Testing of Rosenbrock Solvers for EXA2Green

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February 18, 2015

In point 4 of the COSMO-ART roadmap M13-M36, we have 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 "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 the 0-dim-boxmodel. The document closes with conclusions and an estimation of the new solver's potential E2S improvement for the extended testbed.

1 Basics of rosenbrock_posdef_h211b_qssa

In early 2013, G. Fanourgakis, J. Lelieveld and D. Taraborelli have 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 periof 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. [5] 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 intransparant "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-d boxmodel and with the repository revision number 220. It deals with a variable CHI function. The initial conditions represent a chemical mixture right above Paris as it is configured for the very first timestep for the extended box model. The time step size, in which the

function "INTEGRATE" is called, is chosen as TSTEP = 120 sec, the total integration time is TEND = 3600 sec. This leads to a total of 30 calls of the function "INTEGRATE. [1]

The code was produced with the respective executables in bin/kpp. After the code was produced by KPP, a back-up file for kpp_Main.f90, stored in backup_files_serial_integrator_tests/, was copied to the current directory. This file includes the tuning of the parameters and the additional writing out of the wall clock time and the number of timesteps. All tests are run with scalar relative and absolute tolerances of rtol $=10^{-2}$ and atol $=10^{-2}$ and in non-autonomous mode, i.e. $f = f(t, y)$ depends on t.

Reference Solution As a reference solution we took a run with Ros4 solver using KPP-2.2.1 and scalar relative 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,

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

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

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

with $T = 3600$ sec. As a reference solution we take a run with the Rosenbrock4 solver, using KPP version 2.2.1, and scalar absolute and relative tolerances of atol=10^{-2} and rtol=10^{-2}.

Speedup As an estimate for the serial speedup, we investigate the accumulated **number of timesteps** and the **wall clock 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 3dimensional simulation in COSMO-ART.

```
starttime = MPI_WTIME()
CALL INTEGRATE( TIN = T, TOUT = T+DT, ISTATUS_U = ISTATE, &
     RSTATUS_U = RSTATE, &
     ICNTRL_U = (/ 0,1,3,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 /) )

endtime = MPI_WTIME()
T = RSTATE(1)

meantime = meantime + endtime - starttime
n_tsteps = n_tsteps + ISTATE(3)

    if (nbit == 0) then
       time_first_call = meantime
       n_tsteps_first_call = n_tsteps
    end if
nbit = nbit + 1
```

[1] We have been discussing in detail, what this actually means! As it has been presented in the first part of this document, the splitting approach is an essential source of stiffness and stiffness is the reason, why the chemical simulations are so time consuming. The more stiffness present, the more time steps will be necessary. The way this test was set up means, i.e. TSTEP=120 sec and TEND=3600 sec, we only have perturbed initial concentrations for the very first of the 30 function calls of the "INTEGRATE" function. Therefore, only the first measurement can give a qualitative estimate for performance improvements for future 3d runs with COSMO-ART!

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 1a, the results in table **??**.

In 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 differ to those of [ref0] and [ref1], especially in the number of timesteps per function call. At this point, it also gets clear, that the time measurements we take, are not linear with the number of time steps, taken: the 158 timesteps taken in [ref0] need even more time, than the 313 timesteps token in [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 $k = 2$. As mentioned before, this new control mechanism is already implemented in the baseline in KPP-2.2.1. There $b = 1$ and $k = 4$ are chosen for Ros4.

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 1a and **??**.

3.2.3 [posdef<1:2>]

The tests [posdef1] - [posdef2] test all options of positive definition using Ros4, no QSSA and no linear interpolation. Note, that is absolutely intransparant, what this option actually does! Parameters and results can be seen in table 1b and **??**.

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 varied from 10^{-9}, 10^{-6}, 10^{-3} and 10^{0}. Parameters and results can be seen in table 1c and **??**.

3.2.5 [opt_<int>_<mode>]

The parameters for these tests are 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 it has been seen in the previous QSSA tests, best choices for INCNTRL(6) seem to be 2 or 3 - we now choose 2. We both tested Ros4 and Rodas3 in combination with above mentioned settings. Parameters and results can be seen in table 1d and **??**.

	[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		

(a) Parameters for tests [ref0]-[ref2].

