Testing of Rosenbrock Solvers for Exa2Green

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In point 4 of the COSMO-ART roadmap M13-M36, we had promised an *"Integration of algorithmic changes, which were demonstrated in the PRACE 2IP WP8 to improve KPP solver performance (up to a factor 2 for the ODE solver)."* This document first outlines the fundamentals of the new solver, which will be denoted by "rosenbrock_posdef_h211b_qssa". Then, technical details concerning the integration of the solver into KPP-2.2.1 are explained. The following section presents tests for the new solver. Different configurations of the solver are being compared with respect to the speedup and the accuracy of the solution. All tests are carried out by means of a zero-dimensional box model.

1 Basics of rosenbrock_posdef_h211b_qssa

In early 2013, G. Fanourgakis, J. Lelieveld and D. Taraborelli had announced a new integrator, that combines the quasi-steady-state approach with the Rosenbrock integrator and a new time-stepping algorithm. G. Fanourgakis noted that the "*scheme is very efficient and significantly reduces the number of iterations that the Rosenbrock implit ODE solver requires. At the same time the accuracy of the integrator remains almost unaffected.*"

The new integrator combines several features:

1. **Time-step control:** A new adaptive time-stepping algorithm for the integration of ODEs, as recommended by Söderlind [3].
2. **Stiffness reduction:**
   (a) Quasi-Steady-State Approximation (QSSA)
   (b) A linear interpolation of the rate coefficients.
3. **Positive definition**: Artificial preservation of positivity to improve stability.

1.1 Time-step control

Classic Rosenbrock solvers usually determine the time step size h_{n+1} by means of

$$h_{n+1} = h_n(\epsilon/r_n)^{1/k},$$

with the tolerance parameter ϵ, the error estimate r_n, $k = p + 1$ and p the order of convergence. The new integrator uses a more sophisticated step size controller algorithm H211b, as introduced by Söderlind [3]. Different than the one mentioned before, it also makes use of the error estimates of the previous time steps. The size of the timesteps is determined by

$$h_{n+1} \quad = \quad h_n(\epsilon/r_n)^{1/(bk)}(\epsilon/r_{n-1})^{1/(bk)}(h_n/h_{n-1})^{-1/b}.$$

According to Söderlin [3], the optimal parameters are $b = 1$ and $k = 2$. Note, that this new time-step control is already implemented in the baseline.

1.2 Stiffness reduction

1.2.1 Quasi-Steady-State Approximation (QSSA)

A reduction fot the stiffness of the set of ODEs is accomplished via the simplest QSSA formula,

$$\begin{aligned} P(t,y) - D(t,y)\, y &= 0 \\ \Rightarrow y &= P(t,y)/D(t,y), \end{aligned}$$

i.e. for some species, we assume that the amount being destructed $D(t,y)\ y$ equals the amount being constructed $P(t,y)$ at some time. After an induction period of τ_{ind}, those species are assumed to be in a quasi-stationary state. Sportisse and Djouad [4] have shown, that the error of using a QSSA is acceptable, if $|(P-L)/(P+L)| \leq 10^{-2}$. Turanyi et al. [6] have further shown, that the time within the QSSA species reach a quasi steationary steady state τ_{ind} is estimated to be about 10 times the longest QSSA species lifetime, τ_{QSSA}^{max}. The QSSA option can be turned on/off in ICNTRL(6). The respective threshold value for QSSA species lifetime τ_{QSSA}^{max} can be adjusted in RCNTRL(10).

```
!    ICNTRL(6)  -> 0 no QSSA
!                  1 QSSA
[...]
!    RCNTRL(10) -> thres_tau, threshold value for QSSA species lifetime
```

Further, undocumented options for QSSA seem to exist, as can be seen later in the code:

```
!~~~> Choice of QSSA
    IF (ICNTRL(6) == 0) THEN                [...no QSSA...]
ELSEIF (ICNTRL(6) == 1) THEN ! DAE QSSA            [...]
ELSEIF (ICNTRL(6) == 2) THEN ! Plain QSSA          [...]
ELSEIF (ICNTRL(6) == 3) THEN ! Iterated QSSA       [...]
ELSEIF (ICNTRL(6) == 4) THEN ! Extrapolated QSSA   [...]
ELSEIF (ICNTRL(6) == 5) THEN ! Extrapolated QSSA   [...]
```

1.2.2 Linear interpolation of rate coefficients

A second step to reduce stiffness is aimed at by using a linear interpolation scheme to smoothly vary the rate coefficients. It has been seen, that the abrupt change in the photolysis rate coefficients during night/day transitions significantly increase the stiffness of the ODEs. A linear interpolation scheme has been added to interpolate rate coefficients during the time splitting interval, which eventually may lead to a decrease in stiffness.

