PDR Model Benchmark

M. Röllig
&
N. P. Abel, T. Bell, F. Bensch, J. Black, G. J. Ferland, B. Jonkheid, I. Kamp,
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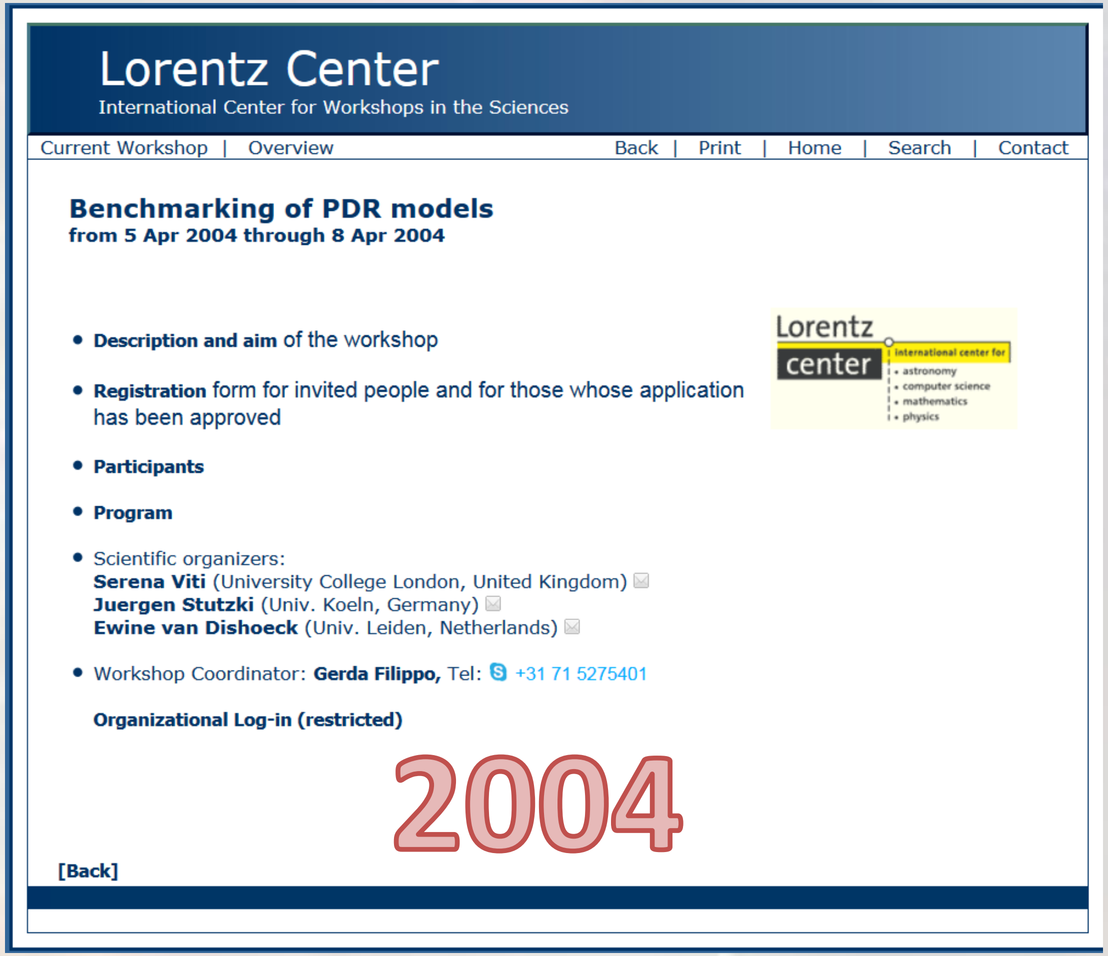
E. Roueff, G. Shaw, M. Spaans, A. Sternberg, J. Stutzki, W.-F. Thi,
E. F. van Dishoeck, P. A. M. van Hoof, S. Viti, M.G. Wolfire

PDR Model Benchmark



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Benchmarking of PDR models
from 5 Apr 2004 through 8 Apr 2004

- **Description and aim** of the workshop
- **Registration** form for invited people and for those whose application has been approved
- **Participants**
- **Program**
- Scientific organizers:
  Serena Viti (University College London, United Kingdom)
  Juergen Stutzki (Univ. Koeln, Germany)
  Ewine van Dishoeck (Univ. Leiden, Netherlands)
- Workshop Coordinator: **Gerda Filippo**, Tel: +31 71 5275401

Organizational Log-in (restricted)

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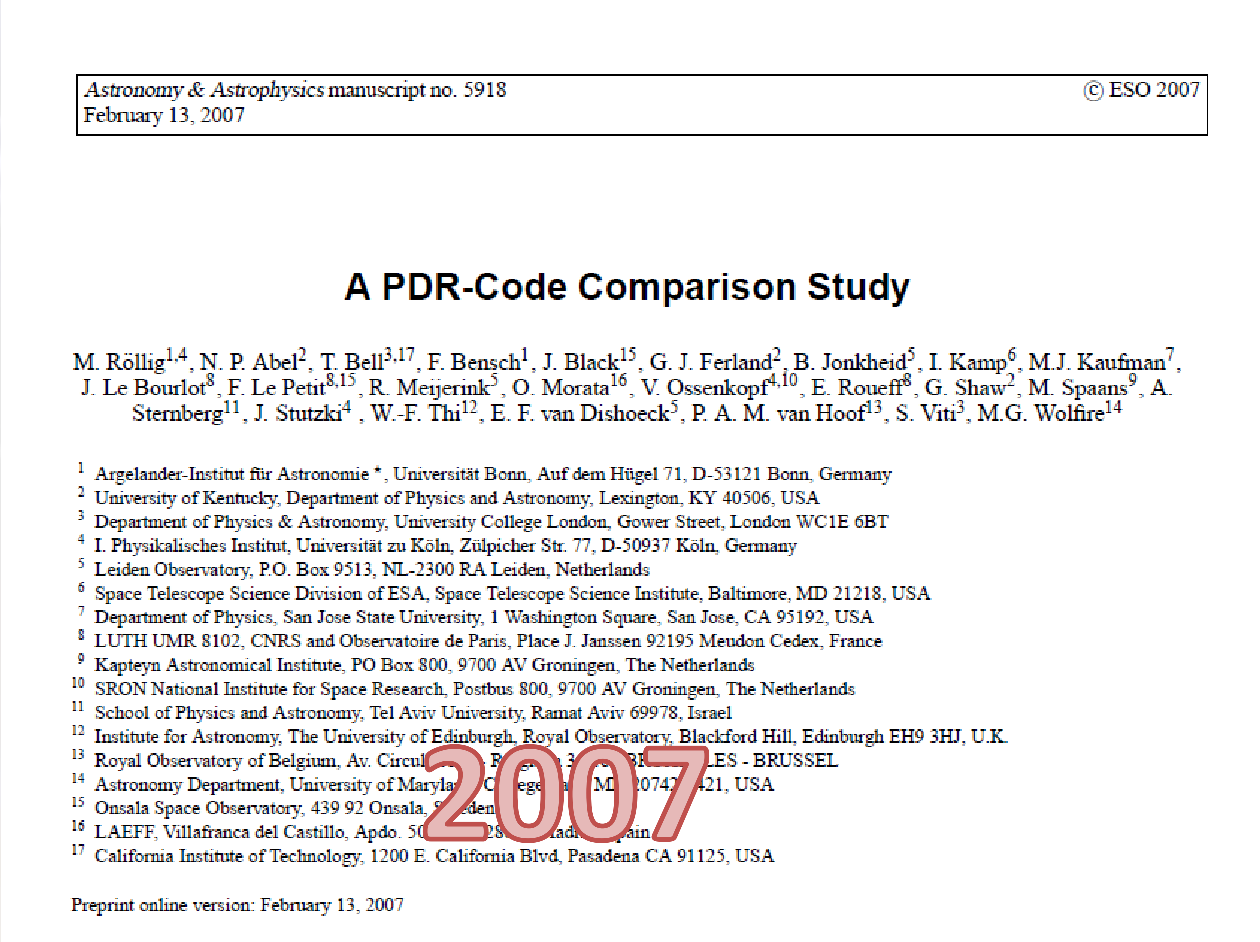

Astronomy & Astrophysics manuscript no. 5918
February 13, 2007

A PDR-Code Comparison Study

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13 Royal Observatory of Belgium, Av. Circul ... LES - BRUSSEL
14 Astronomy Department, University of Maryla ... 21, USA
15 Onsala Space Observatory, 439 92 Onsala, ... den
16 LAEFF, Villafranca del Castillo, Apdo. 50 ... ain
17 California Institute of Technology, 1200 E. California Blvd, Pasadena CA 91125, USA

Preprint online version: February 13, 2007

Participating Models

Model Name	*Authors*
Aikawa	*H.-H. Lee, E. Herbst, G. Pineau des Forets, J. Le Bourlot, Y. Aikawa, N. Kuboi*
Bensch	*H. Störzer, B. Köster, M. Zilinsky, U. Leuenhagen, S. Jeyakumar, F. Bensch*
CLOUDY	*Gary J. Ferland, Peter van Hoof, Nick P. Abel, Gargi Shaw*
COSTAR	*I. Kamp, F. Bertoldi, G.-J. van Zadelhoff*
HTBKW	*D. Hollenbach, A.G.G.M. Tielens, M.G. Burton, M.J. Kaufman, M.G. Wolfire*
KOSMA	*H. Störzer, B. Köster, M. Zilinsky, U. Leuenhagen, S. Jeyakumar, M. Röllig*
Lee96mod	*H.-H. Lee, E. Herbst, G. Pineau des Forets, E. Roueff, J. Le Bourlot, O. Morata*
Leiden	*J. Black, E. van Dishoeck, D. Jansen and B. Jonkheid*
Meijerink	*R. Meijerink, M. Spaans*
Meudon	*J. Le Bourlot, E. Roueff, F. Le Petit*
Sternberg	*A. Sternberg, A. Dalgarno*
UCL_PDR	*S. Viti, Wing-Fai Thi, Tom Bell*

Benchmark Calculations

- standard chemistry:
  - 31 species
    H, H^+, H_2, H_2^+, H_3^+, O, O^+, OH^+, OH, O_2, O_2^+, H_2O, H_2O^+, H_3O^+, C, C^+, CH, CH^+, CH_2, CH_2^+, CH_3, CH_3^+, CH_4, CH_4^+, CH_5^+, CO, CO^+, HCO^+, He, He^+, e^-
  - UMIST06 database
  - elemental abundances: He=0.1, C=$1.0\text{x}10^{-4}$, O=$3.0\text{x}10^{-4}$
  - PAH's switched off
- standard radiation field
  - normalized to Draine field (1978)
  - cosmic-ray ionization: $\zeta=5\text{x}10^{-17}\ s^{-1}$
  - visual extinction: $A_V=6.289 \times 10^{-22} \times N_{Htotal}$
  - dust attenuation: $\tau_{UV}=3.02 \times A_V$

Benchmark Calculations

Requested output

For the species: H, H_2, C^+, C, CO, O, O_2, CH, OH, e^-

1. local absolute volume densities (cm^{-3}) vs. depth
2. column densities (cm^{-2}) vs. depth
3. dissociation/ionization rates (s^{-1}) vs. depth for H_2, C, CO
4. local cooling/heating rates (erg s^{-1} cm^{-3})
   fine structure lines of CII(158m), OI(63µ, 146µ), and CI(610µ, 370µ), and photoelectric grain heating
5. gas and dust temperature for models F5-F8

Benchmark Calculations

F1 completed by all 12 groups

F2-F4 complete by 10 groups

F5-F8 completed by 8 groups (some with numerical 'noise')

CLOUDY used different chemical network

KOSMA/Bensch used spherical geometry

results for Lee96mod are for $t=10^8$ yrs

F1 T=const $n=10^3\ cm^{-3}$, $\chi=10$	**F2** T=const $n=10^3\ cm^{-3}$, $\chi=10^5$
F3 T=const $n=10^{5.5}\ cm^{-3}$, $\chi=10$	**F4** T=const $n=10^{5.5}\ cm^{-3}$, $\chi=10^5$
F5 T=variable $n=10^3\ cm^{-3}$, $\chi=10$	**F6** T=variable $n=10^3\ cm^{-3}$, $\chi=10^5$
F7 T=variable $n=10^{5.5}\ cm^{-3}$, $\chi=10$	**F8** T=variable $n=10^{5.5}\ cm^{-3}$, $\chi=10^5$

Benchmark Calculations

F1 completed by all 12 groups

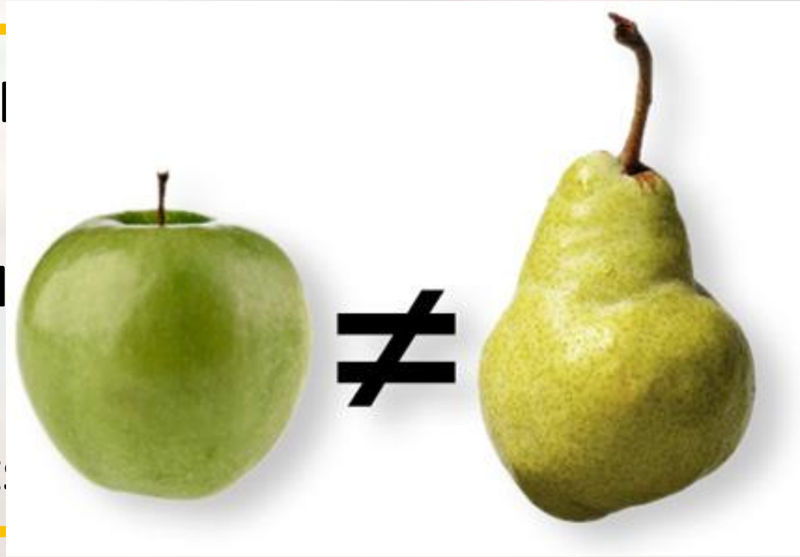
F2-F4 complete by 10 groups

F5-F8 completed by 8 groups (some with numerical ‘noise’)

CLOUI … work

KOSM … try

result … rs



F1 T=const $n=10^3\ cm^{-3}$, $\chi=10$	**F2** T=const $n=10^3\ cm^{-3}$, $\chi=10^5$
F3 T=const $n=10^{5.5}\ cm^{-3}$, $\chi=10$	**F4** T=const $n=10^{5.5} cm^{-3}$, $\chi=10^5$
F5 T=variable $n=10^3\ cm^{-3}$, $\chi=10$	**F6** T=variable $n=10^3\ cm^{-3}$, $\chi=10^5$
F7 T=variable $n=10^{5.5}\ cm^{-3}$, $\chi=10$	**F8** T=variable $n=10^{5.5} cm^{-3}$, $\chi=10^5$

