Complexity reduction of astrochemical networks:
a topological approach

S. Bovino

Institut für Astrophysik Göttingen

October 8, 2012

What we know

- Chemistry is one of the most important ingredients
- Chemistry is one of the bottleneck of a simulation
- Solving chemistry $\longrightarrow$ set of stiff coupled ODE's
- We need reduction techniques

How to reduce the ODE's system?

1. Reducing the # reactions in the RHS (most heavy part of the problem) (Dr. Grassi's talk)
2. Reducing the dimensionality (remove species$\rightarrow$# ODE's decreases) (this talk)

Methods

Reducing dimensionality: *A priori* methods

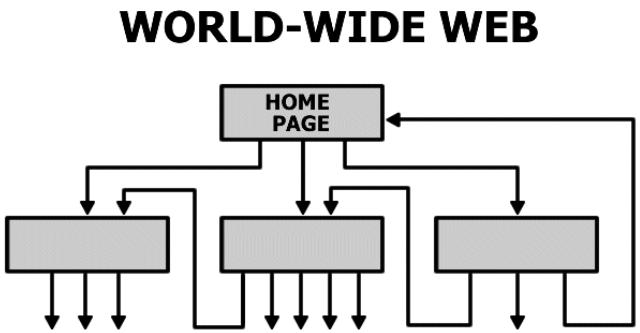
- Preselect important species (by physical assumptions) [e.g. Nelson+ 1999]
- Linear subset [e.g. Glover+ 2010]
- Lumping methods [e.g. Okino+ 1998]
- SVD, PCA, ...
- Topology-based methods

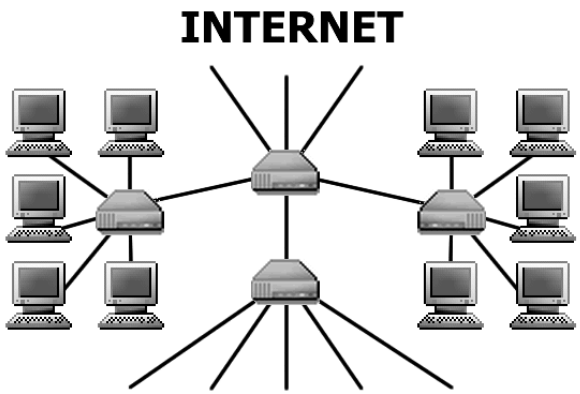
What does it mean topology?

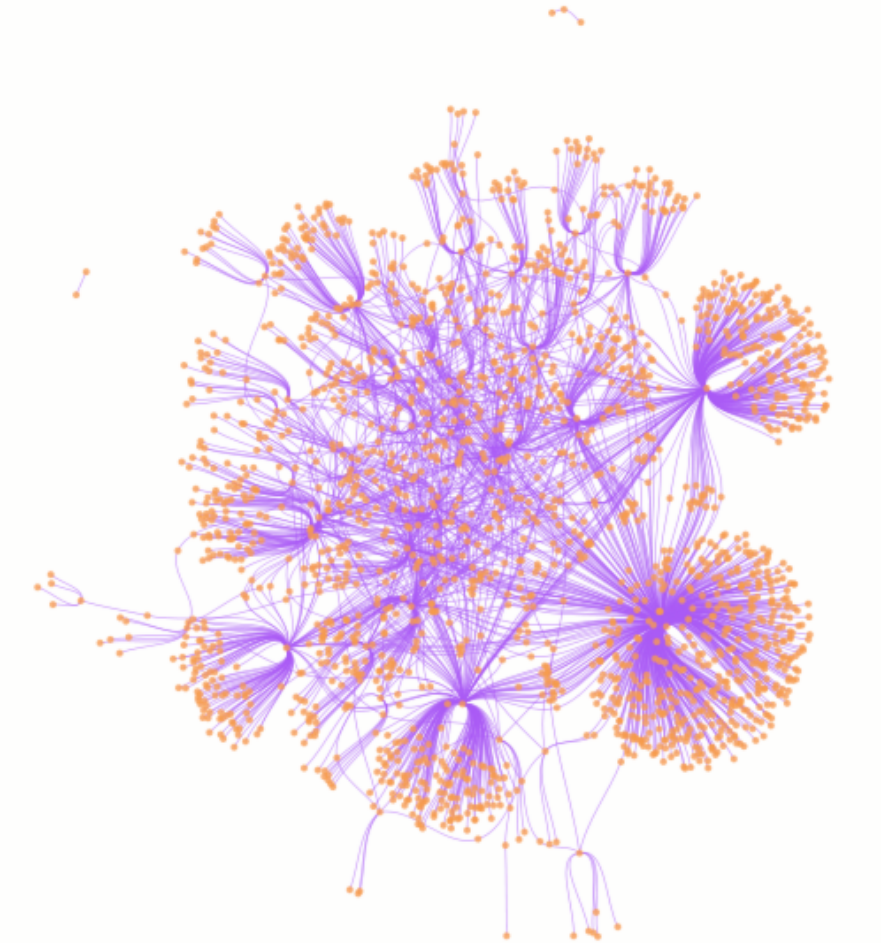
Topology is a usually schematic description of the arrangement (geometrical) of a network, including its nodes and connecting lines.

