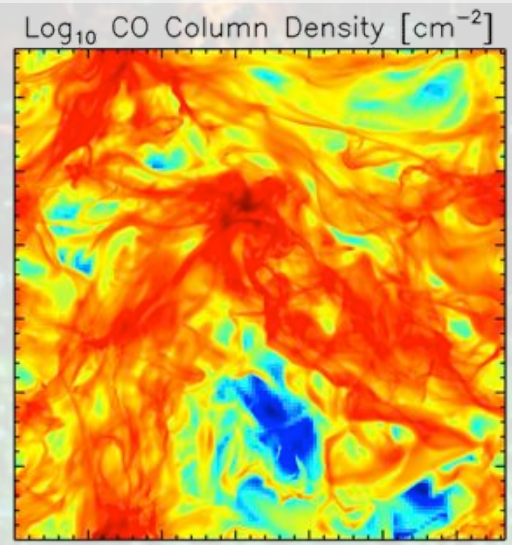
KROME + RAMSES: Integration of Chemistry with Fluid Dynamics

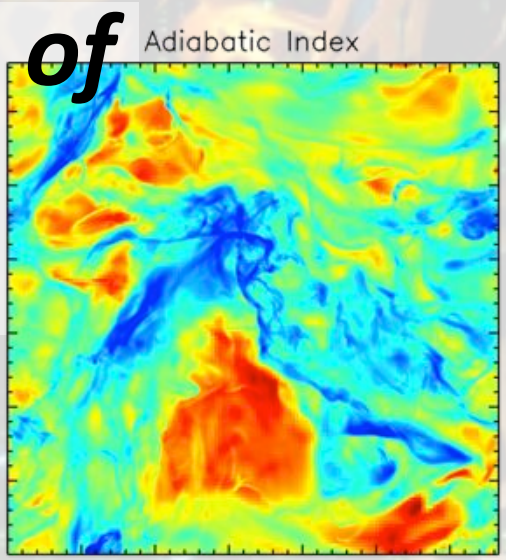
KROME Bootcamp, Göttingen, September 2014

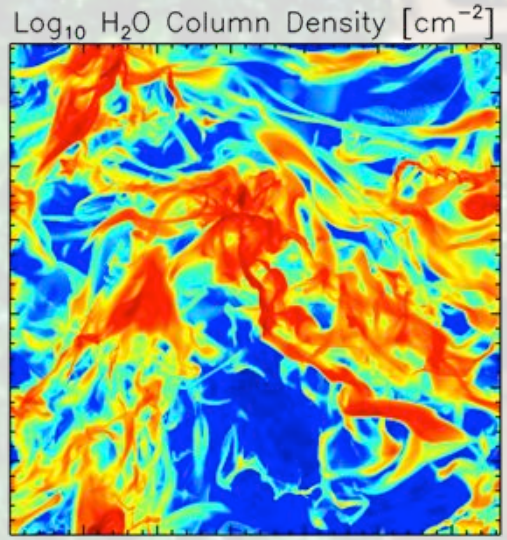
Troels Haugbølle

troels.haugboelle@snm.ku.dk

Centre for Star and Planet Formation
Natural History Museum
University of Copenhagen







Sapere Aude

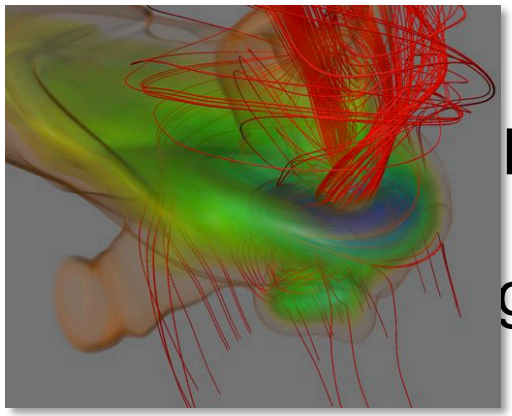
PRACE

CENTRE FOR STAR AND PLANET FORMATION

A research centre for cosmochemistry, astrophysics and astronomy

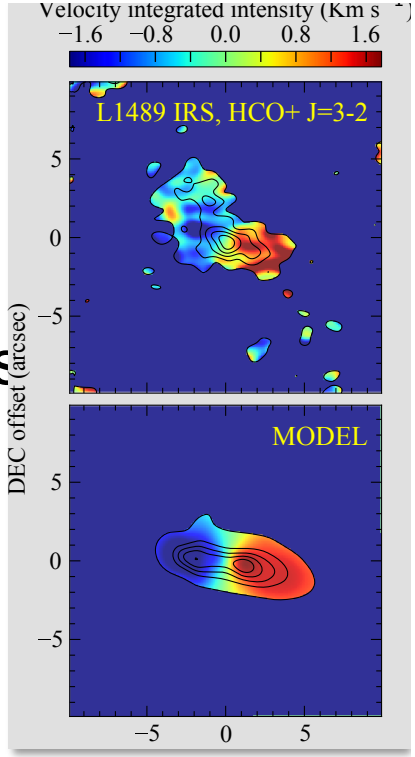
STARPLAN

Chemistry + Fluid Dynamics A Happy Union ?