Benchmark Calculations

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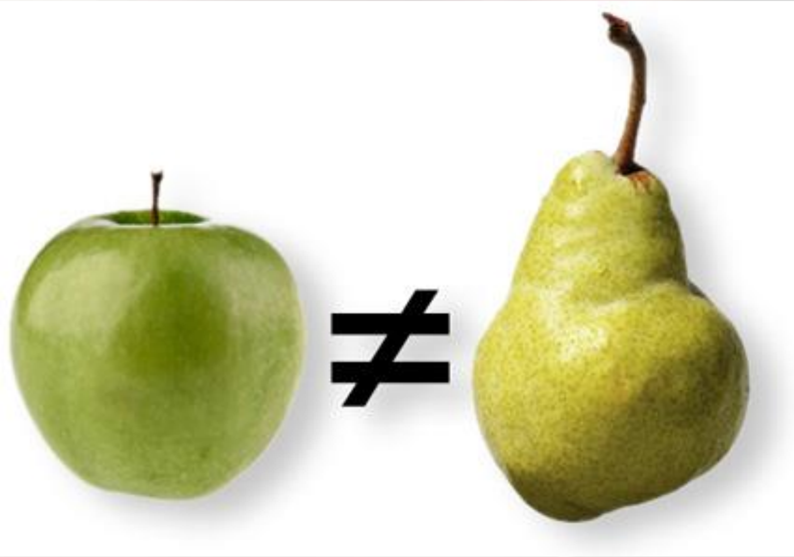


CLOU … work

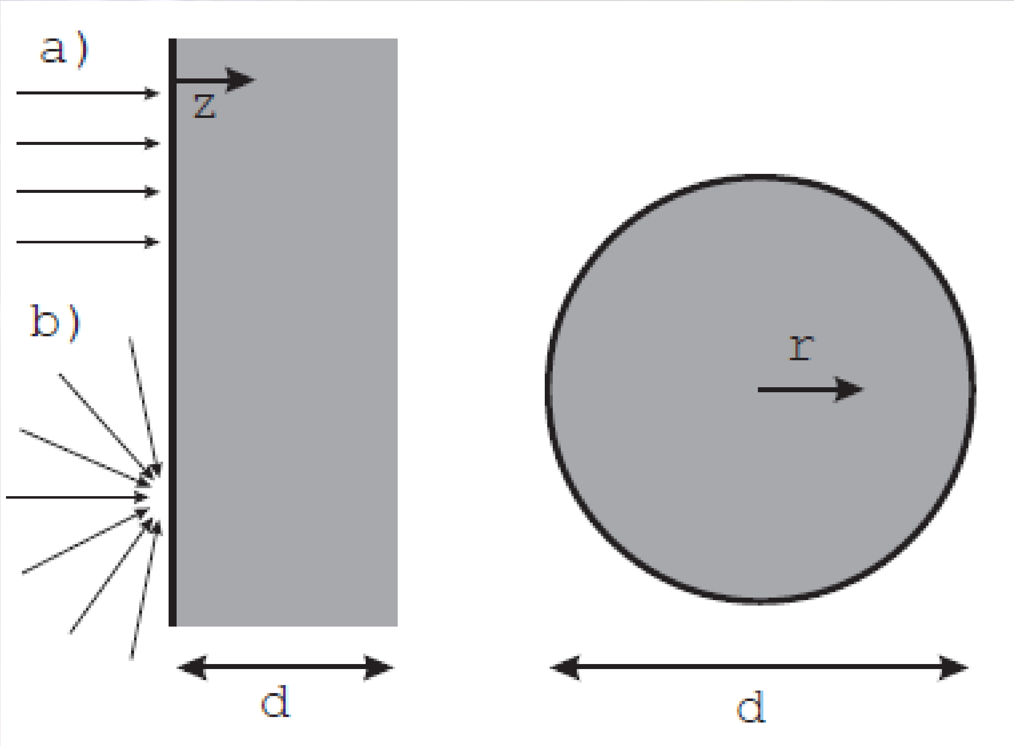
KOSM … try

result … rs

Comparable?

H_0: PDR models are all alike?

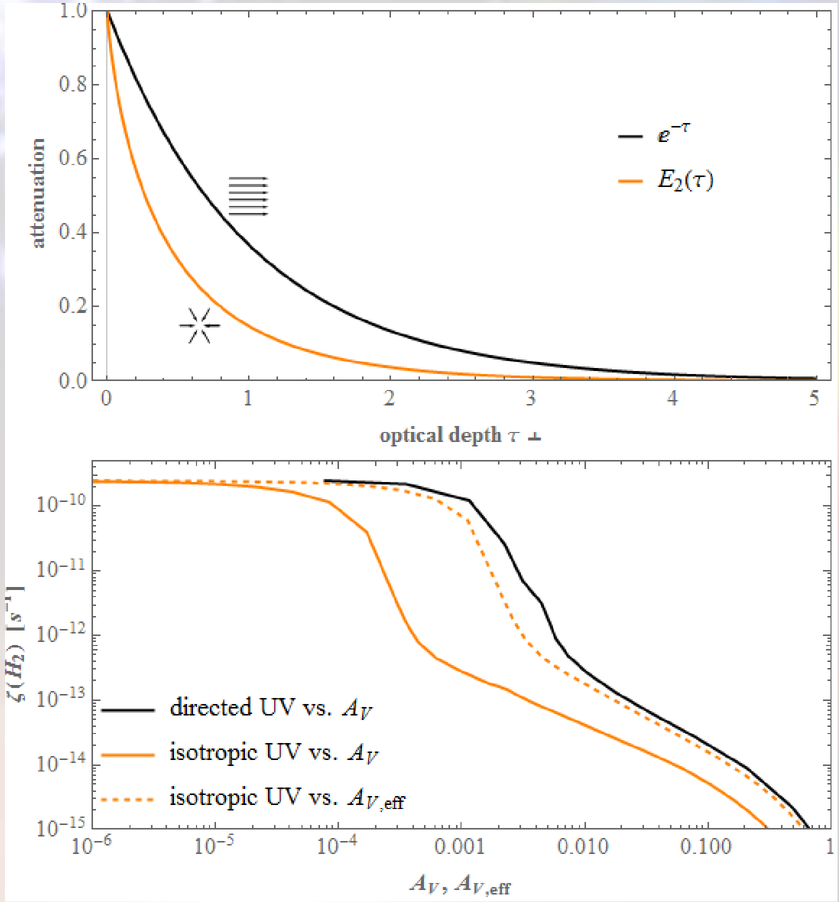
- Different model geometry complicates things
- When is a spherical cloud comparable to a plane-parallel slab? (semi-infinite, illuminated from both sides,…)



Comparable?

~~H_0~~: PDR models are all alike?

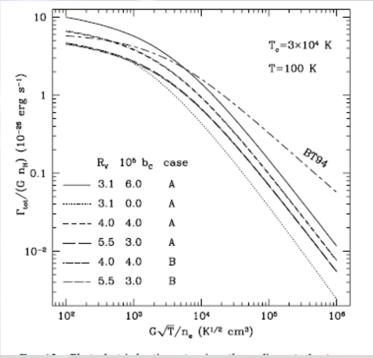
- Different model geometry complicates things
- When is a spherical cloud comparable to a plane-parallel slab? (semi-infinite, illuminated from both sides,…)
- Basic concepts such as A_V and column density change meaning in isotropically illuminated clouds

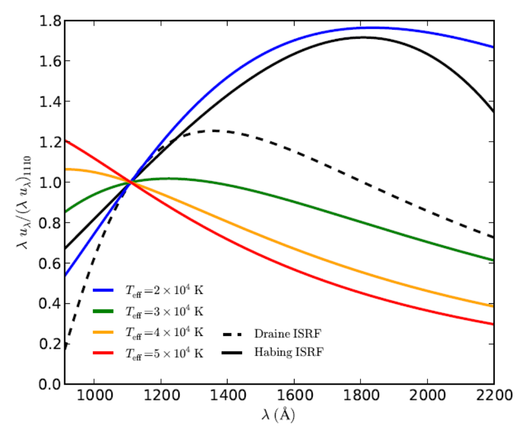


Comparable?

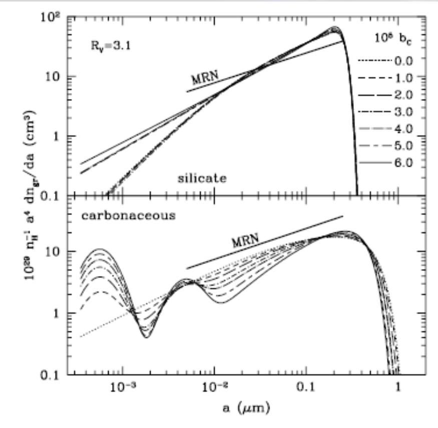
- FUV ≠ FUV
- Hardwired parts of the models can not simply be replaced → ~~Self-consistency~~
- Time-dependence/steady-state
- Dust treatment
- Approximations vs. detailed treatment
- Radiative transfer, scattering, shielding
- H_2 physics/chemistry (H_2^*, formation)
- Rate coefficients
- Heating/cooling

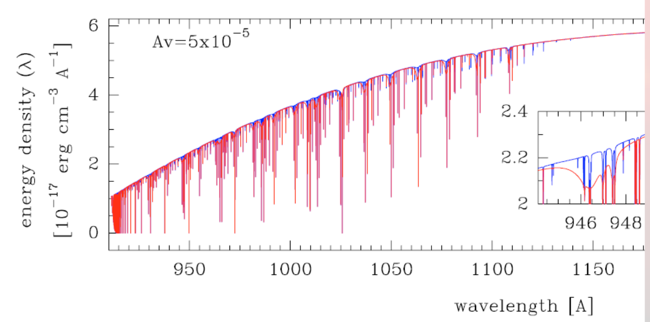
Weingartner & Draine 2001, ApJSS 134





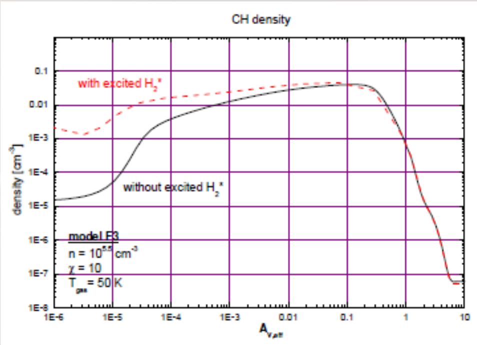
Baczynski et al. 2015





Goicoechea et al. 2007

Weingartner & Draine 2001, ApJ 548



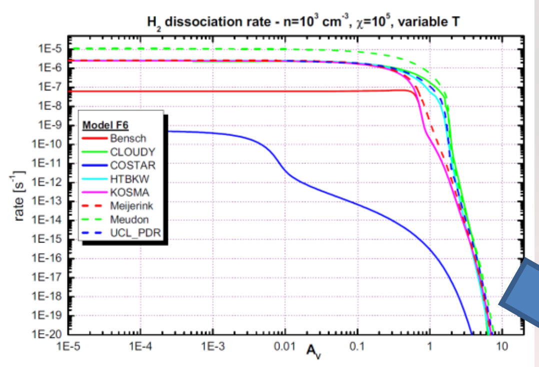
Röllig et al. 2007

Comparable

- **Crippling**: all codes had to limit their capabilities in various areas to allow comparison
- **Playground problems**: Simple & reduced problem setup to minimize impact of hidden factors
- Analysis focused mainly on **chemistry** and **shielding** in the isothermal model setups.

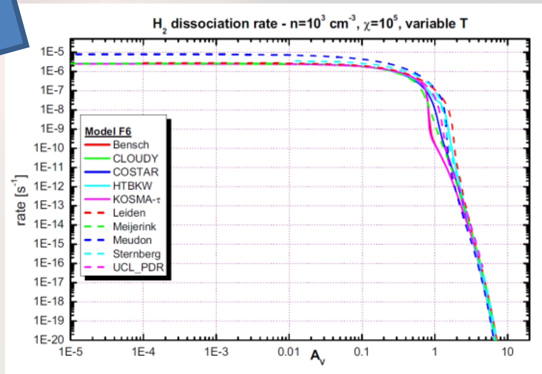
Benchmark Data Archive

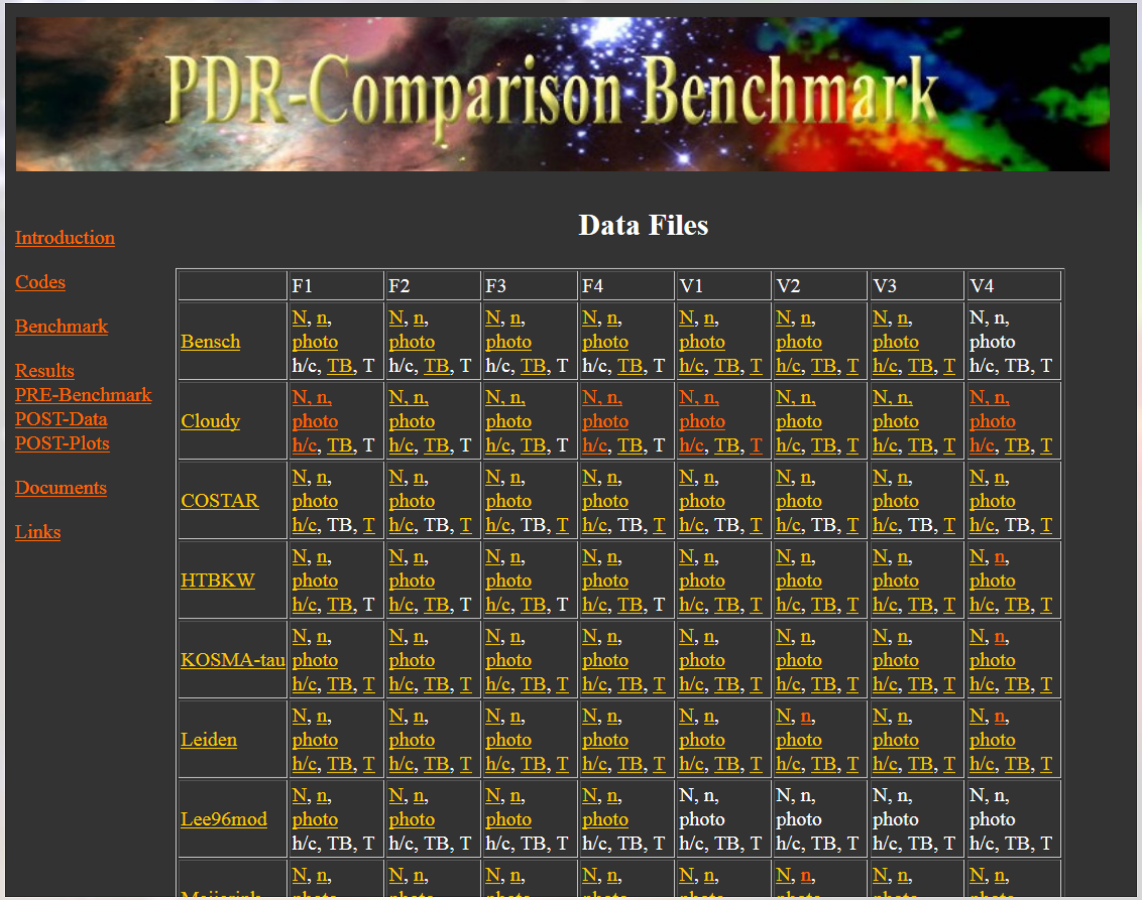
- All the results (data files, plots, documents) have been published on a website.



