Parallelization of TM4 for shared memory computers and integration of KPP in TM4

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Parallelization of TM4 model with OpenMP

What is OpenMP?

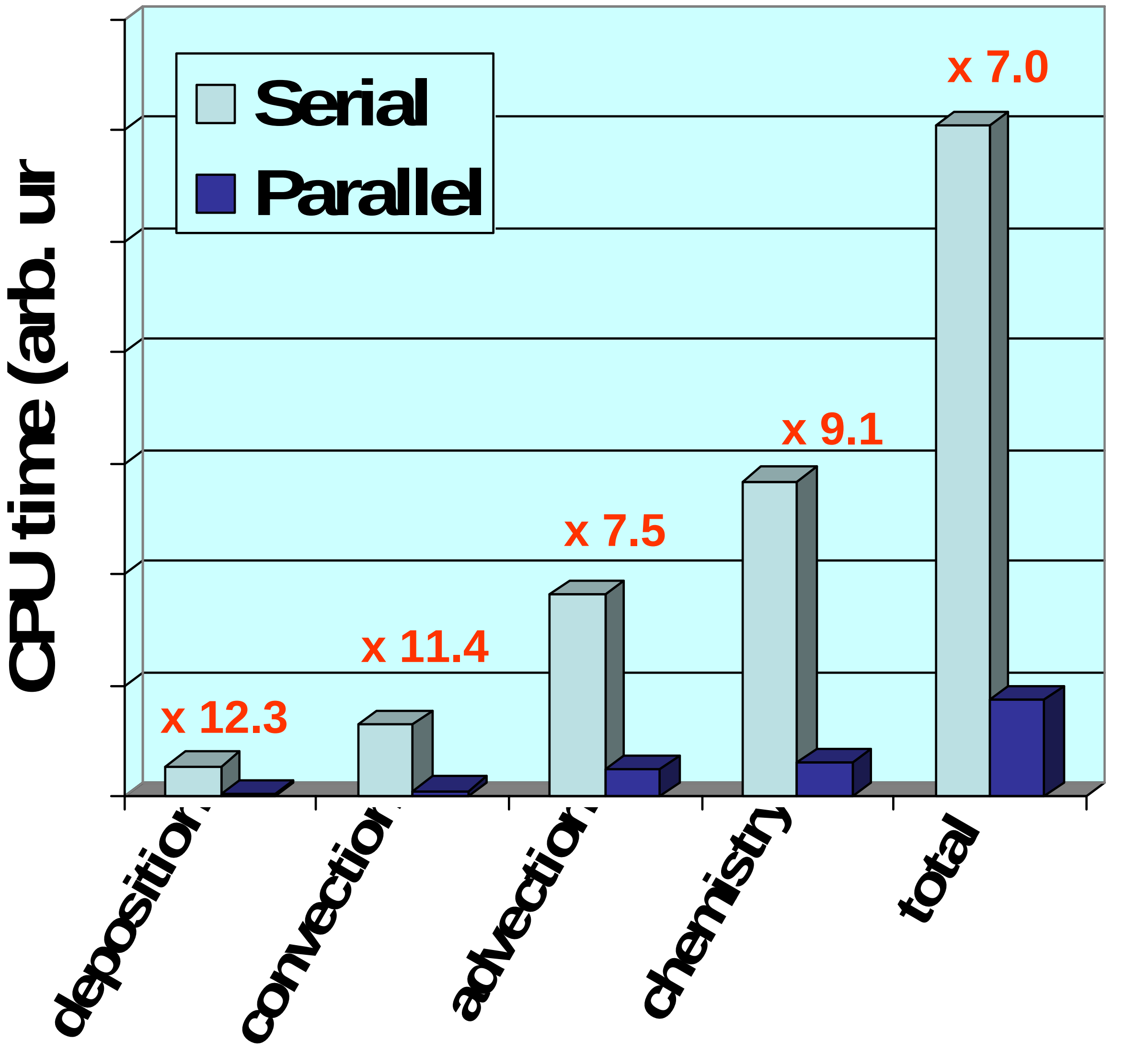
Defacto standard API for writing shared memory parallel applications in C, C++, and Fortran

OpenMP API consists of:

- Compiler Directives
- Runtime subroutines/functions
- Environment variables

```
!$OMP PARALLEL
!$OMP DO
DO I=1,100
A(I) = A(I) + B
ENDDO
!$OMP END DO
!$ OMP END PARALLEL
```