ha[KROME]s

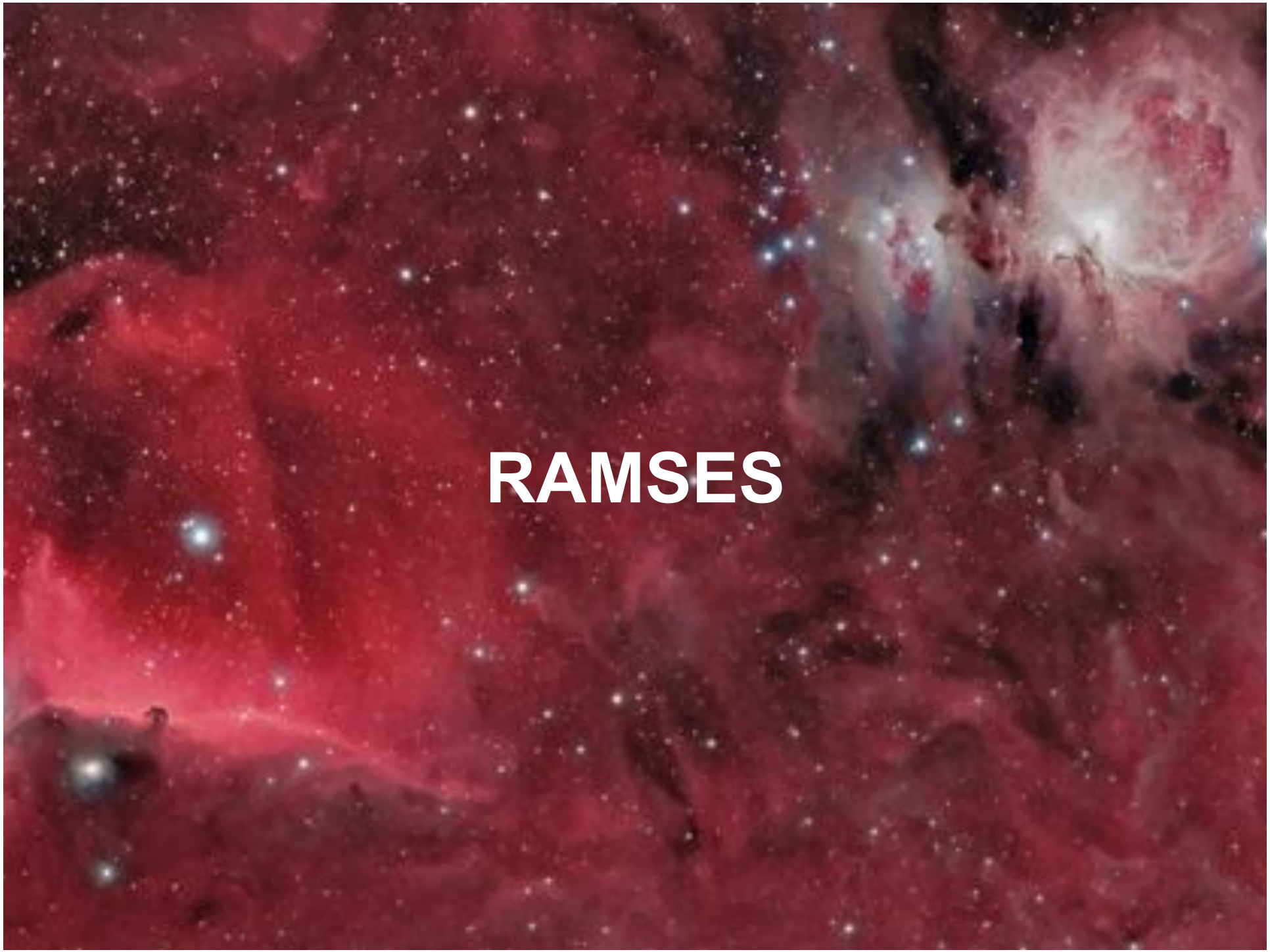
gl[better science through chemistry]n



- With the completion of ALMA, precise astrochemistry models are becoming ever more important:
  - Model➔Chemical Abundance➔Synthetic Observations

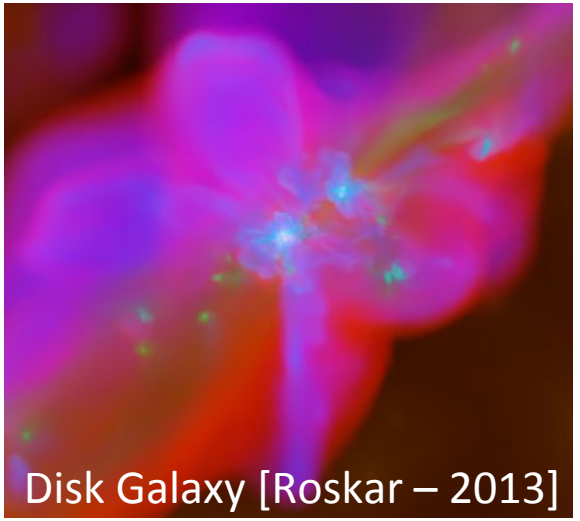
But

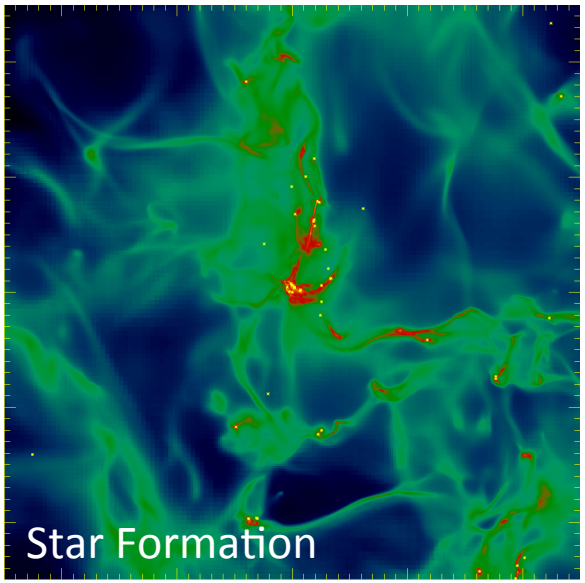
- What are the ingredients in a proper model?
- What are the pitfalls?