Networks as directed graph /1

Directed graph network examples





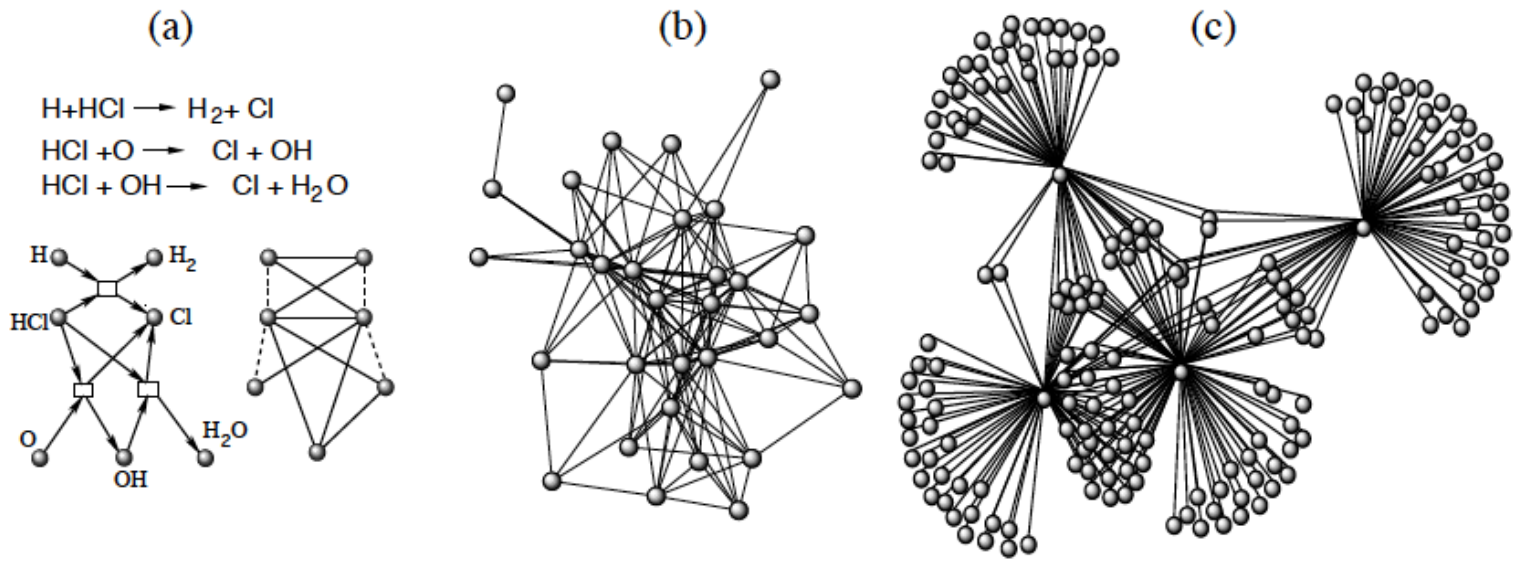


Networks as directed graph /2

Astrochemical networks

NODES $\longrightarrow$ chemical species

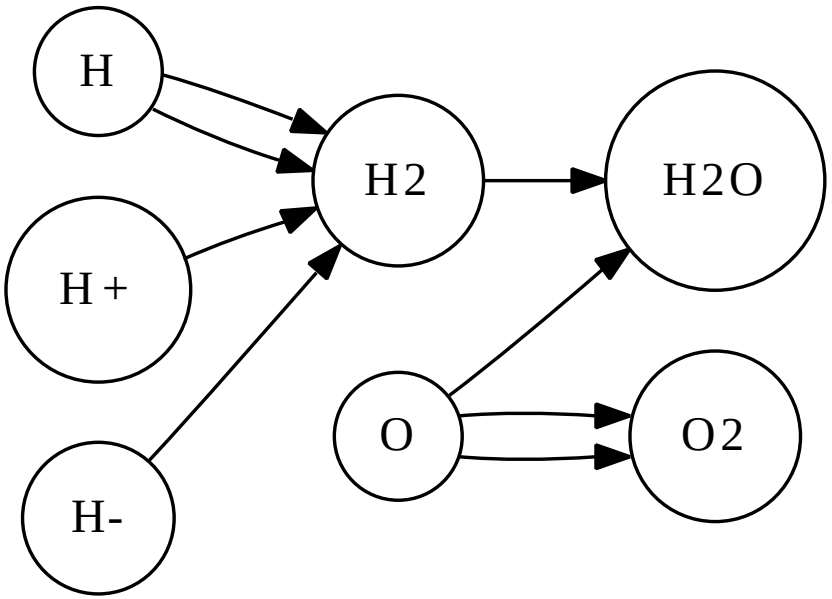
EDGES $\longrightarrow$ conversion between chemicals



