Microphysics and chemistry in hydrodynamical numerical simulations

Part I: Overview

Wednesday 28th October, 2015
Gandalf School

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Motivation: Why chemistry?

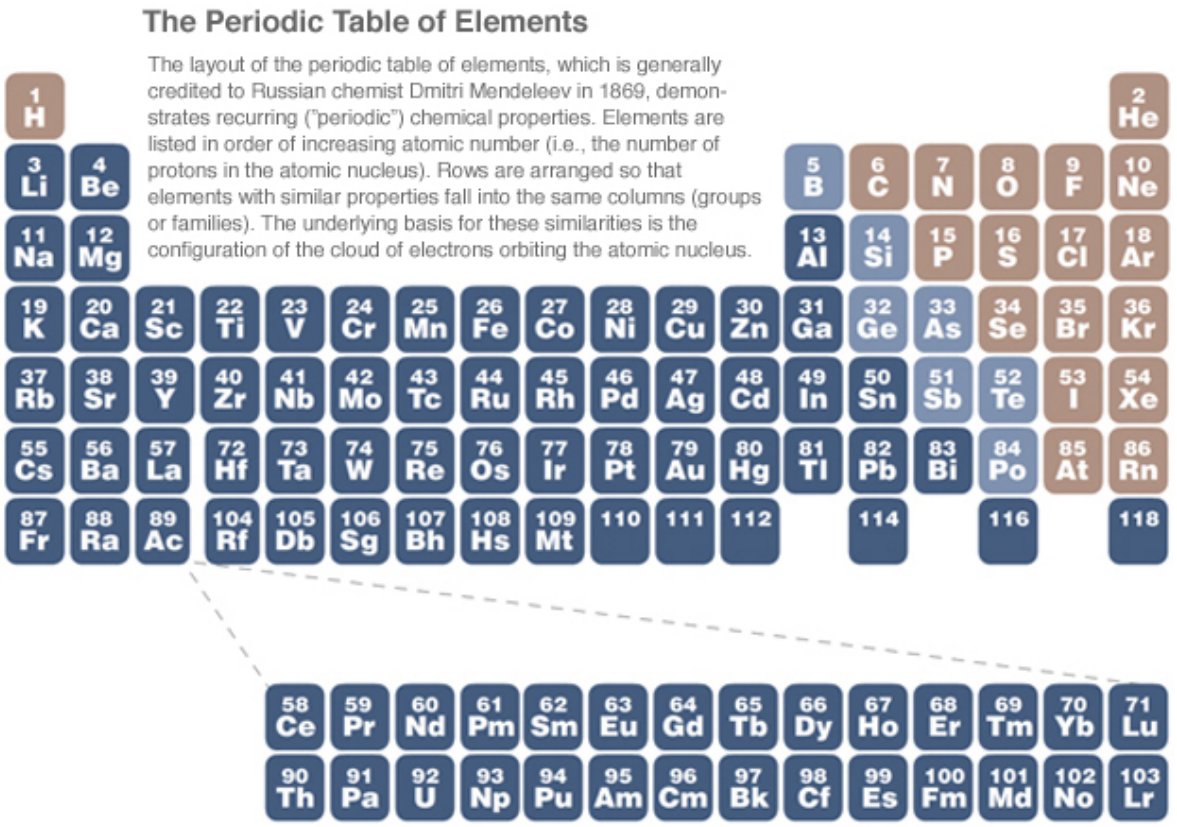
Modelling:

- chemistry and cooling determine the equation of state
- the equation of state of the gas regulates gravitational instabilities and fragmentation

Comparison with observations:

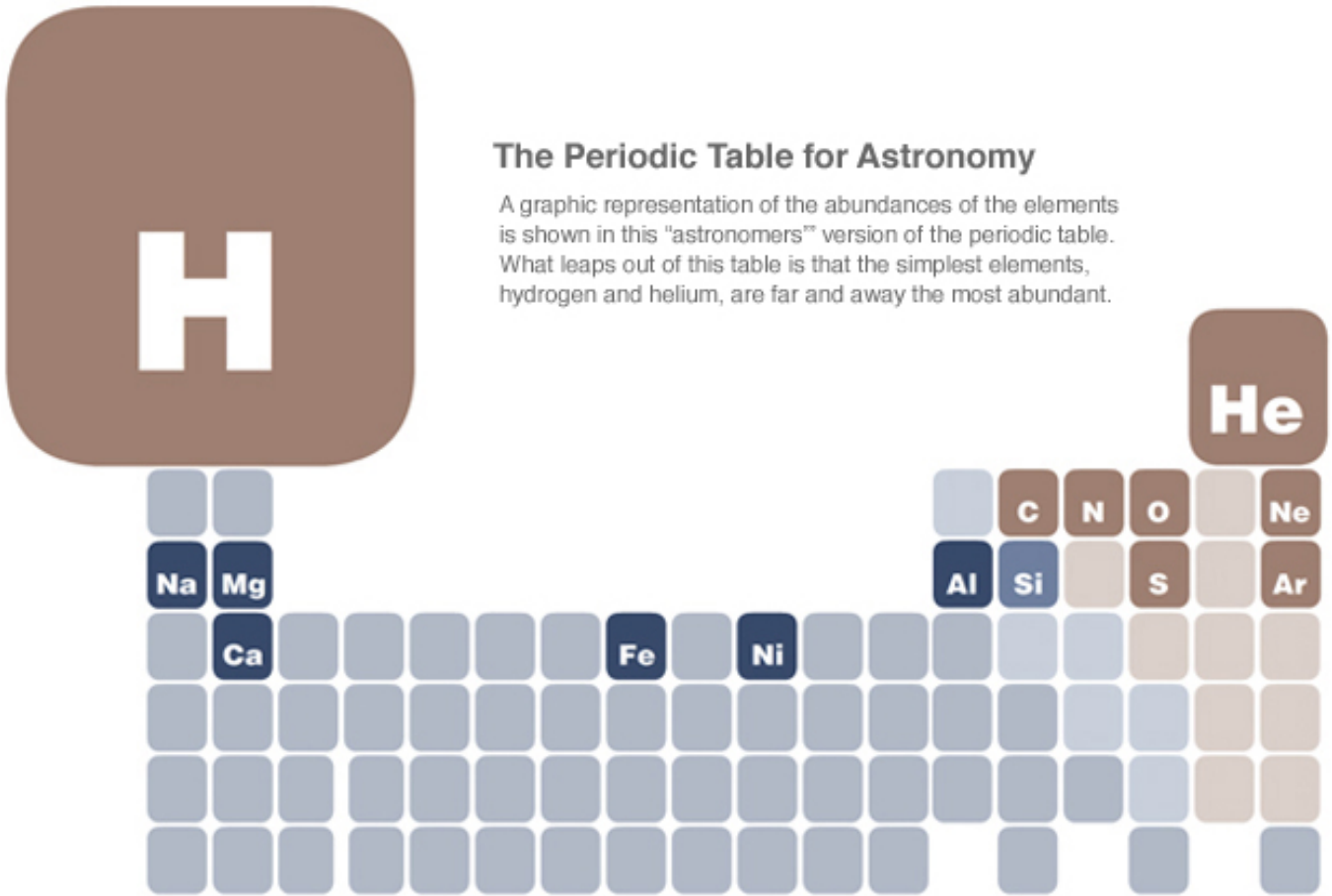
- Astrophysical objects are observed through the line emission of different atoms, ions, and molecules
- A comparison with hydro simulations requires to include these species in the chemical modelling