In the code, this option is controlled by an integer called i_do_lin_interp. This function can only be called in the non-autonomous mode, i.e. if $f = f(t,y)$ depends on t.

```
IF (.NOT.Autonomous) THEN
if (i_do_lin_interp==1) then
!CALL Update_SUN()
        CALL Update_RCONST()
        else if (i_do_lin_interp==2) then
            do i=1, Nreact
             x = rconst_dt(i) - rconst_prev(i)
             rconst(i) = rconst_prev(i) + x * delta/period
            enddo
endif
END IF
```

1.3 “Positive definite“ option

Last, an “positive definite” option has been added, so that enables an artificial preservation of positivity of the solution. Typically, this approach, is encountered as “clipping”, i.e. setting negative concentration values to zero. For stability reasons, an artificial preservation of positivity is advantageous. However, this approach is not mass-conserving. More elaborate techniques ensure positivity through additional postprocessing steps, such as a projection onto a non-negative simplex. Methods favoring positivity (as introduced by Sandu [2]) present computationally less costly alternatives.

Details (with missleading comments...) can be found in the code:

```
! positive definite following a suggestion from Adrian
! see "MAX(Ynew,ZERO)" for details
[...]
  IF (posdef==1) THEN
      Y = MAX(Ynew,ZERO) ! new value is positive definite:
  ENDIF
[...]
  IF (posdef==2) THEN
      Y = MAX(Ynew,ZERO) ! new value is positive definite:
  ENDIF
```

This option can be turned on/off in ICNTRL(5).

```
!    ICNTRL(5)  -> 0 no posdef, 1 posdef out of time loop,
!                  2 posdef every substeps
```

2 Integration into KPP-2.2.1

The original rosenbrock_posdef_h211b_qssa solver had been designed for KPP version 2.1. However, for the COSMO-ART baseline we had decided to stick to KPP version 2.2.1. For the sake of comparability, the original code of the new solver was slightly adapted and integrated into KPP version 2.2.1. The modified code is held in the repository’s subfolder kpp-2.2.1_with_Prace_Integrator.

Following modifications to kpp-2.2.1 had to be made:

- **int/**
  - add rosenbrock_posdef_h211b_qssa.f90
  - add rosenbrock_posdef_h211b_qssa.def
- **int/rosenbrock_posdef_h211b_qssa.f90:**
  - rename variable lin_interp into i_do_lin_interp
- **src/gen.c**:
  - add function GenerateFun_Split()

3 Tests

All tests were carried out by means of the 0-dim box-model using the repository revision number 265. The utilized chemical mechanism is RADM-KA (Regional Acid Deposition Model Version Karlsruhe), a slightly amended version of the chemical mechanism RADM2 by Stockwell et al. [5]. RADM-KA comprises 194 reactions and 83 chemical species, whereas one species is held constant. This mechanism was chosen in accordance to the baseline scenario, the collaborators had agreed upon in May 2015 (redefinition of the COSMO-ART baseline).

The tests are set up on a three-dimensional discrete computing domain with $66 \times 56 \times 31$ grid cells, i.e. a total of 114 576 independent 0-dim boxes are being solved. The initial conditions for each box were extracted from realistic COSMO-ART model runs from a computing domain of the same dimension, centered above Paris at high noon (12am), April 13th, 2010. Initial conditions for all species therefore vary for each of the 114 576 0-dim boxes, but all represent a polluted atmosphere above Paris. The model supports variable photolysis conditions, which allows to locally adapt the rate constants. Temperature is kept constant over all boxes. The total integration time is set to one hour, with integrator restarts at every 120 seconds, again in accordance with the baseline. In total, the function INTEGRATE is therefore called 30 times.

In the tests presented here, no external disturbances due to advection, diffusion or further effects are taken into account, as it would be the case in a real air quality model. In fact, only the very first initial conditions represent a realistic set-up with perturbed initial conditions, as those initial values were extracted from realistic, three-dimensional air quality model runs. Since in our tests, the chemical species are not exposed to any perturbation throughout the simulation, they equilibrate with elapsing time. Hence, the systems will be less stiff in the following 29 INTEGRATE function calls. However, the number of timesteps necessary for the solution of the chemical kinetics is strongly influenced by the degree of stiffness. Therefore, only the measurements for the very first call of the INTEGRATE function can give a qualitative estimate for performance improvements for future three-dimensional runs within COSMO-ART.