(R. V. Solé & A. Munteanu 2007)

Topology-based reduction /1

- *a priori* method
- using network topology to determine most "active" chemical species
- degree, 2^{nd} degree, betweenness centrality, ...
- (see Jolley+ 2010, 2012; Barabasi+ 20**)



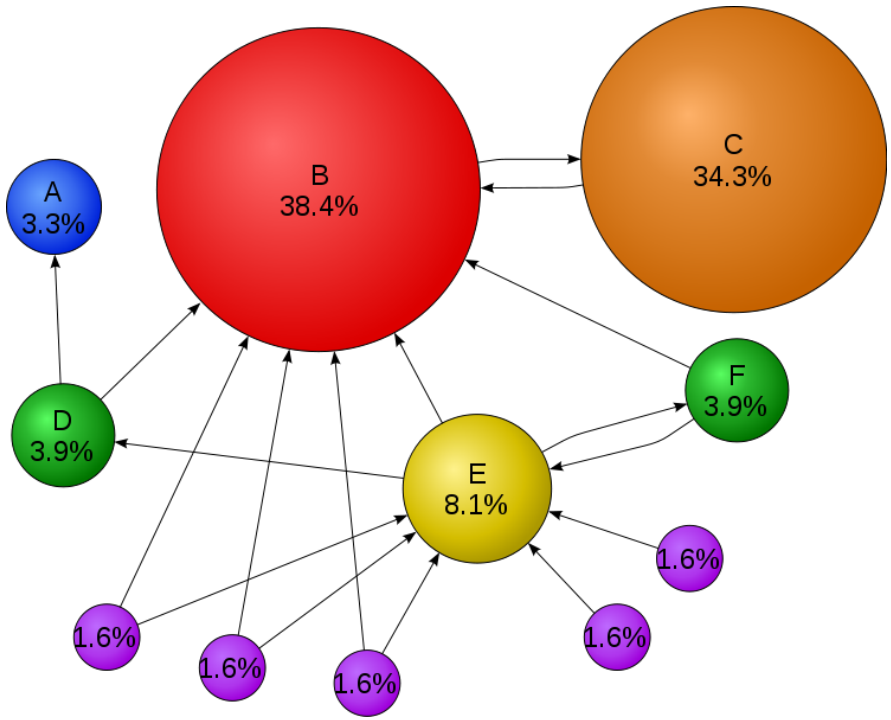
	1^{st}	2^{nd}
H_2	5	8
O	3	6
H	2	10
H_2O	2	8
O_2	2	6
H^+	1	5
H^-	1	5

Topology-based reduction /2

2nd degree follows "The SOCIAL NETWORK rule"

What is it important?

To know people (nodes) who are in touch with many other people
Similar to **PageRank** algorithm of Google



Topology-based reduction /3

Our approach

- Evaluate the 2^{nd} degree of each node
- Ranking of the species based on the 2^{nd} degree
- Choose a threshold:
  - taking a fraction of the largest 2^{nd} degree
  - taking the smallest 2^{nd} degree of one of the most abundant species (above a given initial threshold)
- Cut the species (and then reactions involving them) below the threshold
- We reduced the dimensionality of the problem!