Standard periodic table



http://chandra.harvard.edu/xray_astro/chemistry.html

Astronomers periodic table



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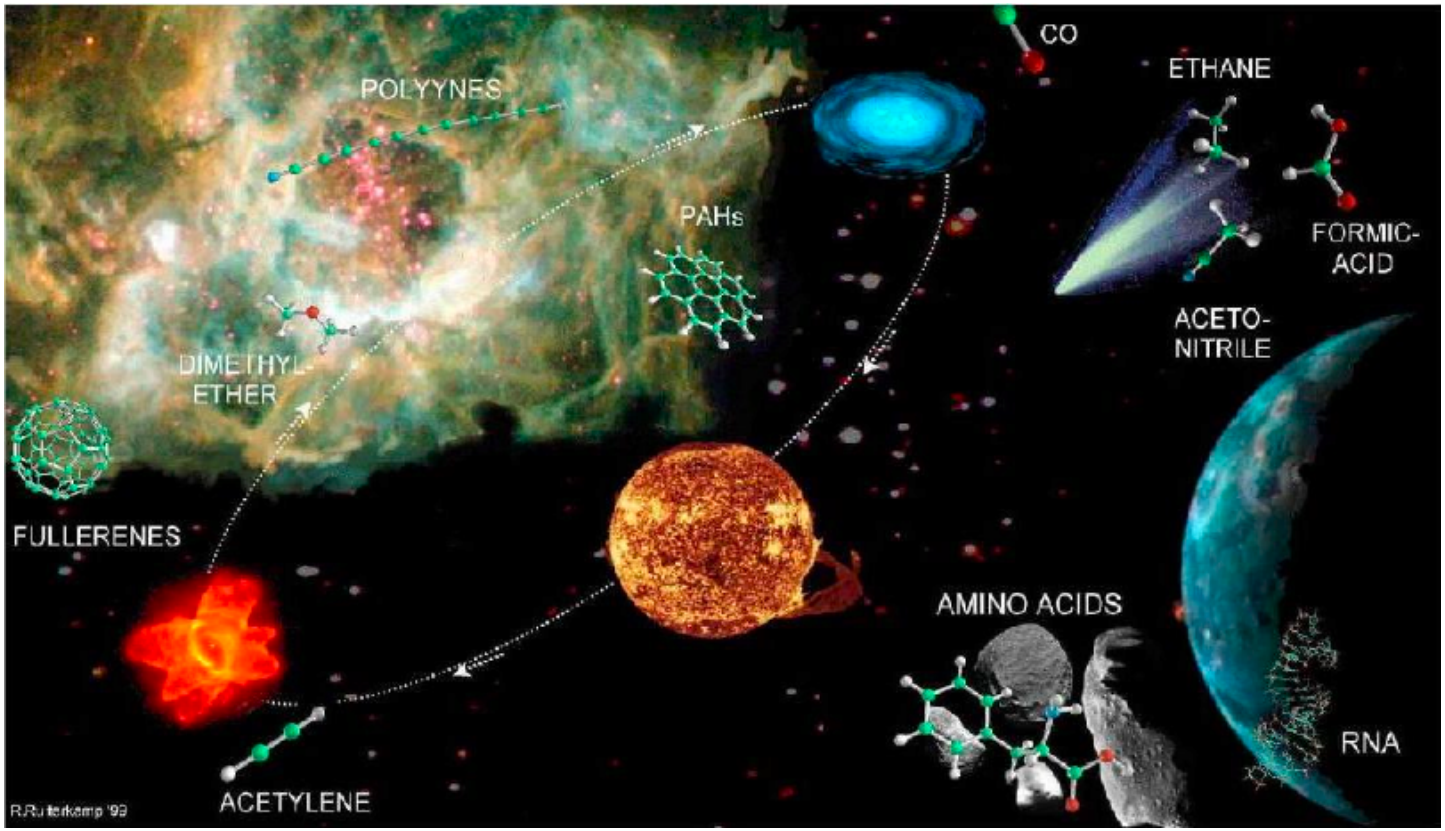
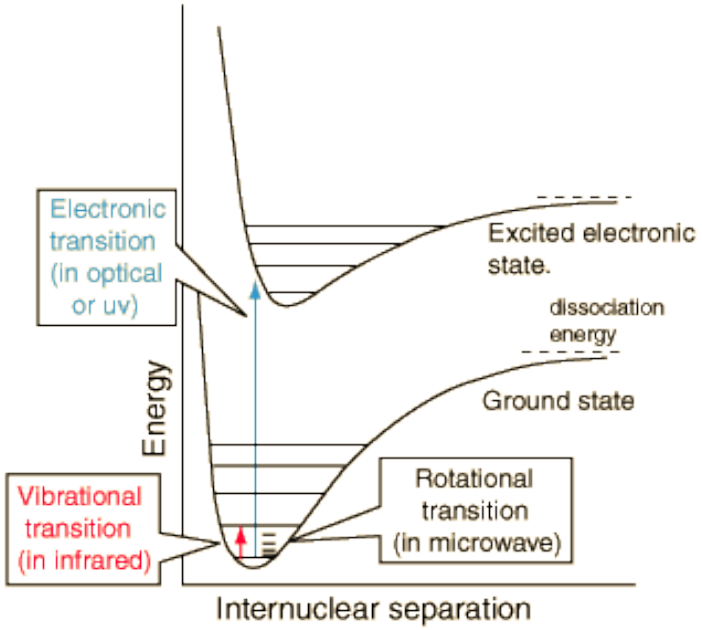
Observations

