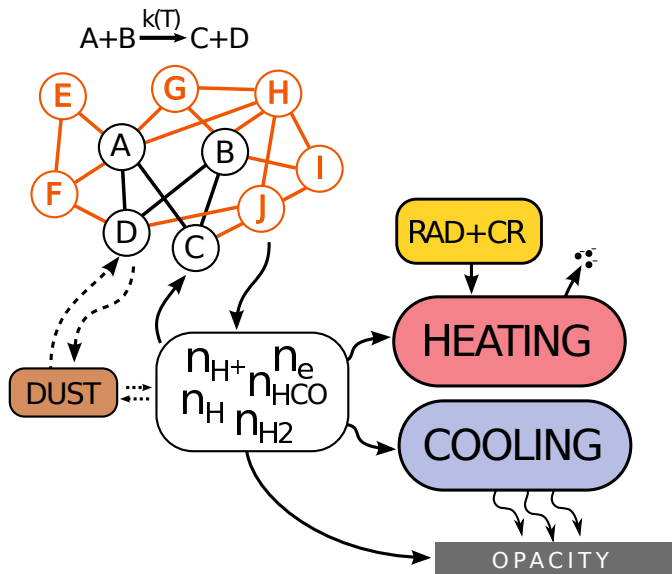
Chemistry, the full story (10/24)



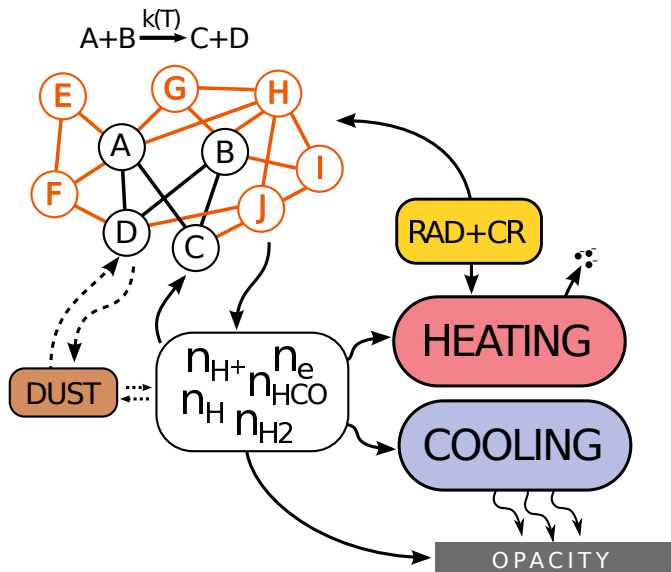
Chemistry, the full story (11/24)



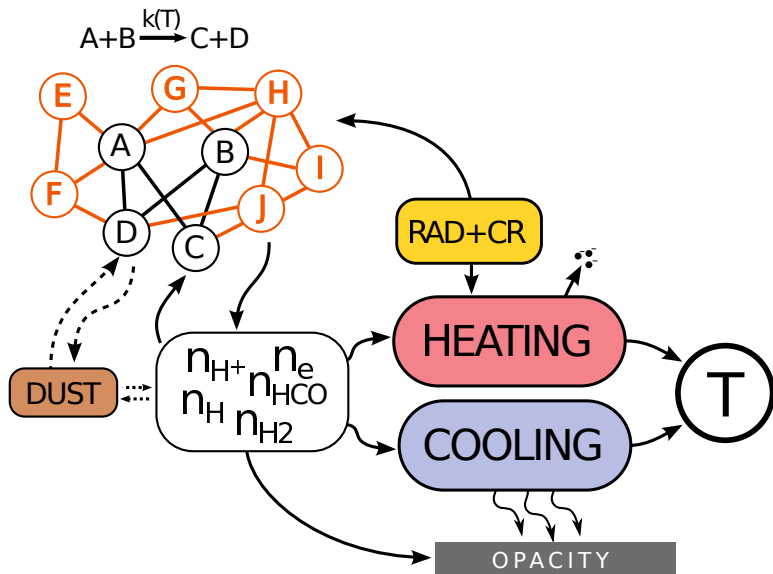
Chemistry, the full story (12/24)



