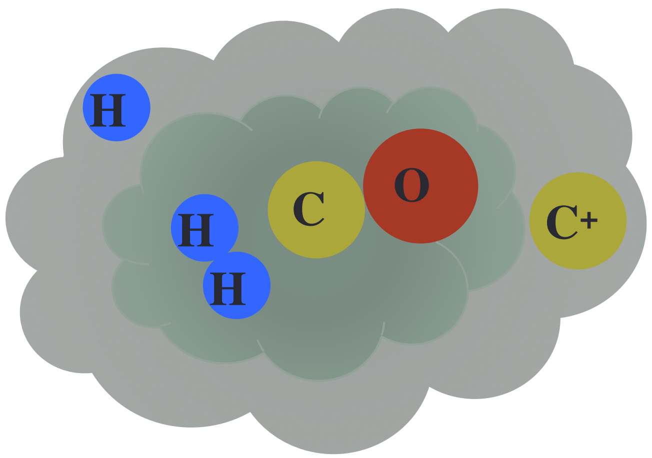

Chemistry in Athena++

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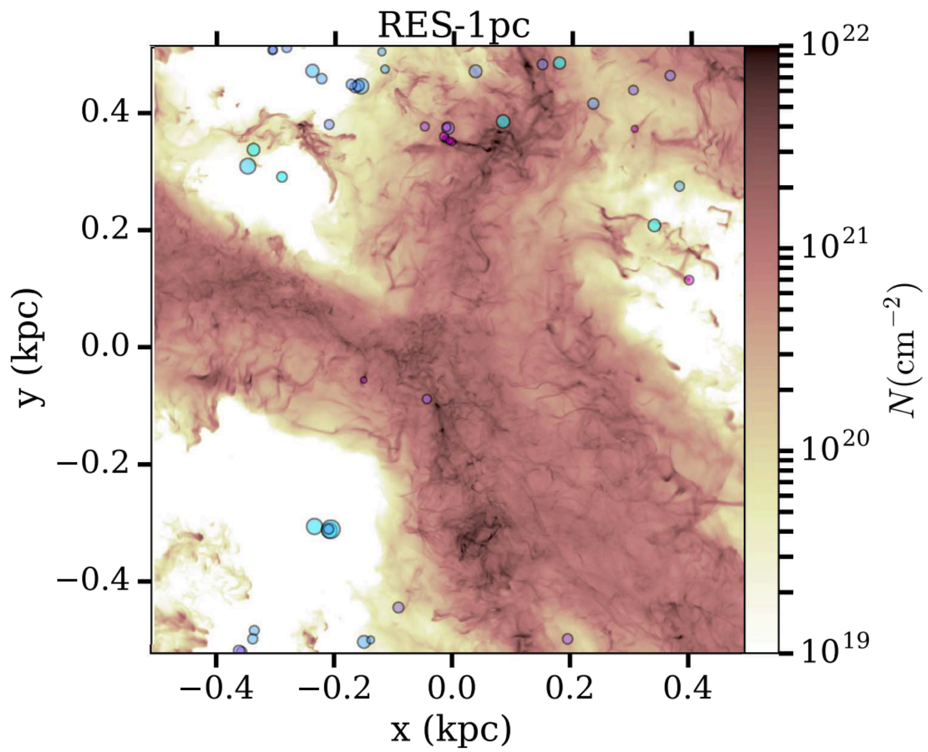
Max Planck Institute for Extraterrestrial Physics (MPE)

