Next generation astrochemistry

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September 2015

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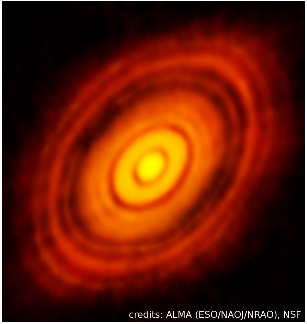
KROME
better science through chemistry

ISM chemistry

Why chemistry/microphysics? (in numerical simulations)

"Chemistry has been termed by the physicist as the messy part of physics" (F. Soddy)

- 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
- comparison with observations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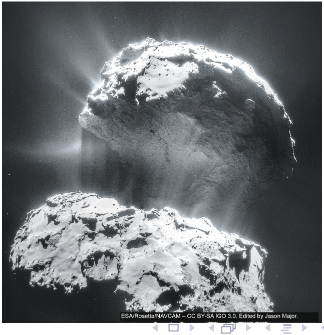
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ISM chemistry/2

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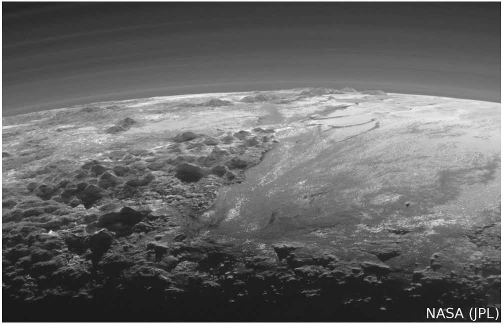
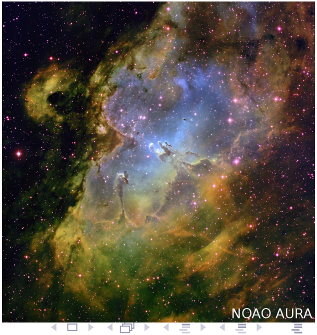


NASA (JPL)

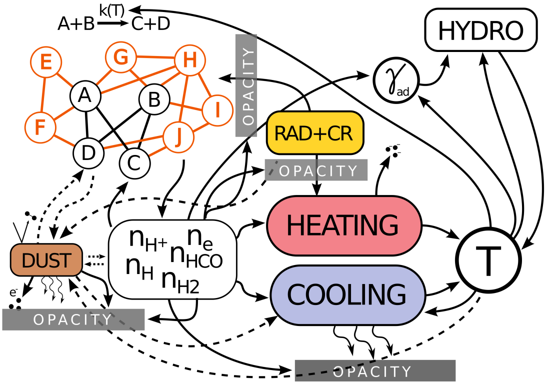


NOAO AURA

ISM chemistry/3

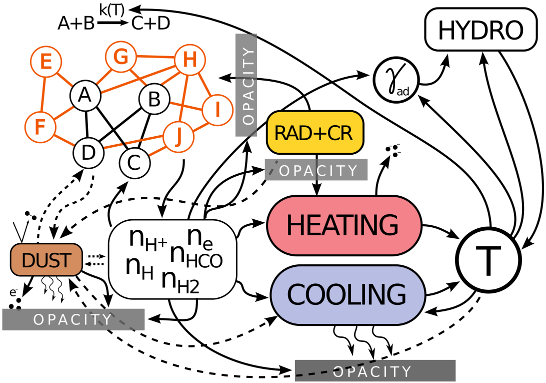
Troubles with chemistry/microphysics (in numerical models)

- very CPU demanding (solving stiff ODEs+)
- has a non-linear/complex behaviour (e.g. MC)
- connected with (and influenced by) many physical processes
- has to be coupled with hydro-codes (already demanding)



Ingredients

- chemistry (i.e. “pure” chemical reactions, $\mathrm{CO^+ + e^- \rightarrow C + O}$)
- photochemistry (several levels of complexity, $\mathrm{CO} + \gamma \rightarrow \mathrm{C} + \mathrm{O}$)
- thermal processes (cooling/heating, ro-vib cooling)
- consistent opacity (based on chemical/dust composition, non-local)
- dust (from “passive” interaction to coupled evolution)



