

ASIS v1.0: an adaptative solver for the simulation of atmospheric chemistry

Daniel Cariolle^{1,2}, Philippe Moinat¹, Hubert Teyssède^{3,†}, Luc Giraud⁴, Béatrice Josse³, and Franck Lefèvre⁵

¹Climat, Environnement, Couplages et Incertitudes, UMR5318 CNRS/Cerfacs, Toulouse, France

²Météo-France, Toulouse, France

³Centre National de Recherches Météorologiques, UMR3589 CNRS/Météo-France, Toulouse, France

⁴Institut National de Recherche en Informatique et en Automatique, Talence, France

⁵Laboratoire Atmosphères, Milieux, Observations Spatiales, CNRS/UPMC/UVSQ, Paris, France

[†]deceased, April 2013

The authors would like to thank the referees for their comments and suggestions on this manuscript. We detail below the responses to the comments and the modifications that we intend to introduce in the revised manuscript.

1. Response to general comments

1a. Accuracy and efficiency of the ASIS solver compared to Rosenbrock's.

Referee 1. First, from the paper it is not so clear why a new solver is needed. In fact, in the paper there are comments which may make the CTM modeller decide to stick to solvers like Rosenbrock. In particular I would like to see a more detailed comparison against Rosenbrock concerning run time and accuracy, for small and large numbers of chemical species.

Referee 2. It isn't clear to me though, why such an expensive solver should be preferred over similarly expensive solvers available through open source packages such as KPP which can provide comparable accuracy and runtimes.

Referee 3. I would also like more discussion of computational cost - the timestep is discussed in detail, but is rarely then compared to the overall run-time. It is certainly interesting to see where the timestep changes, but in terms of usability it would be handy to know exactly how much more time it took.

In section 3 we have discussed in detail the accuracy of the ASIS solver compared to Rosenbrock's and Gear's type algorithms. We show that for a given relative tolerance value, Rtol, ASIS has comparable accuracy to those schemes. For low values of Rtol ASIS needs shorter timesteps to maintain comparable accuracy. For the values of Rtol that we believe small enough for atmospheric model simulations (in the range 1 to 3 %), the timesteps of ASIS and those of higher order schemes are comparable, but since ASIS requires less computation the CPU time should be comparable or lower.

We have investigated further this point and we report below several tests performed within the Matlab environment.

The following table gives the mean timesteps and CPU time for different box model configurations (the FLUX case of section 3) performed using ASIS and the ode23s code.

	Rtol	Mean timestep	CPU
ASIS	0,001	4,4	25,5
ASIS	0,01	23,3	6,4
ASIS	0,025	49,9	4,8
Ode23s	0,001	39	58,9
Ode23s	0,01	44	50,1
Ode23s	0,025	46	49,9
Ode23s+J	0,001	39	6,6
Ode23s+J	0,01	44	6,2
Ode23s+J	0,025	46	6,1

If ode23s is used without providing a subroutine for the computation of the Jacobian of the chemical system the ode23s code is much slower than ASIS, by a factor 2 to 10. This is because the ode23s code computes by differentiation an approximation of the Jacobian. It requires more iterations with the subroutine that computes the chemical tendencies and the CPU cost is rather high.

If the routine that computes the Jacobian is provided to ode23s, the CPU cost decreases significantly (lines Ode23+J of the table) and becomes comparable to the CPU used by ASIS. At low tolerance ode23s+J is faster than ASIS, at higher tolerance the costs of ASIS and ode23s+J are comparable.

The important point to mention is that within the Matlab environment the CPU cost does not come from the linear algebra parts of the algorithms but from the evaluation of tendencies and Jacobian matrices. Therefore it

is very dependant upon the chemical system and the details of the programming of the associated subroutines.

The situation is quite different within the Fortran environment. With the Fortran version of ASIS the CPU cost for the calculation of the Jacobian (the matrix M of eq. 7) is negligible compared to the linear algebra computations. This is because the compiler handles efficiently the associated subroutine (fill_matrix) that contains frequent indirect addressing. It is not possible to evaluate if this is also the case with all the codes based on Rosenbrock's algorithm, but if it is so ASIS should perform well when the mean time steps are comparable since it needs less linear algebra computations.

In conclusion we cannot give a general statement on the computational cost of ASIS compared to Rosenbrock's solvers. It is too dependant on the computational environment, on the details of the coding of the tendencies and the Jacobian matrices associated with the chemical scheme, and on the chemical scheme itself in particular the number of species and its stiffness.