Athena++ workshop, UNLV, March 2019

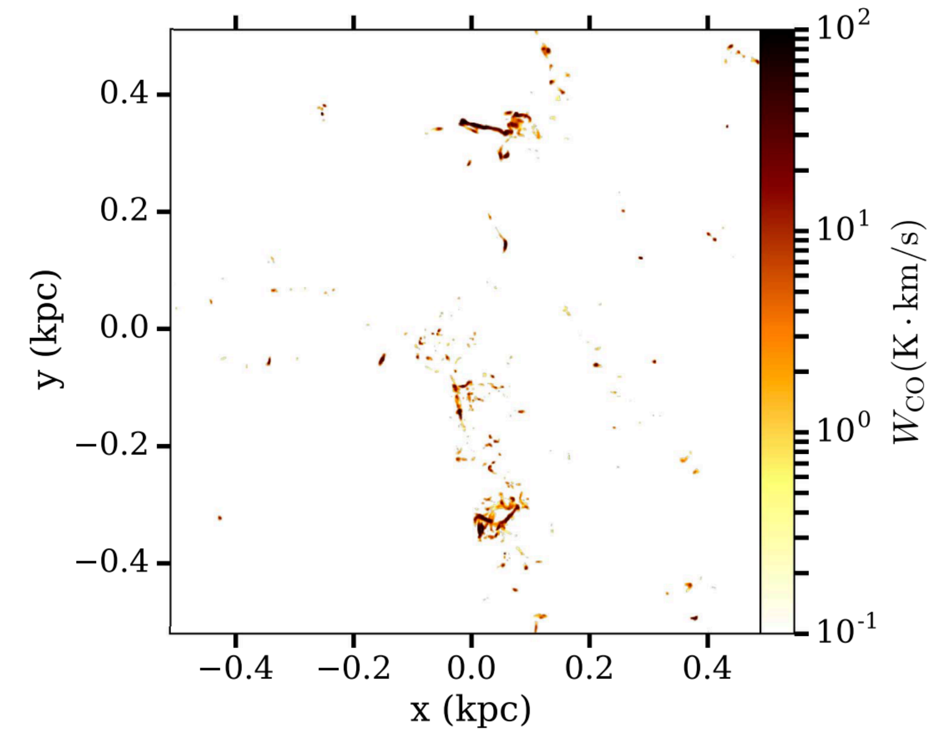
Max-Planck-Institut für
extraterrestrische Physik

An application of chemistry

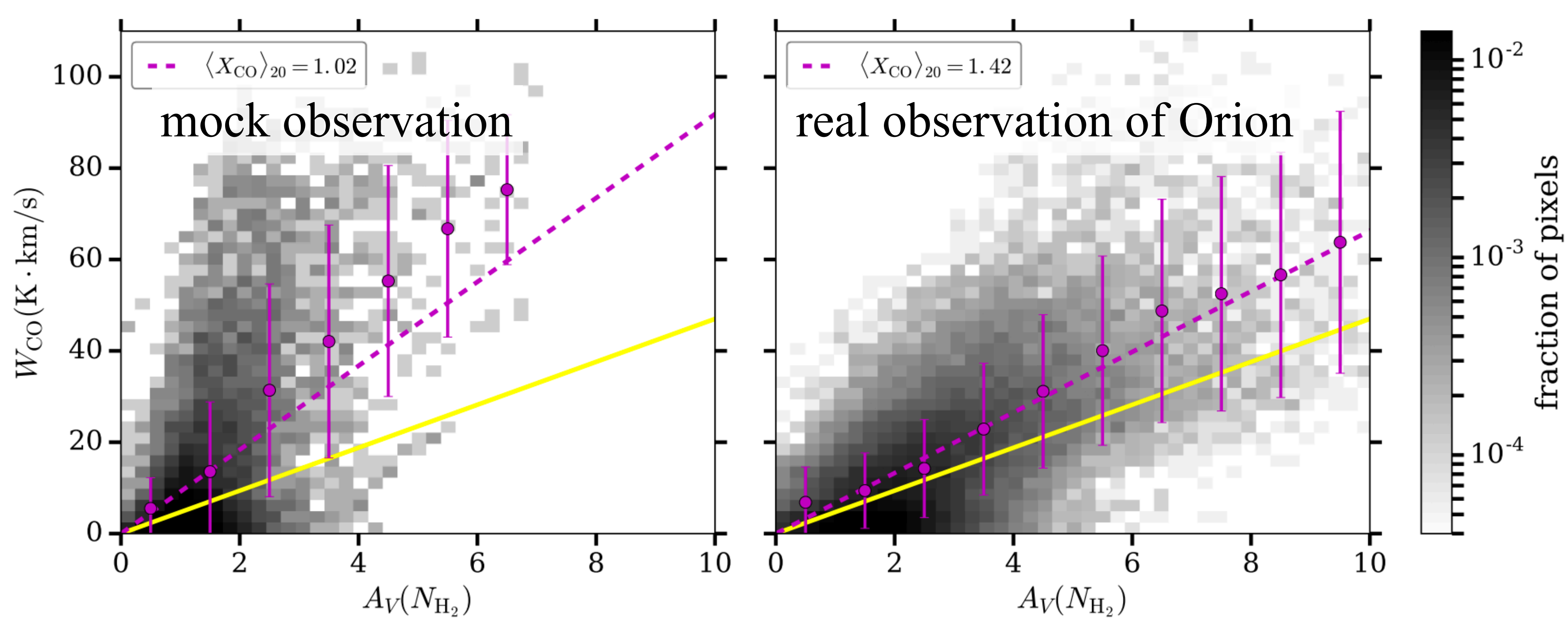


simulation

chemistry →



mock observation



Gong, Ostriker and Kim (2018), The X_{CO} Conversion Factor from Galactic Multiphase ISM Simulations

