



The Xgear Project

A New Era for Astrochemical Modelling?

Xgear started life as the desire for a wrapper programme written in C that could collect parameters for running astrochemical models using derivatives of the HMC (hot molecular core) NEWGEAR Fortran code initially developed by Tom Millar and collaborators in the early 1980s, and as further developed by Helen Roberts from 1998. The HMC code utilises DLSODE: the Double precision Livermore Solver for Ordinary Differential Equations (Hindmarsh 1983; Radhakrishnan and Hindmarsh 1993).

The initial goal of the Xgear Project is to enable astrochemical models to be run easily and consistently, with full user control over the many parameters that must be specified to run a model. These parameters can be defined on the command line and/or in a plain text configuration file. However, in the longer term the building a PHP-MySQL front-end to Xgear is envisaged, so that models can also be setup and run using a client web interface to a (remote) Xgear application server or cluster. The results from running sets of models covering various parts of parameter space could then be stored in a database for subsequent querying. Other enhancements could include alternative model engines to the variants of HMC and the inclusion of additional processes such as gas-grain interactions. Chemical reaction rates can be taken from UFA 2006: the new UMIST database for astrochemistry (Woodall, Agundez, Markwick and Millar 2006), which replaced Rate99: The UMIST database for astrochemistry (Le Teuff, Millar and Markwick 2000), or other reaction networks. Initially, the code for Xgear will be made publicly available under the terms of the GNU General Public License. The code is expected to compile successfully under Linux, Unix and OS X, for both 32- and 64-bit platforms. Please see www.xgear.eu for the current status of the Xgear project.