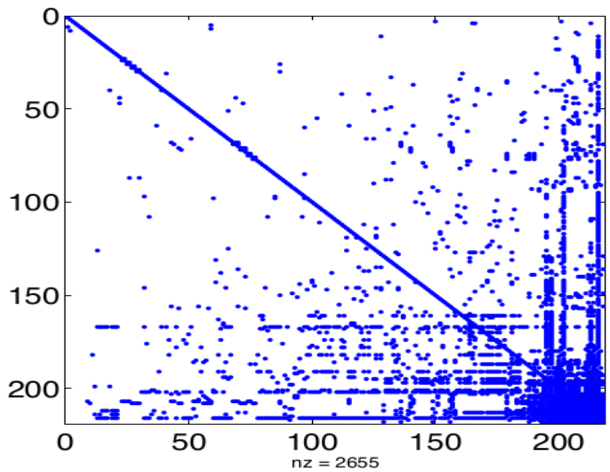
OpenMP parallelization



Integration of KPP in TM4 (and TM5)

Kinetic PreProcessor (KPP) provides a suite of stiff numerical integrators

- It provides a large collection of stiff numerical integrators
- It allows to easily incorporate additional solvers
- It has been successfully integrated with major models (ECHAM5/MESSy, CMAQ, GEOS-Chem, WRF-Chem)
- It prepares highly efficient routines for sparse LU decomposition and substitution (sparse linear algebra) that are specific to the particular sparsity of the simulated chemical mechanism



Chemical kinetics are remarkably parallel between grid cells, so there is abundant data parallelism

Description of a Chemical mechanism

$NO + O_3 \rightarrow NO_2 + O_2$

$O + O_2 + M \rightarrow O_3 + M$

$NO_2 + h\nu \rightarrow NO + O$

$NO_2 + O \rightarrow NO + O_2$

$Rate_1 = k_1 [NO][O_3]$

$Rate_2 = k_2 [O][O_2][M]$

$Rate_3 = J [NO_2]$

$Rate_4 = k_3 [NO_2][O]$

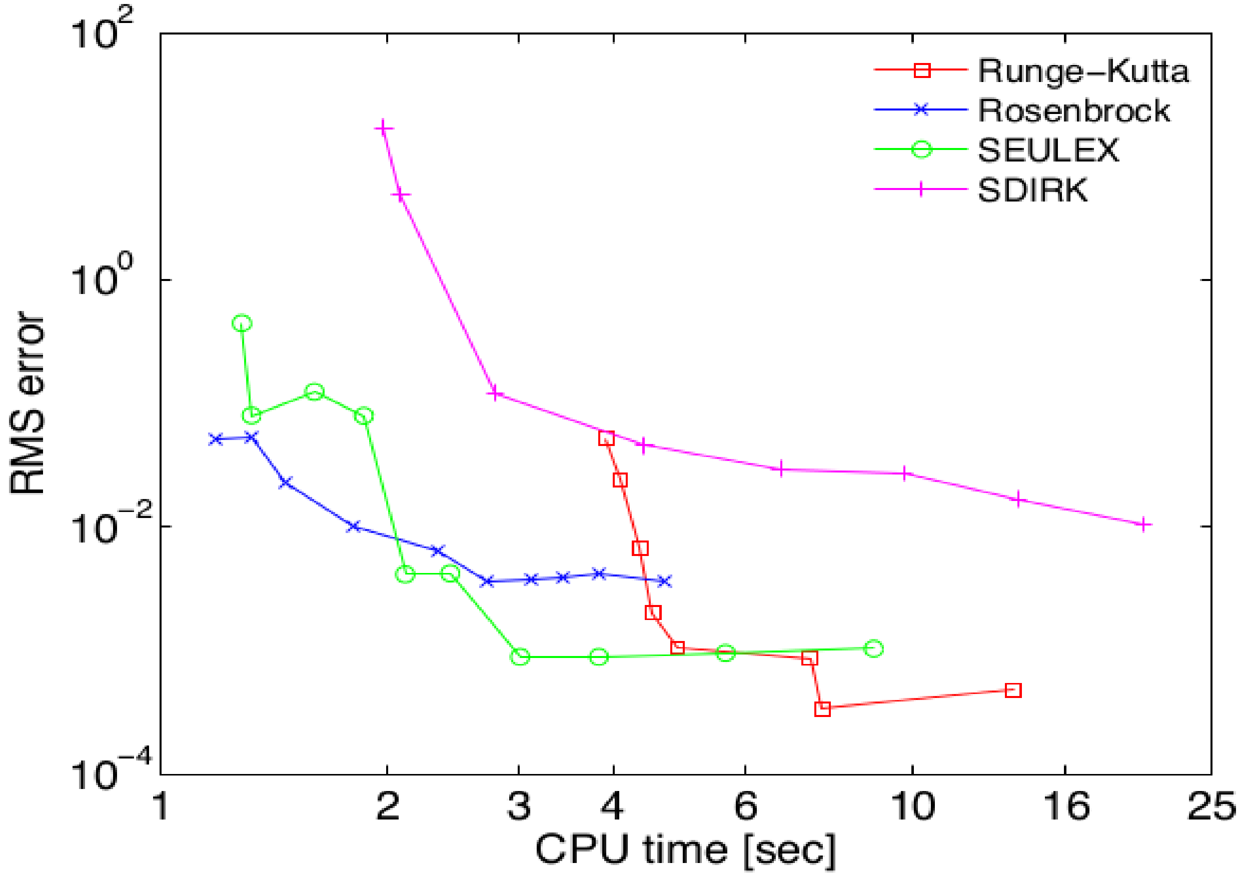
$$\frac{d[NO]}{dt} = J[NO_2] + k_3[NO_2][O] - k_1[NO][O_3]$$