Our objective is to offer an alternative to existing solvers having in mind that ASIS should be rather effective at the rather high tolerance error that can be used by most atmospheric models. Its formulation is not complex so it can be easily coded within the environment of existing models with the help of the example available on line (see the following comment 1.d). Our approach is to avoid the use of external pre-processors that are often judged not user-friendly by modellers because the generated code has to be adapted to the chemical models (see discussion in section 7).

It is clear that if a modeller uses already an implementation of a Rosenbrock solver like KPP, the effort to turn to ASIS might be too high compared to the expected benefit. But many models do not use solvers based on Rosenbrock's or Gear's methods and we believe that ASIS could be an interesting and simple alternative for them.

In the revised manuscript we will give some indications of the CPU time to run the ASIS code and discuss the difficulty to evaluate a priori the relative efficiency of the solvers.

1b. References of other solvers

Referee 1. There are no references given in the introduction to the general literature on chemical or differential equation solvers. An introduction should sketch the starting point of the work - the state-of-the-art - and in this way clarify how the new developments described in the paper advance this present knowledge and models. I suggest that the

authors add a section with references discussing the current status concerning solvers in relation to chemistry models. Several references are provided later on in the paper, but the current list is not very extended and could be expanded somewhat.

The references to existing algorithms, solvers, and their use by chemical models are given in section 2 in connection to the discussion of the numerical treatment of the species tendency equations. By doing so we believe that the reader better sees which class of solver is associated with a given treatment of the equations. In the manuscript we give reference to the most widely used explicit (CHEMEQ, TOWSTEP) and implicit (SIS, QSSA, Rosenbrok's and Gear's) schemes.

Our objective is not to make an exhaustive review article on numerical methods and solvers but to illustrate the specificity of our scheme compared to existing solvers.

In the revised manuscript we will briefly review in the introduction the main class of solvers, and we will give in section 2 additional references on chemical models and their associated solvers.

1c. Duration of the numerical simulations

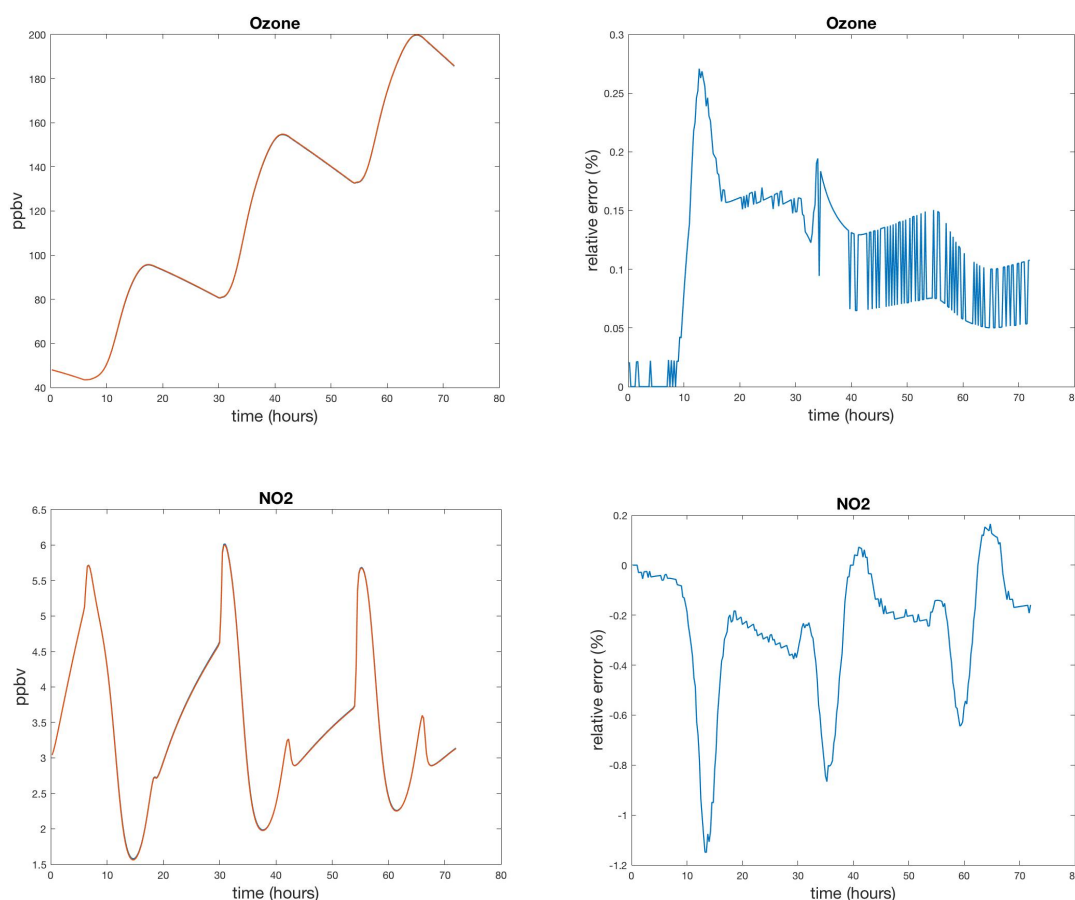
Referee 2. I find it a shame that only 3 month simulations are performed with the global models using the ASIS scheme. It would be very interesting to know what effect the replacement of the chemical solver would have on many other features of global atmospheric chemistry, such as the global oxidising capacity and related aspects such as the methane lifetime and tropospheric ozone budget.