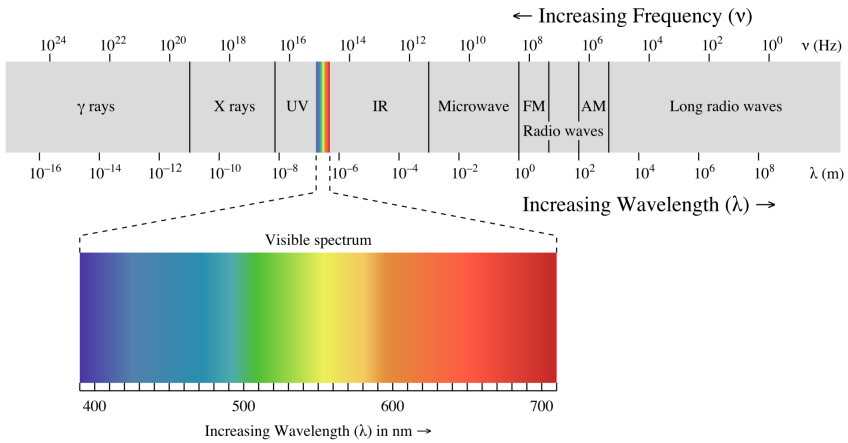
- More than 180 molecules, including organic molecules such as sugars and alcohols, have been discovered in space



Observations (cont'd)
How do we observe molecules?

through emission/absorption lines!





fact to know:

- the internal energy is *quantized*

$$E_t = E_{el} + E_{vib} + E_{rot}$$

radio	m/cm	
microwave	mm	10^{-3} m
infrared	μm	10^{-6} m
visible	nm	10^{-9} m
ultraviolet	Å	10^{-10} m

Observations (cont'd)
what do we observe?

In the last decade astrochemistry had access to powerful instruments

Observations via atom/molecule transitions

- electronic transitions $\rightarrow$ Vis/UV (Hubble Space Telescope)
  - H_2 + atoms observed directly
  - large oscillator strengths[1], minor species can be detected
- vibrational transitions $\rightarrow$ IR (Spitzer, Herschel)
  - both gas and solids observed
  - ices, silicates, oxides, PAH mid-far IR
  - molecules without permanent dipole moment (e.g. H_3^+, CH_4, CO_2)
  - moderate oscillator strengths
- rotational transitions $\rightarrow$ sub-mm (Herschel, ALMA)
  - bulk of interstellar molecules
  - high sensitivity to low abundances (down to 10^{-11} x_H)

[1] probability of photon absorption/emission between energy levels

Observations: starburst galaxy M82

Images from three of NASA's Great Observatories: Hubble, Spitzer, and Chandra

- hot hydrogen (orange)
- cool gas and dust (red)
- X-ray gas emission (blue)
- optical light from stars (yellow-green)

http://chandra.harvard.edu/xray_astro/chemistry.html

Observations (cont'd)
additional information

Molecules are excellent diagnostics of the physical conditions and processes in the regions where they reside [2]

- excitation and abundances are determined by collision
- collisions depend on
  - gas temperature
  - density
  - radiation

[2] E. Van Dishoeck

Chemistry bottlenecks

$$\frac{dn_i}{dt} = \overbrace{\sum_{lm} k_{lm}(T) n_l(t) n_m(t)}^{formation} - \overbrace{\sum_{j} k_{ij} n_i(t) n_j(t)}^{destruction} \quad (1)$$

$$\frac{dT}{dt} = \frac{\gamma(n_i) - 1}{k_B \sum_i n_i} (\Gamma(n_i, T) - \Lambda(n_i, T)) \quad (2)$$

(i) Stiffness $\rightarrow$ need for implicit solvers
- widely varying time scales
- very stiff problems $\rightarrow$ computationally intensive
- accurate and efficient solver

(ii) Network complexity $\rightarrow$ need for reduction techniques
- *a-priori* $\rightarrow$ reduce ODEs number (T. Grassi, **SB**+, MNRAS 2013)
- *on the fly* $\rightarrow$ reduce RHS terms (T. Grassi, **SB**+, MNRAS 2012)

(iii) Rates availability and accuracy
- basic information

(iv) Connected with many physical processes
- very CPU demanding
- hydro-chemistry-radiation strongly coupled

Chemistry bottlenecks

- Chemical network & Rate accuracy
- Network complexity
- Stiffness
- Connected with many physical processes

Chemical network: piece by piece

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^+, C^{3+}, CH^- ...)?
isomers (HOC^+, HCO^+, ...)?
isotopes ($^{12}C^{16}O$, $^{13}C^{16}O$, ...)?
fancy stuff (dust, PAH, ...)?