RAMSES

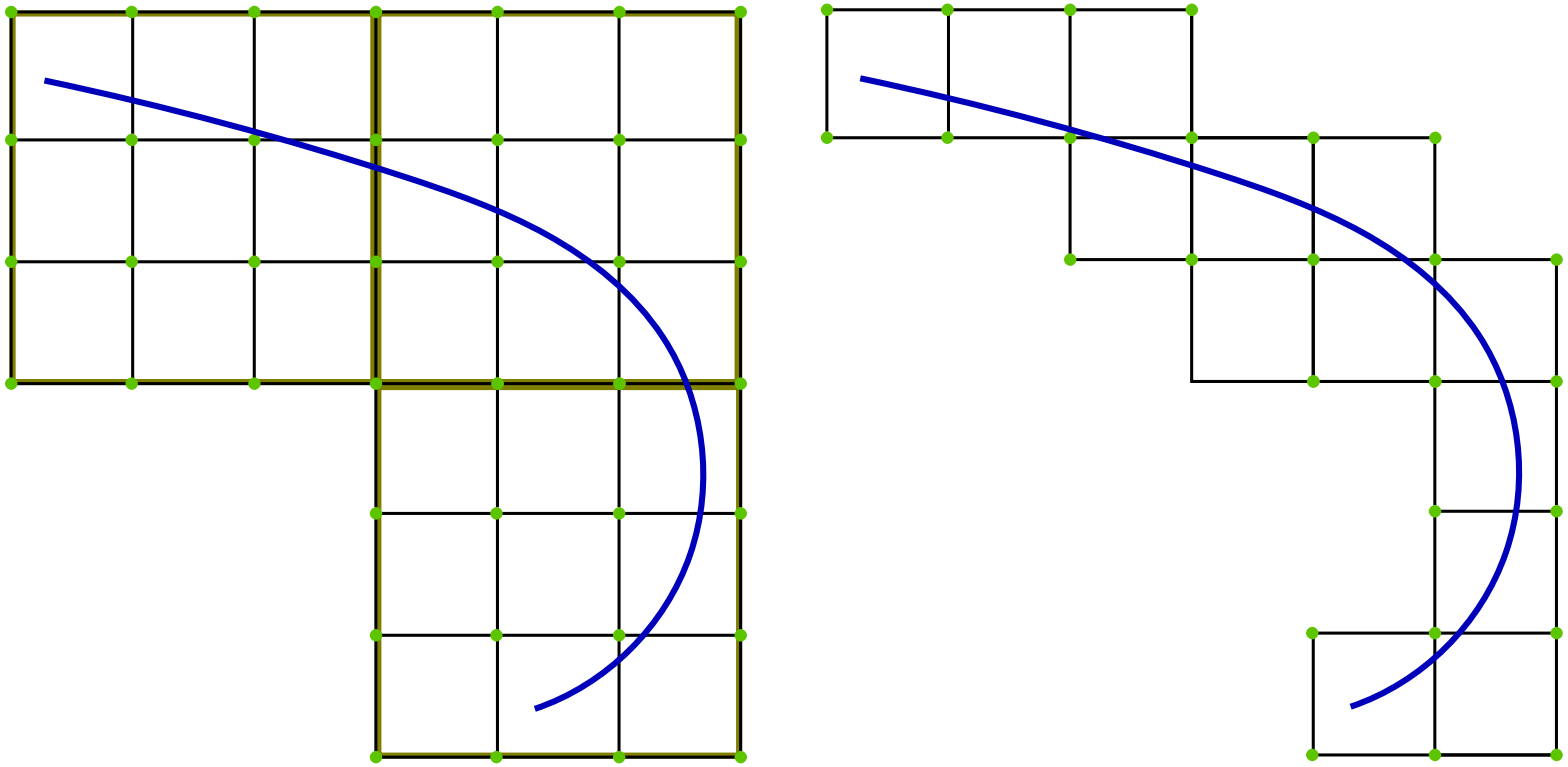
RAMSES

- RAMSES is a *well established* AMR code originally written for Cosmology, but now applied in many other astrophysical contexts.
- Written by Romain Teyssier in 2002, it is public, and used by a large number of groups.
- https://bitbucket.org/rteyssie/ramses
- The AMR structure is a fully threaded oct-tree.
- The code can model a mixture of cell based fluids and particles. It has many physics modules: MHD, Selfgravity, collisionless particles, sink particles, cooling tables, cosmic rays, radiative transfer, feedback, …
- Parallelization is (OpenMP)+MPI (public) or OpenMP+MPI (our version), and the code scales to well over 10.000 cores.


Disk Galaxy [Roskar – 2013]


Star Formation

Tree-Based Adaptive Mesh Refinement



- A patch based AMR structure is much better at adapting to complex flows, like turbulence
- CPU overhead is larger; hard to vectorize efficiently due to linked list structure

Fluid dynamics

- RAMSES includes solvers for HD and MHD with passive scalars
- Implementation based on a second order MUSCL scheme
- Many different Godunov solvers
  - LLF – HLL – HLLC – HLLE – HLLD - ROE
- Different Slope limiters
  - Minmod, Monotonized central, ultrabee, superbee
- MHD is constrained transport with staggered fields, and 2D Riemann solvers for the *EMF*
- Recently, non-thermal energy components have been added in to the second-order predictor-corrector time update

Refinement Criteria

- Jeans / Truelove Criteria
  - If the Jeans length is not resolved, collapse becomes unphysical

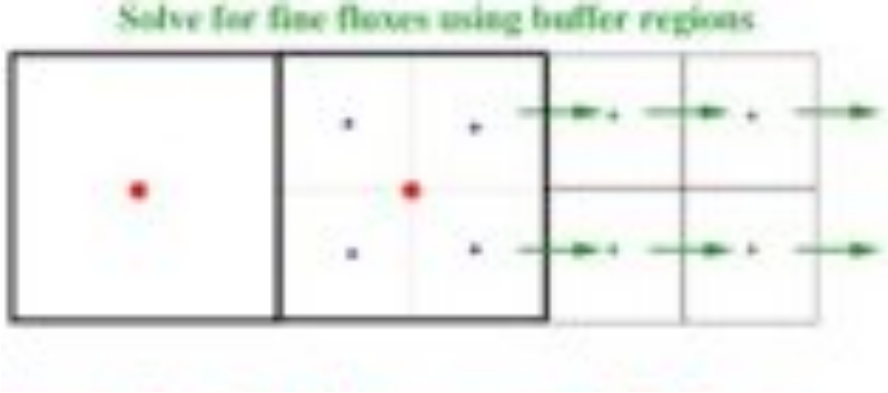
- Gradients, in particular it is possible to refine on passive scalar gradients

- Mass Refinement (Quasi-Lagranian)
  - Related to Jeans. F.x. refine every time density goes up with 4 to have same Jeans resolution on all levels

- Geometrical (zoom)
  - Only allow code to refine in specific region

Godunov and AMR Refinement

- Interpolation to finer meshes
  - Creation of new cells
  - On-the-fly boundary cells
- Averaging to coarser levels
  - Destruction / derefinement
  - Filling of the threaded tree
- Flux correction at boundaries
  - Relatively easy for volume fluxes
  - Tricky for EMF at edges
- Different interpolators
  - Conservative / internal energy
  - Apply different slope limiters



(from talk by Romain Teyssier)

Physics

- HD / MHD: State-of-the-art; many solvers
- Self-Gravity: Conjugate gradient or Multigrid methods
- Cooling & Heating:
  - Cooling for cosmology, high-T, implicit solver, UV & cosmic ray heating
  - Moment based radiative transfer. Coupling to energy equation.
- Particles: DM (collisionless), tracers, sinks
- Sink particles: Based on a clump finder algorithm, can feedback on the gas (Supernovae, winds)
- Metals as passive tracers


COUPLING
RAMSES TO KROME

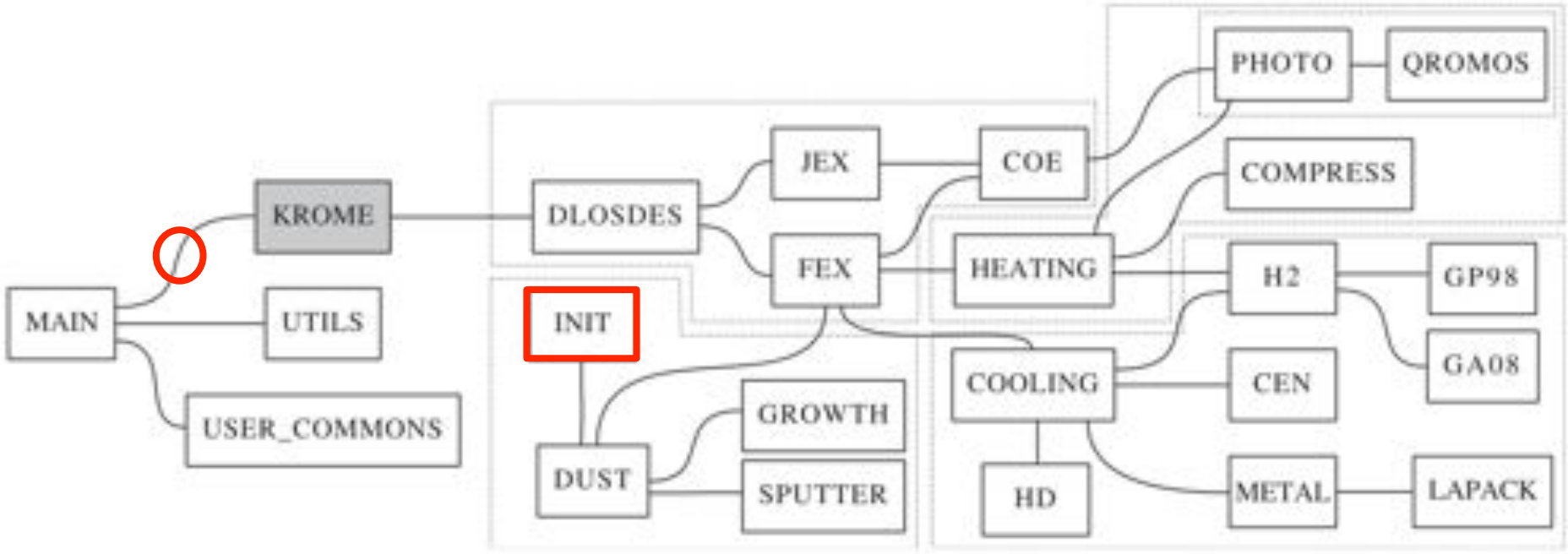


Figure 5. Pictorial view of the graph representing subroutine and modules in the KROME package. *MAIN* is the framework program, *KROME* (greyed) is the main module of KROME, while the other modules are explained in detail within the text.