Equations

Concentration for species i: $s_i = \frac{\rho_i}{\rho}$

$$\frac{\partial s_i}{\partial t} = -\frac{1}{\rho}\mathbf{v}\cdot\nabla(\rho s_i) + K_i$$

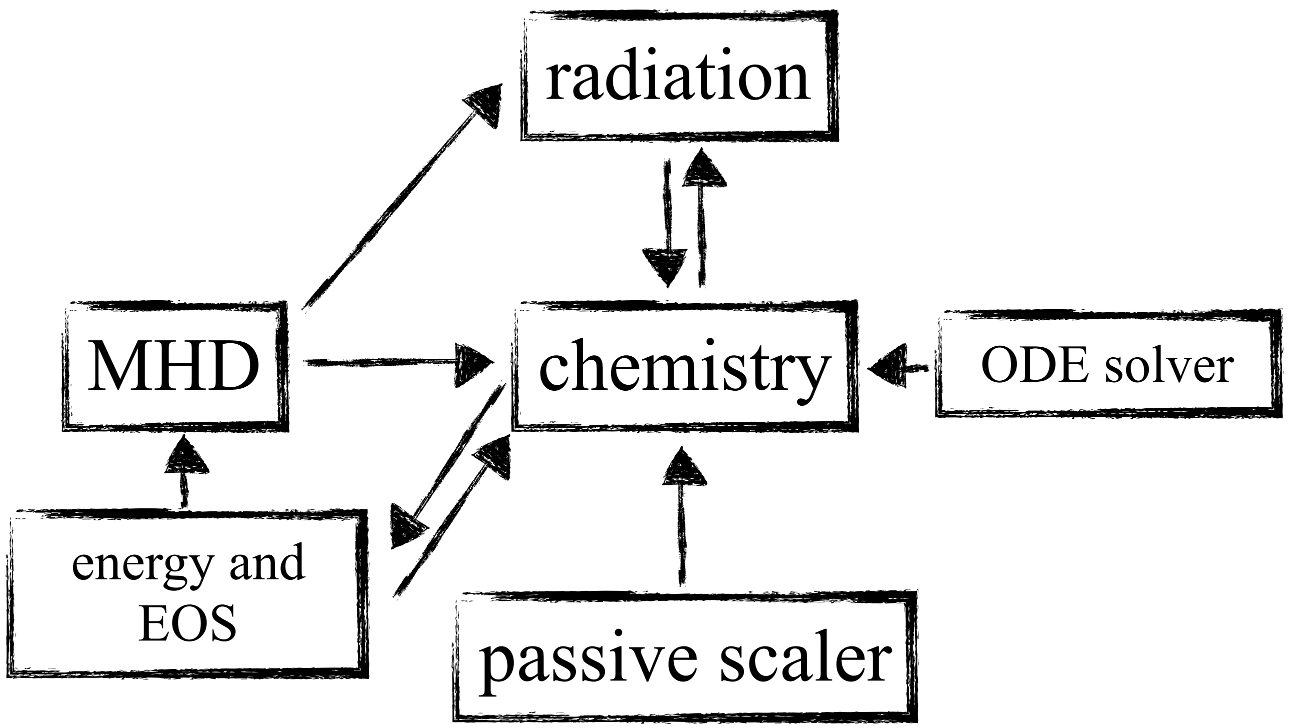
chemical reaction rates
$K_i(\mathbf{s}, \rho, T, G, ...)$
G: radiation field

$$\frac{\partial}{\partial t}\left[\left(\frac{1}{2}\rho v^2 + \frac{P}{\gamma - 1}\right) + \nabla\cdot\left(\frac{1}{2}\rho v^2 + \frac{\gamma}{\gamma-1}P\right)\mathbf{v}\right]$$
$$= \Gamma - \Lambda$$

heating and cooling
$\Gamma, \Lambda(\mathbf{s}, \rho, T, G)$

$$P = \frac{R}{\mu}\rho T$$

mean molecular weight $\mu(\mathbf{s})$



Post-processing chemistry

Concentration for species i: $s_i = \dfrac{\rho_i}{\rho}$

$$\frac{\partial s_i}{\partial t} = -\frac{1}{\rho}\mathbf{v}\cdot\nabla(\rho s_i) + K_i$$