Problem 2 - edges (reactions)

bimolecular ($OH^+ + e^- \rightarrow O + H$)?
photochemistry ($H^- + \gamma \rightarrow H + e^-$)
cosmic rays ($CO + CR \rightarrow C + O$)
cosmic rays secondary ($CO + CRP \rightarrow C + O$)
3-body ($H + H + H_2 \rightarrow H_2 + H_2$)

you can always expand a chemical network

Bare minimum chemical network

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you can always expand a chemical network

Bare minimum chemical network/2

	H	H^+	H^-	e^-	γ	CR
H						
H^+	*x*					
H^-	*x*	*x*				
e^-	*x*	*x*	*x*			
γ	*x*	*x*	*x*	*x*		
CR	*x*	*x*	*x*	*x*	*x*	

chemical reactions “commutes”

$$H^+ + e^- \rightarrow H + \gamma$$
$$e^- + H^+ \rightarrow H + \gamma$$

Bare minimum chemical network/3

	H	H^+	H^-	e^-	γ	CR
H						
H^+	x	*x*			*x*	*x*
H^-	x	x	*x*	*x*		
e^-	x	x	x	*x*	*x*	*x*
γ	x	x	x	x	*x*	*x*
CR	x	x	x	x	x	x

some pairs are impossible (e.g. $H^- + H^-$)

Bare minimum chemical network/4

	H	H^+	H^-	e^-	γ	CR
H	*x*	*x*				
H^+	x	x			x	x
H^-	x	x	x	x		
e^-	x	x	x	x	x	x
γ	x	x	x	x	x	x
CR	x	x	x	x	x	x

some reactions lead to species $\notin$ subset (e.g. $H^- + H \rightarrow H_2 + e^-$)

Bare minimum chemical network/5

	H	H^+	H^-	e^-	γ	CR
H	x	x	✓	✓✓	✓	✓
H^+	x	x	✓	✓	x	x
H^-	x	x	x	x	✓	✓
e^-	x	x	x	x	x	x
γ	x	x	x	x	x	x
CR	x	x	x	x	x	x

final set of reactions

Bare minimum chemical network/6

Final network

$H + e^-$	$\rightarrow$	$H^+ + 2e^-$	collisional ionization
$H + e^-$	$\rightarrow$	$H^- + \gamma$	radiative attachment
$H + \gamma$	$\rightarrow$	$H^+ + e^-$	photoionization
$H + CR$	$\rightarrow$	$H^+ + e^-$	CR ionization
$H^+ + e^-$	$\rightarrow$	$H + \gamma$	recombination
$H^+ + H^-$	$\rightarrow$	$H + H$	mutual recombination
$H^- + \gamma$	$\rightarrow$	$H + e^-$	electron photodetachment
$H^- + H$	$\rightarrow$	$2H + e^-$	collisional detachment
$H^- + CR$	$\rightarrow$	$H + e^-$	CR detachment

Chemical Network & Rate accuracy - Basics

The core of the problem:

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

$$k(T) = \left(\frac{8k_BT}{\pi\mu}\right)^{1/2} \frac{1}{(k_BT)^2} \int_0^\infty \sum_{\nu' j'} \sigma_{j'\nu' \leftarrow j=0\nu=0}(E) e^{-E/k_BT} E dE$$

$$flux = k(T) n_{\mathrm{A}}(t) n_{\mathrm{B}}(t)$$

$$\Downarrow$$

ODEs

- $k(T) \rightarrow$ rate coefficients in $\mathrm{cm}^3\ \mathrm{s}^{-1}$ or $\mathrm{cm}^6\ \mathrm{s}^{-1}$ or s^{-1}
- $n(t) \rightarrow$ concentrations in cm^{-3}

Rate accuracy-Methods
in gas-phase

How to determine $k(T)$?

- Experimentally (lucky)
- Langevin (estimate)
  - valid for ion-molecule reactions
  - "exothermic", i.e. without barrier
  - temperature independent
- *ab initio* calculations (not always available)
  - solving the Schrödinger equation (2nd order coupled PDEs)

How to retrieve $k(T)$?

- Databases (KIDA, UMIST, . . .)
- Literature search (best, but time-consuming)
- Educated guess (also strongly discouraged)

