# Some Case Studies for TM Integration and TM Optimization

Youn-Kyung Kim, Kyoko Makino,
Johannes Grote, and Martin Berz

Department of Physics, UIUC
Department of Physics and Astronomy, MSU

# Integration of Linear ODEs of Markus Neher

Markus Neher presented three test cases for linear ODEs which can illustrate certain aspects of validated integration. He studied with **AWA** and compared with **COSY-VI** with and without **QR Preconditioning**.

Linear ODEs are interesting because they are **easy for AWA**, and COSY-VI's advantage to handle higher order dependence on initial condition is irrelevant. But they are a **challenge for COSY-VI** because only first order terms in initial conditions appear, resulting in extreme sparsity.

We show results of other computation modes with COSY, namely curvilinear preconditioning **(PC-CV),** blunted preconditioning **(PC-BL),** and blunted shrinkwrapping **(SW-BL).**

Both codes use automatic step size control. COSY order 17, AWA order 20, and modes 1 through 4; frequently mode 4, the "intersection of QR decomposition and interval-vector" is best. All runs on a 450MHz Pentium III processor. Source code is available from Kyoko Makino

Integration was performed until $t = 1000$ or until failure for initial box

$$(1, 1, 1) + 10^{-6} \cdot [-1, 1]^3.$$

# Linear Example 1: Pure Contraction

$$B_1 = \begin{pmatrix} -0.6875 & -0.1875 & 0.08838834762 \\ -0.1875 & -0.6875 & 0.08838834762 \\ 0.08838834762 & 0.08838834762 & -0.875 \end{pmatrix} \approx \begin{pmatrix} -\frac{1}{2} & 0 & 0 \\ 0 & -\frac{3}{4} & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

| Mode | t max | Steps | Width | CPU |
|---|---|---|---|---|
| AWA #1 | 85.36 | 262 | 3.1e+1 | 1.86sec |
| AWA #2 | 1000 | 1216 | 2.5e-35 | 6.92sec |
| AWA #3 | 76.35 | 245 | 5.3e-23 | 1.71sec |
| AWA #4 | 1000 | 1216 | 1.4e-35 | 6.87sec |
| VI PC-QR | 1000 | 1437 | 1.1e-17 | 48.09sec |
| VI PC-CV | 1000 | 1386 | 9.0e-18 | 48.61sec |
| VI PC-BL | 1000 | 1410 | 1.2e-15 | 51.45sec |
| VI SW-BL | 1000 | 1423 | 1.4e-15 | 50.32sec |
| VI Naive | 713 | 14143 | 3.2e308 | 90.72sec |

## Linear Example 1: Pure Contraction

We notice in the previous example that the box width of COSY reaches about $10^{-16}$, but does not decrease further. This is because of the default value of the sweeping variable of COSY's TM arithmetic, which is set to about $2.2 \cdot 10^{-20}$. If this is set to $10^{-40}$, we obtain the following results:

| Mode | t max | Steps | Width | CPU |
|---|---|---|---|---|
| AWA #1 | 85.36 | 262 | 3.1e+1 | 1.86sec |
| AWA #2 | 1000 | 1216 | 2.5e-35 | 6.92sec |
| AWA #3 | 76.35 | 245 | 5.3e-23 | 1.71sec |
| AWA #4 | 1000 | 1216 | 1.4e-35 | 6.87sec |
| VI PC-QR | 1000 | 1633 | 3.1e-38 | 53.73sec |
| VI PC-CV | 1000 | 1463 | 4.1e-38 | 53.22sec |
| VI PC-BL | 1000 | 1620 | 3.8e-36 | 56.41sec |
| VI SW-BL | 1000 | 1726 | 6.3e-36 | 63.20sec |
| VI Naive | 713 | 14143 | 3.2e308 | 93.13sec |

# Linear Example 2: Pure Rotation

$$B_2 = \begin{pmatrix} 0 & -0.7071067810 & -0.5 \\ 0.7071067810 & 0 & 0.5 \\ 0.5 & -0.5 & 0 \end{pmatrix} \approx \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

| Mode | t max | Steps | Width | CPU |
|---|---|---|---|---|
| AWA #1 | 1000 | 2549 | 3.5e-6 | 12.69sec |
| AWA #2 | 1000 | 2549 | 3.5e-6 | 13.13sec |
| AWA #3 | 1000 | 2549 | 3.5e-6 | 12.52sec |
| AWA #4 | 1000 | 2549 | 3.5e-6 | 13.35sec |
| VI PC-QR | 1000 | 2021 | 3.5e-6 | 73.40sec |
| VI PC-CV | 1000 | 2046 | 3.5e-6 | 76.96sec |
| VI PC-BL | 1000 | 2021 | 3.5e-6 | 73.57sec |
| VI SW-BL | 1000 | 2030 | 3.5e-6 | 74.77sec |
| VI Naive | 625 | 12368 | 1.9e308 | 97.83sec |