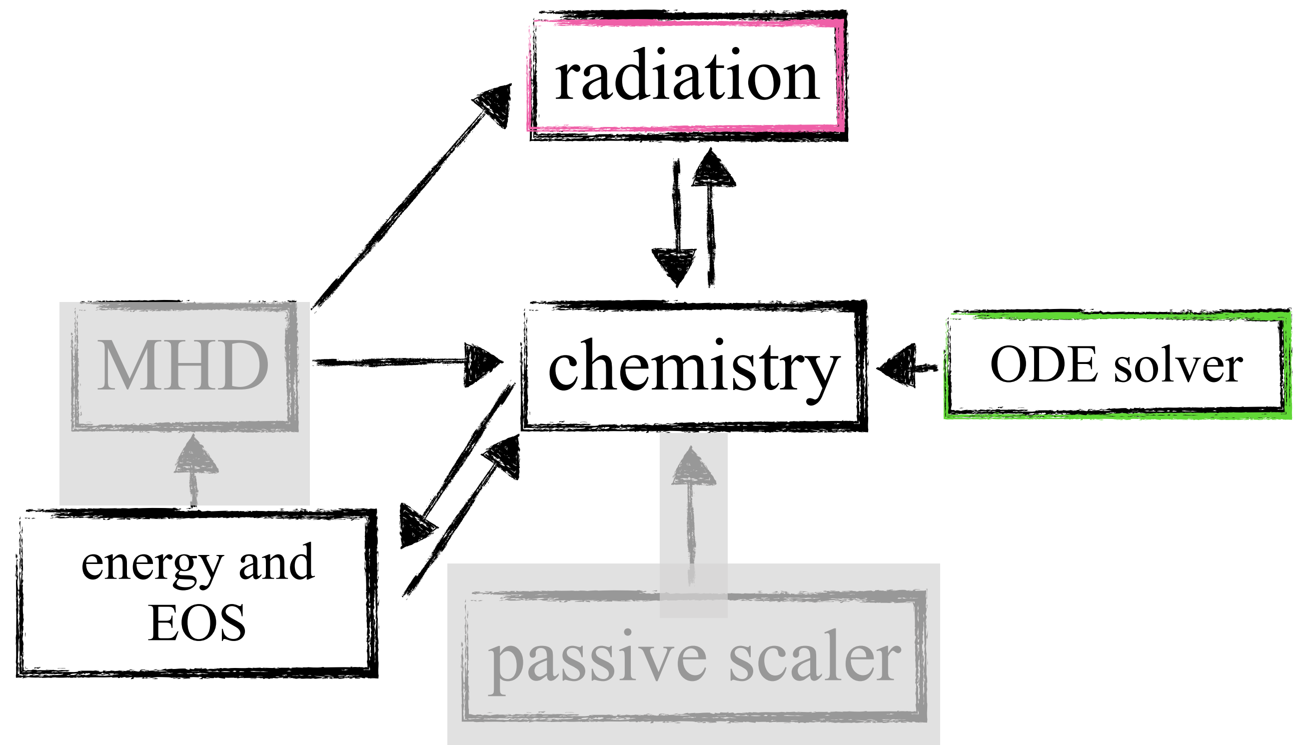
chemical reaction rates
$K_i(\mathbf{s}, \rho, T, G, ...)$
G: radiation field

$$\frac{\partial}{\partial t}\left[\left(\frac{1}{2}\rho v^2 + \frac{P}{\gamma - 1}\right) + \nabla\cdot\left(\frac{1}{2}\rho v^2 + \frac{\gamma}{\gamma - 1}P\right)\mathbf{v}\right]$$
$$= \Gamma - \Lambda$$

heating and cooling
$\Gamma, \Lambda(\mathbf{s}, \rho, T, G)$

$$P = \frac{R}{\mu}\rho T$$

mean molecular weight $\mu(\mathbf{s})$



$$\frac{\mathrm{d}s_i}{\mathrm{d}t} = K_i$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{\Gamma - \Lambda}{c_v}$$

$$G = G(\mathbf{s}, \rho)$$

Running chemistry on Athena++

- Download CVODE library

https://computation.llnl.gov/projects/sundials/cvode

sundials

SUNDIALS: SUite of Nonlinear and DIfferential/ALgebraic Equation Solvers

CVODE

- Checkout the chemistry branch on Athena++ GitHub page

Your branches

chemistry Updated a minute ago by munan 0 | 185 New pull request

- Configure

$./configure.py -pp --chemistry=gow16 --radiation=six_ray --cvode_path=/usr/local -mpi …

-pp	--chemistry=gow16	--radiation=six_ray	--cvode_path=/usr/local	-mpi
post-processing flag (skip the MHD task-list)	chemical network	Radiation solver (six_ray, loc_jeans, const)	CVODE library path	Radiation and chemistry are parallelized