Chemistry bottlenecks

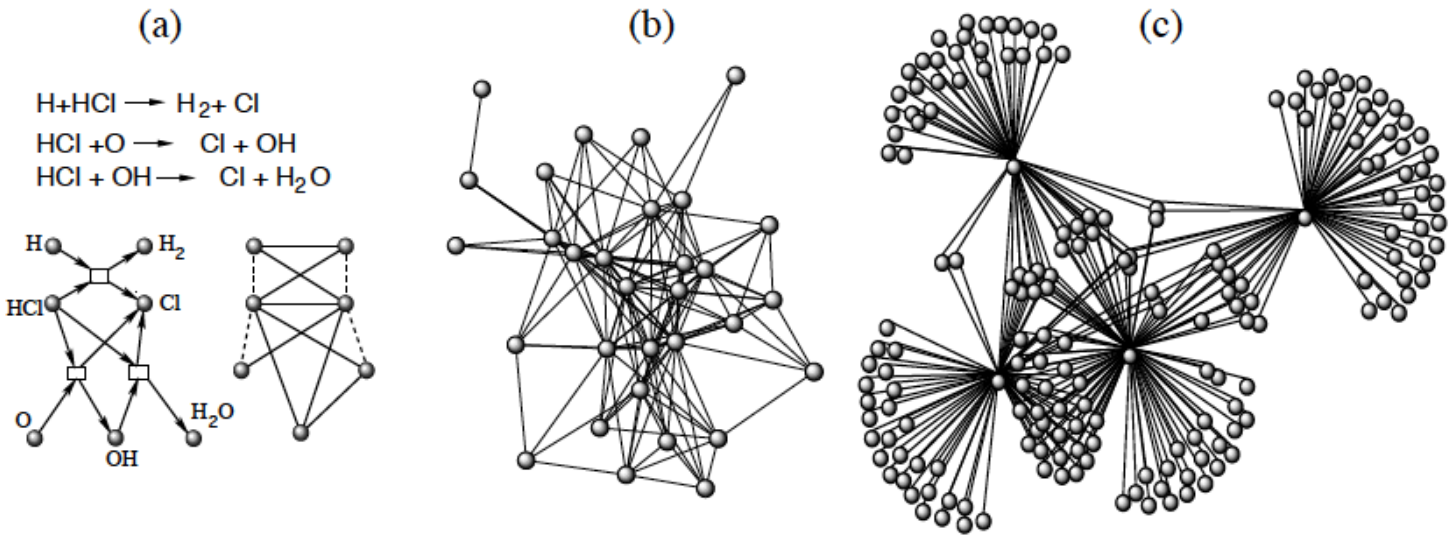
- Rate accuracy
- Network complexity
- Stiffness
- very CPU demanding

Networks as directed graph

Astrochemical networks

NODES $\rightarrow$ chemical species

EDGES $\rightarrow$ conversion between chemicals



- need for chemical network reduction techniques
  - *a-priori* based on topological properties (T. Grassi, **SB**+, MNRAS 2013)
  - *on the fly* based on the most important fluxes (T. Grassi, **SB**+, MNRAS 2012)

R. V. Solé & A. Munteanu 2007

Chemistry bottlenecks

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Stiffness

DIFFERENT DEFINITIONS EXIST: a problem is stiff if

- in particular: fastly reacting components arrive in a very short time in their equilibrium and the slowly changing components are more or less fixed, i.e. stiff
- it contains widely varying time scales, i.e., some components of the solution decay much more rapidly than others.
- the step-size is dictated by stability requirements rather than by accuracy requirements.
- if explicit methods don't work, or work only extremely slowly.
- More generally, a problem is stiff if the eigenvalues of the Jacobian of f differ greatly in magnitude

Explicit vs Implicit methods

- Explicit: in order to evaluate y_{n+1}, we use information from time step n
- Forward Euler's method reminder$\rightarrow y_{n+1} = y_n + hf(t_n, y_n)$

it is a single-step method!

$\downarrow$

each new time step computation as an initial value problem

Let's introduce the *implicit* methods:

- Backward Euler's method: $y_{n+1} = y_n + hf(t_{n+1}, y_{n+1})$ implicit
- it is an algebraic equation to be solved for y_{n+1}

Chemistry bottlenecks

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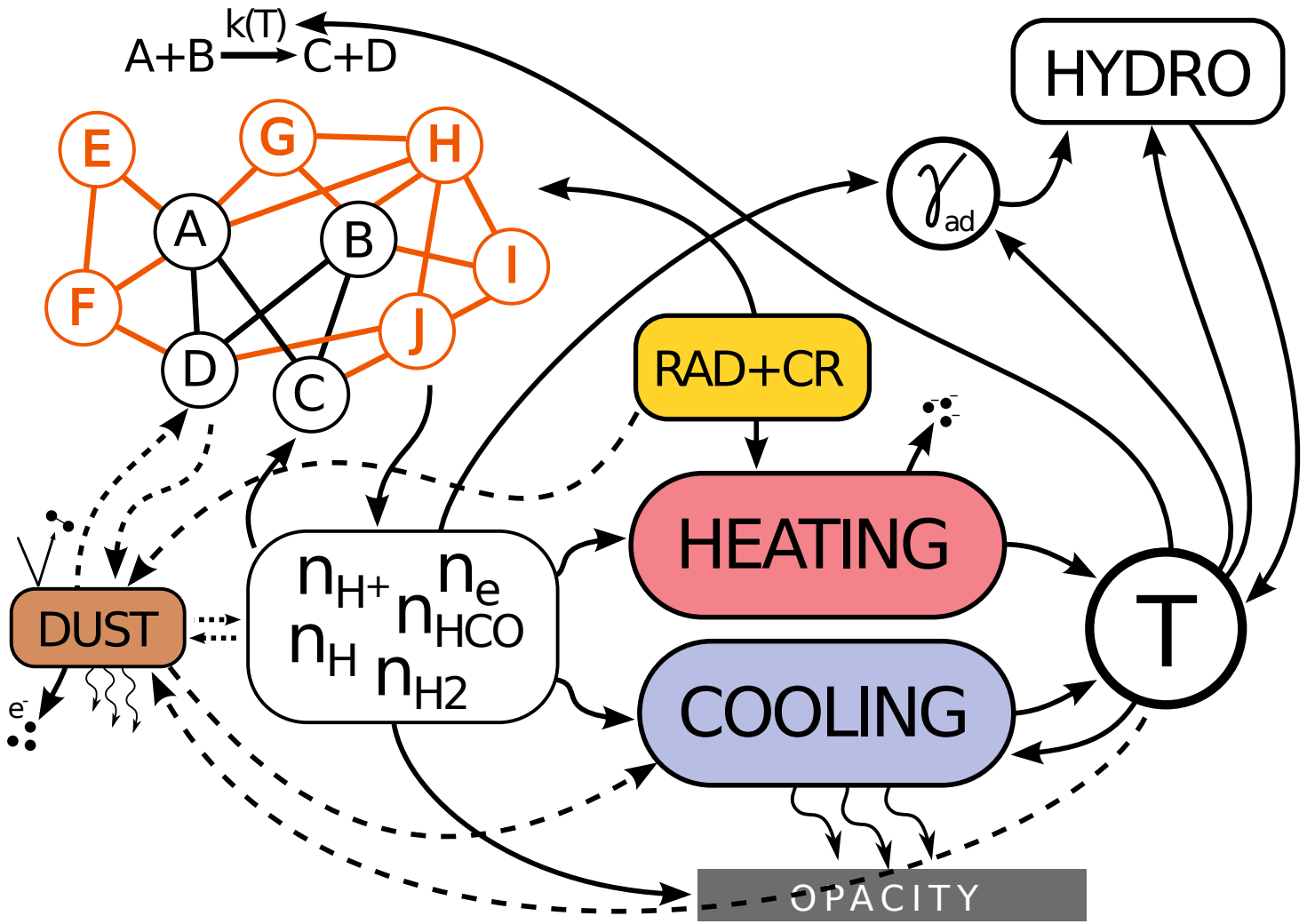
The microphysics