Referee 3. The run length is also a bit short for most cases. The 1 day simulations for the box model are very short, especially when it appears that the A2 case is diverging from the R1/G1/A1 cases. Have these simulations been run for longer, and if so, how do the results of A2 (& A3) evolve? Also, A3 is not plotted at all, but these settings are then used for the MOCAGE simulations. The A3 results should also be included in the plots in Figures 1 & 2 (or plotted separately with a larger scale if required).

The GCM lengths are slightly better (3 months and 150 days), but still short. Are there plans to do longer runs with a full evaluation and budget analysis? The results presented here have highlighted deficiencies in the existing models, but a full analysis on longer simulations would be required to properly validate ASIS, as opposed to this paper which describes its implementation.

The objective of the reported simulations is to present the characteristics of the ASIS solver in terms of accuracy and adaptability to various chemical schemes and situations.

The 1-day simulation with the box model is long enough to evaluate the accuracy of the solver. We have extended the simulations up to 3 days for the FLUX case and the results obtained are fully consistent with the 1-day simulation. The next figures show for example results of the time evolution of O_3 and NO_2 concentrations in a 3-day extension of the A3 experiment (with the largest tolerance, 0.025) and its relative difference with an extended G1 experiment.



As can be seen there is no specific trend in relative differences between the species, the differences remain in the range of the chosen relative tolerance. In the revised manuscript we will include in figure 1 the results of experiment A3.

The 3D simulations illustrate the benefit of using a solver like ASIS that has a controlled accuracy and is mass conserving. The 3-month simulation with MOCAGE is short, but long enough to point out the benefits from the ASIS use. We agree that a more fully validation of

MOCAGE+ASIS would require longer simulations, in particular to assess the impact of ASIS on the longer-lived species. This is however beyond the scope of this article. Multiyear simulations of MOCAGE+ASIS are planned in the near future along with simulation of the C-IFS model (Flemming et al., 2015) with the RACMOBUS chemical scheme.

1d Code availability

Referee 1. - p29, code availability: "The ASIS code is property of the CERFACS and includes libraries that belong to other holders." Does this imply any restrictions if other parties want to use the code? Is there a kind of license for using the code?

Referee 2. if the authors do not seriously intend to make their code generally available to the community, and are content with limiting its use to in-house applications, differentiating their product from other alternatives in this way is arguably outside the scope of the manuscript.

After discussions with the holders of the different parts of the code it was agreed that the 0D Fortran code used in section 3 will be made generally available on the CERFACS's server.

1e . Synthesis of the simulations

Referee 3. Due to the large number of tests performed it was a little difficult to keep track of the settings used in each case. I would recommend giving a master table (or tables) giving the configuration for each shorthand used in the plots (e.g. R1, G1, A1, A2, A3, A4, MR, MA, EB, ASIS etc.) and what the settings are used for each (e.g. values for ATOL, RTOL, using ode23s, ode15s, DGEVS, GS, GMRES etc.), the experiment run (e.g. FLUX, STRATO, MOCAGE, Mars Box Model, LMD Mars GCM etc.), and also the chemistry scheme used (e.g. RACMOBUS, Mars). This would be especially helpful for comparing between sections, as it can be difficult to pick out this mass of information from the text.

We will extend table 4 to give the information required by Referee 3.

2. Response to specific comments

All the typos and english shortcomings will be addressed in the revised manuscript and are not detailed hereafter.

Equally, we will improve the quality of the figures as suggested by referee 3.