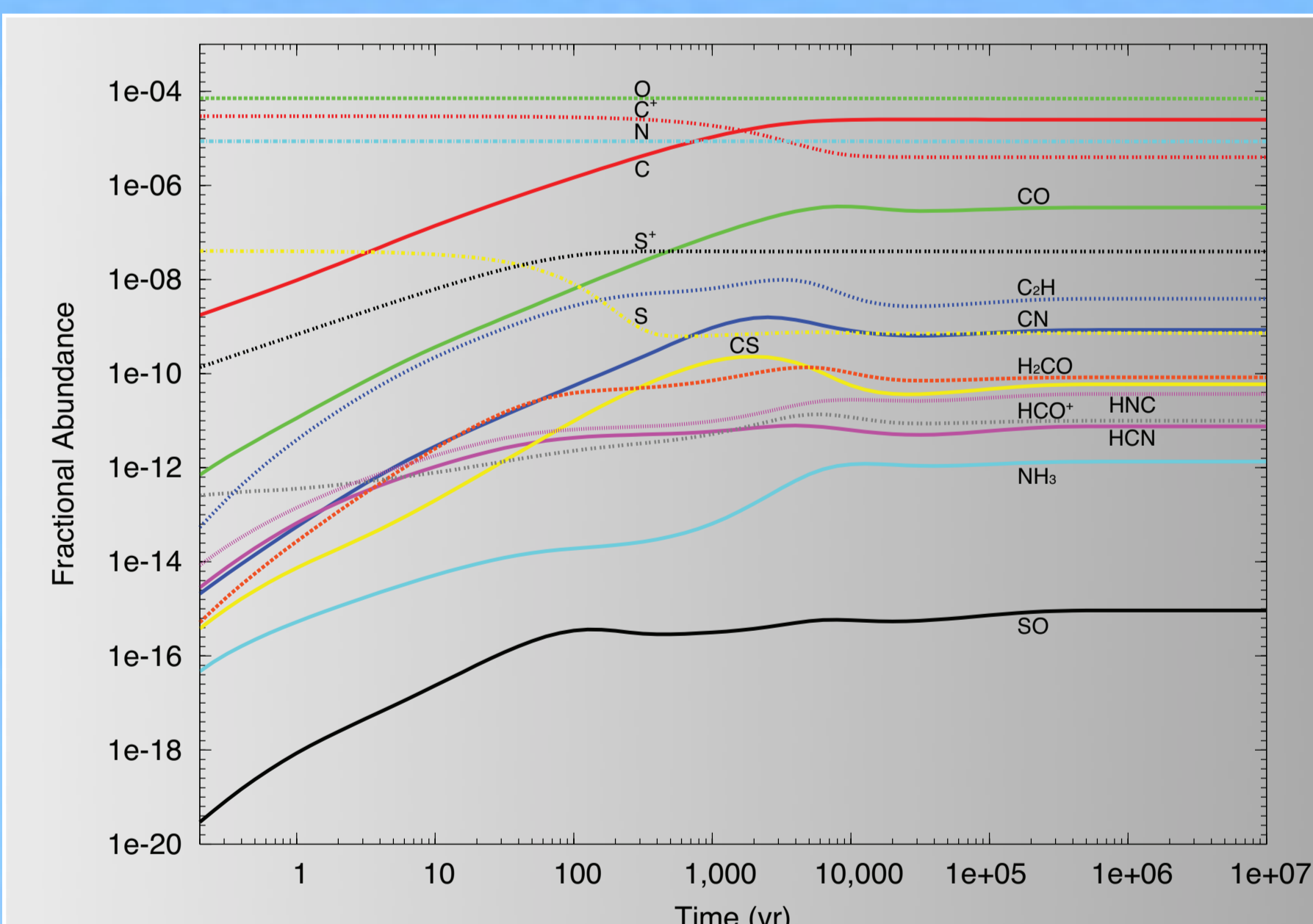


Fig. 1: Example output data showing fractional abundances varying over time for a model where $A_V = 3$ mag, cosmic ray ionisation = $20\times$, UV field = $40\times$ and initial abundances = $0.2\times$ local ISM values (from Ruffle et al. 2007).

The Genesis of HMC

The basic approach to time-dependent chemical modelling of interstellar clouds at UMIST was initiated by Graeme Watt in 1983. He used the reaction set of Prasad and Huntress (1980, 1982) and the GEAR ordinary differential equation (ODE) solver of Hindmarsh (1974) to calculate what later became called 'pseudo-time-dependent models', one-point models in which the physical conditions are fixed and the chemistry evolves with time. Tom Millar used a modified version of this code to work on circumstellar envelopes (CSEs) with Lida Nejad around the same time and also did some work with Lida on dark cloud chemistry. Lida wrote the original DELOAD code during this period, which reads a species and rate file and generates another Fortran program to calculate the rate of each reaction and the rate of change of number density of each species.

The first chemical models for a hot molecular core (HMC) source were published by Brown, Charnley and Millar in 1988. This was a comprehensive model in that it followed a collapse phase with accretion, the warm-up and desorption of ice species and the subsequent evolution of the hot gas. However there was no fundamental change to the HMC code at this point - it was still one-point in nature - although