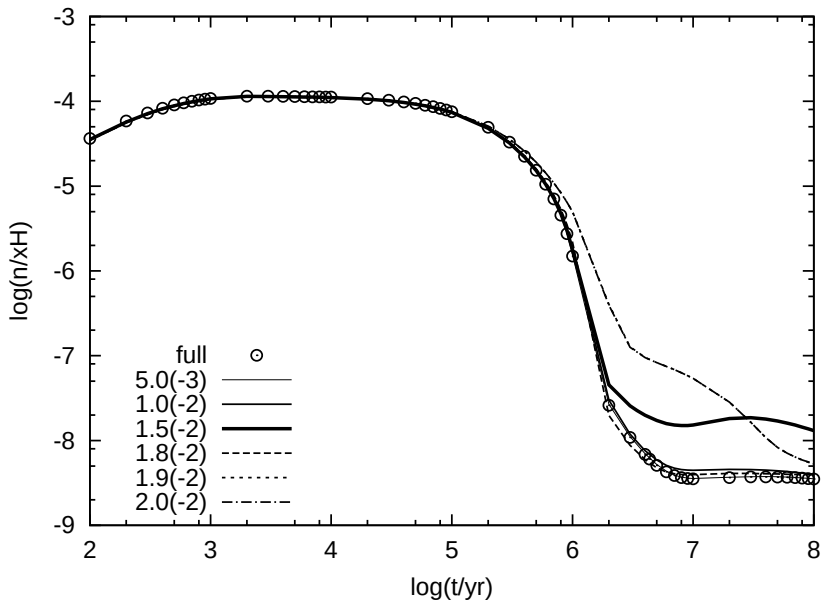
2nd degree Application /1

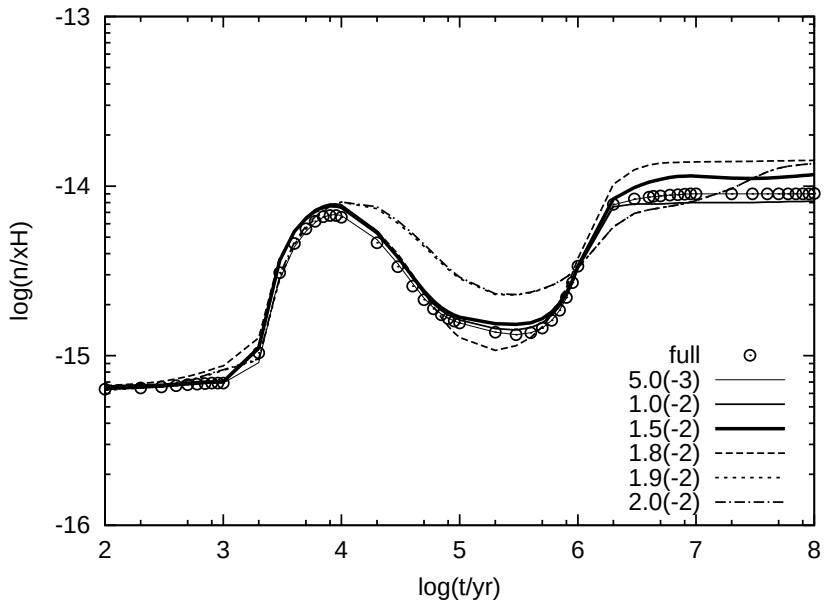
Application I: one-zone large network

- UMIST2008, Wakelam&Herbst 2008
- species: 454
- reactions: 4431
- one-zone
- no cooling
- $T = 10$ K
- $\zeta_{\mathrm{CR}} = 1.3 \times 10^{-17}$ s^{-1}
- $A_v = 10$

2nd degree Application /2

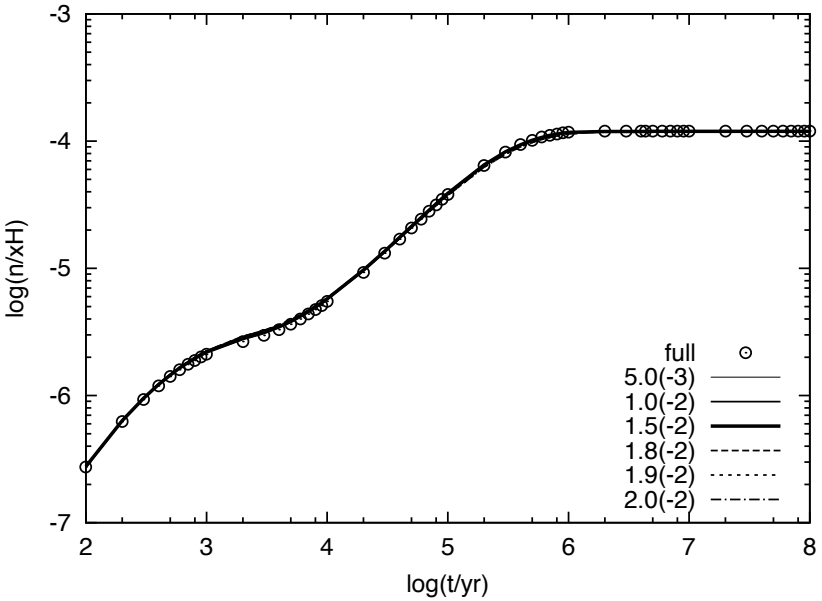
Application I: one-zone results ($x_{\rm C}(t)$, $x_{\rm O}(t)$)