Referee 3. p2 line 30: I'm confused by "It is also desirable to let to the user a minimum of free parameters to tune". Do you mean "desirable to give the user"?

Yes, the idea is to give to the user a choice in a limited number of parameters that control the accuracy of the solution.

Referee 1. p3, line 25: The second term on the left is diagonal. Please explain why ? Diagonal in which space?

$L(t, C)$ being completely explicit, the matrix $(I + L(t, C) \delta t)$ is diagonal by construction.

Referee 1. p3, line 27: "mass conservation is not maintained". Can you add a reference or text book? Is it possible to describe in one line how the reader may understand that there is no conservation of mass?

The mass conservation is not maintained when the species tendencies associated to a given reaction are different after time discretisation. This is for instance the case with the simple BDF scheme. We will recall this in the revised manuscript.

Referee 3. p4 line 18: I think you mean "Sandu and Sander (2006)", although I can't find this reference in the reference list. I assume it is Sandu, A. and Sander, R.: Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1, Atmos. Chem. Phys., 6, 187-195, doi:10.5194/acp-6-187-2006, 2006. I haven't gone through and double-checked all the other references, but I suggest that the authors do so.

Yes this is the right reference. We will double-check again all the other references.

Referee 1. p5, line 27: Why is $\beta \geq 1$ required? Should this be $\beta > 0$?

$\beta > 0$ is enough from a mathematical point of view, but to better discriminate between implicit and explicit parts for the species tendencies $\beta > 1$ is more appropriate. We have tested values for $\beta > 1$ but not investigated $0 < \beta < 1$.

Referee 1.- Fig.6. The colour scale is unclear: Does the colour between 1 and 2 mean there are two substeps or one substep? I assume “number of sub-timesteps” can only take integer values.

The first colour (dark blue) corresponds to 1 sub-timestep. The colour scale intervals should be read] lower value, higher value].

The number of sub-timesteps can of course only take integer values. However we show interpolated values from model levels (which are function of ground pressure) to pressure levels (50hPa and 540hPa) and interpolated values are generally not integers.

Referee 3. p22 line 1: Do you mean “4.7 times”? Is this a mean over the whole 3-month run?

Yes it is 4.7 times, calculated over the 3-month run.

Referee 1. p25, line 32: “4 times smaller”. How can I see this from the figure 12, which has a scale ranging between -30 to 30%?

In order to highlight differences obtained during the day, the colour scale of Figure 12 is limited to maximum and minimum values of $\pm 30\%$. This is now mentioned in the legend. The related text in the body of the manuscript will be modified as follows:

“Regarding OH, the GCM results confirm the poor description of the HOx chemistry by the EB scheme at the terminators. At night, OH values calculated by EB are more than 30% smaller than with ASIS”.

Referee 3.

p26 Figure 11: When is this from - is it a snapshot from the start/middle/end of the 150-day run?

It is a snapshot at the end of the 150-day run, now indicated in the revised legend of Figure 11.

page 27 Figure 12: Similarly for Figure 11 - when is this from with respect to the start of the run. Is it the same as for Figure 11?

Yes similarly to Figure 11 this is a snapshot at the end of the 150-day run. This will be indicated in the revised legend of Figure 12.

Referee 1. p28: I was wondering if ASIS could be used for adjoint (4D-Var) type of applications?

In theory, the adjoint of the ASIS code can be developed. It requires that all the intermediate calculations (sub-timesteps, matrix M evaluations,

...) be stored. Then the adjoint of the successive linear operators can be derived if a direct method (for instance based on a LU decomposition) is used to solve the linear systems (eq. 7). The situation is more complex if an iterative solver is used.

However we do not plan to develop the adjoint of the ASIS code, we are alternatively exploring ensemble methods (Emili et al., 2016) for assimilation applications.

References

Emili, E., Gürol, S., and Cariolle, D.: Accounting for model error in air quality forecasts: an application of 4DEnVar to the assimilation of atmospheric composition using QG-Chem 1.0, *Geosci. Model Dev.*, 9, 3933-3959, doi:10.5194/gmd-9-3933-2016, 2016.

Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.-M., Diamantakis, M., Engelen, R. J., Gaudel, A., Inness, A., Jones, L., Josse, B., Katragkou, E., Marecal, V., Peuch, V.-H., Richter, A., Schultz, M. G., Stein, O., and Tsikerdekis, A.: Tropospheric chemistry in the Integrated Forecasting System of ECMWF, *Geosci. Model Dev.*, 8, 975-1003, doi:10.5194/gmd-8-975-2015, 2015.