very messy!



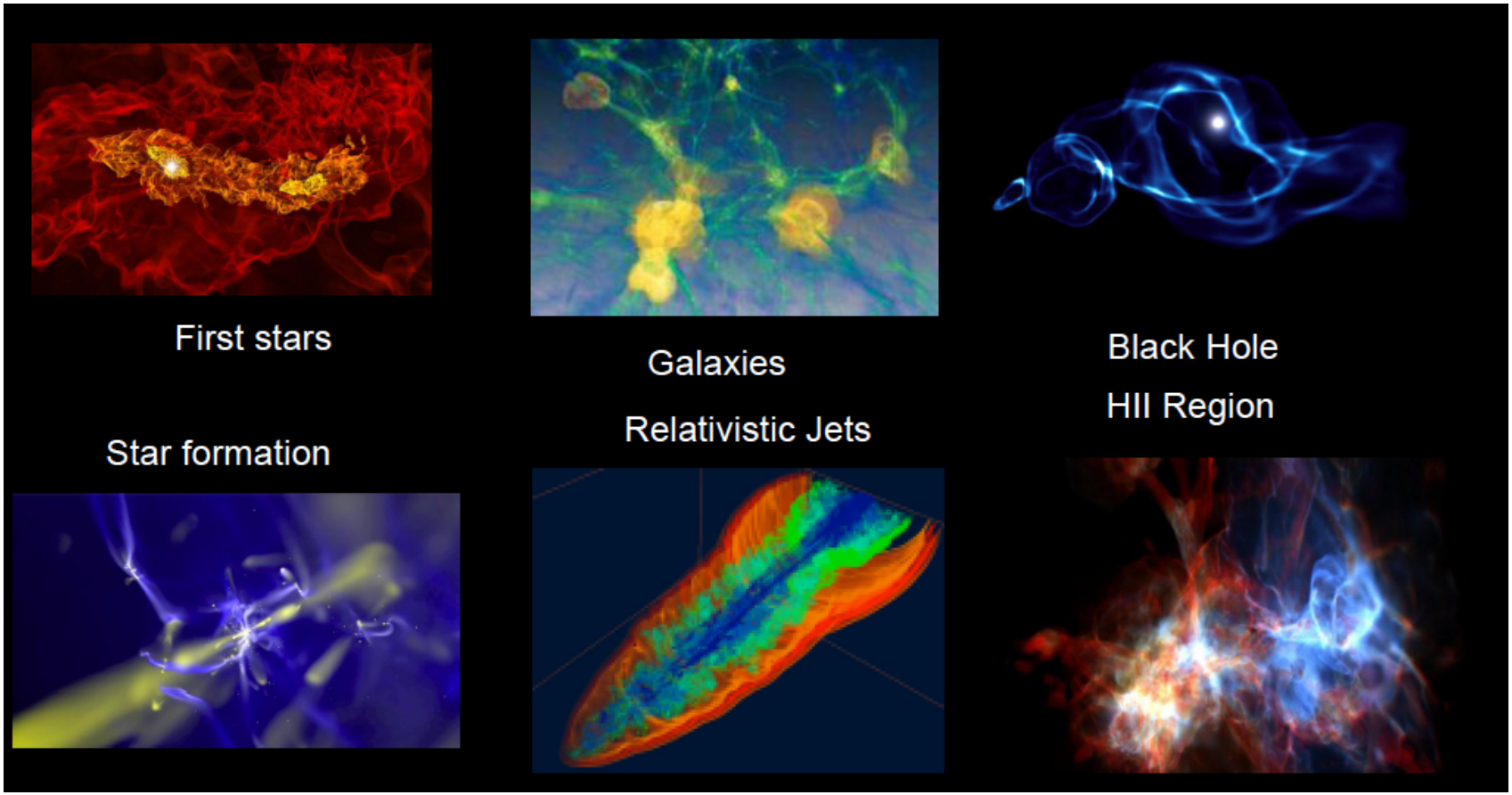
To recap

- chemistry is everywhere in our Universe
- observations provide spectra from electronic/rot./vib. transitions of different species
- chemistry essential for comparison with observations
- chemistry is troublesome
- chemistry coupled with many physical processes
- chemistry is computationally expensive but with the current machine power can be included (even large networks)

Chemistry-hydrodynamics coupling

Goals:

- hydro: Model the growth of structure in the universe
- chemistry: Model $\rightarrow$ Chemical abundances $\rightarrow$ Synthetic observations



Chemistry-hydrodynamics coupling (cont'd)

- What are the ingredients for a proper model? (tomorrow's talk)
- What are the pitfalls?