Running KROME with a *framework code* is easy:

`./krome -ramses -useN –network …`

the files, ready for integration, are left in **`./build`**

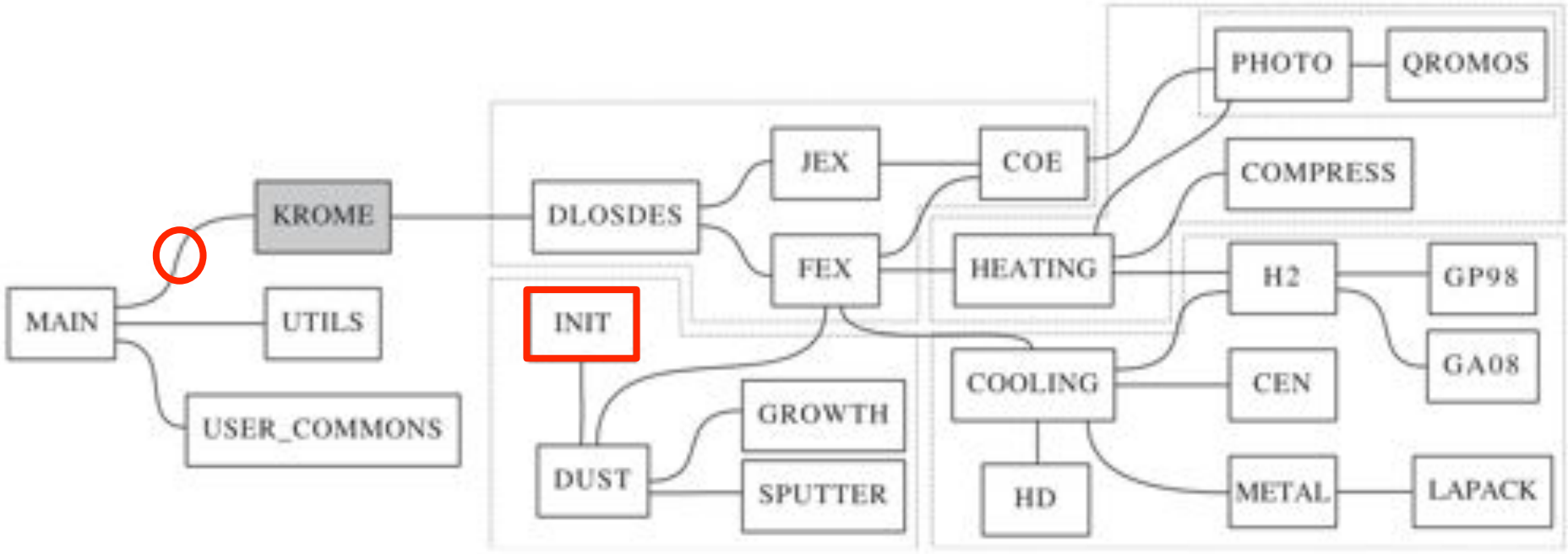


Figure 5. Pictorial view of the graph representing subroutine and modules in the KROME package. *MAIN* is the framework program, *KROME* (greyed) is the main module of KROME, while the other modules are explained in detail within the text.

KROME couples through the energy equation as a source term:

$$\frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot \boldsymbol{F} = \boldsymbol{S}$$

$$\frac{\partial (\rho e)}{\partial t} + \nabla \cdot [(\rho e + P)\boldsymbol{v}] = S_e$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = (\gamma - 1)\frac{\Gamma(T, \bar{n}) - \Lambda(T, \bar{n})}{k_\mathrm{b} \sum_i n_i}$$

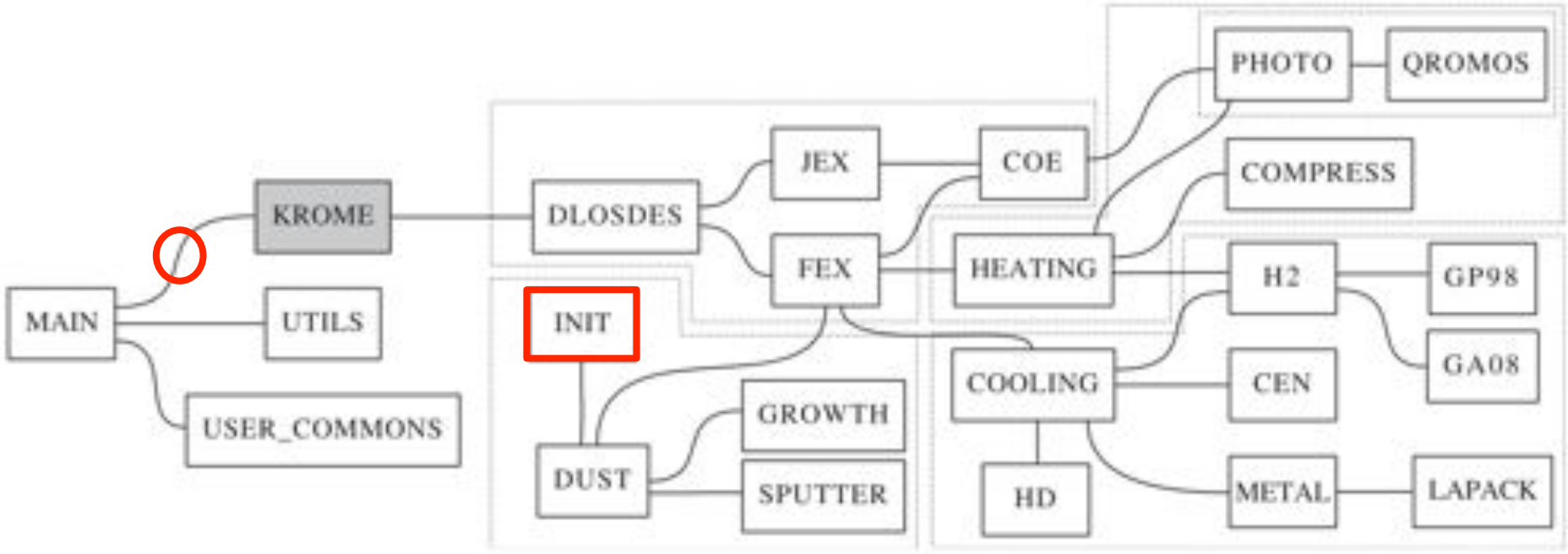


Figure 5. Pictorial view of the graph representing subroutine and modules in the KROME package. *MAIN* is the framework program, *KROME* (greyed) is the main module of KROME, while the other modules are explained in detail within the text.