	[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

(b) 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

(a) 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	

(b) 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, 6
RCNTRL(1:9, 11:20)	0.0
RCNTRL(10)	10^{-9}, 10^{-6}, 10^{-3}, 10^{0}

(c) 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(6)	2			
ICNTRL(4, 5, 6:20)	0			
RCNTRL(1:7, 11:20)	0.0			
RCNTRL(8)	1.0			
RCNTRL(9)	2.0			
RCNTRL(10)	1.0			

(d) 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]	0.1912E-07	8	0.1654E+02	4	0.1008E+0	142	0.3025E+03
[ref1]	0.1912E-07	13	0.2719E+02	10	0.2173E+02	304	0.6518E+03
[ref2]	0.1912E-07	13	0.3656E+01	10	0.2886E+01	304	0.8658E+02
[timestep_1_2]	0.1911E-07	7	0.1938E+01	3	0.1232E+01	95	0.3697E+02
[timestep_1_4]	0.1911E-07	9	0.4089E+01	4	0.1526E+01	127	0.4578E+02
[linint1]	0.1912E-07	13	0.2383E+02	10	0.1867E+02	304	0.5602E+03
[linint2]	NaN	NaN	NaN	NaN	NaN	NaN	NaN
[posdef1]	0.1912E-07	13	0.3452E+01	10	0.3835E+01	304	0.1151E+03
[posdef2]	0.1912E-07	13	0.5945E+01	10	0.3948E+01	304	0.1184E+03
[QSSA2_1E-9]	0.1911E-07	13	0.5109E+01	10	0.3340E+01	304	0.1002E+03
[QSSA3_1E-9]	0.1911E-07	13	0.3645E+01	10	0.2919E+01	304	0.8758E+02
[QSSA6_1E-9]	NaN	NaN	NaN	NaN	NaN	NaN	NaN
[QSSA2_1E-6]	0.1912E-07	13	0.3713E+01	10	0.3404E+01	304	0.1021E+03
[QSSA3_1E-6]	0.1912E-07	13	0.3680E+01	10	0.2915E+01	304	0.8746E+02
[QSSA6_1E-6]	NaN	NaN	NaN	NaN	NaN	NaN	NaN
[QSSA2_1E-3]	0.1912E-07	13	0.6157E+01	7	0.2896E+01	21	0.8689E+02
[QSSA3_1E-3]	0.1912E-07	13	0.3687E+01	7	0.2126E+01	216	0.6377E+02
[QSSA6_1E-3]	NaN	NaN	NaN	NaN	NaN	NaN	NaN
[QSSA2_1E0]	0.1911E-07	13	0.3548E+01	6	0.2534E+01	187	0.7603E+02
[QSSA3_1E0]	0.1911E-07	13	0.3811E+01	6	0.1864E+01	187	0.5592E+02
[QSSA6_1E0]	NaN	NaN	NaN	NaN	NaN	NaN	NaN
[opt_ros4_a]	0.1906E-07	7	0.1901E+01	2	0.6882E+00	66	0.2065E+02
[opt_rodas3_a]	0.1902E-07	9	0.2225E+01	2	0.6513E+00	68	0.1954E+02
[opt_ros4_na]	0.1906E-07	7	0.2036E+01	2	0.7403E+00	66	0.2221E+02
[opt_rodas3_na]	0.1902E-07	9	0.2630E+01	2	0.8170E+00,	68	0.2451E+02

Table 1: Results for all tests on Piz Daint.

4 Conclusions

All results are only discussed with regard to option a) first call only. This decision has been guided by the comment in footnote 4.

Discussion measurements on Piz Daint Table 1 shows the results for measurements carried out on PizDaint at CSCS. All tests led to very small erors $< 10^{-6}$. The integrator [ref2] led to results, which were approx. 3 times faster than [ref0] and more than 7 times [ref1]. Again, both tests of the new time stepping algorithm are significantly faster than the reference [ref0], also faster than [ref1] and [ref2]. Best performance was achieved with $b = 1$ and $k = 2$, which was approximately 10x faster than the reference [ref0]. Further, all QSSA tests with ICNTRL(6) = 2 or 3 were faster than the reference. All other choices for ICNTRL(6) led to very (>> reference*10) long computing times. These tests have therefore only been executed partly. The fastest results could be achieved with the parameters chosen in accordance to the poster by Taraborelli et al. [1], including a QSSA assumption (ICNTRL(6) = 2) and $\tau_{QSSA}^{max} = 1$ sec and the new time stepping control h211b with $b = 1$ and $k = 2$ in autonomous mode. Both Rodas3 and Ros4 led to comparable results in terms of performance.

References

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