All in one

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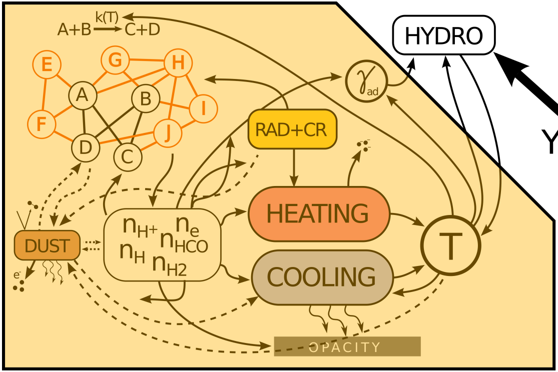
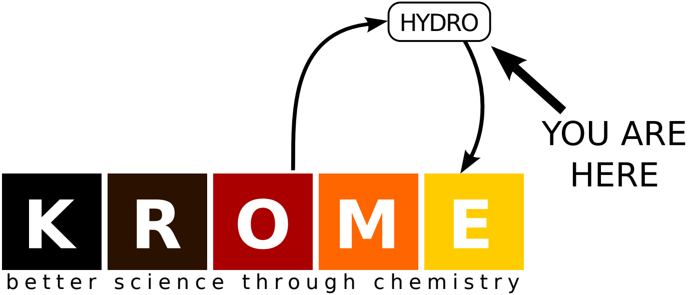


YOU ARE HERE

KROME



What is KROME?

- Python pre-processor creates *ad hoc* F90 modules
- Chemistry, dust-related physics, cooling, heating, photoionization, . . .
- Open source, `kromepackage.org`, Grassi+2014 (MNRAS)
- Highly optimized, “fast” solver (DLSODES)
- Can be coupled to hydrocodes, RAMSES, Enzo, FLASH, Gasoline, . . .
- growing comunity, 2 computational schools

Prototypical problem

Context: turbulent molecular clouds

- Star-forming regions
- Complex structures at all scales
- Molecular richness (mainly H-C-O, but also F-S)
- Large CO variability
- CH^+ and SH^+ unexpected abundances
- CO-to-H_2 conversion factor still under investigation

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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

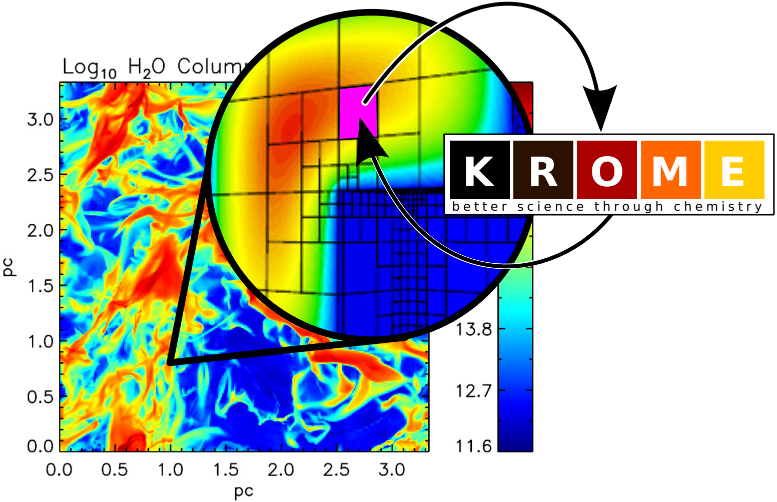
RAMSES-CPH (powered with KROME)

- Non-equilibrium H-C-O chemistry (+CRs, +photo)
- Fully coupled thermochemistry (on-the-fly fine-structure +tables)
- Consistent adiabatic index (state-of-the-art partition functions)
- Dust chemistry (H_2 catalysis), dust cooling/photoheating.
- Workaround: local density-based photochemisty, i.e. $A_v = f(n_{\rm tot})$
- Optional: access to photochemistry-based opacity (RT-ready)
- Testing: more dust chemistry (H-C-O) + dust tables

Model specs

- MHD/HD
- $\simeq 3.3 \times 3.3 \times 3.3$ pc
- Turbulence: Mach 11 @ 10 K
- $\langle n_{\rm tot}\rangle \simeq 10^3$ cm^{-3}
- $\langle B\rangle \simeq 7\ \mu$G
- > 18 Mcells
- 4.7 Myr $\simeq 3.5\,\tau_d \simeq 4.5\,\tau_{ff}$
- ~ 300 rates, ~ 40 species

Cell-by-cell



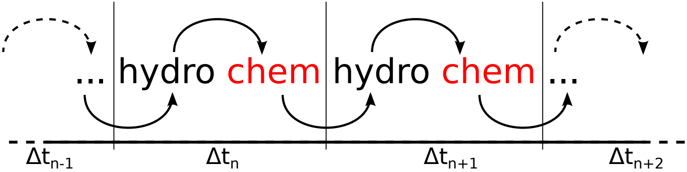
- A set of one-zone models: one for each ijk-th cell (this case $\gtrsim 18\text{M}$).
- i.e. the ijk-th cell doesn't see the neighbourhoods.