BEFORE

AFTER





PDR-Comparison Benchmark

Introduction
Codes
Benchmark
Results
PRE-Benchmark
POST-Data
POST-Plots
Documents
Links

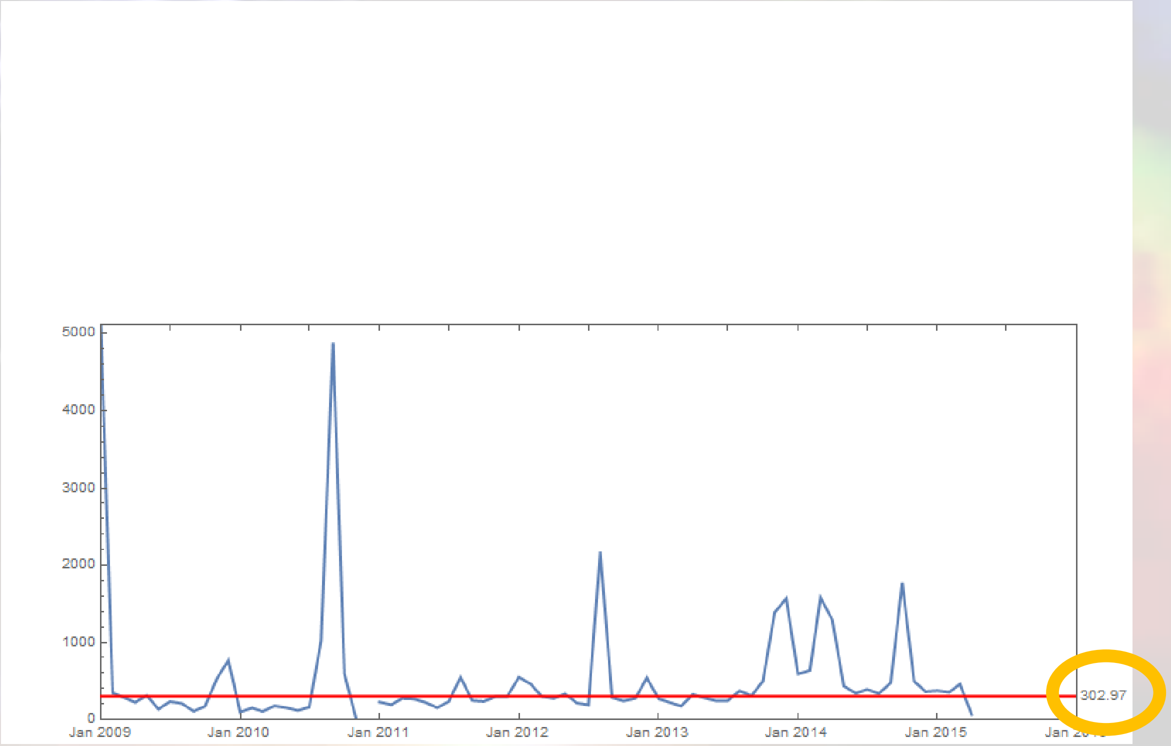
Data Files

	F1	F2	F3	F4	V1	V2	V3	V4
Bensch	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
Cloudy	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
COSTAR	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
HTBKW	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
KOSMA-tau	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
Leiden	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
Lee96mod	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T	N, n, photo h/c, TB, T
[illegible]	N, n,	N, n,	N, n,	N, n,	N, n,	N, n,	N, n,	N, n,

http://www.astro.uni-koeln.de/pdr-comparison/

Benchmark Data Archive

- All the results (data files, plots, documents) have been published on a website.
- Surprising archive traffic (2009-15)



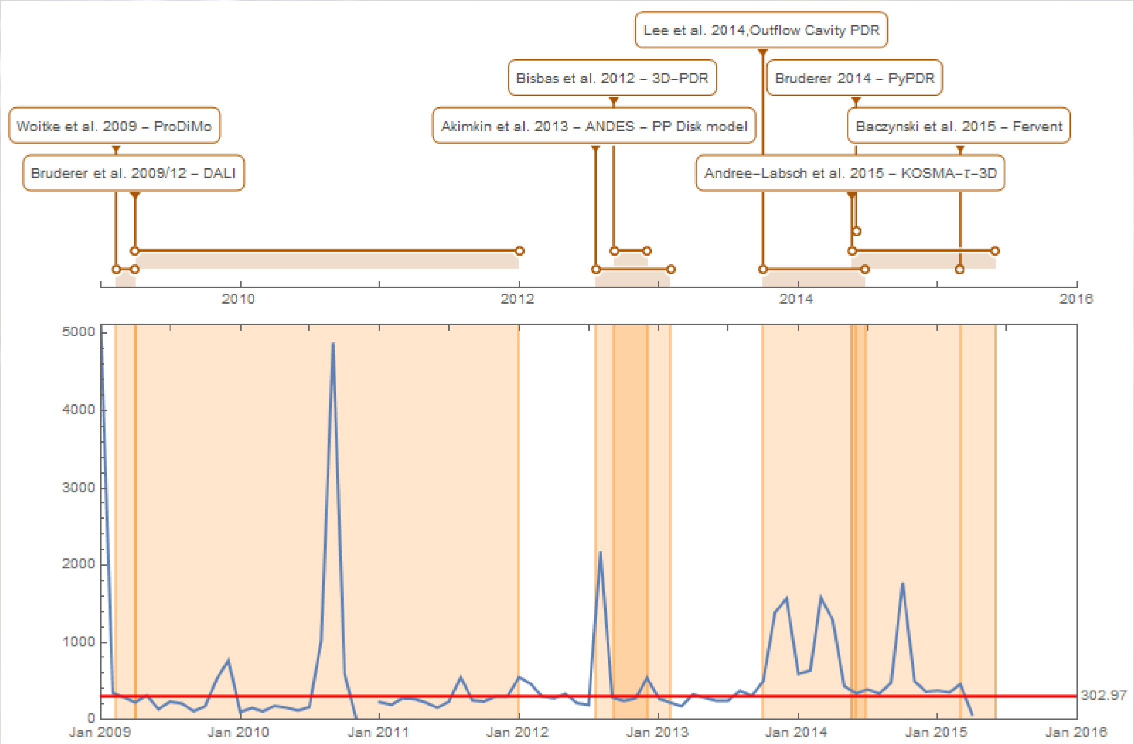
300/month

http://www.astro.uni-koeln.de/pdr-comparison/

Benchmark Data Archive

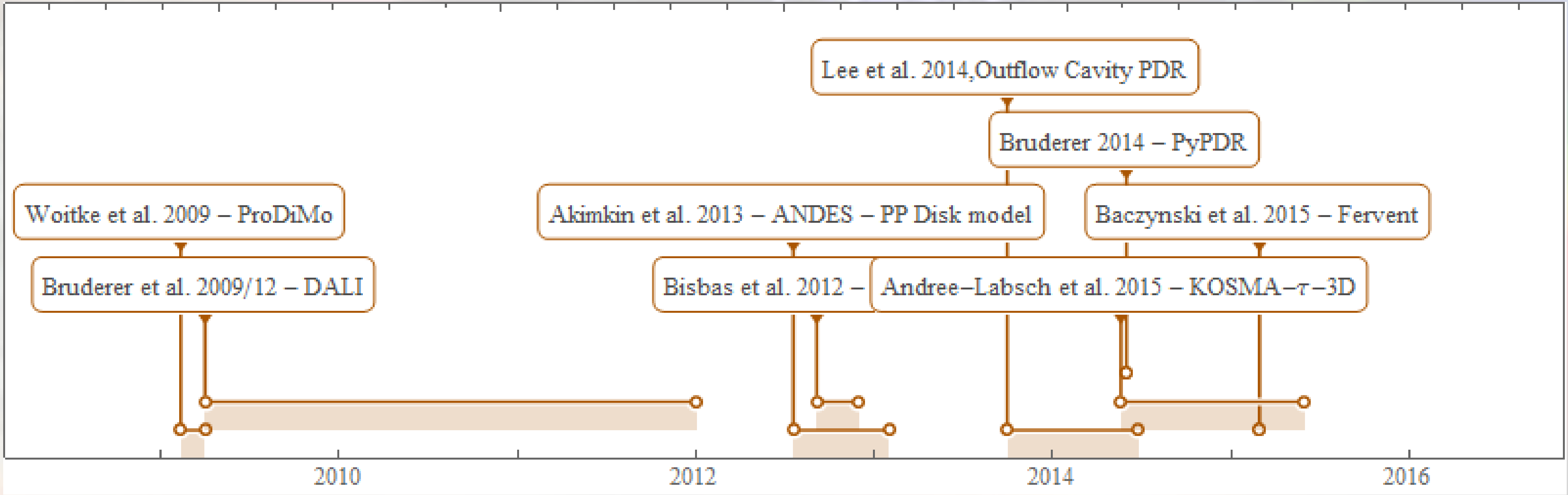
- All the results (data files, plots, documents) have been published on a website.
- Surprising archive traffic (2009-15)
- Modelers use the benchmark data to benchmark their new models against.

Mission accomplished!



http://www.astro.uni-koeln.de/pdr-comparison/

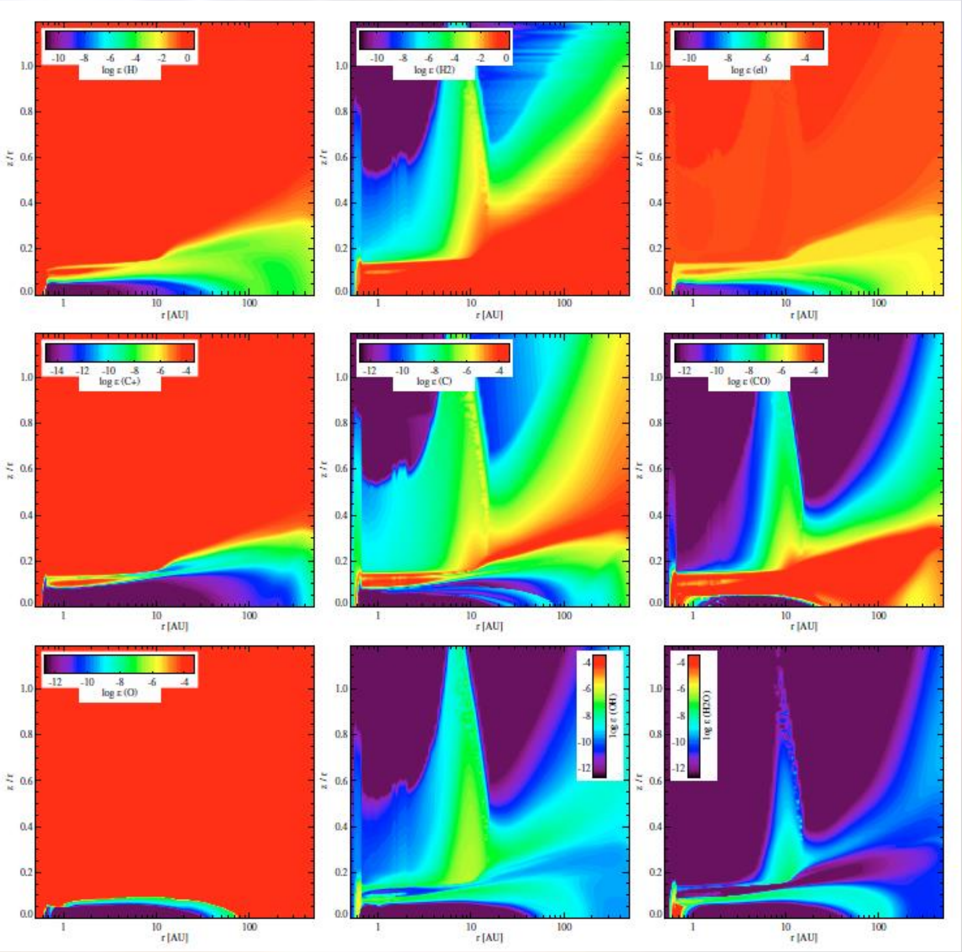
New kids on the block



Protoplanetary **Di**sk **Mo**del

Woitke, Kamp & Thi, A&A 501, 383–406 (2009)

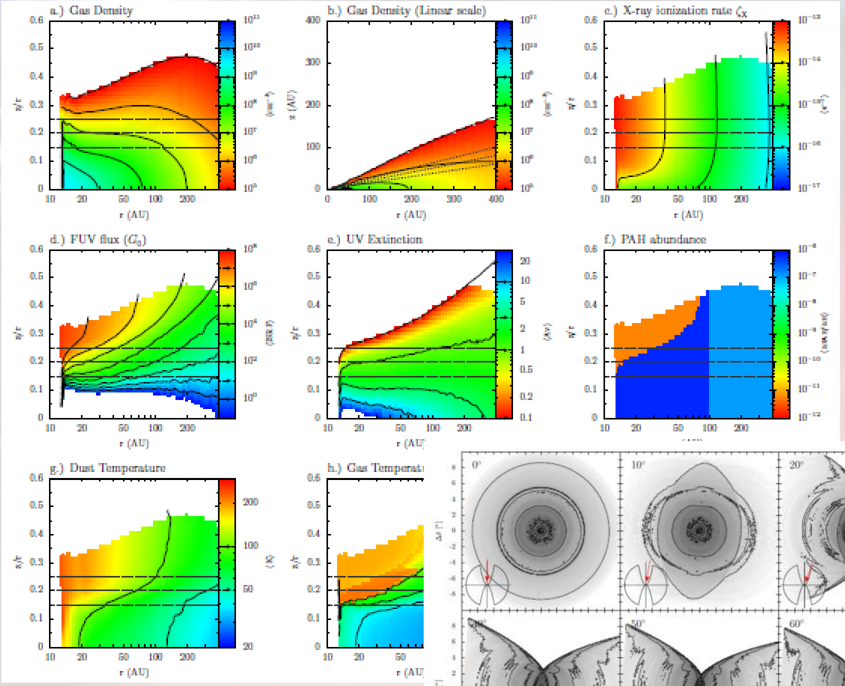
- Based on COSTAR (Kamp, Bertoldi, van Zadelhoff)
- 1+1 D model: physical, thermal and chemical structure of protoplanetary disks.
- 2D dust continuum radiative transfer,
- Gas-phase and photo-chemistry, ice formation/evaporation
- X-ray-driven chemistry and heating via H_2 ionization
- hydrostatic disk structure in axial symmetry