- Regression tests

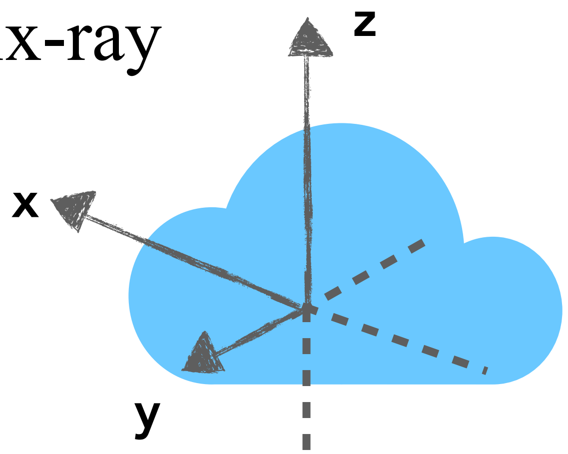
$./run_tests.py chemistry (problem generator that reads Athena4.2 VTK output)

Current code implementations

- CVODE

Dense matrix solver: computational cost ~ N_s^3

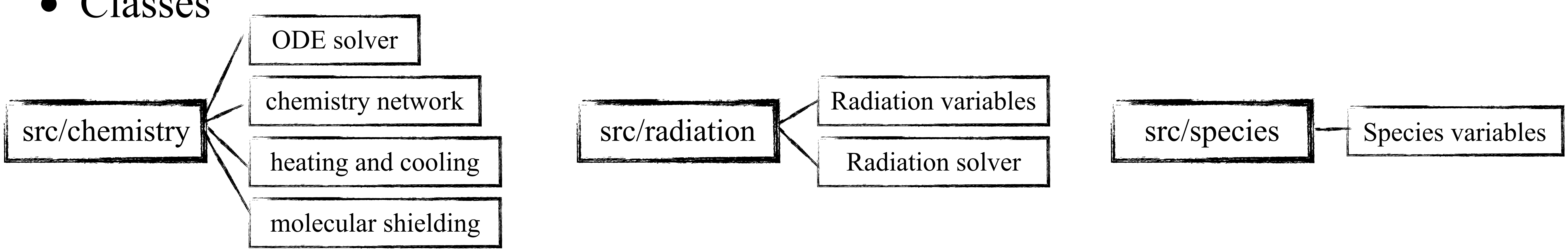
- Six-ray



$$G = \frac{1}{6}\sum G_i$$
$$G_i = G_0 \exp(-\sigma N_i)$$

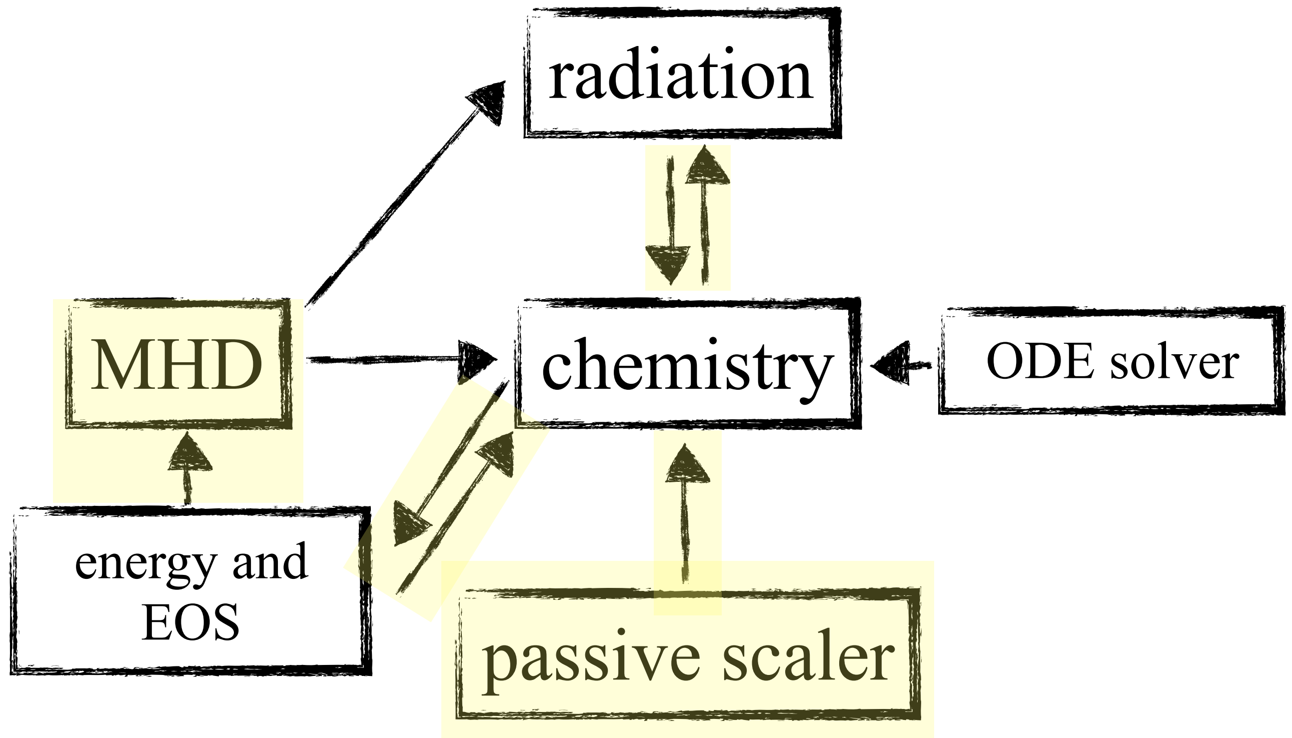
Fast compared to chemistry, pretty good approximation for the turbulent ISM.