Operator-splitting approach

Status of a single cell:

$$\begin{aligned}\bar{s}_{ijk}(t) &= \left\{\rho_{ijk}(t), \bar{v}_{ijk}(t), T_{ijk}(t), \bar{n}_{ijk}(t), \ldots\right\} \\ \bar{n}_{ijk}(t) &= \left\{\mathrm{H}, \mathrm{H}_2, \mathrm{C}^+, \mathrm{e}^-, \mathrm{CO}, \ldots\right\}_{ijk}(t)\end{aligned}$$

Cell time-stepping:



At time t for the ijk-th cell:

$$\bar{s}_{ijk}(t+\Delta t) = \mathbf{T}\,\bar{s}_{ijk}(t) = \mathbf{H}\,\bar{s}_{ijk}(t,\bar{s}) + \mathbf{K}\,\bar{s}_{ijk}(t) + \ldots$$

The chemical network

Chemical network = Cauchy's problem

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \overbrace{\sum_{lm} k_{lm}(T)n_l(t)n_m(t)}^{\textit{formation}} - \overbrace{n_i(t)\sum_{j} k_{ij}(T)n_j(t)}^{\textit{destruction}} \qquad [\times N \approx 40]$$

$$n_{i,0} \equiv n_i(t=0)$$

Extra equations → less flexibility

$$\frac{\mathrm{d}T}{\mathrm{d}t} = HEAT(T,\bar{n}) - COOL(T,\bar{n}) \qquad [+1]$$

$$k_{lm}(t) \propto \int_{E_0}^{\infty} I(E,t)\sigma(E)\mathrm{d}E$$

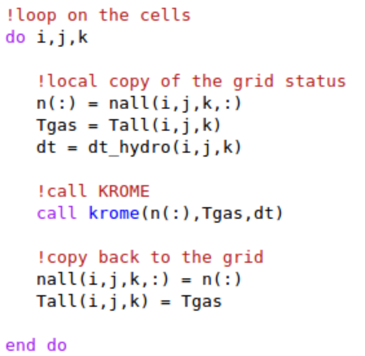
$$\gamma_{ad}(t) = f_\gamma(T,\bar{n})$$

$$\ldots$$

$$\begin{tikzcd}
\mathrm{n_i} \arrow[loop left] \arrow[d] & \mathrm{k(T)} \arrow[l] \\
\Lambda \arrow[r, shift left] & \mathrm{T} \arrow[l, shift left] \arrow[u]
\end{tikzcd}$$

Calling KROME “serially”

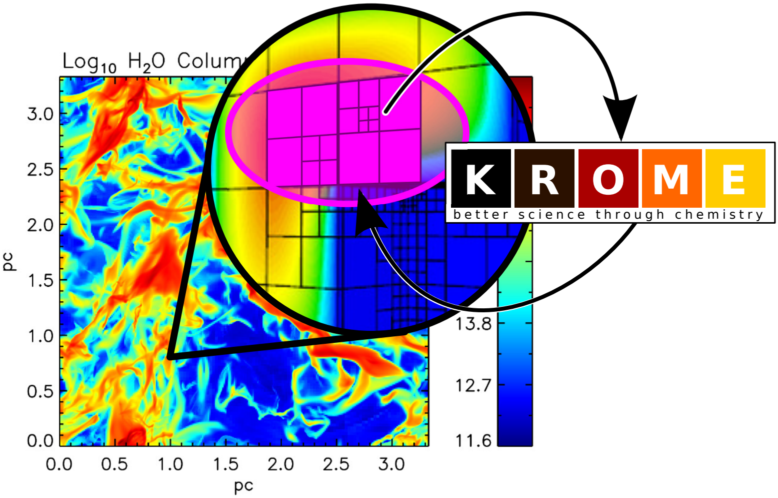
How to call to KROME cell-by-cell (from FORTRAN)



```
!loop on the cells
do i,j,k

   !local copy of the grid status
   n(:) = nall(i,j,k,:)
   Tgas = Tall(i,j,k)
   dt = dt_hydro(i,j,k)

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

   !copy back to the grid
   nall(i,j,k,:) = n(:)
   Tall(i,j,k) = Tgas

end do
```