KROME couples through the energy equation as a source term:

- KROME has to be initialized. This happens in the initialization of cooling and heating in *cooling_module.f90*

- Time evolution and cooling and heating due to the chemical composition is calculated in the thermal energy hook: *cooling_fine.f90*

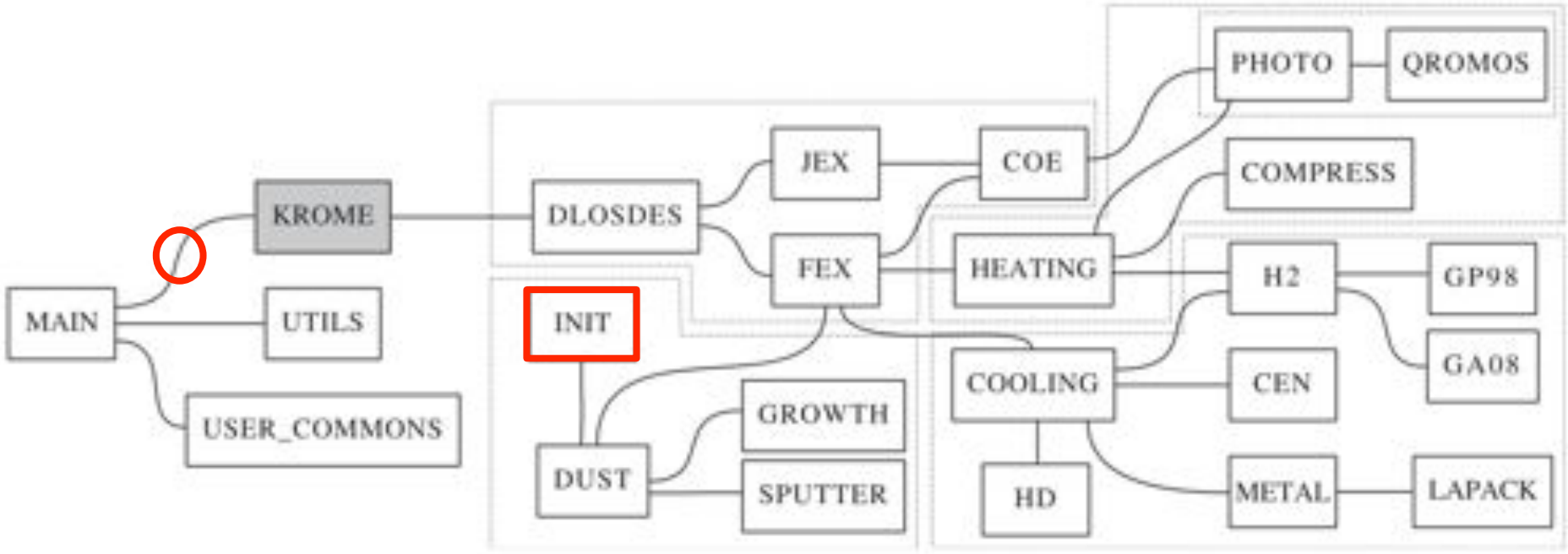


Figure 5. Pictorial view of the graph representing subroutine and modules in the KROME package. *MAIN* is the framework program, *KROME* (greyed) is the main module of KROME, while the other modules are explained in detail within the text.

Is that ALL there is to chemistry integration ?

Issues and Outstanding Questions

- In Astro Chemistry

  You need to know what you don't know!

  applies heavily. You need to know what are the relevant reactions for your physical setup.

- Timescales and thermal conduction
- Adiabatic Index
- Local Conservation of abundances
- Performance and parallelization

Issues and Outstanding Questions

- In Astro Chemistry

You need to know what you don't know!

applies heavily. You need to know what are the relevant reactions for your physical setup.

- Ionization, MHD, and thermal conduction

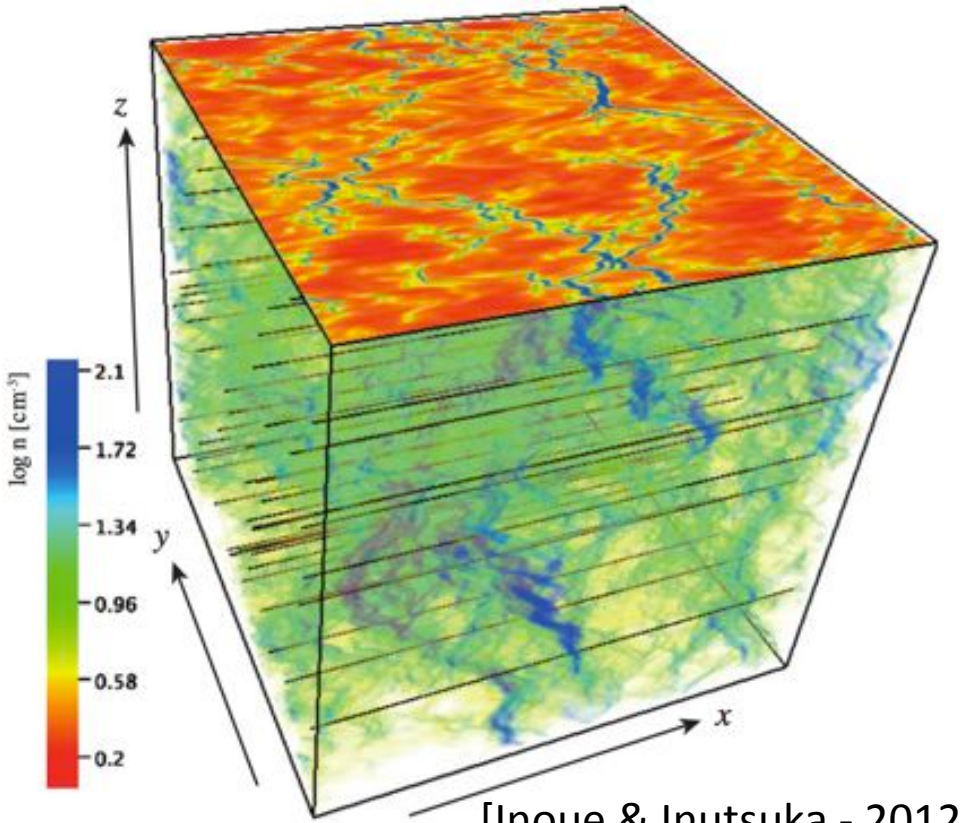
$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \boldsymbol{v}) = f_i(n_j, N_j, T, G_0)$$

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot \left(p + \frac{B^2}{8\pi} + \rho \boldsymbol{v} \otimes \boldsymbol{v} - \frac{\boldsymbol{B} \otimes \boldsymbol{B}}{4\pi} \right) = 0,$$

$$\frac{\partial e}{\partial t} + \nabla \cdot \left\{ \left(e + p + \frac{B^2}{8\pi} \right) \boldsymbol{v} - \frac{\boldsymbol{B} \cdot \boldsymbol{v}}{4\pi} \boldsymbol{B} \right\} = \nabla \cdot \kappa \nabla T - L(n_i, N_i, T, G_0),$$

$$\frac{\partial \boldsymbol{B}}{\partial t} = \nabla \times (\boldsymbol{v} \times \boldsymbol{B}),$$

$$\rho = \sum_i m_i n_i,$$



[Inoue & Inutsuka - 2012]

Issues and Outstanding Questions

- In Astro Chemistry

  You need to know what you don't know!

  applies heavily. You need to know what are the relevant reactions for your physical setup.

- Timescales and thermal conduction

- Adiabatic Index:
  - Only when $\gamma < 4/3$ gravitational collapse will proceed
  - Changes in the adiabatic index are crucial for the
    - formation of protostars
    - stability of accretion disks
- The *effective* adiabatic index may be different due to cooling and heating! F.x. ISM has $\gamma_{eff} < 1$

Issues and Outstanding Questions

- In Astro Chemistry

  You need to know what you don't know!

  applies heavily. You need to know what are the relevant reactions for your physical setup.