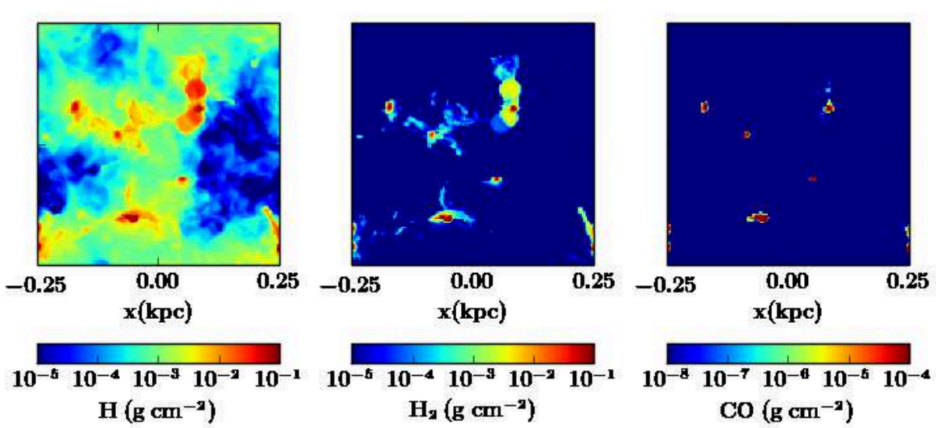
- Classes



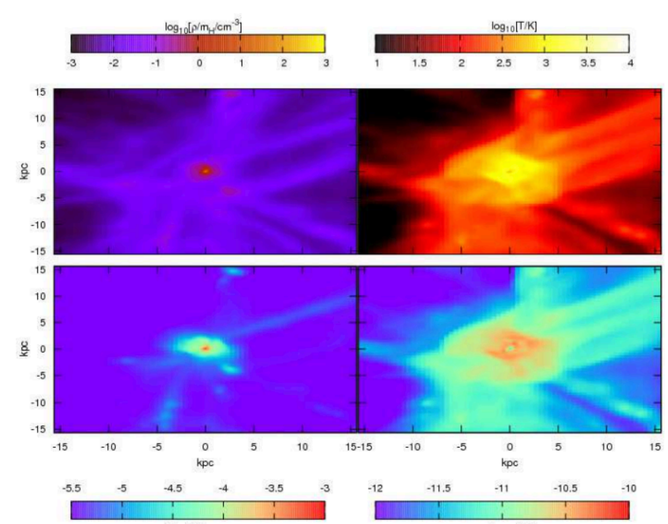
- Task-list

The goal: general time dependent chemistry

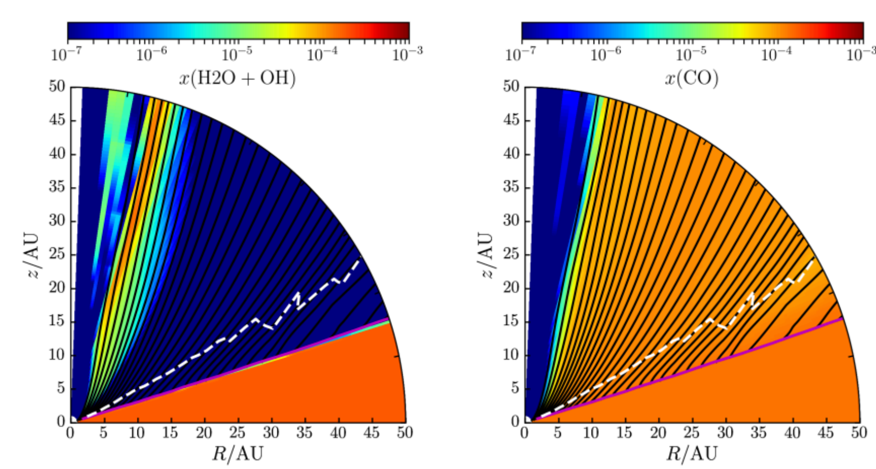




Walch+ 2014, FLASH



Grassi+ 2012, KROME



Wang+ 2018, Athena++

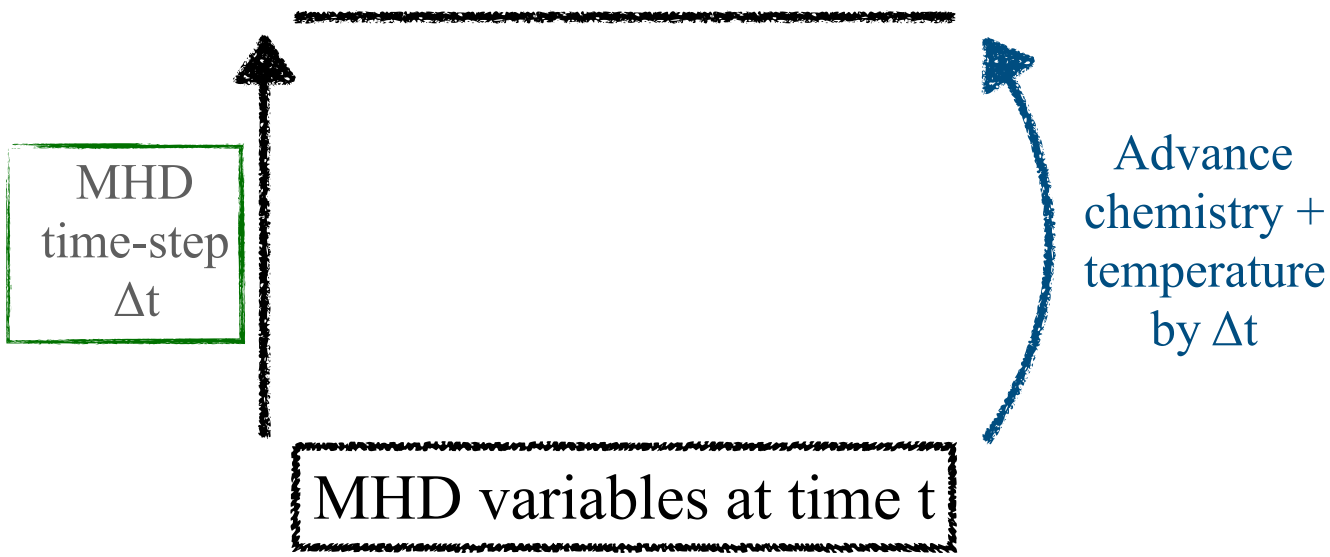