$$\frac{d[NO_2]}{dt} = k_1[NO][O_3] - J[NO_2] - k_3[NO_2][O]$$

$$\frac{d[O]}{dt} = J[NO_2] - k_2[O][O_2][M] - k_3[NO_2][O]$$

$$\frac{d[O_3]}{dt} = k_2[O][O_2][M] - k_1[NO][O_3]$$

Investigation of the performance (efficiency) of implicit time stepping algorithms



H. Zhang *et al*., *Atmosphere* **2**, 510 (2011)

Integration of KPP in TM4 (and TM5)

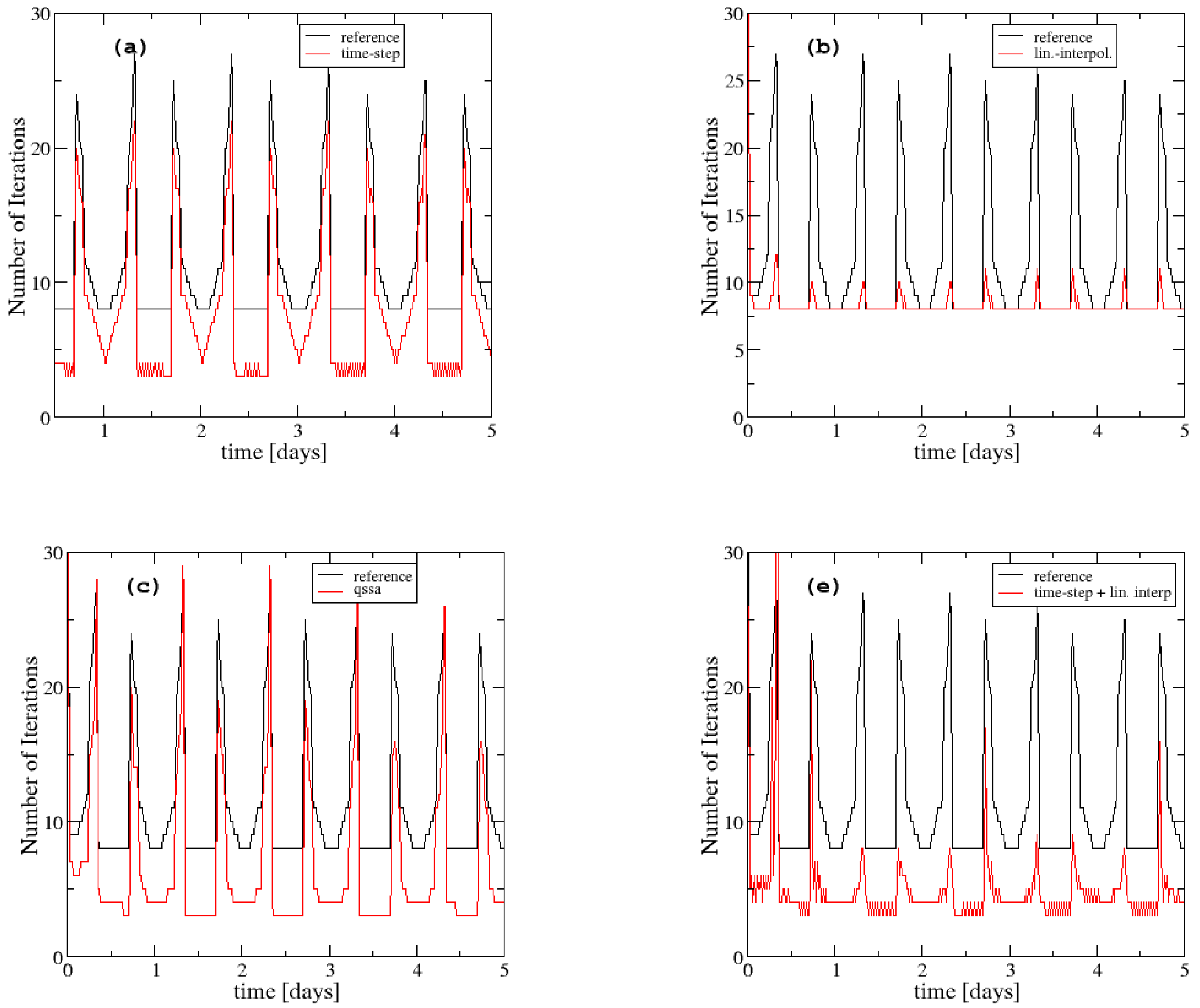
- Integration of KPP in TM4
- Evaluation of EBI and Rosenbrock algorithms in terms of accuracy and efficiency (Box model and TM4)
- Implementation of EBI in the KPP package (if necessary)