The simulation is being monitored by means of 8 key chemical species (NO, NO2, NO3, HO, H2O2, HCHO, OP1, O3), and observed at the gridpoint located right above Paris.

The source code for the simulation of the chemical kinetics was generated by KPP. To this end, first a KPP executable was produced in bin/kpp. After the Fortran code was generated by KPP, backup files containing modifications needed for the benchmarking (tuning of parameters, statistics output) of the different solvers are copied to the current directory. All tests are run with scalar relative and absolute tolerances of rtol $=10^{-2}$ and atol $=10^{-2}$ on one node of Piz Dora at CSCS (12-core Intel Haswell CPUs (Intel® Xeon® E5-2690 v3)).

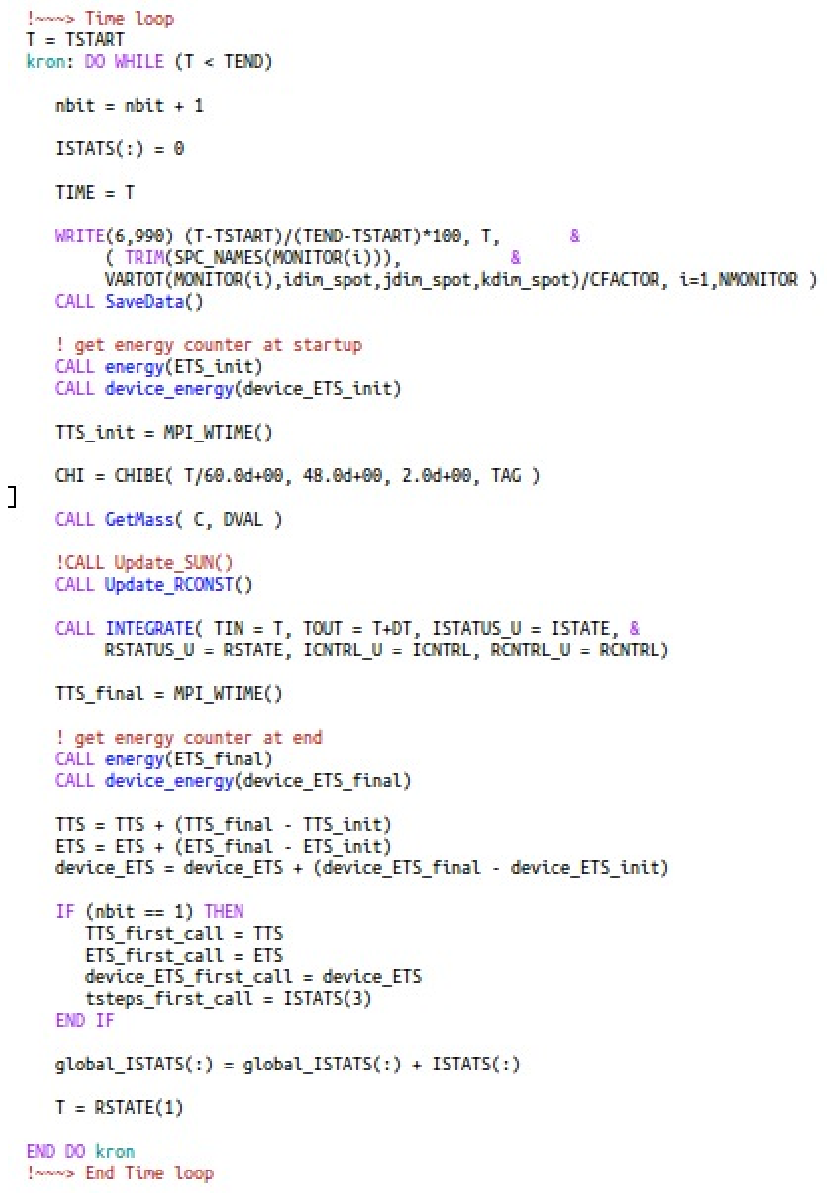
Reference Solution As a reference solution, we took a run with the Rosenbrock4 solver using KPP-2.2.3 (as it corresponds to the solver used in the original COSMO-ART baseline) and scalar and absolute tolerances of rtol $=10^{-2}$ and atol $=10^{-2}$.