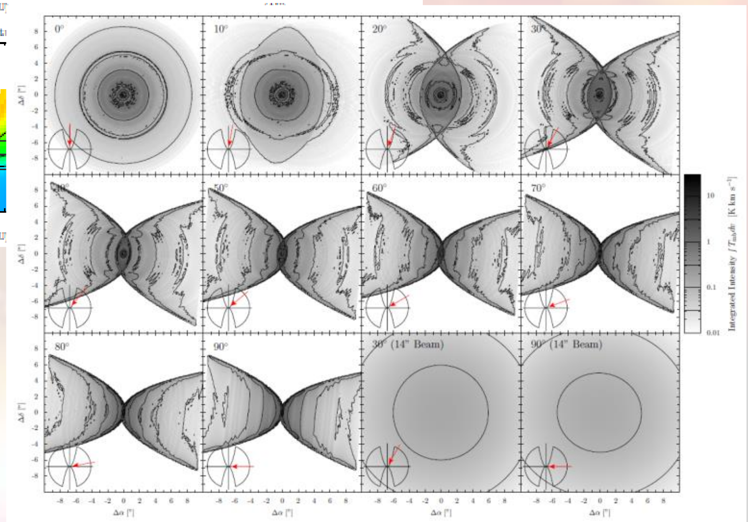


DALI

Bruderer, van Dishoeck, Doty, Herczeg, A&A 541, A91 (2012)

- Flexible geometry, pp-disks, envelopes
- Steady state & t-dependent chemistry
- gas-phase & simple surface hydrogenation
- X-ray induced chemistry
- PAH chemistry & H_2^*
- Photodissociation using shielding rates
- MC continuum RT
- ‘escape formalism’ for molecular excitation
- ray tracing for emission

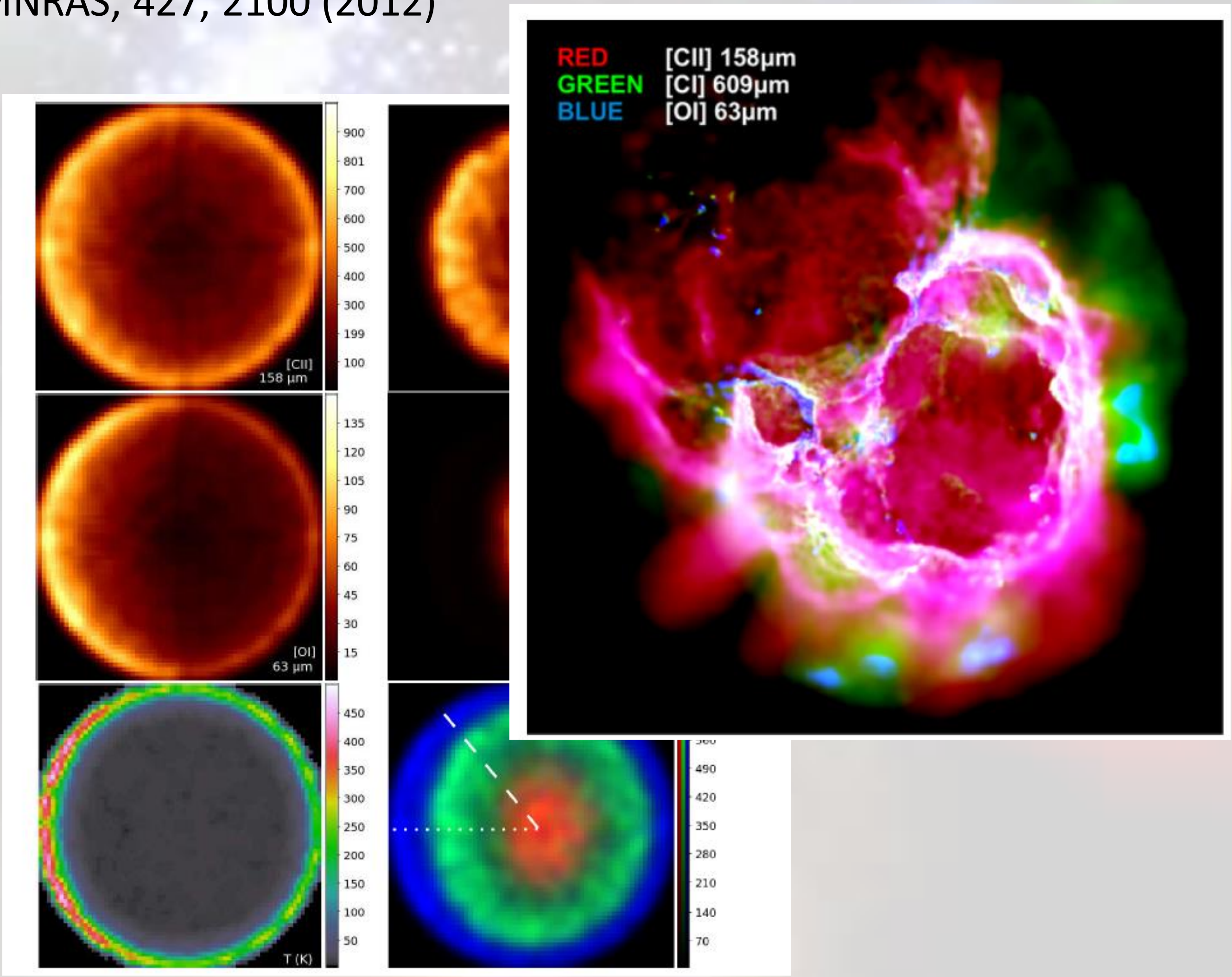




3D-PDR

Bisbas et al. MNRAS, 427, 2100 (2012)

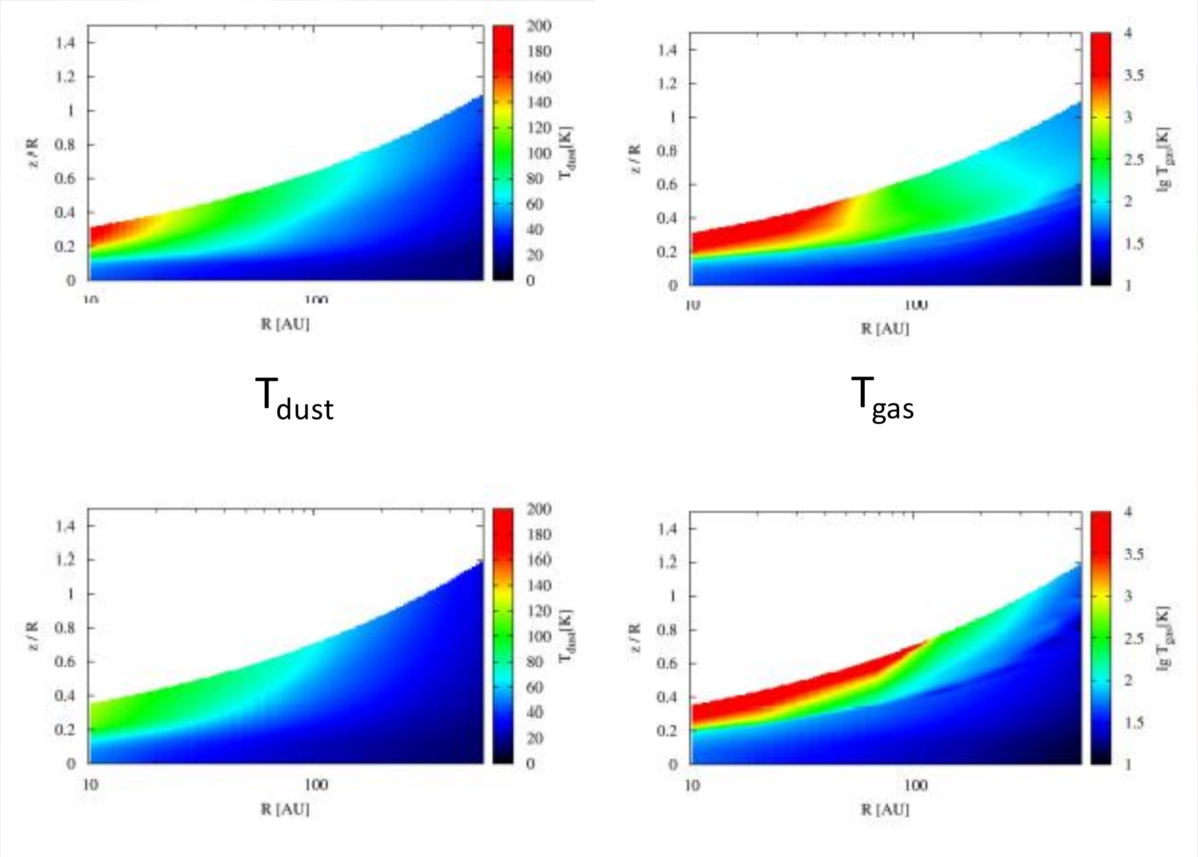
- 3D-PDR code (arbitrary geometry)
- HEALPIX-based ray tracing
- Further development of UCL_PDR
- Cooling by C^+,C,O,CO
- 2-lev approximation of H_2
- Small (33 spec.) , time dependent chemistry
- CO and H_2 PD using shielding rates



Accretio**N** disk with **D**ust **E**volution & **S**edimentation

Akimkin et al., ApJ 766:8 (24pp), (2013)

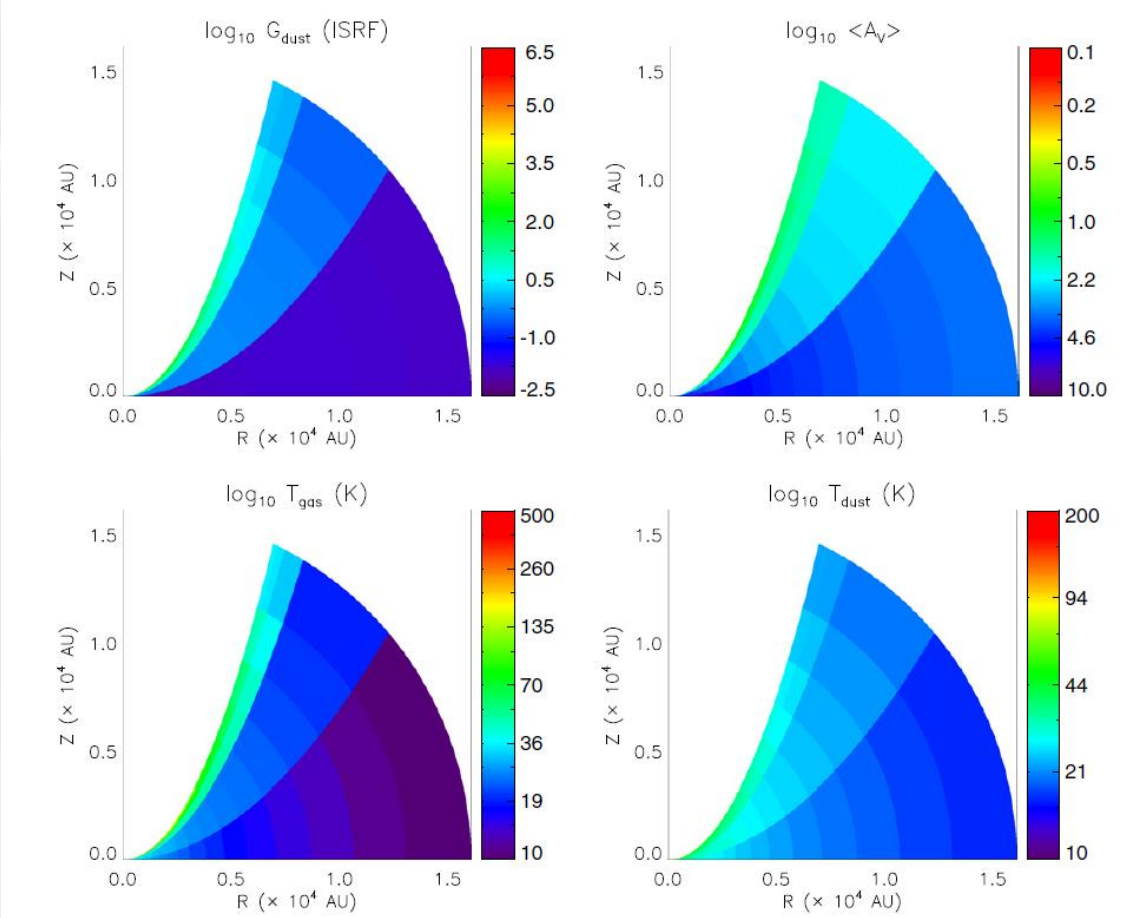
- Hydrostatic, quasi-static disk
- 1+1D freq.-dependent continuum RT
- dust growth (coagulation & fragmentation) and sedimentation
- chemical evolution using an extended gas-grain network with UV/X-ray-driven processes surface reactions
- Explicit PD rate computation
- gas thermal energy balance