Improving the performance of the Rosenbrock solvers

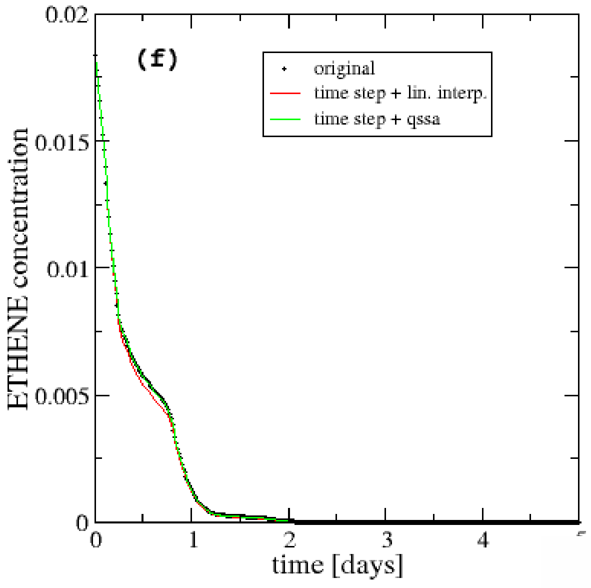
D. Taraborrelli, G. S. Fanourgakis, R. Sander, B. Steil, A. Pozzer and J. Lelieveld, "**Swift integration of atmospheric chemical mechanisms**", *(in preparation*)’

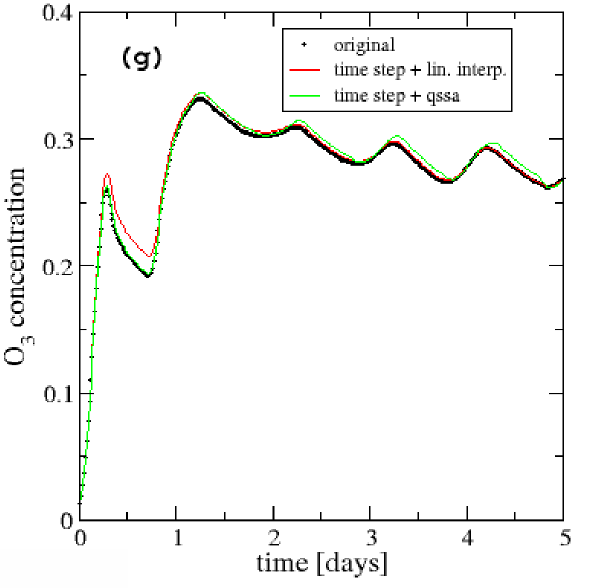
- A new adaptive time-stepping algorithm for the integration of ODEs
- A quasi steady state approximation (QSSA) that applies at the beginning of the integration period (transient phase) aiming also to reduce the stiffness of the ODEs.
- A linear interpolation scheme that interpolates the rate coefficients aiming to reduce the stiffness of the ODEs