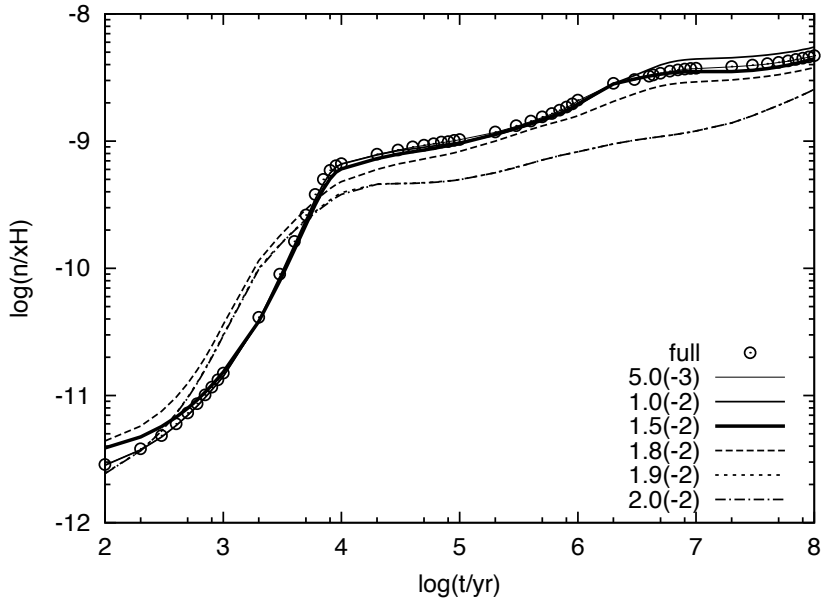




2nd degree Application /3

Application I: one-zone results ($x_{\rm CO}(t)$, $x_{\rm OH}(t)$)





speed-up = x3

2nd degree Application /4

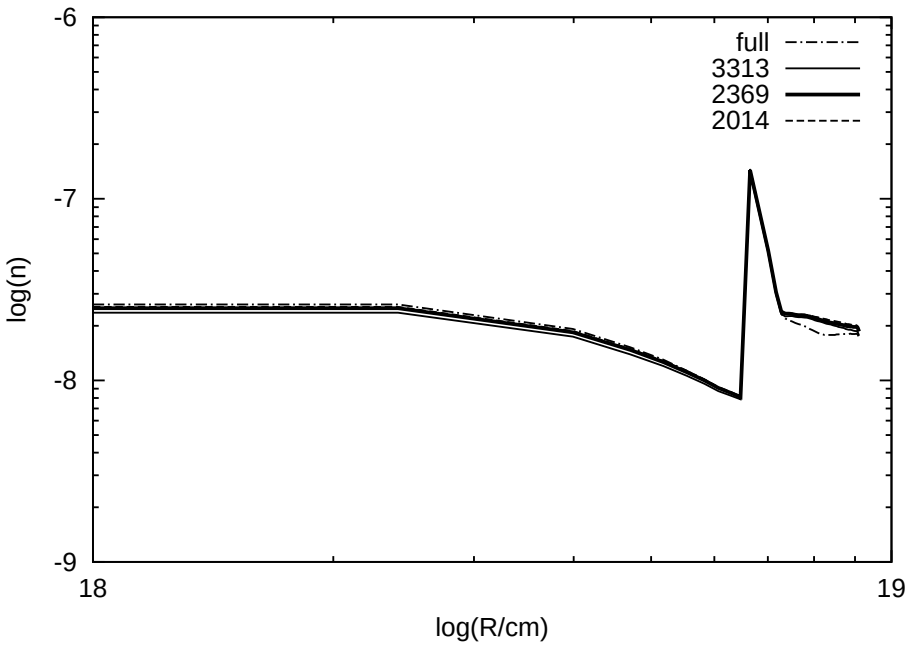
Application II: 1D Lagrangian code, VERY PRELIMINARY TEST