- Timescales and thermal conduction

- Adiabatic Index

KROME solves: $$\frac{\mathrm{d}T}{\mathrm{d}t} = (\gamma - 1)\frac{\Gamma(T, \bar{n}) - \Lambda(T, \bar{n})}{k_\mathrm{b} \sum_i n_i}$$

with the adiabatic index computed according to the KROME "-gamma" switch: constant, FULL, ROT, VIB, EXACT

But what about ***YOUR*** code ? A variable adiabatic index should be implemented, including in the (M)HD solvers, and all places that convert between pressure and internal energy

```
!##########################################################
SUBROUTINE find_mhd_flux_vec(qvar,cvar,ff,vel)
.........
  !! compute the 1D MHD fluxes from the conservative variables
  !! the structure of qvar is : rho, Pressure, Vnormal, Bnormal,
  !! Vtransverse1, Btransverse1, Vtransverse2, Btransverse2
  IMPLICIT NONE

  INTEGER :: i , ivar, ib
.........
  ! Local variables
  entho = one/(gamma-one)
  d=>qvar(:,1); P=>qvar(:,2); u=>qvar(:,3); A=>qvar(:,4)
  v=>qvar(:,5); B=>qvar(:,6); w=>qvar(:,7); C=>qvar(:,8)
  ecin = half*(u*u+v*v+w*w)*d
  emag = half*(A*A+B*B+C*C)
#ifdef KROME
  etot = P / (merge(qvar(:,ichem),gamma,chemistry) - one) + ecin + emag
#else
  etot = P*entho+ecin+emag
#endif
  Ptot = P + emag
  du   = d*u

  ! Compute conservative variables
.........


  ! Compute fluxes
  ff(:,1) = du
.........
  do ivar = 9,nvar
#ifdef KROME
     if (ivar .ne. ichem) then
#endif
        ff(:,ivar) = du*qvar(:,ivar)
#ifdef KROME
     else  ! Make sure effective adiabatic index has zero flux
        ff(:,ivar) = zero
     endif
#endif
  end do

  call trace_api('find_mhd_flux_vec(qvar,cvar,ff,vel)','exit',3)
END SUBROUTINE find_mhd_flux_vec
!##########################################################
```

Adiabatic Index

Example extract from local CPH version of RAMSES :

- KROME returns adiabatic index as a passive scalar
- All pressures computed from internal energy or vice versa use passive scalar
- Update Godunov solvers to work with changing adiabatic index
- Make sure refinement and interpolation is ok

Issues and Outstanding Questions

- In Astro Chemistry

  You need to know what you don't know!

  applies heavily. You need to know what are the relevant reactions for your physical setup.

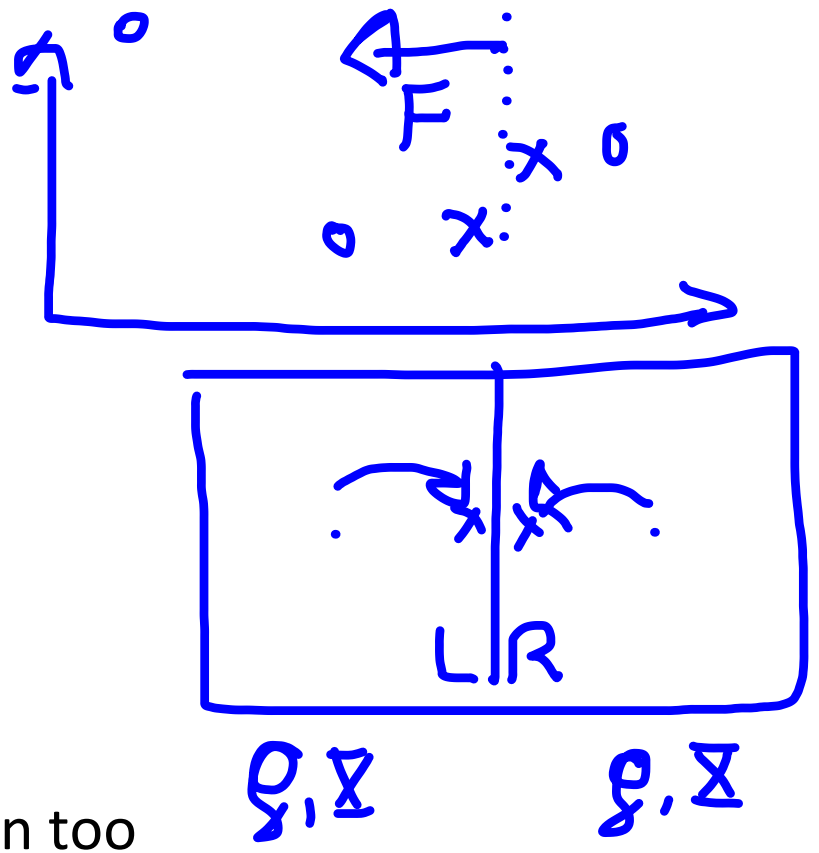
- Timescales and thermal conduction

- Adiabatic Index

- Multi-fluid Advection and Conservation of Abundances [Plewa and Müller 1999]

Multi-fluid Advection
Conservation of Abundances

- Flux conservation ensures *global* conservation of species
- Slope limiter induces large *local* error in species (≈30% errors)
- Simple fix: Renormalize in each step
- Solution: Renormalize interpolated abundances making them sum to 1
- Important at coarse-fine interpolation too



$$\varphi_i^{\#} = \frac{1}{\sum_{n=1}^{N_X} X_{i,n}^{\#}}, \quad \mathcal{X}_{i,n}^{\#} = \varphi_i^{\#} X_{i,n}^{\#}$$

[Plewa and Müller 1999]

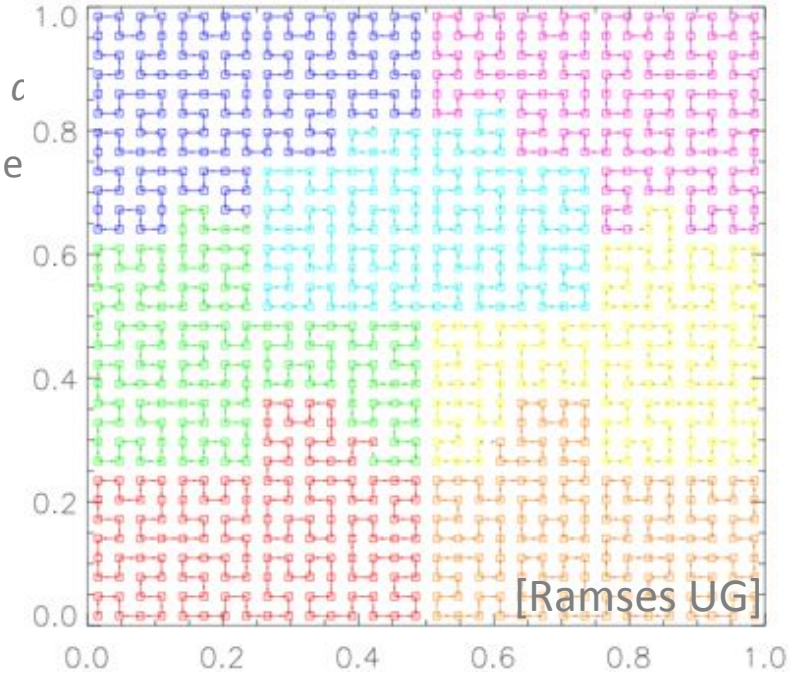
Issues and Outstanding Questions

- In Astro Chemistry

  You need to know what you c

  applies heavily. You need to know what are the rele reactions for your physical setup.