Towards time dependent chemistry

- Passive scaler, advection of chemical species

- Merge the species class with the **passive scaler class**.

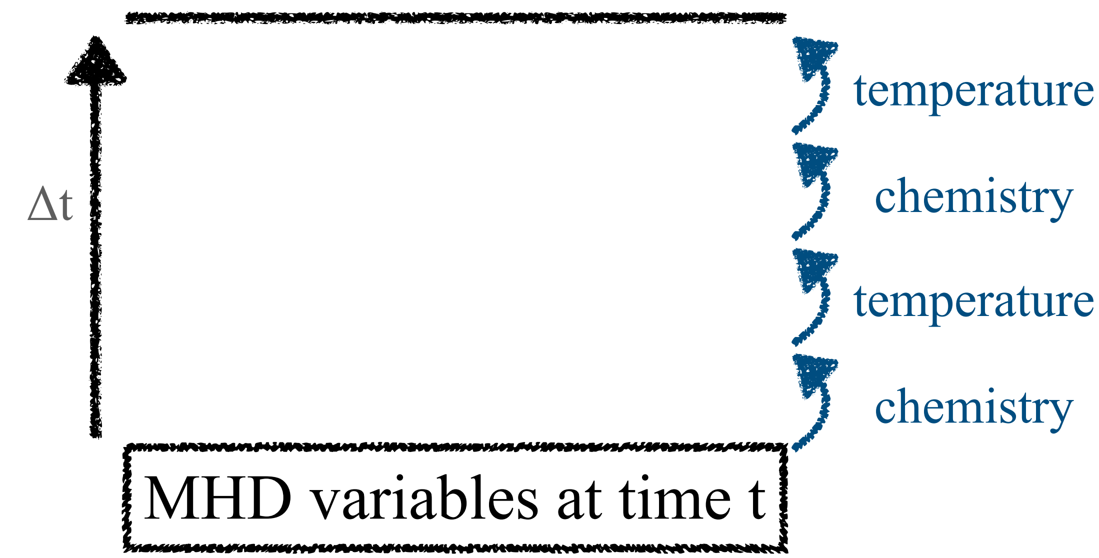
- Conservation of elemental abundances: **normalise the fluxes in the advection step** (Glover+ 2010).