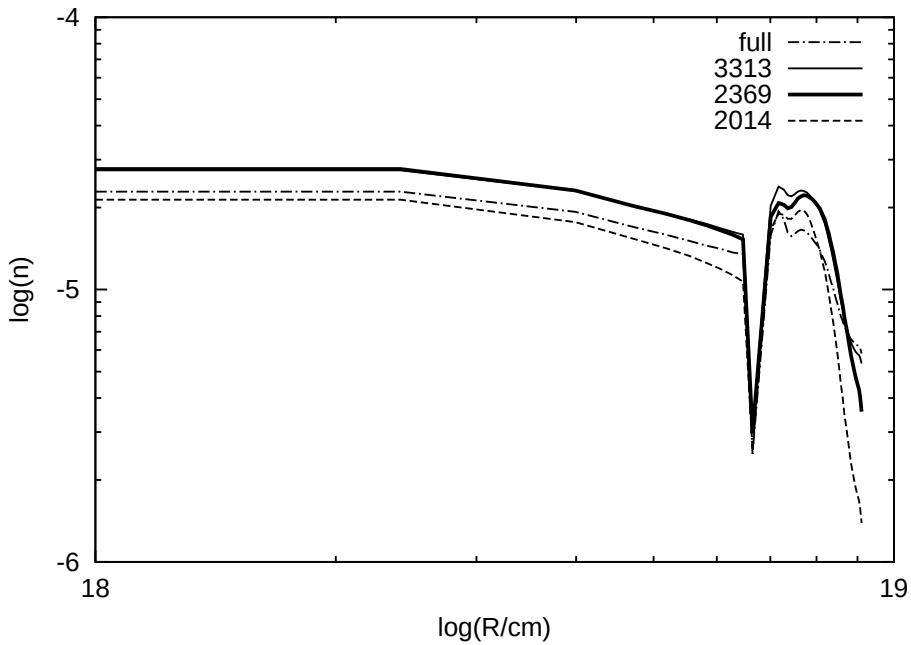
- Lagrangian
- Cooling, Heating, UV field
- Dust accretion
- Dust destruction (see Grassi+ 2011)
- Shocks (collapse in the near future)

- species: 455
- reactions: 4431
- no cooling, no dust physics
- we only include CHEMISTRY
- T_{ej}=10^4 K, T_{amb} = 10 K
- $\rho_{amb} = 10^{-22}$ g/cm^3
- $\rho_{ej} = 10^{-20}$ g/cm^3
- # cells = 50, fireballs = 10
- R = 1 pc, $t_{final} = 10^6$ ys

2nd degree Application /5

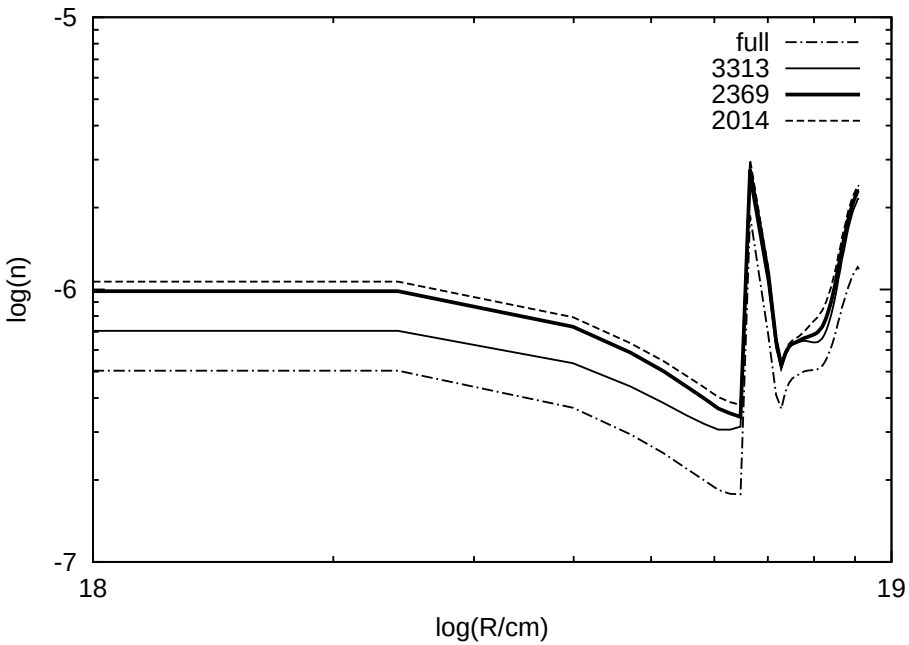
Application II: 1D results ($n_{\mathrm{H}^+}(t_{final}, R)$, $n_{\mathrm{CH}}(t_{final}, R)$)