# Linear Example 3: Contraction and Rotation

$$B_3 = \begin{pmatrix} -0.125 & -0.8321067810 & -0.3232233048 \\ 0.5821067810 & -0.125 & 0.6767766952 \\ 0.6767766952 & -0.3232233048 & -0.25 \end{pmatrix} \approx \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix}$$

| Mode | t max | Steps | Width | CPU |
|---|---|---|---|---|
| AWA #1 | 77.05 | 262 | 3.8e14 | 1.54sec |
| AWA #2 | 1000 | 3501 | 3.0e-6 | 19.23sec |
| AWA #3 | 114.15 | 340 | 2.5e14 | 2.09sec |
| AWA #4 | 1000 | 3501 | 3.0e-6 | 19.45sec |
| VI PC-QR | 1000 | 2772 | 3.0e-6 | 100.11sec |
| VI PC-CV | 1000 | 2769 | 3.0e-6 | 107.30sec |
| VI PC-BL | 1000 | 2746 | 4.7e-6 | 101.61sec |
| VI SW-BL | 1000 | 2728 | 1.2e-5 | 102.01sec |
| VI Naive | 546 | 10799 | 1.9e308 | 97.10sec |

## Linear ODE Integration - Conclusions

Studying the numerical experiments shows the following results:

- The COSY preconditiong methods based on QR, Curvilinear, and Blunting, all show qualitatively the same behavior as the QR mode of AWA. The latter is known to have error growth similar to the non-validated integration for autonomous linear ODEs. Thus the three **COSY** modes achieve the **same behavior as AWA** for these examples.
- As expected, the **naive COSY** method does not have favorable behavior, and terminates prematurely with box overflow. This is similar to the situation with the AWA parallelepiped or AWA interval vector modes.
- The number of **integration steps** of all methods are rather similar.
- The COSY **CPU times** are 5-10 times higher than those of AWA. An internal auditing shows that because these ODEs are so simple, most of the CPU time is spent in the floating point linear algebra tools. Porting of these tools to FORTRAN from COSY language (which is signficiantly more expensive for floating point arithmetic) should help substantially.

## TM Global Optimization with COSY-GO

During TM03, Youn-Kyung and Johannes showed some live runs for a 2D global optimization problem using **COSY-GO**. This was a two-dimensional projection of a six dimensional function, the so-called **normal form defect function**.

These functions and their range play an important role in stability theory, and much information can be found in the papers of the MSU group. The functions are known to have significant cancellation, which makes validated treatment **hard**. They also have very many local extrema, which makes validated treatment **a necessity**.

At TM03 we did not yet know how to run **GlobSol**, which we do now thanks to Baker. For purposes of speed, the engine to evaluate the function was ported to GlobSol from the F77 version of the COSY tools. Youn-Kyung is happy to provide the specific normal form defect function used in this study to anyone interested.

We show results for CPU time, maximum list size, and total number of investigated boxes that were studied for the problem of finding the mimimum of the function over the domain $x_i \in [-0.1, +0.1]$ for $i \leq d$, $x_i = 0.1$ for $i > d$, as a function of the dimension $d$.

## COSY-GO Results

Tolerance on the sharpness of the resulting minimum is $10^{-10}$.For the evaluation of the objective function, Taylor models of order 5 were used. For the range bounding of the Taylor models, Makino's LDB with domain reduction was being used.

| Dimension | CPU-time needed | Max list | Total # of Boxes |
|---|---|---|---|
| 2 | 5.747071 sec | 11 | 31 |
| 3 | 38.48828 sec | 44 | 172 |
| 4 | 346.8604 sec | 357 | 989 |
| 5 | 3970.746 sec | 2248 | 6641 |
| 6 | 57841.94 sec | 17241 | 49821 |

## GlobSol Results

For the computations, GlobSol's maximum list size was changed to $10^6$, and the CPU limit was set to 10 days. All other parameters affecting the performance of GlobSol were left at their default values.

| Dimension | CPU-time needed | Max list | Total # of Boxes |
|---|---|---|---|
| 2 | 18810 sec | | 4733 |
| 3 | >562896 sec (not finished yet) | | |
| 4 | >259200 sec (could not finish) | | 63446 (remaining) |
| 5 | > 86400 sec (could not finish) | | 21306 (remaining) |
| 6 | not attempted | | |

We observe that in this example, COSY outperforms GlobSol by many orders of magnitude. However, we are not completely sure if a different choice of parameters for GlobSol could result in better performance.