Two of the prevailing problems are

- adiabatic index (γ)
- the mean molecular weight (μ).
- strongly dependent on the chemical composition of the gas
- used to convert pressure $\rightarrow$ energy $\rightarrow$ temperature

$$p = (\gamma - 1)e, \tag{3}$$

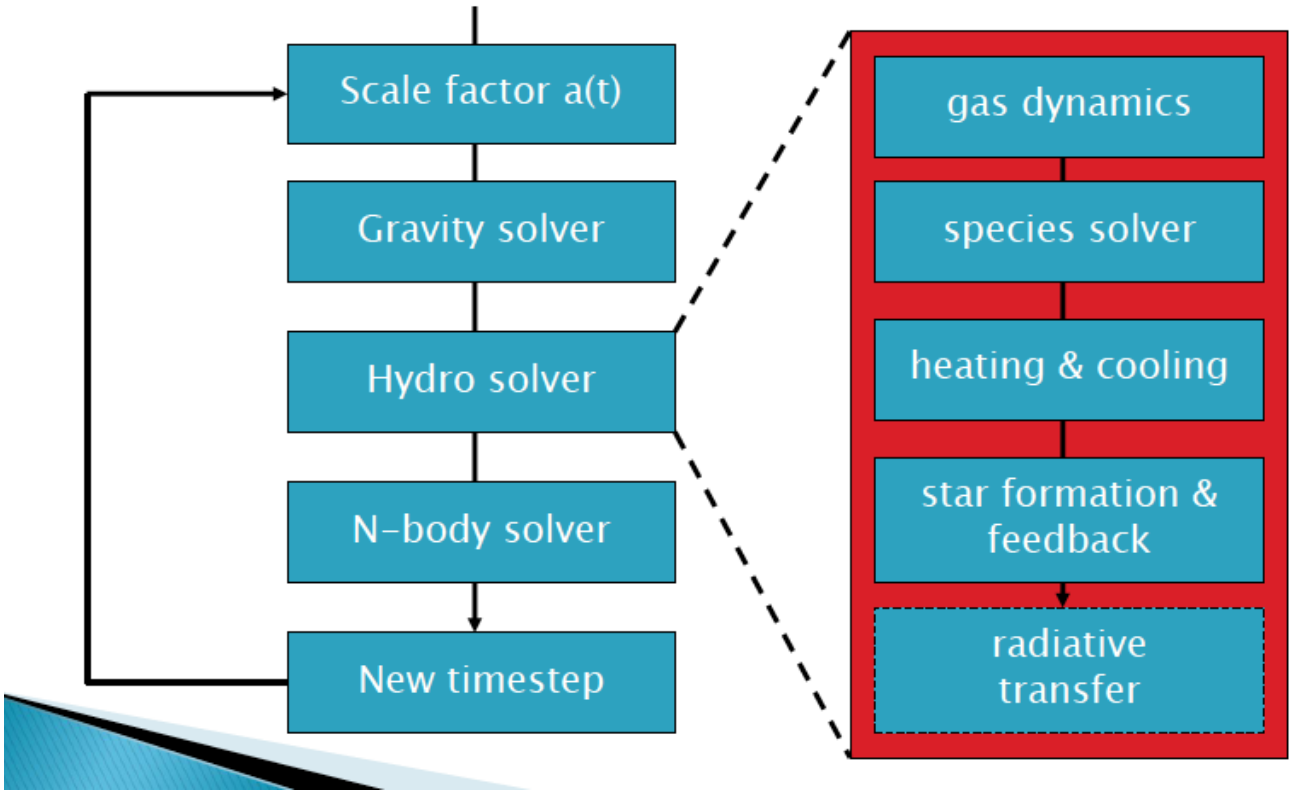
$$e = \frac{k_b T}{(\gamma - 1)\mu m_{\rm H}}, \tag{4}$$

- Multi-fluid Advection and Conservation of Abundances (not for SPH, as mentioned by David)

Chemistry-hydrodynamics coupling (cont'd)