- Timescales and thermal conduction
- Adiabatic Index
- Local Conservation of abundances



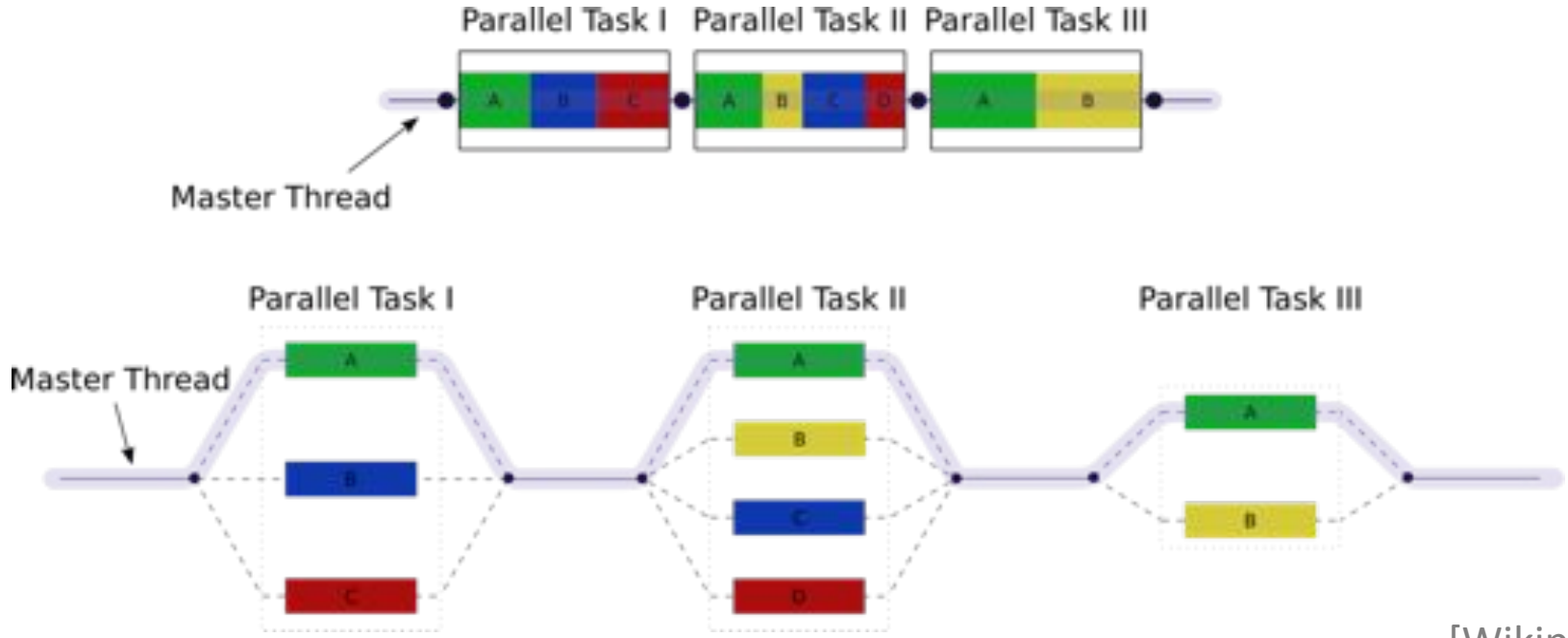
- Performance and parallelization:
  - Traditional parallelization method is MPI
  - Global domain decomposition according to cost of cell or particle updates with e.g. regular domains, or along a space filling curve.
  - Problem: Cost of KROME is highly “non-deterministic”

KROME + OpenMP

- Problem: Cost of KROME is highly “non-deterministic”

t … KROME dt is chemistry dependent … translates to ***different per-cell cost*** $t + dt_{code}$

- OpenMP can alleviate the imbalance by dynamic load balancing inside a node



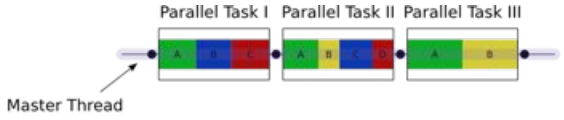
[Wikipedia]

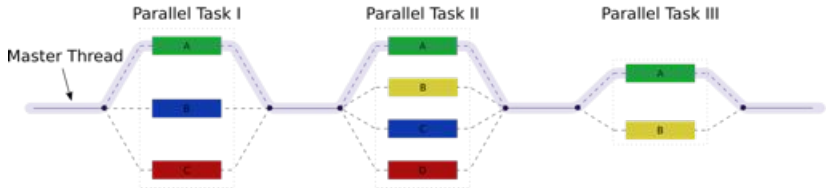
KROME + OpenMP

- Problem: Cost of KROME is highly “non-deterministic”

t … KROME dt is chemistry dependent … translates to ***different per-cell cost*** $t + dt_{code}$

- OpenMP can alleviate the imbalance by dynamic load balancing inside a node





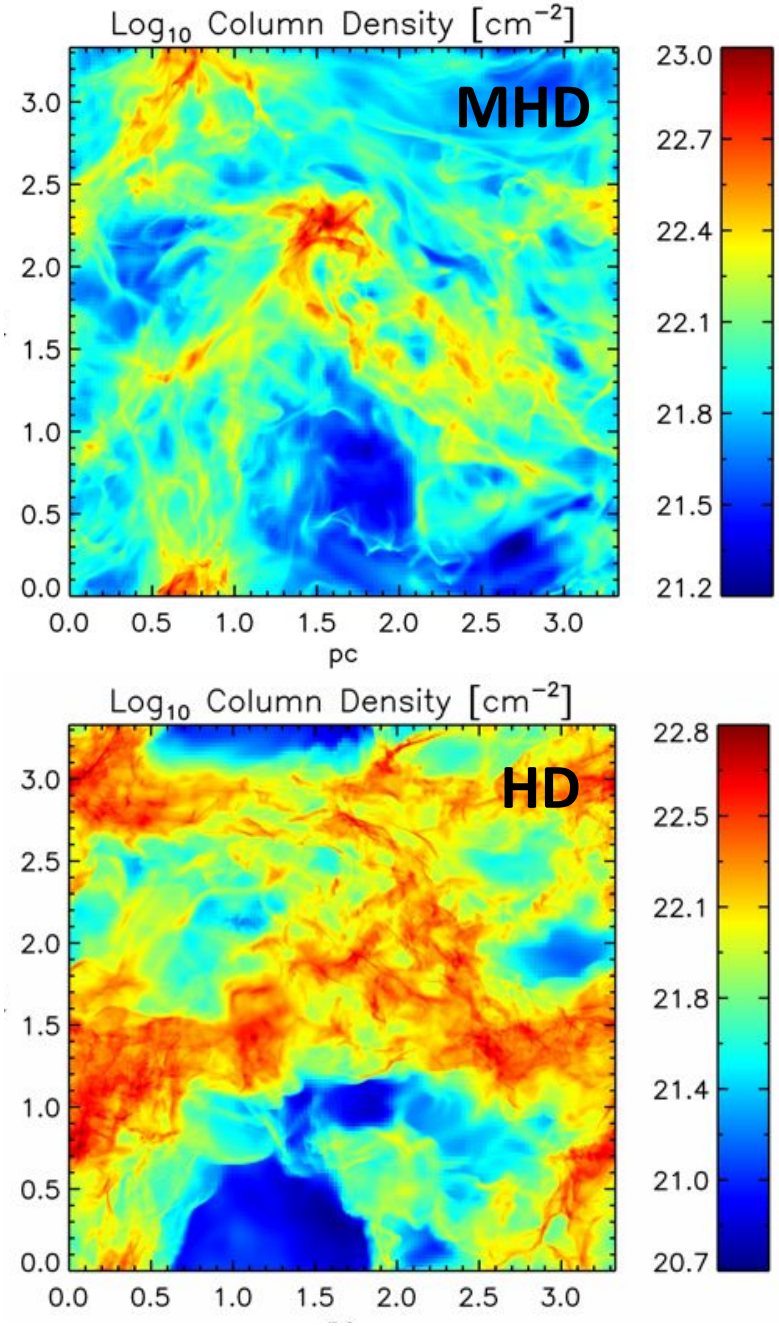
From Shock1D

```
!$omp parallel do private(xx, rhogas, ix) schedule(dynamic,2) ! <- Enable OpenMP
do ix = 1, nx                                                 ! <- Loop over mesh
   xx(:) = x(ix,:) !use local array
   rhogas = rho(ix) !get density
   call krome(xx(:),rhogas,Tgas(ix),dt)                       ! <- Call KROME
   x(ix,:) = xx(:) !get the updated value back
enddo
```