- Heating and cooling: the energy equation and EOS



Same as current post-processing implementation (Grassi+ 2012, Wang+ 2017)

Shall we limit Δt according to heating and cooling rates?



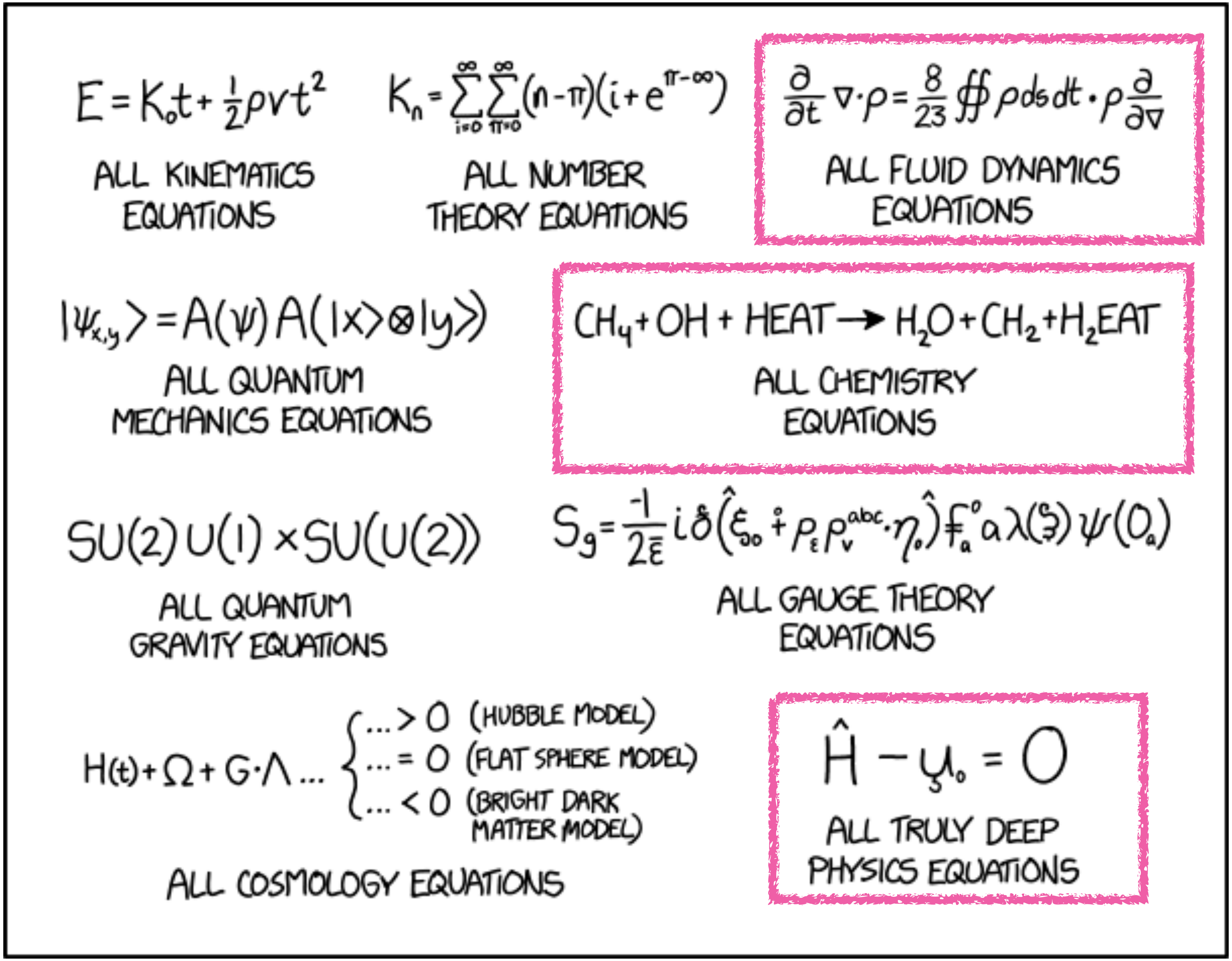
Solve chemistry and temperature separately, sub-cycling: might be faster (Glover+ 2010, Walch+2014)

- Radiation

- Do we simply update radiation field after chemistry (current implementation and literature), or do we need to iterate between chemistry and radiation (for H_2 self-shielding)?

- Performance: cost function for Meshblocks, GPU, AMR

Summary



https://xkcd.com/2034/