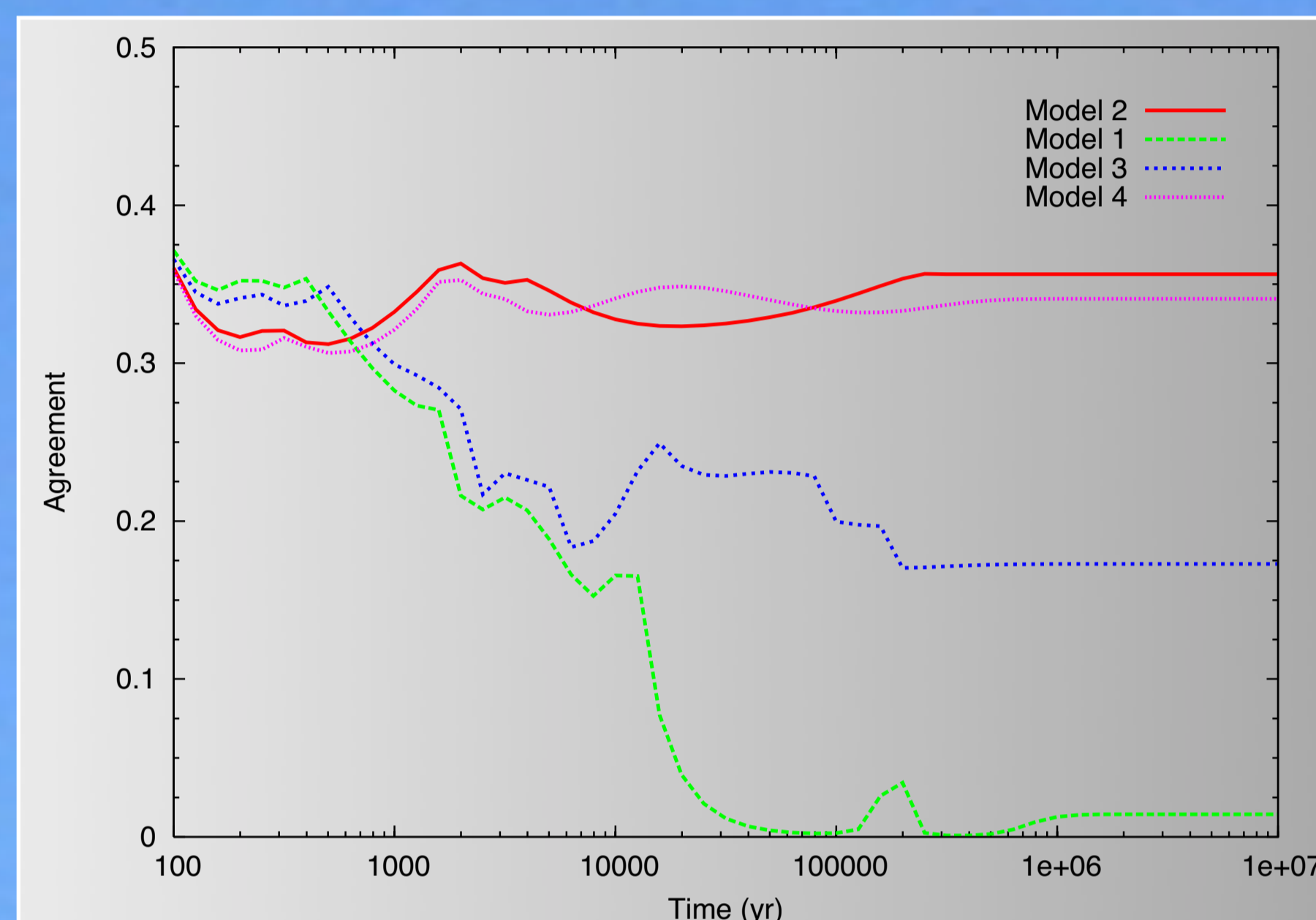


Fig. 2: Example of varying agreement factor over time when observations are compared with models where A_V (mag) and cosmic ray ionisation rates differ, but other parameters are held at constant values (from Ruffle et al. 2007).

the initial conditions and chemical reactions were different. Subsequently, deuterium chemistry was included in the HMC model by Brown and Millar (1989).

During 1991-1995, Steve Charnley and Tom Millar in three papers, with Herbst and Tielens, developed a chemical description of complex organics from simple ice molecules. After this Steve Rodgers (1998) adapted and updated, in terms of the deuterium chemistry, the previous HMC model. By this time the ODE solver NEWGEAR (Hindmarsh 1983) was being used in place of the original GEAR integrator. The next development of the HMC code was by Tom Millar due to a collaboration with Macdonald and Habing at Kent. They were doing a spectral line survey of the HMC G34.3 and Tom developed a multi-point model of the source, with three different physical components and 22 radial points to describe these. Also, the chemistry was more complex. Much of the work during the 1990s was aimed at extending the chemistry and finding quicker more efficient integrators, all based on the original GEAR approach.

Rate99 and Deuterium Chemistry

Helen Roberts then arrived on the scene and substantially developed and updated the HMC code. In 1998 she added Sulphur chemistry to the reaction network (Hatchell, Roberts and Millar 1999) and during 1999-2001 she added doubly deuterated species to the reaction network, as well as adding accretion onto grains (Roberts and Millar 2000). During 2001-2004 Helen updated the reaction network to Rate99: The UMIST database for astrochemistry (Le Teuff, Millar and Markwick 2000), wrote new programmes to generate "complete" deuterium chemistry (doing the same for the Ohio State University chemical network and comparing results), and added grain surface chemistry and thermal desorption and (optional) cosmic ray desorption (Roberts, Herbst and Millar 2003, 2004). Between 2005-2009 HMC was moved to the double precision version of NEWGEAR, the reaction network was updated to be based on UFA 2006: the new UMIST database for astrochemistry (Woodall, Agundez, Markwick and Millar 2006), the ODEs were changed to solve for fractional abundances rather than concentrations (so that density could vary over time), and other non-thermal desorption mechanisms were added (Roberts and Millar 2007).