Embedded protostar with outflow cavity PDR

Lee et al. , ApJSS, 213:33 (23pp), 2014

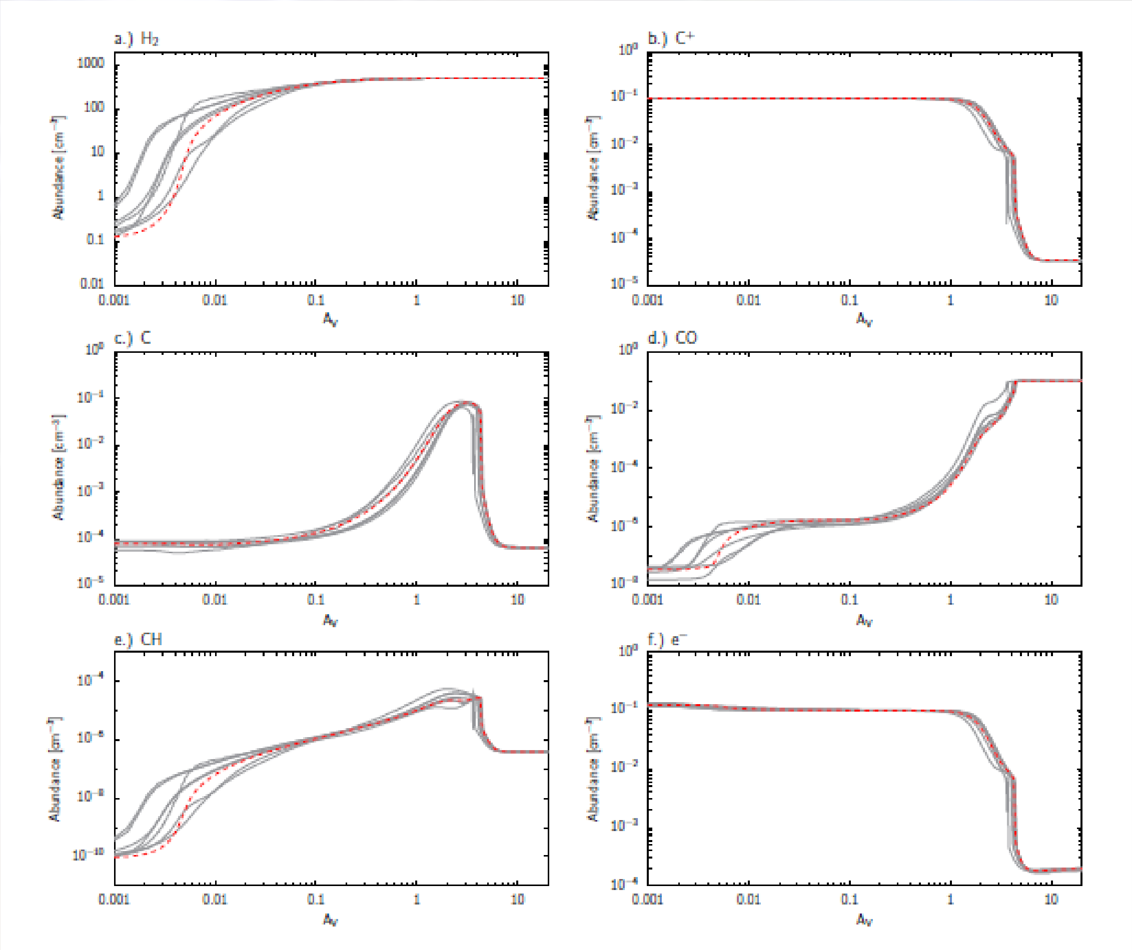
- Custom coordinates based on circular paraboloid
- dust continuum radiative code RADMC-3D $\rightarrow T_d$
- grid-based Monte Carlo RT -> FUV
- RATRAN upgrade: RIG
- Gas+dust chemistry (ALCHEMIC derivate)
- H_2 formation (C&T 2002-10)



PyPDR

Bruderer 2014: http://www.mpe.mpg.de/~simonbr/research_pypdr/index.html

- tiny/minimal PDR code written in Python
- Plane-parallel slab (semi-infinite)
- basic chemistry with about 30 molecules, time dependent
- NLTE excitation of [OI], [CII], [CI], CO, and ^{13}CO using an escape probability approach
- Major heating & cooling processes implemented

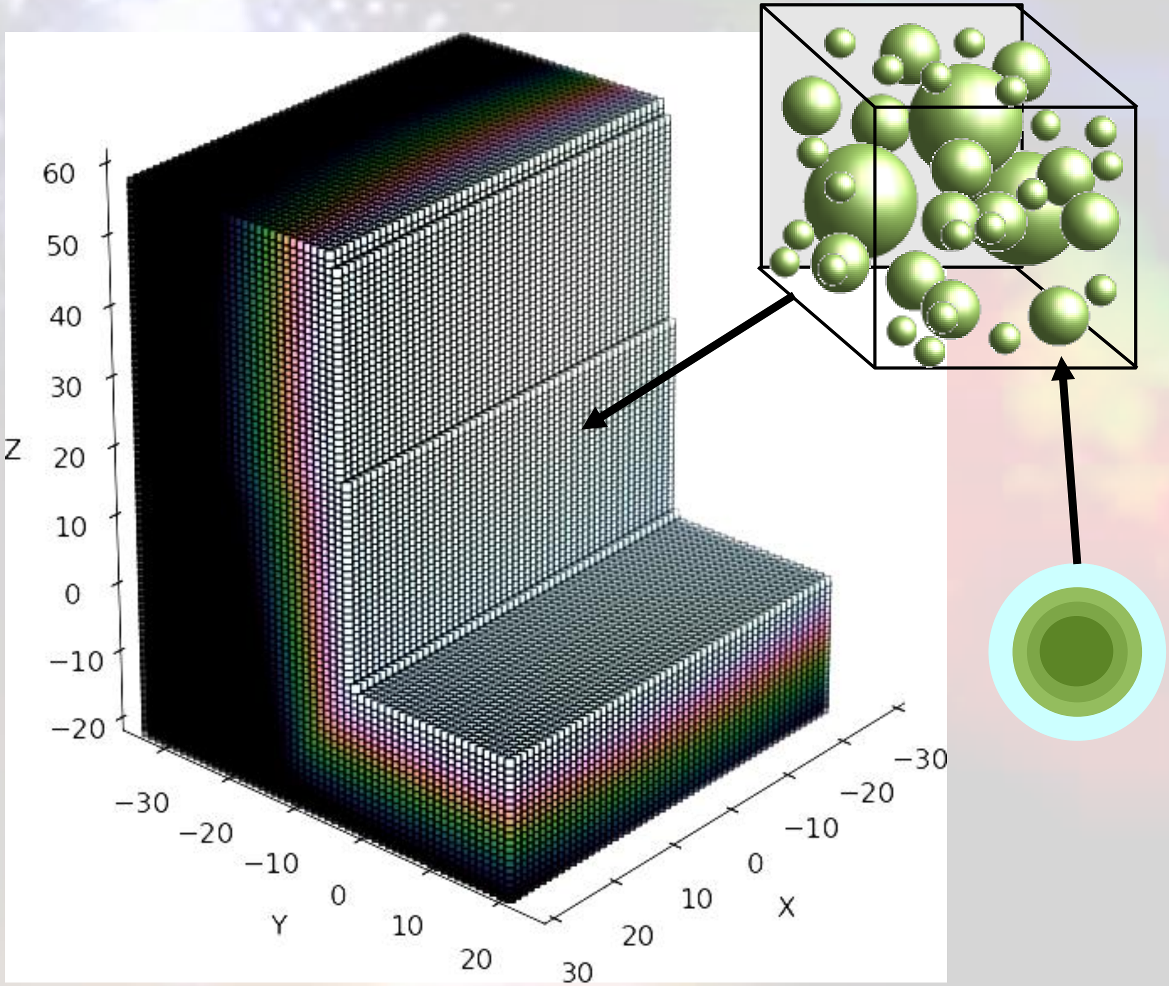


KOSMA-τ 3D

Andree-Labsch et al. , A&A, 2015, submitted

- 3D PDR with arbitrary geometry & velocity structure
- Post-processing of KOSMA clumpy PDR ensembles
- Voxel filled with fractal cloud ensembles
- Stochastic shielding and attenuation
- Ray tracing RT for FUV attenuation and line emission

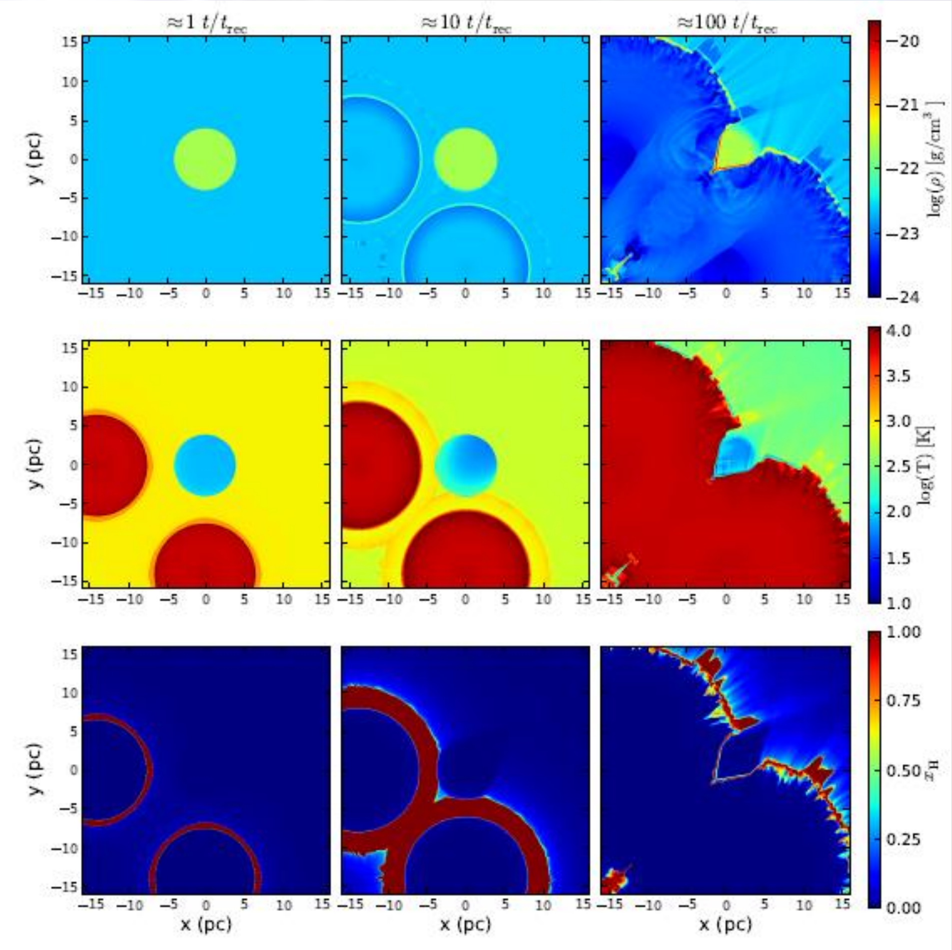
See S. Andree-Labsch's talk



Fervent

Baczynski, Glover, and Klessen. , MNRAS, 2015, submitted

- RT module for the MHD adaptive mesh refinement code FLASH 4.
- Self-consistent, time dependent evolution of energetics, chemistry and density of the ISM
- No scattering or continuum yet
- Only H ionization
- Very small chemistry (NL97 chemical network) H-H_2 transition well reproduced



Benchmark codes keep updating

Cloudy
- Upgrade of atomic & molecular structure
- Enhanced Chemistry (s.s. & t-dep., freeze-out)
- Grain physics/chemistry
- pyCloudy, Cloudy_3D

KOSMA-τ
- Clumpy PDR ensembles
- Dust upgrade & new cont. RT
- New H_2 formation (C&T 2002-10)
- Upgraded chemistry (UDfA12 + isotop., surface chemistry, s2s chemistry)
- Shielding, PD rate scaling, heating,…
- KOSMA-τ 3D

Meijerink
- XDR
- Mechanical heating
- Chemistry

HTBKW
- H_2 treatment (link to Meudon) (Kaufman et al. 2006)
- Merging with HII region (Stardust99)
- Chemistry upgrade (t-dep., surface chem.)
- Dust upgrade (PAHs, VSG,…)
- Coupling to shock-code

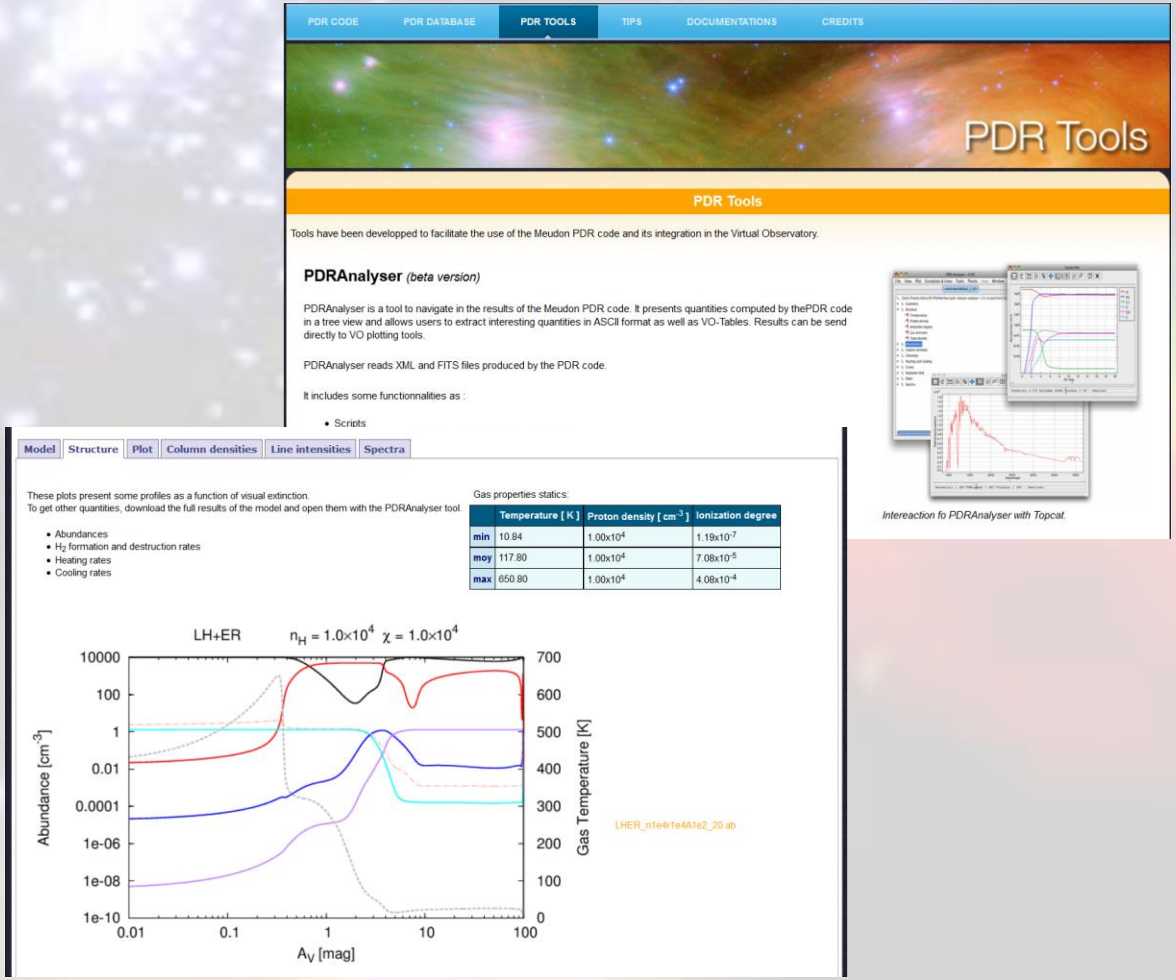
Meudon
- RT upgrade (FUV & line)
- Grain upgrade (composition, growth)
- Stochastic grain chemistry
- H_2 formation (LH & ER processes)
- Stochastic grain heating
- Chemistry upgrade (s2s chemistry,…)

Apologies for all modelling/upgrade efforts not mentioned here!