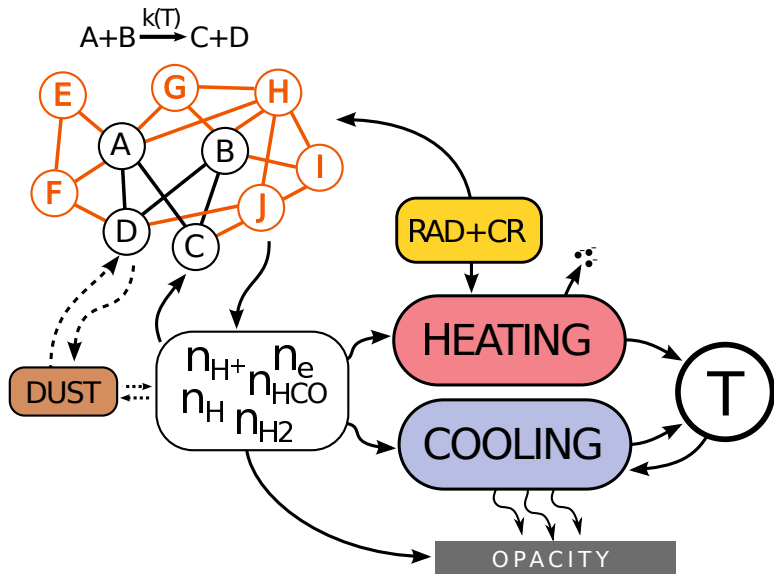
Chemistry, the full story (13/24)



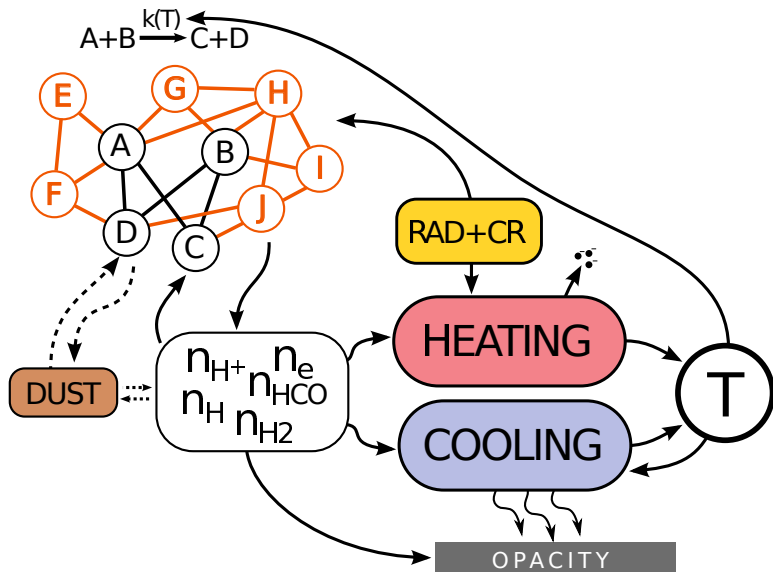
Chemistry, the full story (14/24)



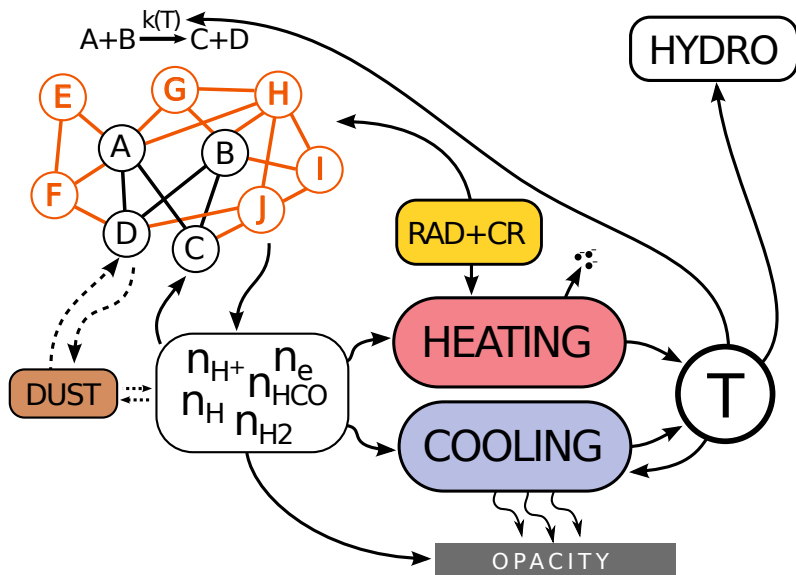
Chemistry, the full story (15/24)