HMC and Circumstellar Envelopes

The core engine of the chemical models of Millar and collaborators, that is, the solution of mathematically-stiff ODEs to obtain molecular abundances, could be adapted for differing physical situations. As mentioned above, in the late 1980s, Nejad and Millar (1987, 1988) produced a model which could be applied to the study of the CSEs around asymptotic giant branch (AGB) stars. Further developments to the chemistry resulted in complex models which contained anions and molecules with up to 23 carbon atoms (Millar and Herbst 1994; Millar, Herbst and Bettens 2000). In 2000, the discovery of benzene in the protoplanetary nebula CRL618 (Herpin and Cernicharo 2000) prompted Paul

Woods to take the HMC code in a different direction, with the development of an appropriate CSE model (Woods et al. 2002), an adaptation of earlier versions of the HMC code. The assumption of a constant mass-loss rate, which is more appropriate for an AGB star, could not safely be assumed, and thus a time-dependent model of a circumstellar torus was created which successfully produced the observed abundance of benzene in CRL618. This model incorporated the cessation of mass-loss at the end of the AGB phase, and the ensuing slow expansion of a high-density torus. In a revision to the model to account for the effect of the rapidly heating star, a simulated X-ray chemistry was also introduced (Woods et al. 2003). Photochemistry is particularly important in the post-AGB phase, and in general molecules can survive in well-shielded regions of ~ 10 magnitudes of extinction. In environments where such high densities are not available, i.e. stars with lower mass-loss rates, molecules are destroyed rapidly (Woods et al. 2005).