Accuracy We estimate the accuracy of the final solution by means of the relative L^2-error to the reference solution $\tilde{c}$ at final integration time,

$$\mathrm{err}_{\mathrm{rel}} = \sqrt{\frac{\sum_{i=0}^{N} \left(\tilde{c}_i(T) - c_i(T)\right)^2}{\sum_{i=0}^{N} \tilde{c}_i^2}}$$

with $T = 3600$ sec. The current way to calculate the relative error is not ideal as we consider only a portion of the full population of chemical species (NO, NO2, NO3, HO, H2O2, HCHO, OP1, O3). However we take into account the most critical chemical species, which are the ones that typically have the biggest error contributions, so the approximation is fine.

Speedup As an estimate for the serial speedup, we investigate the accumulated **number of timesteps** and the **elapsed time** for a) the first function call of the function "INTEGRATE" and b) an average over all function calls "INTEGRATE" and c) in total over all 30 timesteps. It has to be emphasized, that measure a) will give a realistic hint on the estimated speed-up within a three dimensional simulation in COSMO-ART.



```
!~~~> Time loop
T = TSTART
kron: DO WHILE (T < TEND)

   nbit = nbit + 1

   ISTATS(:) = 0

   TIME = T

   WRITE(6,990) (T-TSTART)/(TEND-TSTART)*100, T,        &
        ( TRIM(SPC_NAMES(MONITOR(i))),             &
        VARTOT(MONITOR(i),idim_spot,jdim_spot,kdim_spot)/CFACTOR, i=1,NMONITOR )
   CALL SaveData()

   ! get energy counter at startup
   CALL energy(ETS_init)
   CALL device_energy(device_ETS_init)

   TTS_init = MPI_WTIME()

   CHI = CHIBE( T/60.0d+00, 48.0d+00, 2.0d+00, TAG )
]
   CALL GetMass( C, DVAL )

   !CALL Update_SUN()
   CALL Update_RCONST()

   CALL INTEGRATE( TIN = T, TOUT = T+DT, ISTATUS_U = ISTATE, &
        RSTATUS_U = RSTATE, ICNTRL_U = ICNTRL, RCNTRL_U = RCNTRL)

   TTS_final = MPI_WTIME()

   ! get energy counter at end
   CALL energy(ETS_final)
   CALL device_energy(device_ETS_final)

   TTS = TTS + (TTS_final - TTS_init)
   ETS = ETS + (ETS_final - ETS_init)
   device_ETS = device_ETS + (device_ETS_final - device_ETS_init)

   IF (nbit == 1) THEN
      TTS_first_call = TTS
      ETS_first_call = ETS
      device_ETS_first_call = device_ETS
      tsteps_first_call = ISTATS(3)
   END IF

   global_ISTATS(:) = global_ISTATS(:) + ISTATS(:)

   T = RSTATE(1)

END DO kron
!~~~> End Time loop
```

3.1 Ros4 implementations for different KPP versions

In the first tests [ref0], [ref1] and [ref2], the KPP-2.2.1, KPP-2.2.3 and KPP-2.2.1_with_Prace_Integrator implementations of Ros4 were checked. The parameters for the tests can be seen in table 1, the results in table 7.

In the case of the Prace implementation, no additional options such as QSSA, posdef and linear interpolation were enabled. The results illustrate, that the pure implementation of Ros4 already uses a different time step control mechanism. So the results [ref2] differ to those of [ref0], especially in the number of timesteps per function call. However the number of timesteps between [ref2] and [ref1] are exactly the same as well as the numerical accuracy, only the timings are different. At this point it also gets clear, that the time measurements we take, are not linear with the number of timesteps: the 266 timesteps taken in [ref0] need even more time than the 346 timesteps taken in [ref2].

	[ref0]	[ref1]	[ref2]
KPP version	2.2.1	2.2.3	2.2.1_with_Prace_Integrator
ATOL(:)	1.0d-2		
RTOL(:)	1.0d-2		
ICNTRL(1)	0		
ICNTRL(2)	1		
ICNTRL(3)	3		
ICNTRL(4:20)	0		
RCNTRL(:)	0.0		

Table 1: Parameters for tests [ref0]-[ref2].

3.2 Tests of Rodas3 rosenbrock_posdef_h211b_qssa

In the next set of tests, the new integrator rosenbrock_posdef_h211b_qssa was tested with varying parameters.

3.2.1 [timestep_<b>_<k>]

In these tests, the new time stepping control mechanism is tested only using Ros4, with no linear interpolation, no posdef option and no QSSA. According to Söderlind [3], an optimal choice is given by $b = 1$ and $k = 2$, but $b = 1$ and $k = 4$ were also tested for Ros4. Parameters and results can be seen in table 2 and 7.