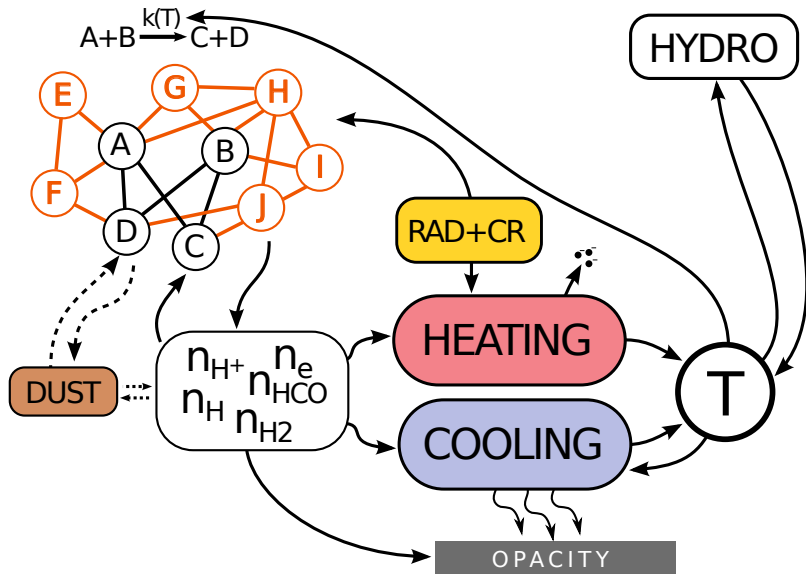
Chemistry, the full story (16/24)



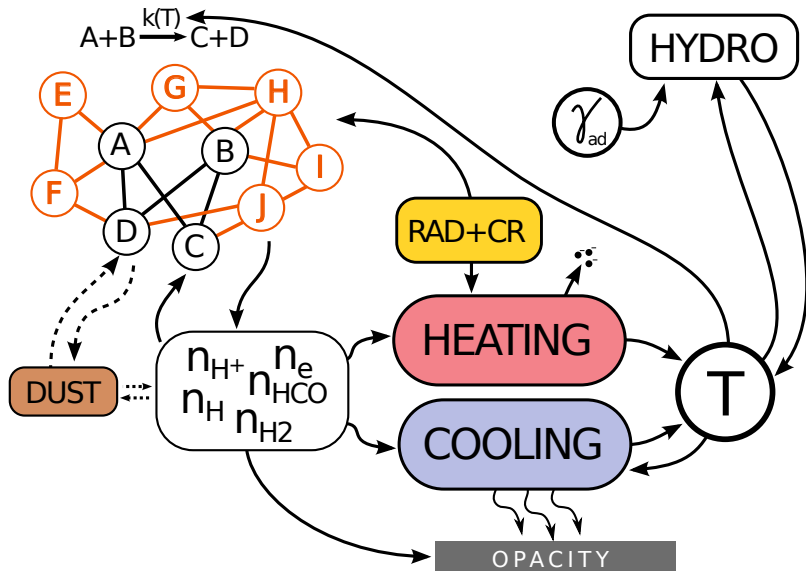
Chemistry, the full story (17/24)



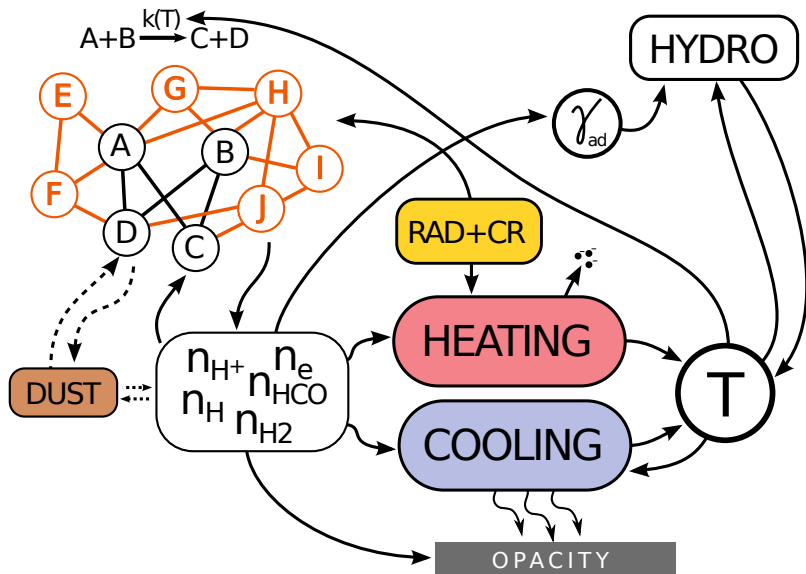
Chemistry, the full story (18/24)