Chemistry couples through the energy equation as a source term

$$\frac{\partial(\rho e)}{\partial t} + \nabla[(\rho e + P)v] = S_e \tag{5}$$



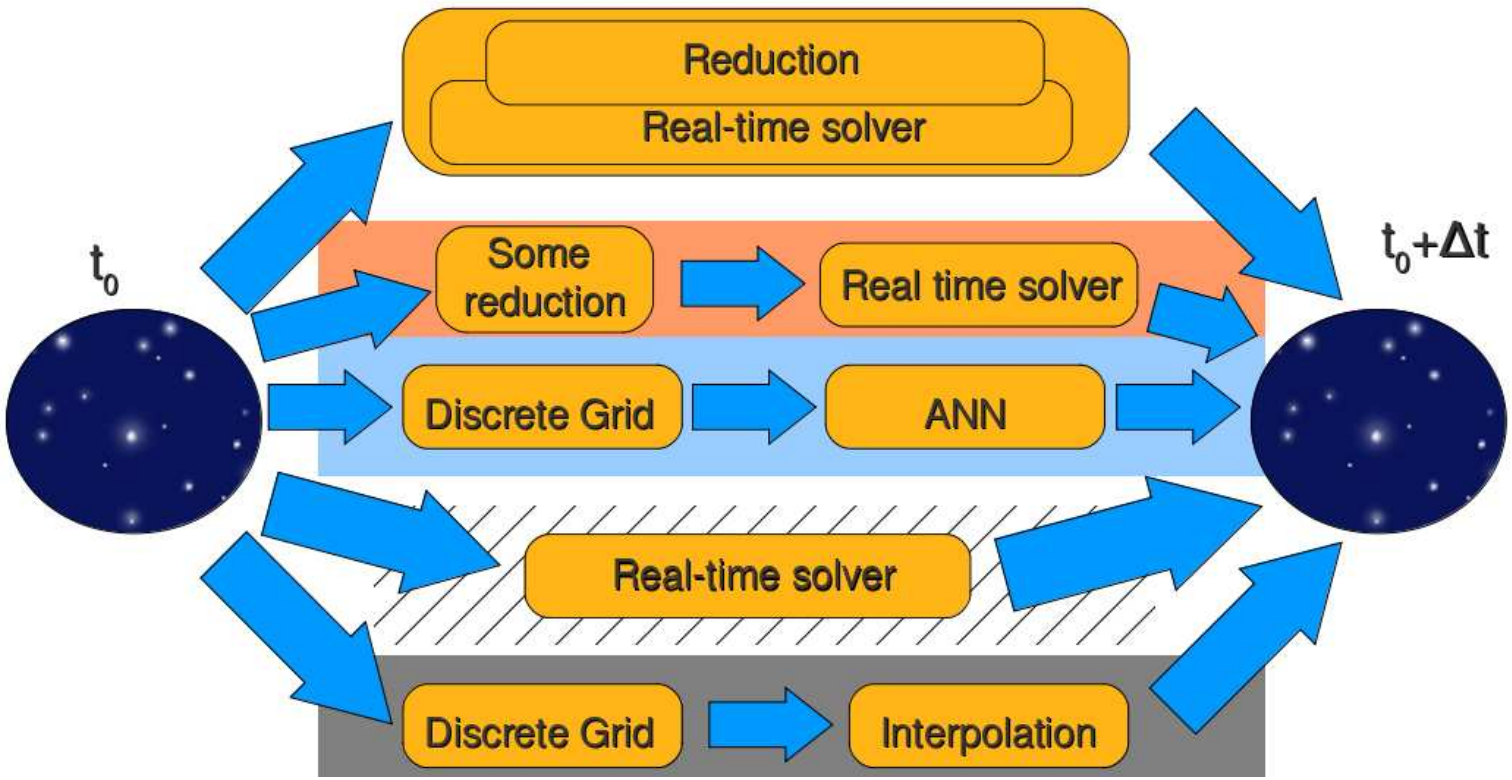
Chemistry-hydrodynamics coupling (cont'd)

Update a gas volume element at any time-step
($\gtrsim 10^6$ particles (gas units), $> 10^4$ time-steps)

- e.g. 1Dhydro+chemistry: $\gtrsim$ 90% of the CPU time
- Most heavy part together with the solution of the Poisson equation

Chemistry-hydrodynamics coupling (cont'd)

Problem: too many reactants (> 400) and too many reactions (> 4000)!
Methods to solve ODE System:



Why KROME?
Motivation

- the chemistry is a complex problem
- no general codes to solve microphysics (in HD)
- only very specific codes around (env-dependent)
- chemistry mostly hard-coded
- often not updated chemistry
- approximations/assumptions (env-dependent) to speed-up
- numerically unstable solvers (sometimes)
- some attempts to have external libraries but not enough

KROME

T. Grassi, **SB**+ MNRAS, 2014

- KROME is a package which helps users to build their own microphysics
- KROME is open source
- KROME is a pre-processor
- the core of KROME is a mix of PYTHON and FORTRAN 90.
- a chemical network is compulsory to run KROME
- to use KROME in your simulations you need to run ./krome first
- users functions are provided to an easy usage
- KROME reduces the hard-coding from the users
- to embed KROME into an external code requires a simple call
  - `call krome(x(:), Tgas, dt)`

Bitbucket and KROME
a happy marriage

Atlassian Bitbucket

KROME
better science through chemistry

KROME is developed and maintained on Bitbucket

What is bitbucket?

Bitbucket is a web-based hosting service for projects that use **distributed revision control system (DRCS)**

- Git
- Mercurial

Main advantages (already discussed by Giovanni)

- it is not a centralized system (there is no central server)
- it is a peer-to-peer network
- you can work without being connected to a network

What does KROME include?

- Solving chemical networks (ODEs+Jacobian+sparsity+tables)
- Several chemical networks provided (from primordial up to $>$5k reacts)
- Photochemistry module per bins
- Cosmic rays (rate approximation, $\alpha\zeta_{CR}$)
- Atomic cooling (H, H^+, He, He^+, He^{++}, as Cen1992)
- H_2^{rv} cooling (GP98+GA08), HD^{rv} (Lipovka+2005), CO cooling
- H_2^{cd} cooling (Martin+98, Glover+Jappsen2007)
- Collisionally induced emission (CIE) cooling (Ripamonti+Abel2004)
- CI, OI, SiI, FeI, and ions cooling (Maio+2007, HM79, at runtime)
- Continuum (Omukai2000, Lenzuni+91)
- Compton Cooling (Cen 1992)
- Chemical heating including H_2 on dust (Omukai2000, HM79)
- Photoheating (ν-dependent, GA08)
- MRN profile for dust ($\propto a^{-3.5}$) for graphite and Si-based
- Dust growth by sticking (Dwek98)
- H_2 formation on dust (Cazaux+Spaans2009)
- patches available for 3D codes: Enzo, Ramses, Flash, Gasoline, and Mocassin, (Gandalf?)

Some work done with KROME

Some nice applications pursued with KROME

- formation of supermassive black holes[3]
- collapse of low-metallicity minihaloes[4]
- formation of primordial stars[5]
- chemical evolution of self-gravitating primordial disks [6]
- formation of the first galaxies[7]
- the formation of very massive stars[8]
- study of ISM star-forming filaments[9]
- turbulent molecular clouds[10]
- galaxy evolution [11]

[3] Latif+, 2014,2015a,b
[4] Bovino+, 2014a
[5] Bovino+, 2014b
[6] Schleicher+, 2015
[7] Prieto+, 2015
[8] Katz+, 2015
[9] Seifried+, 2015
[10] Haugbølle+, 2015
[11] Capelo+, 2015

Thank you for your attention!

DFG Deutsche Forschungsgemeinschaft