3.2.2 [linint<0:2>]

The tests [linint0], [linint1] and [linint2] test all options of using linear interpolation using Ros4, with no posdef option and no QSSA. Parameters and results can be seen in table 3 and 7.

3.2.3 [posdef<1:2>]

The tests [posdef1] - [posdef2] test all options of positive definition using Ros4, no QSSA and no linear interpolation. Parameters and results can be seen in table 4 and 7.

3.2.4 [QSSA<1:6>_<τ_{QSSA}^{max}>]

All options for QSSA using Ros4, no posdef option, and no linear interpolation are tested. The parameter τ_{QSSA}^{max} is tuned with 10^{-9}, 10^{-6}, 10^{-3} or 10^{0}. Parameters and results can be seen in table 5 and 7.

3.2.5 [opt_<int>_<mode>]

The parameters for these tests were chosen in accordance to the results presented on a poster by Taraborelli et al. [1]: "the optimum for speedup and accuracy has been found with Rosenbrock Rodas3 in the autonomous mode, $\tau_{QSSA}^{max} = 1s$ and the H211b controller with $b = 1$ and $k = 2$". As noticed with the previous QSSA tests, best choices for ICNTRL(6) seem to be 2 or 3, which provides equivalent results. For our tests, we considered ICNTRL(6) = 2 as it seems a bit faster. Nevertheless, even if the previous QSSA tests revealed that considering $\tau_{QSSA}^{max} = 1s$ is indeed the best choice in terms of computational speed, it turns out that it is definitely not concerning numerical accuracy ($\sim 10^{-3}$ for $\tau_{QSSA}^{max} = 1s$ versus $\sim 10^{-7}$for $\tau_{QSSA}^{max} \leq 10^{-3}$). Therefore we conducted our experiments by using $\tau_{QSSA}^{max} = 10^{-3}$, instead of $\tau_{QSSA}^{max} = 1s$ considered by Taraborelli et al. [1]. We tested both Ros4 and Rodas3 (in autonomous mode or not) in combination with above mentioned settings. Parameters and results can be seen in table 6 and 7.

	[timestep_1_2]	[timestep_1_4]
KPP version	2.2.1_with_Prace_Integrator	
ATOL(:)	1.0d-2	
RTOL(:)	1.0d-2	
ICNTRL(2)	1	
ICNTRL(3)	3	
ICNTRL(1, 4:20)	0	
RCNTRL(1:7,10:20)	0.0	
RCNTRL(8)	1	1
RCNTRL(9)	2	4

Table 2: Parameters for tests [timestep_<b>_<k>].

	[linint1]	[linint2]
KPP version	2.2.1_with_Prace_Integrator	
ATOL(:)	1.0d-2	
RTOL(:)	1.0d-2	
ICNTRL(2)	1	
ICNTRL(3)	3	
ICNTRL(1, 4:20)	0	
RCNTRL(:)	0.0	
I_DO_LIN_INTERP	1	2

Table 3: Parameters for tests [linint0]-[linint2].

	[posdef1]	[posdef2]
KPP version	2.2.1_with_Prace_Integrator	
ATOL(:)	1.0d-2	
RTOL(:)	1.0d-2	
ICNTRL(2)	1	
ICNTRL(3)	3	
ICNTRL(5)	1	2
ICNTRL(1, 4, 6:20)	0	
RCNTRL(:)	0.0	

Table 4: Parameters for tests [posdef0] and [posdef1] 1.

	[QSSA<1:6>_<τ_{QSSA}^{max}>]
KPP version	2.2.1_with_Prace_Integrator
ATOL(:)	1.0d-2
RTOL(:)	1.0d-2
ICNTRL(2)	1
ICNTRL(3)	3
ICNTRL(1, 4, 5, 7:20)	0
ICNTRL(6)	1, 2, 3, 4, 5
RCNTRL(1:9, 11:20)	0.0
RCNTRL(10)	10^{-9}, 10^{-6}, 10^{-3}, 10^{0}

Table 5: Parameters for tests [QSSA<1:6>_<τ_{ind}>].