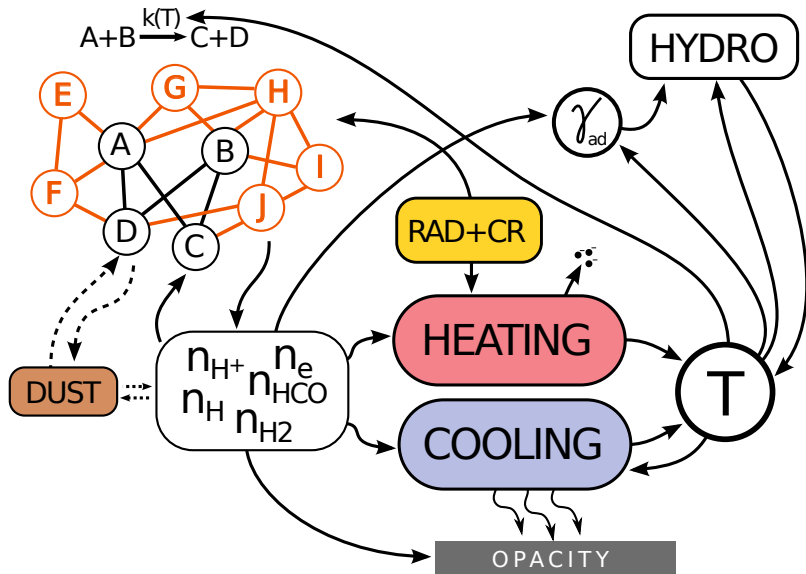
Chemistry, the full story (19/24)



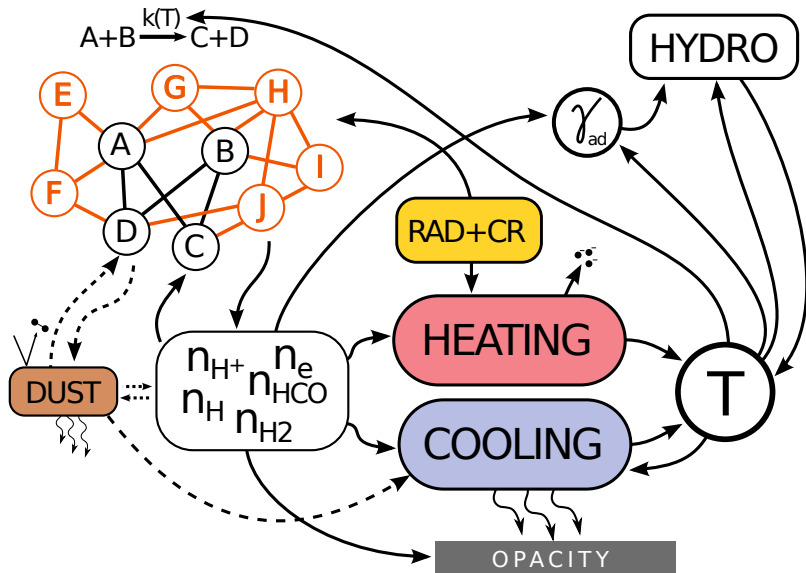
Chemistry, the full story (20/24)