- Read BB Wiki for recommendations of KROME + OpenMP.
- *ALWAYS* use *Intel Inspector* or similar before production.

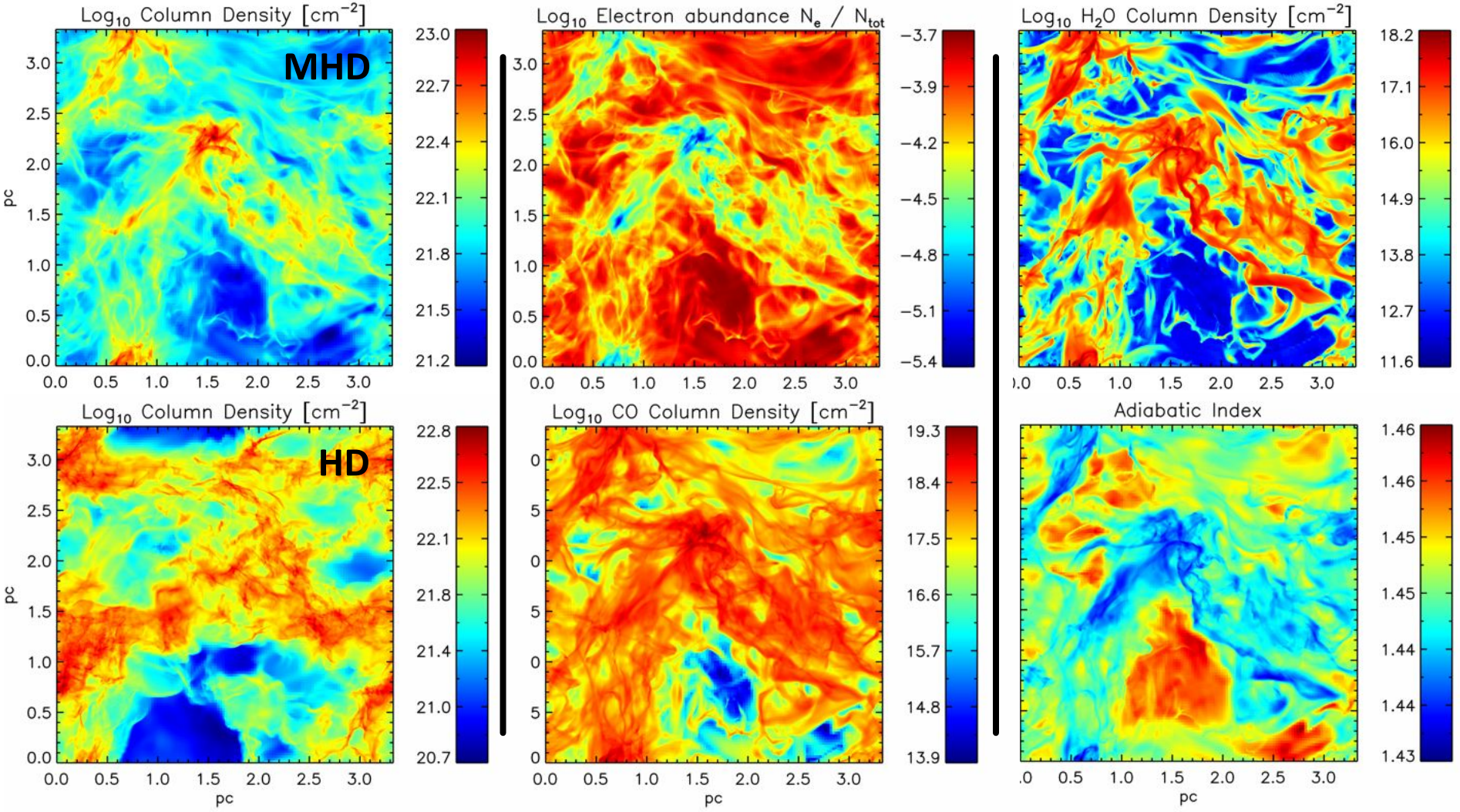

APPLICATIONS

Turbulent Molecular Cloud



- Piece of a molecular cloud: $(3.3\ pc)^3$
- Running with either HD or MHD
- Driven turbulence to Mach=11 @ 10K
- $\langle\rho\rangle = 1000\ cm^{-3}$, $\langle B\rangle = 7\ \mu G$
- Root grid: 128^3
- Refinement on density, and gradients of : ρ, v, P, and B
- More than 18M cells at up to $(4096)^3$
- H-C-O chemistry (COthin network), UV, CRs, Solar abund. Similar to D. Seifried.
- Approx for $A_V=(n_{tot} / 1000)^{2/3}$
- Consis. abundance advection, variable γ
- Evolved over 4.7 Myr = 3.5 dyn. times = 4.5 free-fall times

Turbulent Molecular Cloud



- Large diff. in HD & MHD
- ISM is magnetized
- Affects SFR, IMF

- Most H molecular
- CO effectively formed
- Free ions even @ 10-50K

- Water at threshold density
- Only small changes in γ
- Need dust to go further

Summary

- KROME is ready and viable for complicated chemistry
- It is easy to use KROME with RAMSES, and other framework codes
- If the framework code use a finite volume method, consistent advection should be implemented (simple!), both for fluxes and for interpolation, if AMR.
- A more challenging change is to include a variable adiabatic index. Crucial in combination with self gravity
- We currently only have preliminary results of our molecular cloud models, but first results show promising agreement with literature, but with much higher numerical fidelity and including magnetic fields.
- OpenMP can significantly improve performance of KROME