	[opt_ros4_na]	[opt_ros4_a]	[opt_rodas3_na]	[opt_rodas3_a]
KPP version	2.2.1_with_Prace_Integrator			
ATOL(:)	1.0d-2			
RTOL(:)	1.0d-2			
ICNTRL(1)	0	1	0	1
ICNTRL(2)	1			
ICNTRL(3)	3		4	
ICNTRL(5)	1			
ICNTRL(6)	2			
ICNTRL(4, 7:20)	0			
RCNTRL(1:7, 11:20)	0.0			
RCNTRL(8)	1.0			
RCNTRL(9)	2.0			
RCNTRL(10)	10^{-3}			
I_DO_LIN_INTERP	0			

Table 6: Parameters for tests [opt_<int>_<mode>].

	err_{rel}	#tsteps	CPU time [s]	#tsteps	CPU time [s]	#tsteps	CPU time [s]
		a) first call only		b) in average		c) in total	
[ref0]	0.1906E-06	59	64.296	8	10.726	266	321.770
[ref1]	0.4712E-07	21	26.237	11	14.378	346	431.349
[ref2]	0.4712E-07	21	5.006	11	2.738	346	82.155
[timestep_1_2]	0.5346E-06	47	10.238	6	1.441	183	43.221
[timestep_1_4]	0.8385E-07	22	5.095	8	2.049	258	61.466
[linint1]	0.4712E-07	21	23.730	11	13.023	346	390.689
[linint2]	NaN	NaN	NaN	NaN	NaN	NaN	NaN
[posdef1]	0.4712E-07	21	4.985	11	2.741	346	82.240
[posdef2]	0.4712E-07	21	4.983	11	2.744	346	82.320
[QSSA2_1E-9]	0.5352E-07	21	5.015	11	2.768	346	83.047
[QSSA3_1E-9]	0.5352E-07	21	5.029	11	2.774	346	83.224
[QSSA2_1E-6]	0.5352E-07	21	4.987	11	2.765	346	82.957
[QSSA3_1E-6]	0.5352E-07	21	5.003	11	2.777	346	83.310
[QSSA2_1E-3]	0.5352E-07	21	5.032	11	2.777	346	83.321
[QSSA3_1E-3]	0.5352E-07	21	5.050	11	2.786	346	83.594
[QSSA2_1E0]	0.2264E-03	21	5.051	4	1.215	146	36.464
[QSSA3_1E0]	0.2264E-03	21	5.020	4	1.220	146	36.593
[opt_ros4_a]	0.5421E-06	47	9.805	6	1.383	183	41.475
[opt_rodas3_a]	0.2144E-06	18	3.979	4	1.058	135	31.731
[opt_ros4_na]	0.5421E-06	47	10.175	6	1.461	183	43.839
[opt_rodas3_na]	0.2144E-06	18	4.236	4	1.129	135	33.872

Table 7: Results for all tests on Piz Dora.

4 Conclusion

Table 7 shows the results for measurements carried out on one node of Piz Dora at CSCS using the GNU compiler version 4.9.1. The first observation is that in the case of the pure Prace implementation [ref2] (Ros4 with no additional options such as QSSA, posdef and linear interpolation) already outperforms [ref1] (KPP-2.2.3) by a factor 5 and [ref1] (KPP-2.2.1) by a factor 13 for the time spent in the first call only.

Best performance for total runtime was achieved with $b = 1$ and $k = 2$ representing 183 timesteps and 43 s in total, against 258 timesteps and 61 s with $b = 1$ and $k = 4$. However the time stepping control mechanism is faster with $b = 1$ and $k = 4$ if we consider only the first call, requiring with roughly twice less timesteps than the case $b = 1$ and $k = 2$.

The second point is that the linear interpolation scheme to smoothly vary the rate coefficients is quite costy in this case in terms of performance. However it would actually really make sense during night/day transitions and not in this test simulating a 1h scenario at high noon.

Then, we can see clearly that all QSSA tests with ICNTRL(6) = 2 or 3 are faster than the reference [ref0]. All other choices for ICNTRL(6) led to very (>> reference*10) long computing times or errors, therefore these tests have only been executed partly.

Finally, four configurations have been tested according to the results presented on a poster by Taraborelli et al. [1], by varying only the Rosenbrock solver (Ros4 or Rodas3) and the mode (autonomous or not). The fastest run has been achieved for the Rodas3 solver including a QSSA assumption (ICNTRL(6) = 2), an artificial preservation of positivity of the solution, and the new time stepping control h211b with $b = 1$ and $k = 2$ in autonomous mode. The result is an impressive x 16 reduction in the time spent in the first loop w.r.t. [ref0]. The only difference with the conclusion of Taraborelli et al., is $\tau^{max}_{QSSA} = 10^{-3}$ which was chosen in favor of $\tau^{max}_{QSSA} = 1s$ in order to optimize the numerical accuracy.

References

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