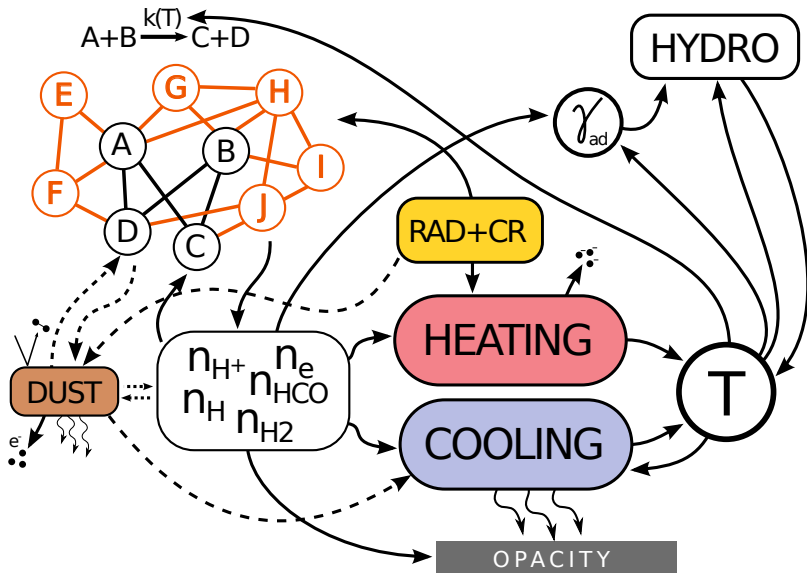
Chemistry, the full story (21/24)



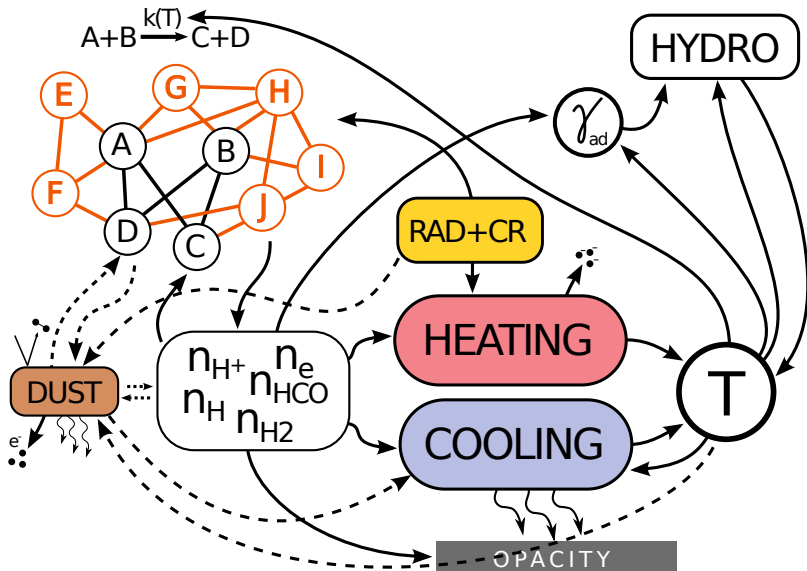
Chemistry, the full story (22/24)



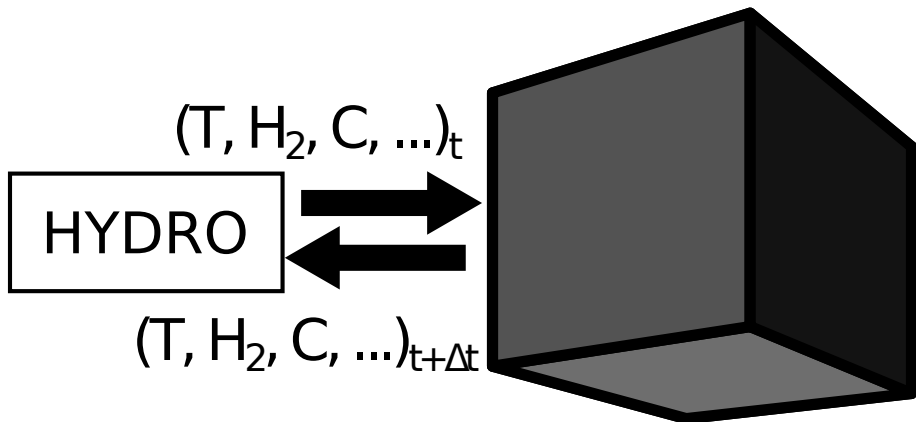
Chemistry, the full story (23/24)



Chemistry, the full story (24/24)



A useful blackbox



```
call krome(x(:), Tgas, dt_hydro)
```



better science through chemistry

a package for astrochemistry

“Any given program, when running, is obsolete”
(Anonymous)



KROME (<http://kromepackage.org/>)