Availability of the Codes/Results

Meudon
http://pdr.obspm.fr/PDRcode.html

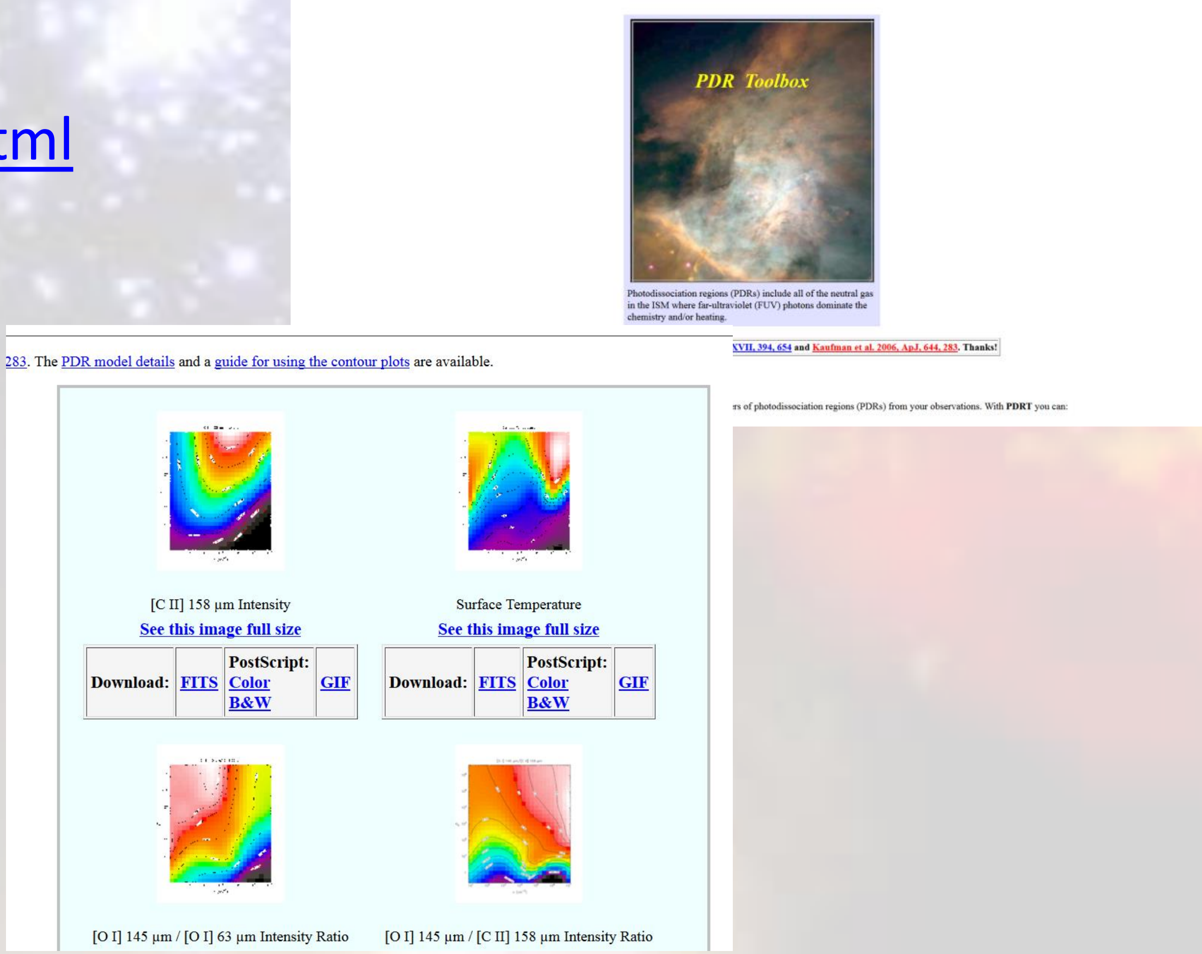
- Code freely available
- PDR Database access (online & download)
- VO integration



Availability of the Codes/Results

HTBKW
http://dustem.astro.umd.edu/pdrt/index.html

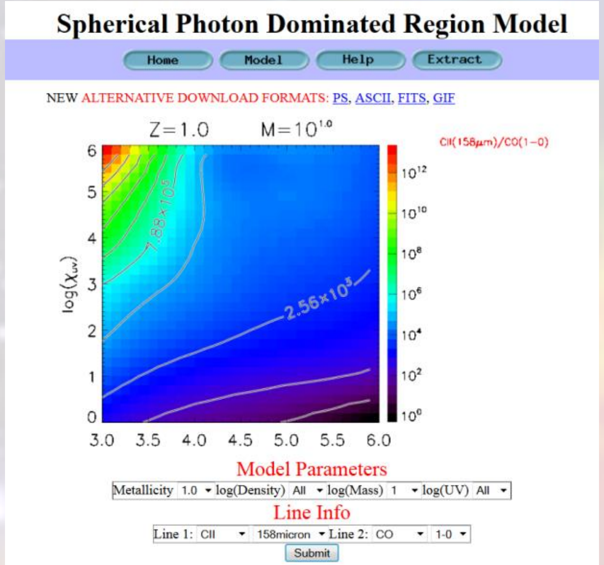
- Browse contour plots from PDR models
- Access desired model plot
- Use Line Ratio Fitting program
- IDL & Python scripting interface for PDR Line Ratio Fit



Availability of the Codes/Results

KOSMA-τ
http://hera.ph1.uni-koeln.de/~pdr/

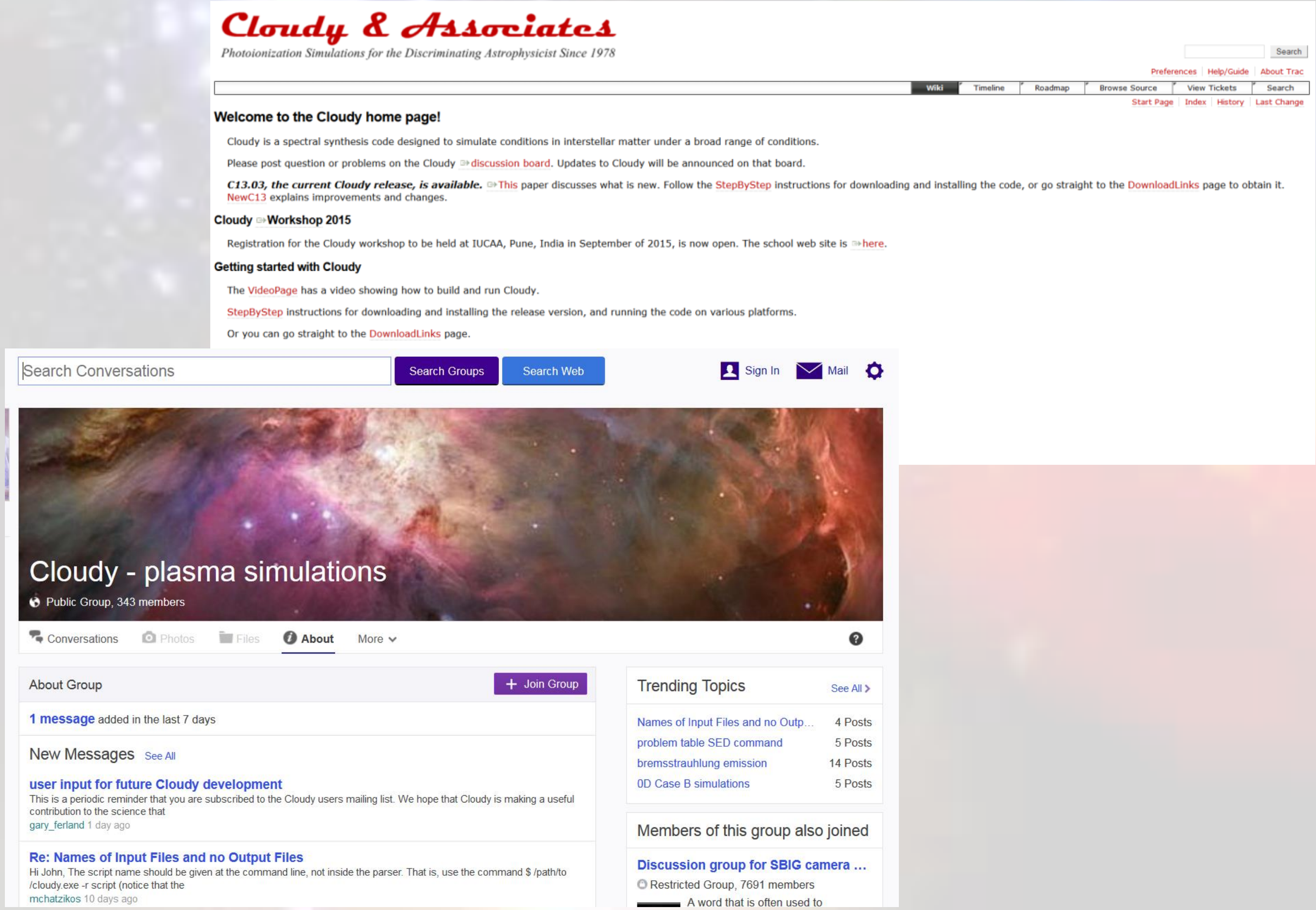
- Browse contour plots from PDR models (interface upgrade to access all results is coming)
- **Isotopic fractionation material** http://www.astro.uni-koeln.de/kosma-tau-downloads
- *Mathematica* script to insert Isotopes into UDfA
- UDfA06 chemistry file including ^{13}C and ^{18}O
- plots



Availability of the Codes/Results

Cloudy
http://www.nublado.org/

- Code freely availably
- User discussion board available



Availability of the Codes/Results

ProDiMo

http://homepage.univie.ac.at/peter.woitke/ProDiMo.html

- Code availably after registration
- Wiki page access for registered users

ProDiMo is a scientific software package in FORTRAN 90 to model protoplanetary disks including gas phase, X-ray and UV-photo-chemistry, gas heating and cooling balance, disk structure and (dust & line) radiative transfer. The following is a preview of the wiki pages for ProDiMo hosted at forge.roe.ac.uk in Edinburgh. **The links do not work (on purpose)!** To get access to the ProDiMo web-pages, the FORTRAN source code, and the IDL visualisation tools, please apply at https://forge.roe.ac.uk/ForgeRegistration.html for a new ProDiMo user account, mentioning my name.

Disclaimer

This code is available on a collaborative basis, meaning ...

- You are not permitted to pass (parts of) the code to anyone else. If another person is interested to join, please tell him/her to follow the same procedure as you have done, namely to apply at https://forge.roe.ac.uk/ForgeRegistration.html for a new ProDiMo user account.
- You have to give all developers of ProDiMo, currently Peter Woitke AND Inga Kamp AND Wing-Fai Thi co-author right, i.e. you should ask us prior to paper submission whether we want to be included as co-authors. If you want to use the X-ray module, you should also give Giambattista Aresu co-autor right.
- If you contribute significant changes to ProDiMo, you get co-author right on all papers that use these changes.
- In order to claim his/her co-author right on a paper going to be submitted, he/she needs to send his/her scientific comments on the paper on timescales of one or two weeks. Otherwise he/she looses that right for this paper.

Remember that, as you can read this wiki page, you have signed up for these conditions.

Welcome to the ProDiMo manual pages

See how to Get_Started here (Code download and compilation - **Note the top of page!**).

See how to Run_ProDiMo here.

Find some more useful Tips_and_Tricks how to run complex disk models and set parameters here.

See how to calculate gas emission lines with RATRAN here.

Check out Known_Problems with some solutions.

Description of Atomic_and_molecular_data and Dust_opacities

Current Work_In_Progress and RefereedPapers using ProDiMo

Program_structure

Availability of the Codes/Results

UCL_PDR

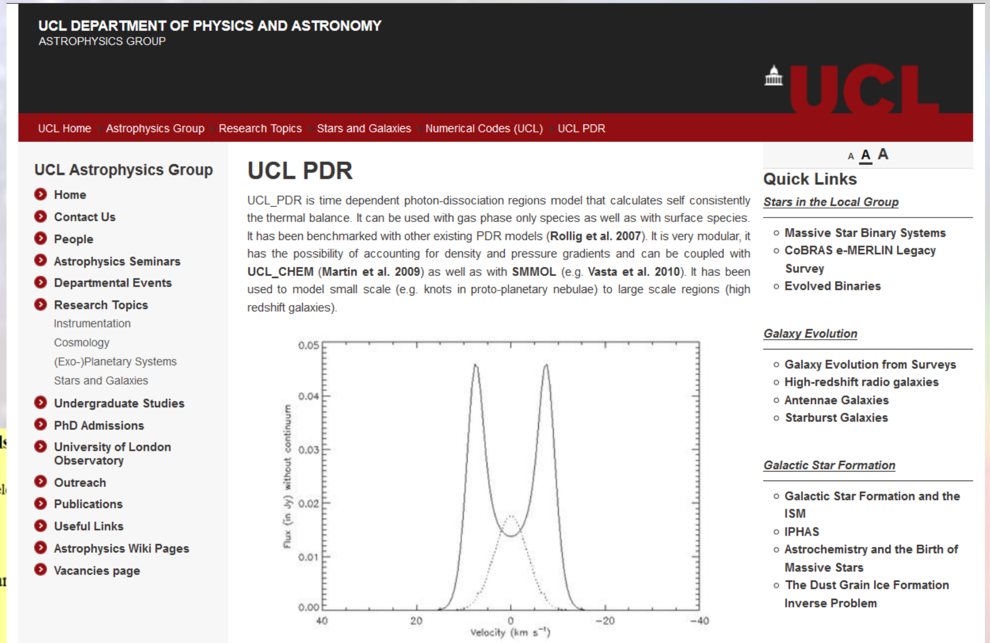
https://www.ucl.ac.uk/star/research/stars_galaxies/codes/uclpdr

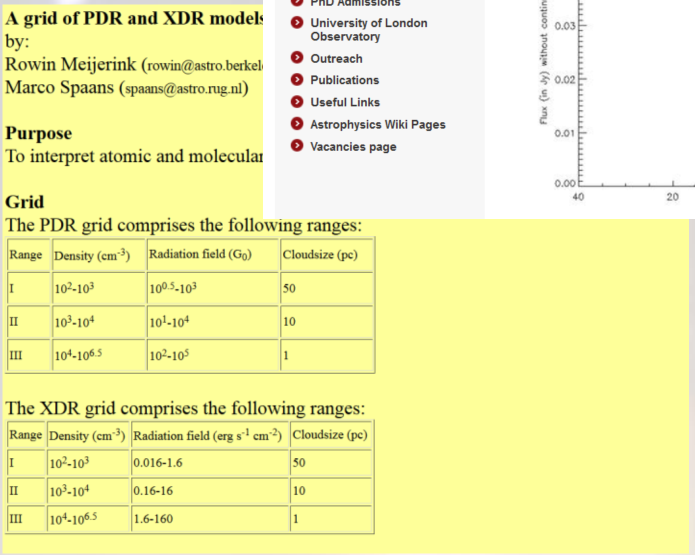
- The code is available on request

Meijerink XDR

http://home.strw.leidenuniv.nl/~meijerink/grid/

- A grid of PDR and XDR models





A grid of PDR and XDR models
by:
Rowin Meijerink (rowin@astro.berkel
Marco Spaans (spaans@astro.rug.nl)