Each cell represents a one-zone model

A single call to rule them all



Log_{10} H_2O Colum
3.0
2.5
2.0
1.5
1.0
0.5
0.0
pc
0.0
0.5
1.0
1.5
2.0
2.5
3.0
pc
13.8
12.7
11.6
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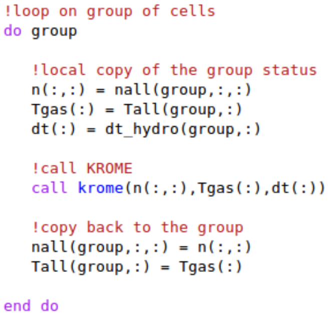
- A set of one-zone models solved within the same solver call

The chemical network (vectorized)

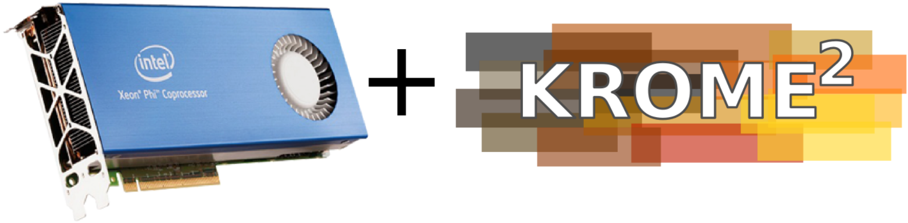
Cell-wise vectorization

$$\begin{cases} \dfrac{\mathrm{d}n_i(:)}{\mathrm{d}t} & = \overbrace{\sum_{lm} k_{lm}(:,T) n_l(:,t) n_m(:,t)}^{formation} - \overbrace{n_i(:,t) \sum_j k_{ij}(:,T) n_j(:,t)}^{destruction} \\ \dfrac{\mathrm{d}T(:)}{\mathrm{d}t} & = HEAT[T(:),\bar{n}(:)] - COOL[T(:),\bar{n}(:)] \\ n_{:,i,0} & \equiv n_i(:,t=0) \end{cases}$$



```
!loop on group of cells
do group

   !local copy of the group status
   n(:,:) = nall(group,:,:)
   Tgas(:) = Tall(group,:)
   dt(:) = dt_hydro(group,:)

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

   !copy back to the group
   nall(group,:,:) = n(:,:)
   Tall(group,:) = Tgas(:)

end do
```

KROME 2 on Xeon-Phi

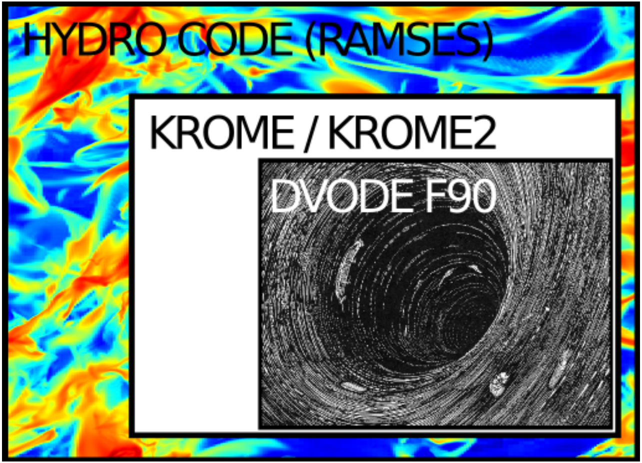


Next step, KROME→KROME 2

- use the MIC architecture for chemistry
- load-balance hydro+chemistry
- KROME is thread-safe* (but not vectorized)
- KROME 2 is OpenMP/MIC-ready
- KROME 2 designed to be vectorized
- KROME 2 has many other features (not relevant here)

*branch openmp

Solver - DLSODES/DVODE F90



- Based on original f77 version
- Flexible solver (too much, probably)
- Not designed to be thread-safe (recently modified)
- +KROME 2: compiles on Xeon-Phi (more tests should be done)

Summary

Conclusions / Future outlook

- Chemistry: complex problem but “easily” vectorizable
- Hydro+chemistry seems to be promising on MIC
- Best strategy (so far): multi-cell vectorization
- Updated (2013) DVODE-F90 solver is thread-safe
- New (< 1 month) KROME 2 is designed for multi-cell strategy
- KROME 2 currently under developement
- TODO: more tests to understand actual scaling

Thank you for your attention!

“My computer’s so fast it finishes an infinite loop in 5 minutes.”
(Anonymous)

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`http://kromepackage.org/`