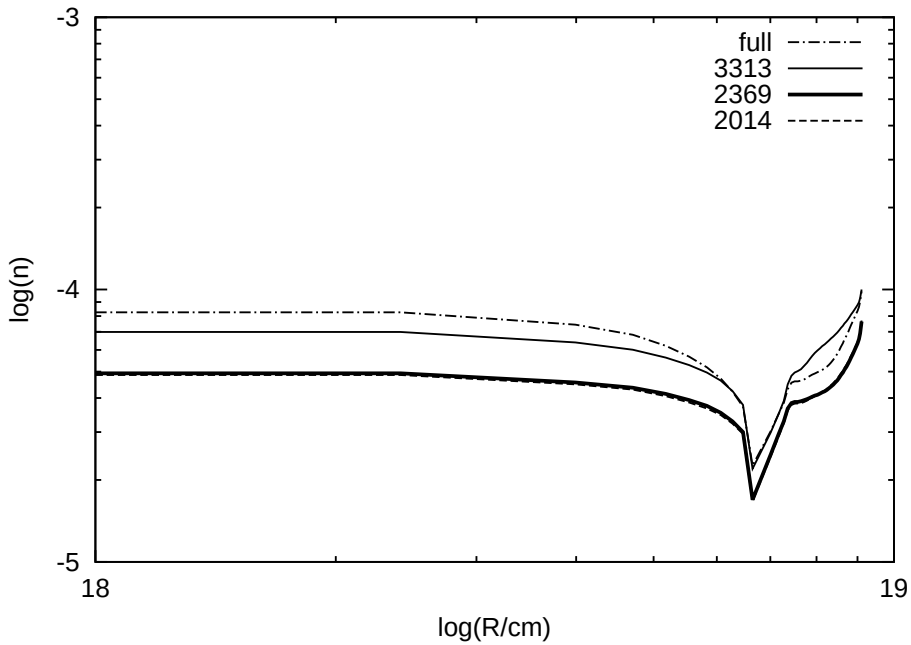




2nd degree Application /6

Application II: 1D results ($n_{C^+}(t_{final}, R)$, $n_O(t_{final}, R)$)





2nd degree Application /7

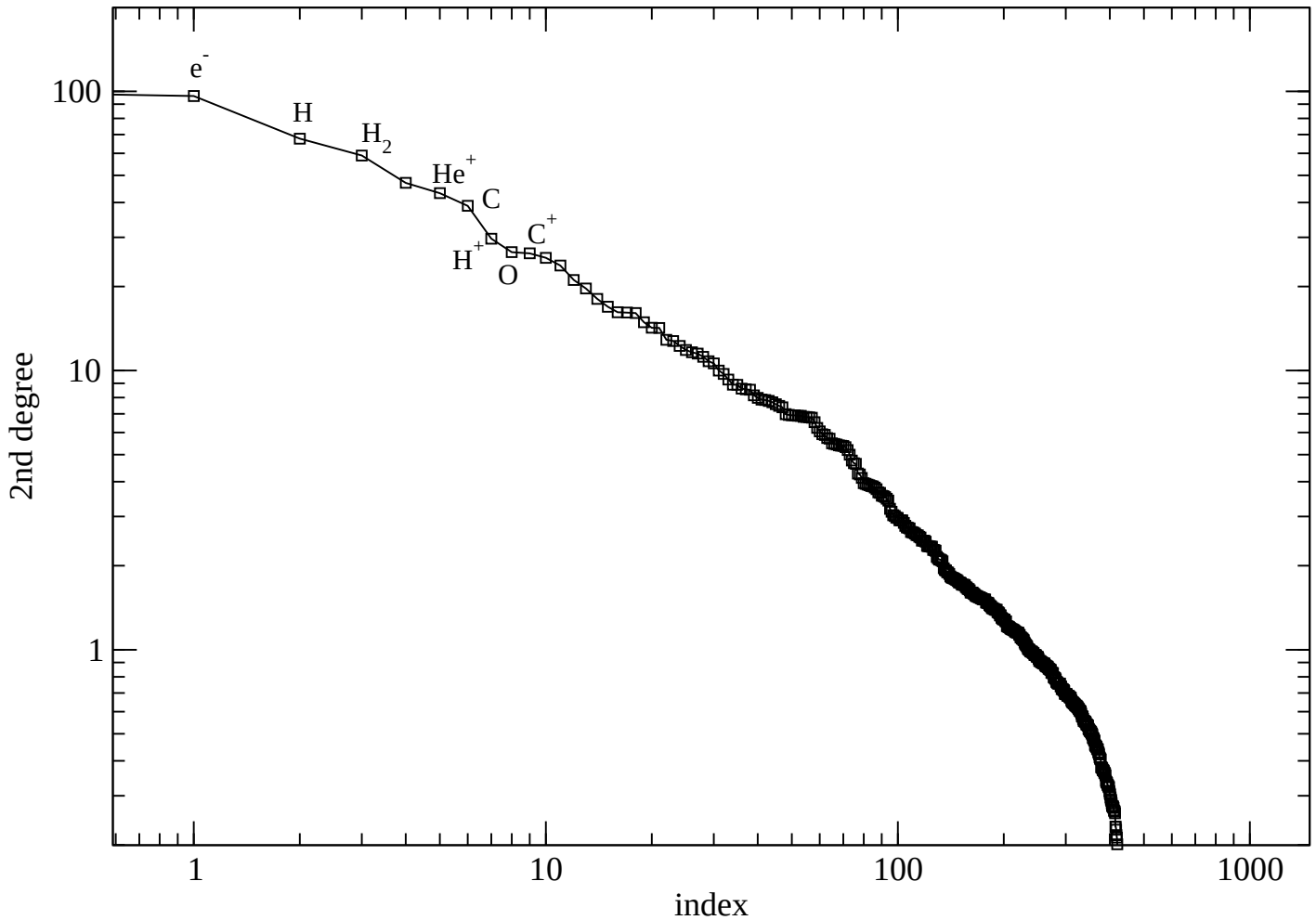
method (# reac.)	CPUtime
full (4431)	1.00
topology (3313)	0.50
topology (2369)	0.37
topology (2014)	0.30