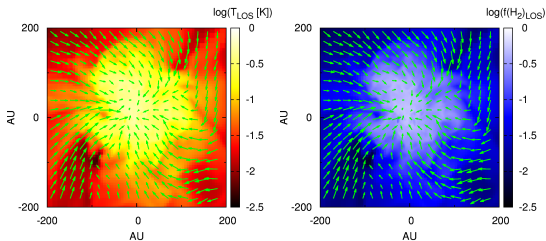
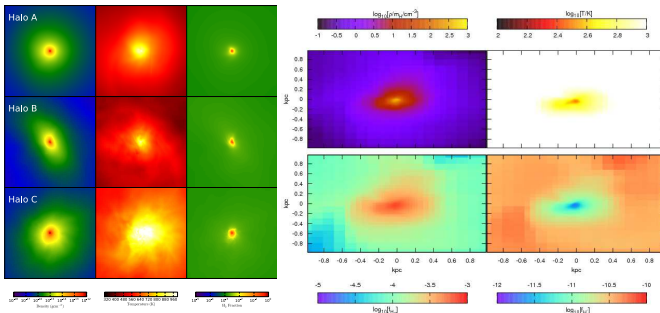
- Python Pre-processor provides Fortran routines
- Creates F90 modules from chemical network and option flags
- Dust evolution, Cooling, Heating, Photoionization, ...
- Open source, bitbucket community
- Highly optimized, fast solvers (DLSODES, DVODE F90)
- Test suite (MC, 1D SNe, planet, 3D and C/C++ wrappers, ...)
- Grassi et al. 2014 ([arXiv:1311.1070](https://arxiv.org/abs/1311.1070)), TG+2011 ([arXiv:1012.1142](https://arxiv.org/abs/1012.1142))

Processes overview

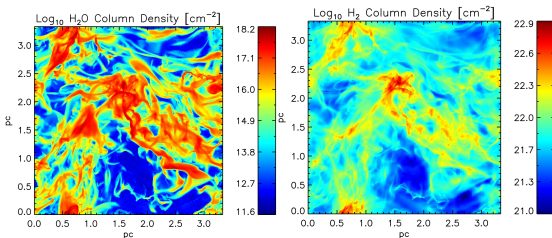
- Solving chemical network (ODEs+Jacobian+sparsity+tables)
- Several chemical networks provided (from primordial up to >5k reacts)
- Photodissociation and photoionisation (ν -dependent xsecs)
- Cosmic rays (rate approximation, $a\zeta_{CR}$)
- Atomic cooling (H, H^+ , He, He^+ , He^{++} , as Cen1992)
- H_2^{ν} cooling (GP98+GA08), HD (Lipovka+2005)
- H_2^{cd} cooling (Martin+98, Glover+Jappsen2007)
- CIE cooling (Ripamonti+Abel2004)
- C, O, Si, Fe, and ions cooling (Maio+2007, HM79, at runtime)
- Continuum (Omukai2000, Lenzuni+91)
- Chemical heating, including H_2 on dust (Omukai2000, HM79)
- Photoheating (ν -dependent, GA08)
- bins in size for dust (graphite and Si-based, incl. optical prop, e.g. Grassi+2011)
- Dust growth by sticking (Dwek98, G+11), thermal sputtering (Nozawa2006)
- H_2 formation on dust (Cazaux+Spaans2009)
- More details in Grassi+2014 (arXiv:1311.1070, MNRAS in press)

KROME in 3D codes (patches)

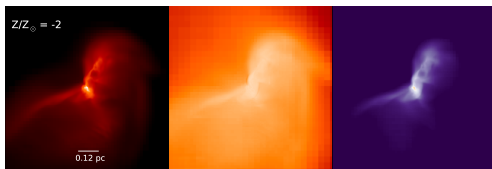
ENZO (S.Bovino, D.Schleicher) + RAMSES (J.Prieto) + FLASH (D.Seifried)



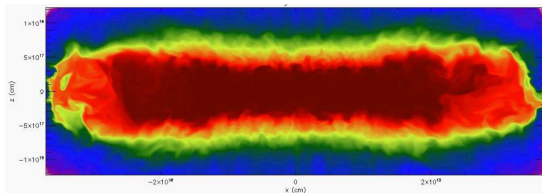
KROME in 3D codes/2



- T. Haugbølle
- RAMSES
- Turbulent MC (MHD)



- S. Bovino+D. Schleicher
- Enzo
- Metal-poor C-rich star



- D. Seifried
- FLASH
- “Filamentology”