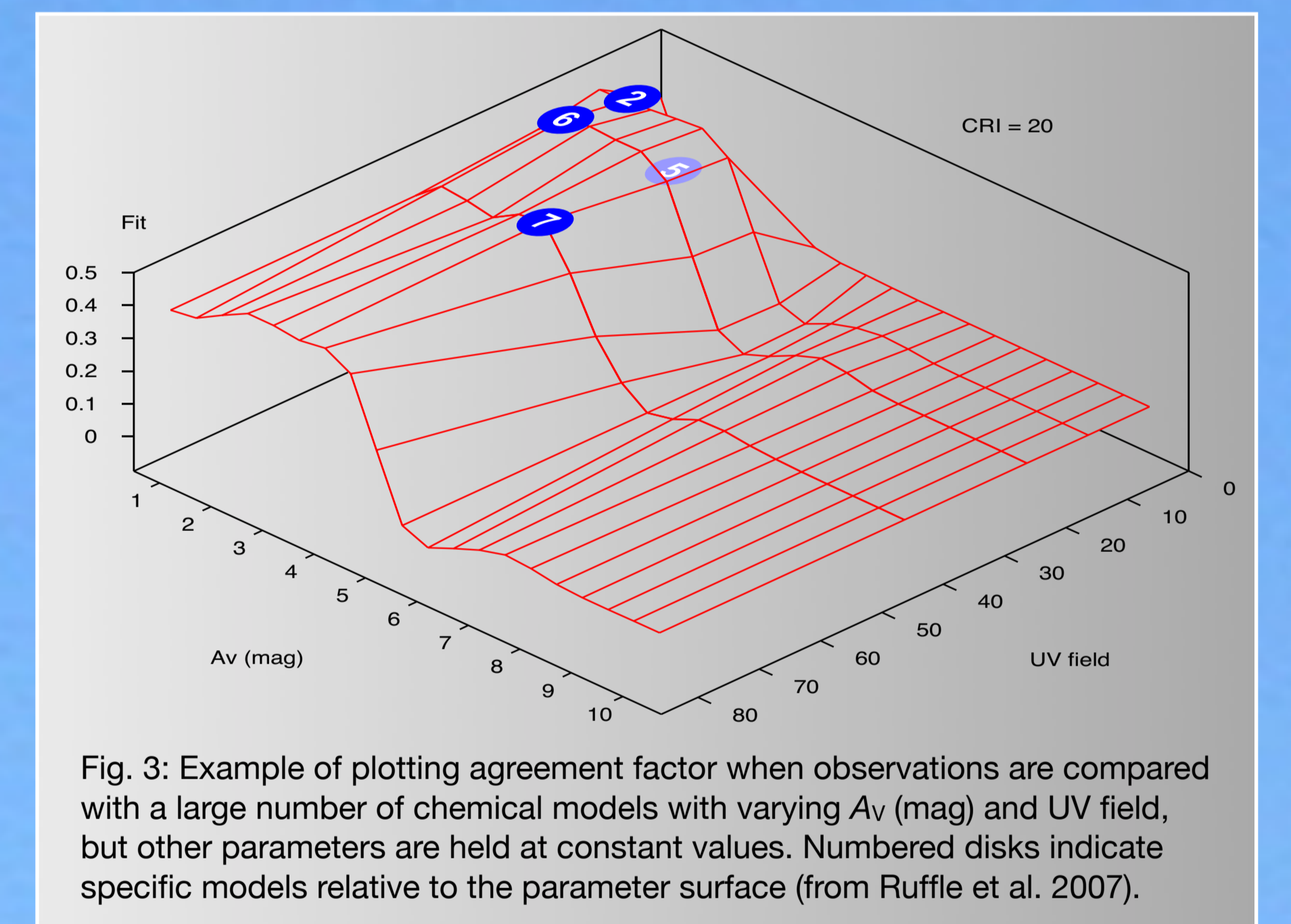


Fig. 3: Example of plotting agreement factor when observations are compared with a large number of chemical models with varying A_V (mag) and UV field, but other parameters are held at constant values. Numbered disks indicate specific models relative to the parameter surface (from Ruffle et al. 2007).

Leiden Benchmarking Workshop

In 2002 Tom Millar organised a workshop in Leiden to compare various (~ 10) time-dependent codes from different groups. Each group ran their model with the same set of initial conditions and then compared results. The codes were not necessarily the same - for example they could differ in the elements they contained, or the reaction sets they used, and the rate coefficients they used, as well as the ODE solver. The workshop was used not to make everyone's models identical but to make sure that the differences could be explained and ensure that they were not due to errors.

```
Source name:      THC-1_north
Species file:    ratefiles/specs.dat
Rate file:      ratefiles/rates.dat
Temperature:    20 K (1 values)
Density n(H2):  10000 cm-3 (1 values)
IA factor:      1.0 5.0 (2 values)
CRI factor:     1.0 10.0 20.0 (3 values)
UV factor:      1.0 20.0 40.0 (3 values)
Extinction (Av): 1.0 2.0 3.0 mag (3 values)
Timescales:    1.0e+07 yr
Gas to dust ratio: 100
Dust density ratio: 3.0
Grain sites density: 7.9e+14 cm-2
Grain radius:   1.0e-05 cm
CRI rate:      1.0e-17 s-1
UV field at 1400 A: 5.0e-17 erg cm-3 A-1
Models to run:  54 (max 100)

Loading species file: ratefiles/specs.dat
Conserved species: 3
Other species:   340
Loading rates file: ratefiles/rates.dat
Number of reactions: 10591
```

Fig. 4: Sample output from Xgear showing extent of parameter space.

Future Developments

The Xgear project - a new era for astrochemical modelling? Well, that might be a little overstated, but coordinating future development of the various versions of the HMC code may well be worth while. A version control system such as CVS would enable individuals to record the history of their source files as they check them into the Xgear repository. In cases where several individuals or groups want to each maintain their own version of HMC, others can import a chosen version and then merge that with codes that they are working on, subsequently checking their new codes into the repository. If you feel that this is worth pursuing, please contact any of the authors of this poster or info@xgear.eu.