Purpose
To interpret atomic and molecular

Grid
The PDR grid comprises the following ranges:

Range	Density (cm^{-3})	Radiation field (G_0)	Cloudsize (pc)
I	10^2-10^3	$10^{0.5}$-10^3	50
II	10^3-10^4	10^1-10^4	10
III	10^4-$10^{6.5}$	10^2-10^5	1

The XDR grid comprises the following ranges:

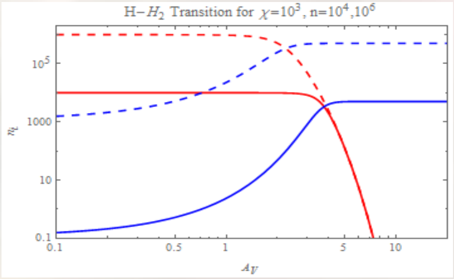
Range	Density (cm^{-3})	Radiation field (erg s^{-1} cm^{-2})	Cloudsize (pc)
I	10^2-10^3	0.016-1.6	50
II	10^3-10^4	0.16-16	10
III	10^4-$10^{6.5}$	1.6-160	1

Model access

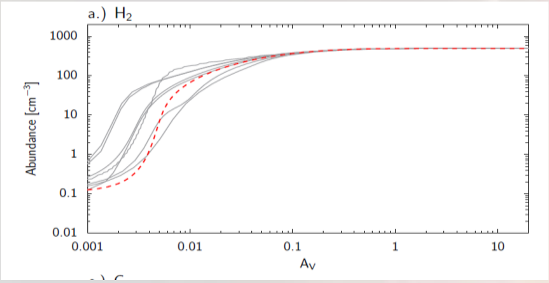
- The conclusion from Benchmark paper still valid:
  ".. observers should not take the PDR results too literally to constrain […] physical parameters like density and radiation field in the region they observe."
- Influence of PDR model input parameters on results difficult to predict – number of crucial model parameters growing
- Fitting model computations to observations requires experience.
- Detailed PDR modelling remains difficult for non-experts
- Easier to collaborate with modeler than to quickly run some PDR models yourself.
- But, …

Model access

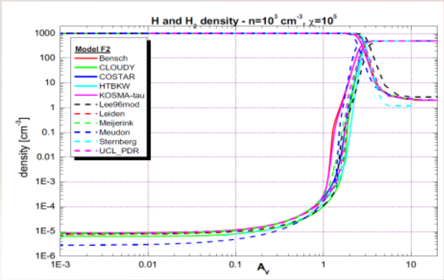
- Simple analysis based on published contour plots/data became much easier thanks to the many ‘public’ outreach efforts.
- Toy models, such as PyPDR span a bridge between simple analytic calculations and full complexity models.



analytic



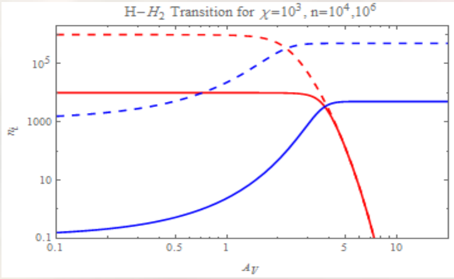
PyPDR



full models

Model access

- Simple analysis based on published contour plots/data became much easier thanks to the many ‘public’ outreach efforts.
- Toy models, such as PyPDR span a bridge between simple analytic calculations and full complexity models.
- If you really want to run models yourself, you have now a number models to choose! Good user-support.



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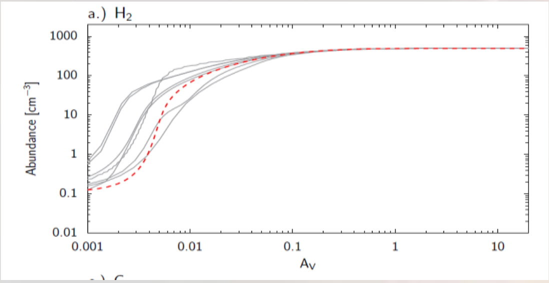
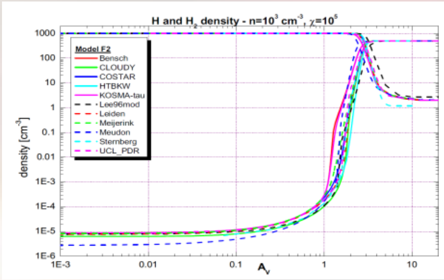


toy



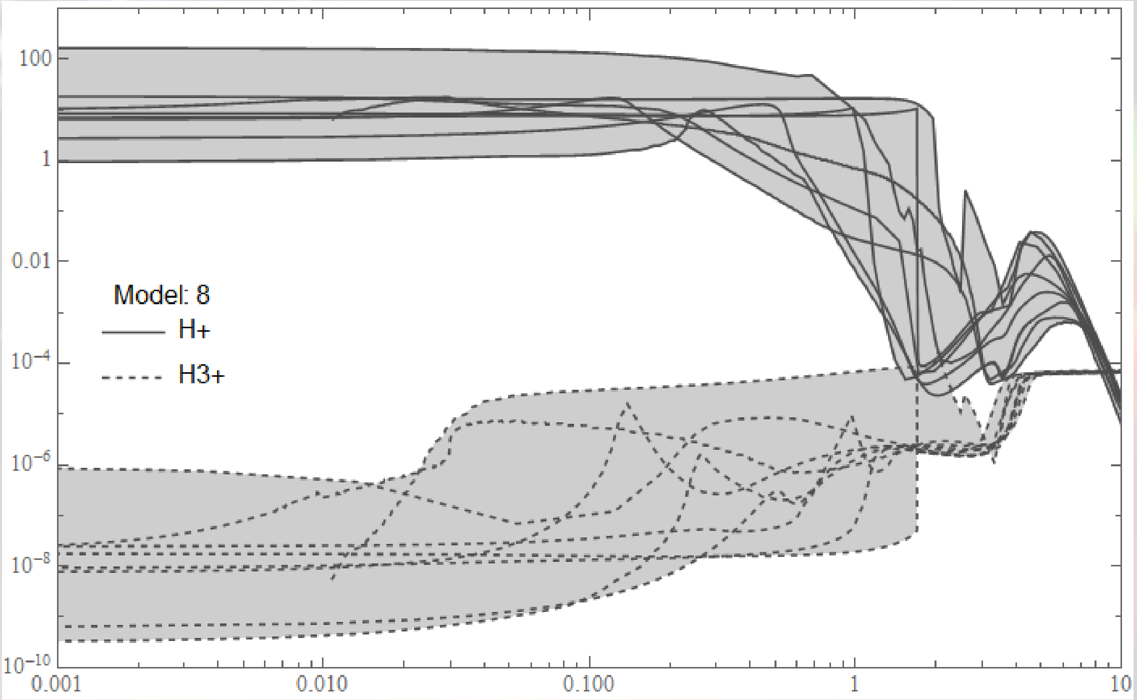
full models

Benchmark V.2?

So much left to do:

- 2007 benchmark left many open issues

Status after the benchmark 2007



$n=10^{5.5}$ cm^{-3}, $\chi=10^5$

Benchmark V.2?

So much left to do:

- 2007 benchmark left many open issues
- Discuss numerics
- New physics/chemistry
- Follow up on CO excitation and C+ workshops
- Benchmark against real world problems
- Exchange of experience, include the new models
- PDR modelling roadmap

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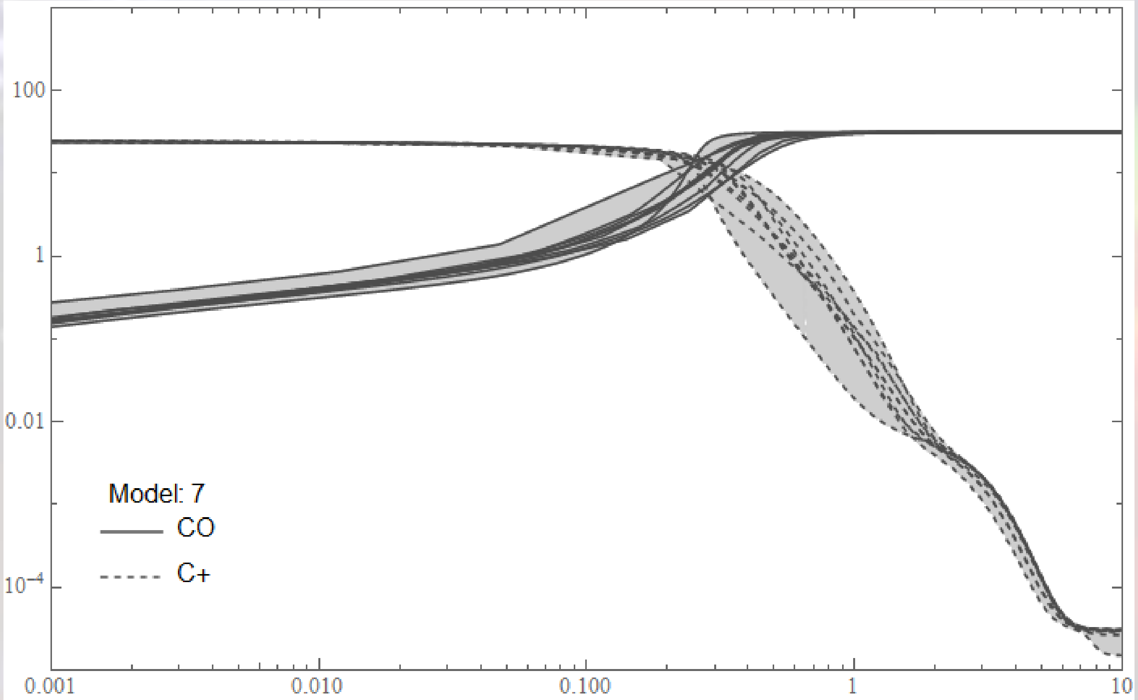

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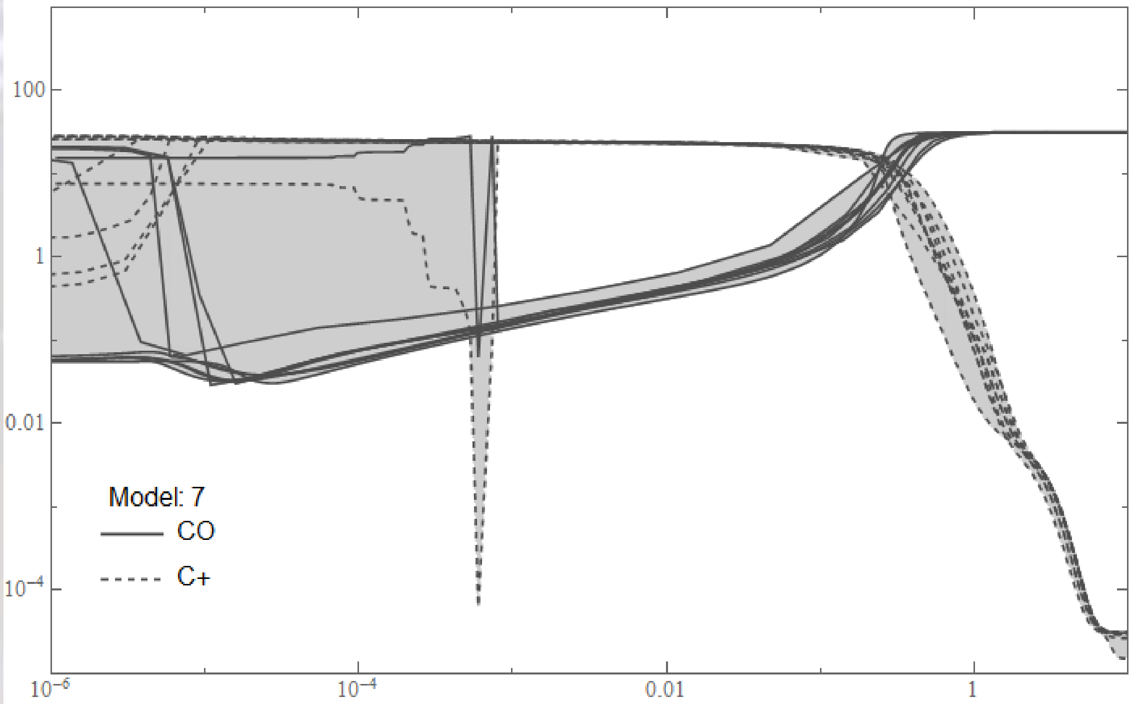

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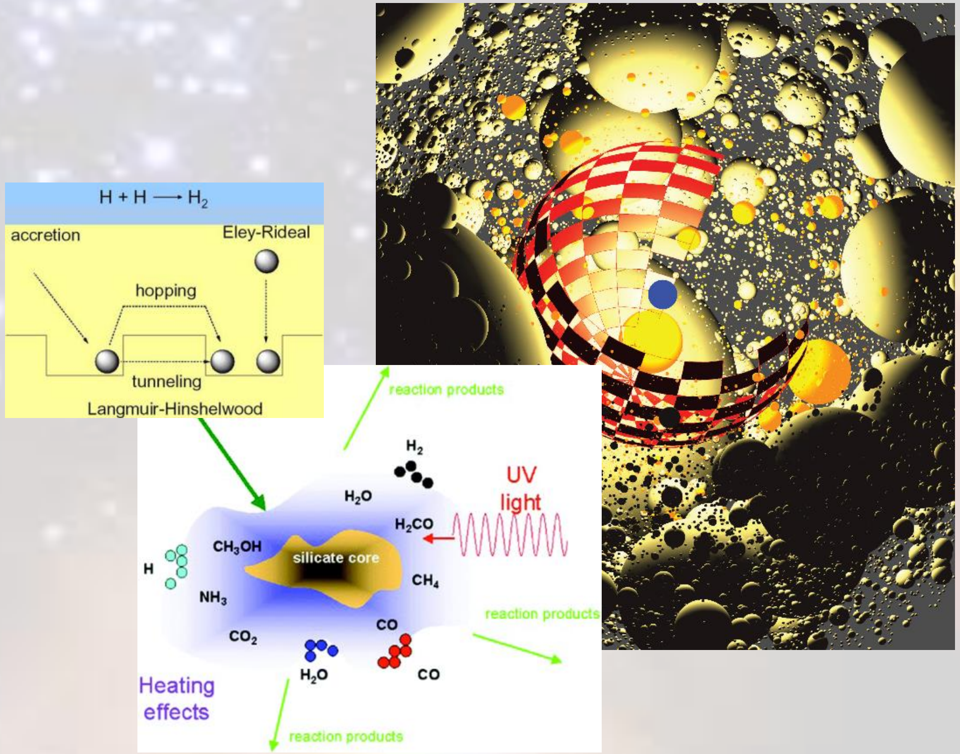