Additional information /1

- Error less than 10%
- We can save 70% of the CPU time (both in one-zone and in 1D)
- Most important $\rightarrow$ we can obtain chemical information on the network, e.g. species cutted: CI/CI^+, Mg/Mg^+, Fe/Fe^+, MgH, HF, C-chains, F and many reactions involving C^+ and He^+.

Additional information /2

Most important HUBS (where most of the information is)

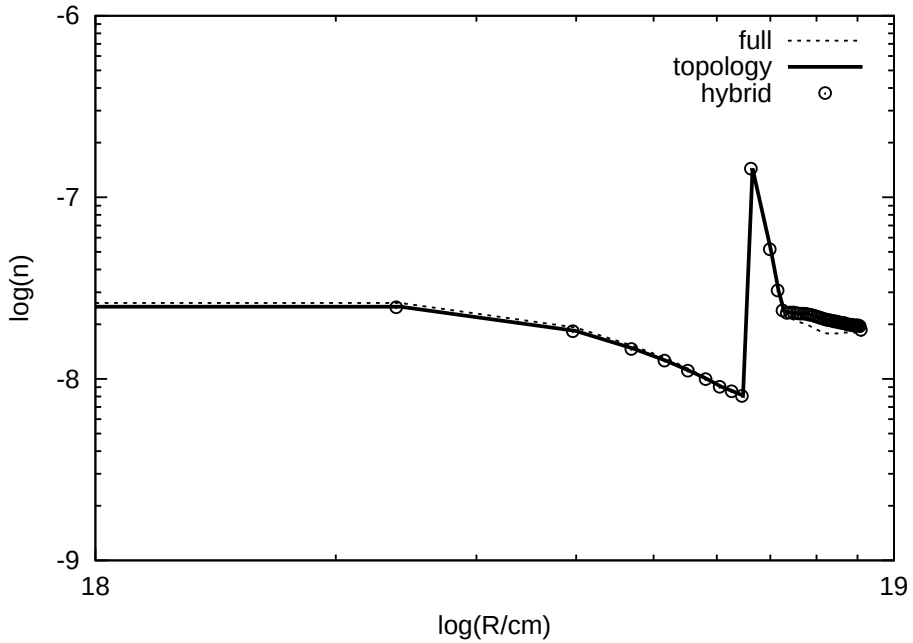


Further considerations

- more accurate tests needed: e.g. including metal cooling
- what about a hybrid method $\longrightarrow$ topology + flux-based?

method	CPUtime
full	1.00
topology-reduction	0.37
hybrid-reduction	0.17

speed-up $\sim$ x10



- changes in species abundances not necessarily means a change in the dynamic!
- Hybrid method (very preliminary) gives additional speed-up!

Summary

- Computational chemistry needs reduction methods
- Topology-based method gives good speed-up, 2x<speed-up<3x
- On-the-fly method works well, 2x<speed-up<10x depending on network's size (Tommaso's talk)
- Coupling *a priori* + "on the fly" reduction methods should save a lot of CPU-time (work in progress)
- All these methods can be applied to smaller network (e.g. Low-Z network with $\sim$ 600 reactions)
- Chemistry problem is SOLVER's dependent (DVODE, DLSODES)
- Work on a specific (special) solver for astrochemical networks! (hard but possible)

Thank you for your attention!

Also thanks to: Dr. T. Grassi (University of Rome Sapienza)
Prof. Dr. D. Schleicher (IfA Göttingen)