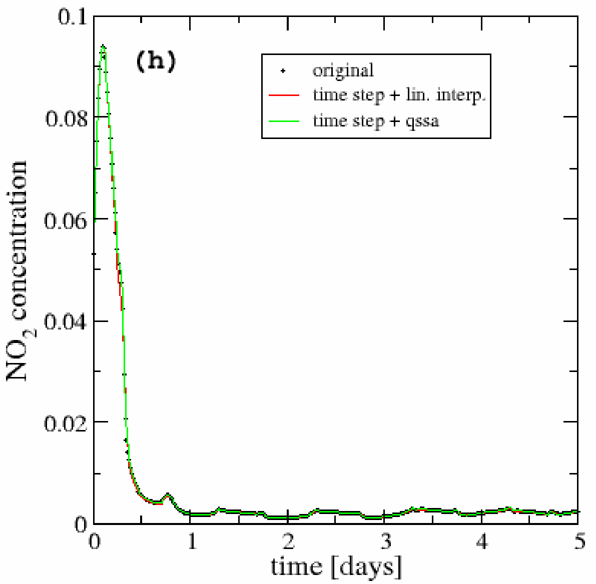
Efficiency of the algorithms



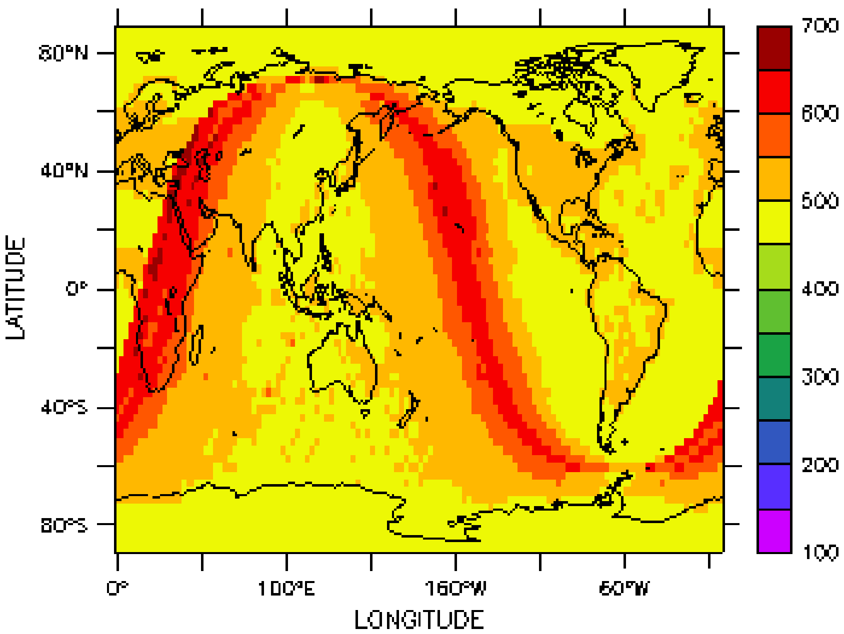
Accuracy of the algorithms



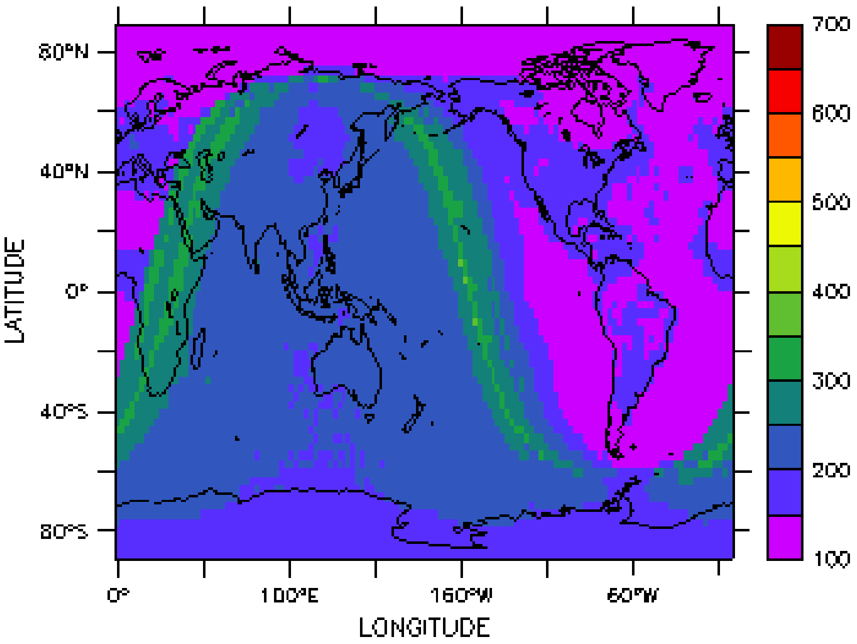




ECHAM/MESSy 3-D model



tot. KPP NSTEPS standard



tot. KPP NSTEPS fast