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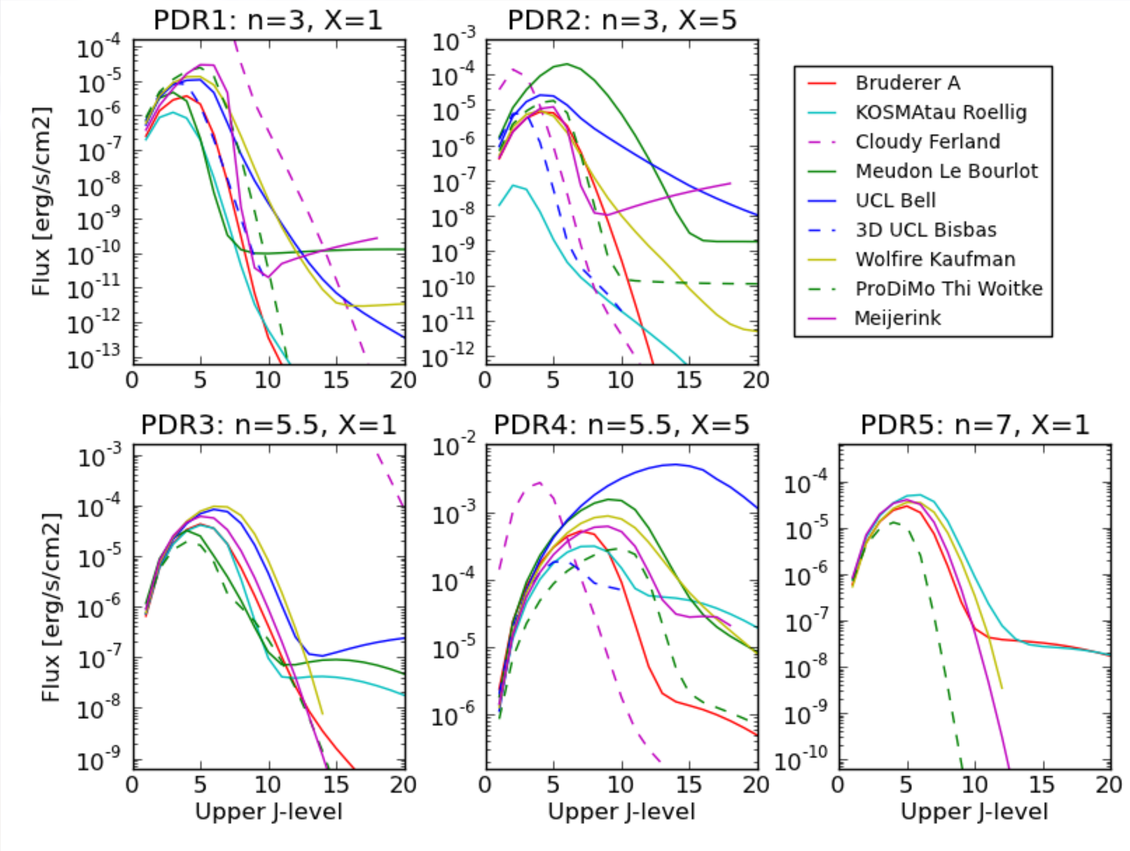

Benchmark V.2!

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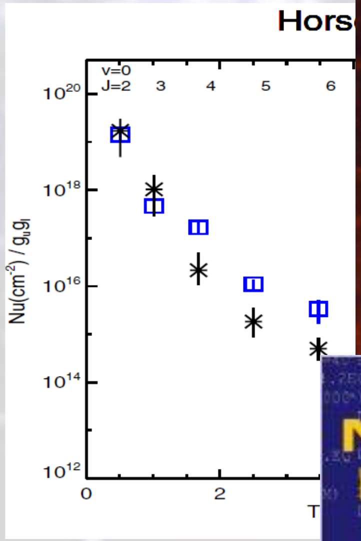
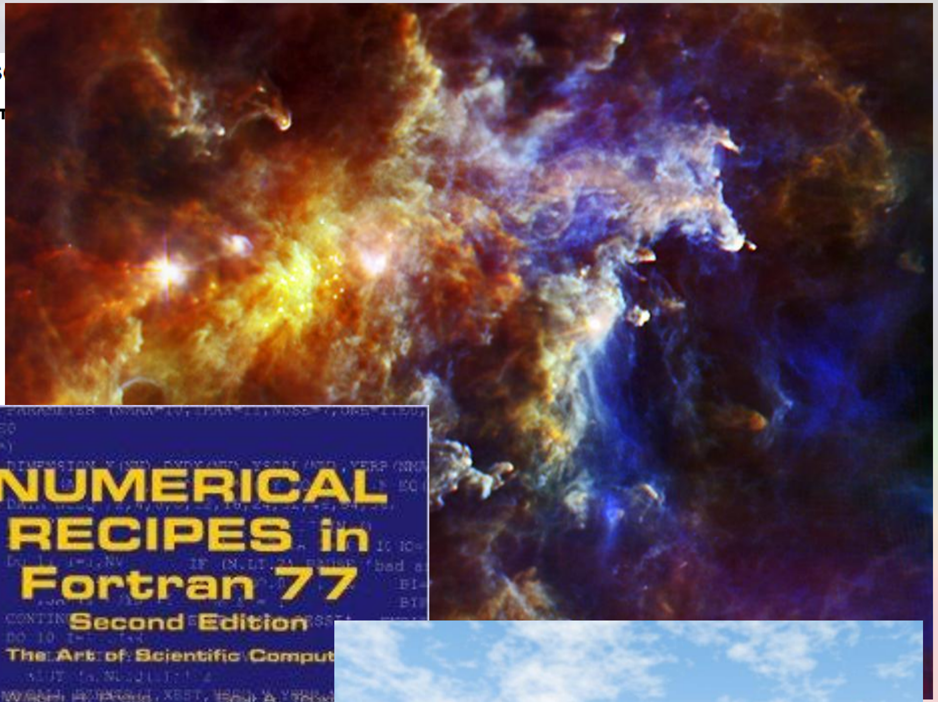
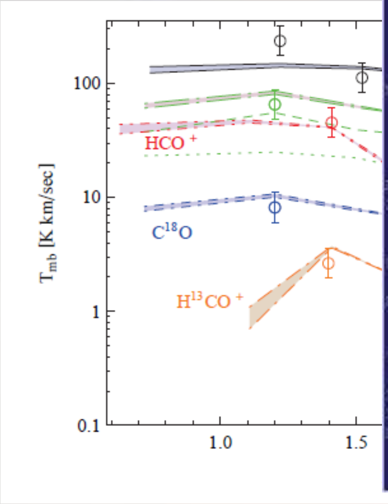
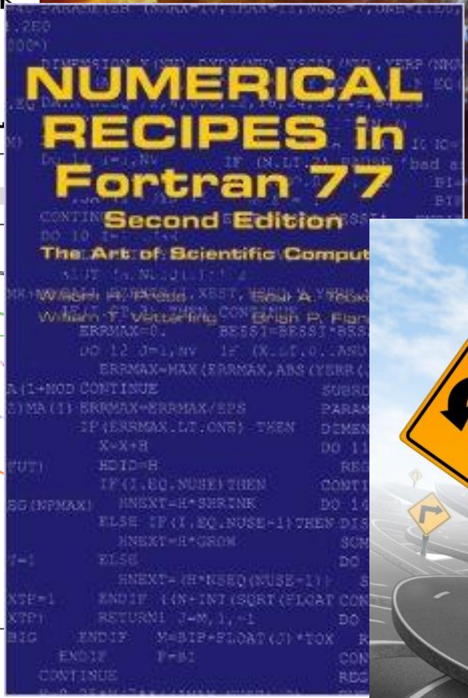
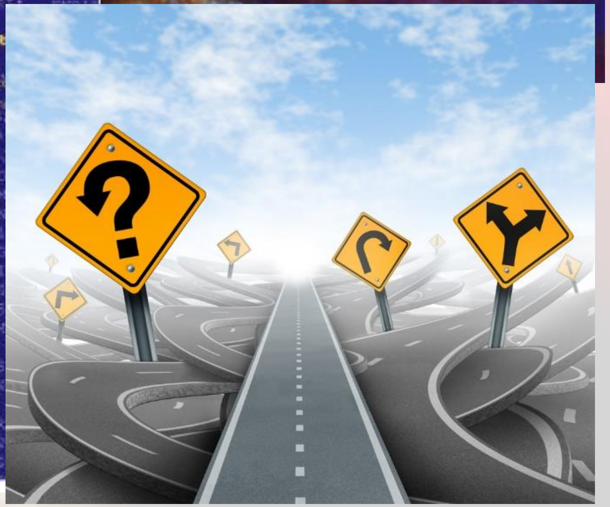






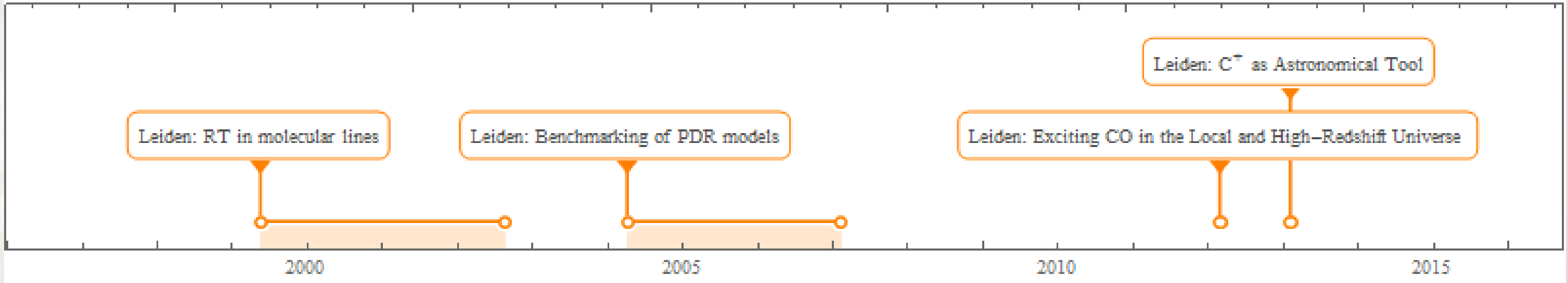




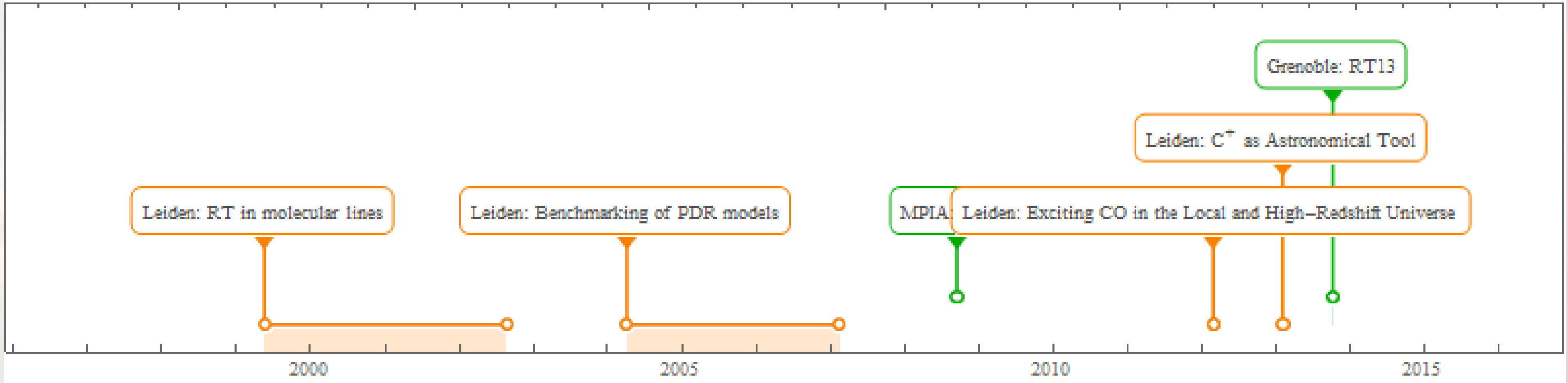
Thank you for the invitation!

Thank you for your attention!

History of Benchmarks



History of Benchmarks



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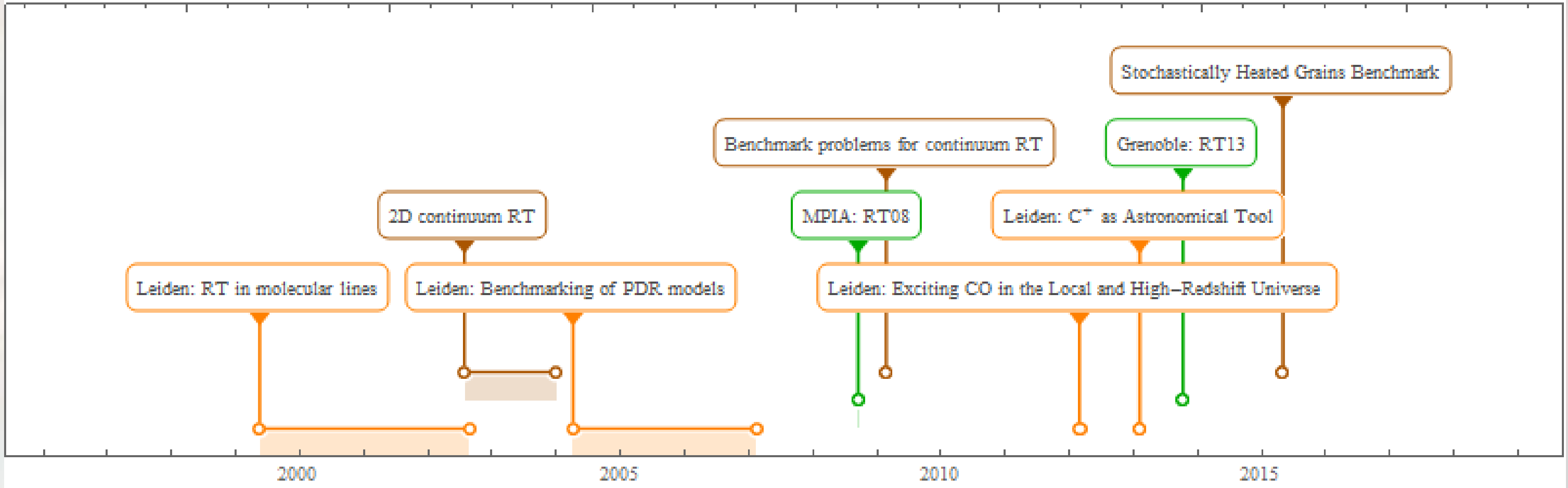

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