Community

“Programming would be so much easier without all the users.”
(Anonymous)

kromepackage.org

KROME**PACKAGE**

[HOME](#)

[ABOUT KROME](#)

[KROME SCHOOLI](#)

[GET KROME](#)

[DOCS](#)

[PAPERS](#)

[PRESS](#)

[ABOUT US](#)

WELCOME TO KROME

(BETTER SCIENCE THROUGH CHEMISTRY)

KROME (bitbucket)

bitbucket.org/tgrassi/krome/

The screenshot shows the Bitbucket web interface for the repository 'KROME' by user 'tgrassi'. The top navigation bar includes 'Dashboard', 'Teams', 'Repositories', and 'Create'. The repository URL is 'https://tgrassi@bitbucket.org/tgra'. The left sidebar lists 'ACTIONS' (Clone, Create branch, Create pull request, Compare, Fork) and 'NAVIGATION' (Overview, Source, Commits, Branches, Pull requests, Issues). The main content area is titled 'Overview' and displays repository statistics: 'Last updated 22 hours ago', 'Website http://kromepackage.org/', 'Language Python', 'Access level Admin', '4 Branches', and '6 Forks'. A description states: 'This is the KROME repository. KROME is a nice and friendly package to model chemistry and microphysics for a wide range of astrophysical simulations. Given a chemical network (in CSV-like format) it automatically generates the routines needed to solve the kinetic of the system, modelled as system of coupled Ordinary Differential Equations. It provides different options which make it unique and very flexible. Any suggestions and comments are welcomed. KROME is an open-source package, GNU-licensed, and any improvements provided by the users is well accepted. See disclaimer below and GNU License in gpl-3.0.txt. KROME is available on http://www.kromepackage.org'. A 'Watching' overlay is visible, showing 'You are watching this repository' and 'Subscribe to notifications about' options. Recent activity shows a commit by Tommaso Grassi: '9725381 alltest skips dev, new md5'.

“Developers! Developers! Developers!” (Steve Ballmer)

• DEVELOPER

• STABLE

• TESTED

kromepackage.org/test

THIS PAGE TESTS THE LATEST BITBUCKET VERSION OF **KROME**

KROME_HOME INFO **BITBUCKET**

KROME: TEST PAGE

Test started :Wed Sep 3 2014, 10:08:21
This changeset :4674be5 ✓
Reference changeset :27dcbe4
Latest "tested" changeset :4674be5 ([download](#)) ✓

| Test name | Status | Time (s) | Test type | Res |
|-----------|--------|----------|-----------|-----|
| compact | ✓ | 0 | regular | ✓ |
| map | ✓ | 55 | regular | ✓ |

KROME - bootcamp 2015

KROME **computational school** | 20-24 July 2015 | Copenhagen
<http://kromepackage.org/bootcamp>

School topics

- Solvers and chemical networks
- Thermal processes and dust
- Optimization and code tuning
- Interfacing KROME to your own code
- Chemistry & synthetic observations
- Exercises with participants
- ★ GRANTS AVAILABLE!

Speakers (preliminary)

S. Bovino (IfA, Goe), **D. Galli** (INAF Arcetri), **T. Grassi** (STARPLAN/NBI, Cph),
T. Haugbølle (STARPLAN/NBI, Cph), **J. Jørgensen** (STARPLAN, Cph), **K. Omukai**
(Tohoku Uni), **D. Schleicher** (IfA, Goe), **D. Seifried** (Hamburg Observatory).

Next steps

- complete dust module (e.g. charge)
- complete surface reactions (adsorption, evaporation, 2body, CR, photo)
- improve Jacobian
- ...

The eternal struggle

EFFICIENCY \longleftrightarrow ACCURACY

Some questions (out of thousands)

- Has your code the right microphysics and/or chemistry?
- What happens to hydrodynamics with fully consistent microphysics (e.g. γ_{ad})?
- What is the smallest set of microphysical processes?
- What is the best realistic/efficient model for each astrophysical environment?
- What is the influence of the rate accuracy on the global model?
- Are chemical networks complete?

Thank you for your attention!

“All models are wrong, but some are useful”
(George Box)



<http://kromepackage.org/>
<http://kromepackage.org/bootcamp>
Grassi et al. 2014 ([arXiv:1311.1070](https://arxiv.org/abs/1311.1070))