To : ???
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Subject : Two-way chemical reaction
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1 Two-way chemical reactions

The two-way chemical reaction simulation is taken as example to see the behaviour or the fully implicit Δ-formulation for reaction terms only. This is particularly of interest for the water quality computations with lots of processes. Example taken from Hundsdorfer and Verwer (2003).

The ODE system reads:

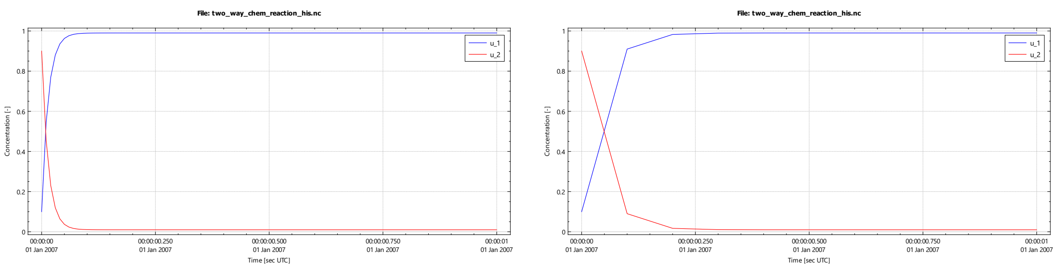
$$\frac{\partial u_1}{\partial t} = -k_1 u_1 + k_2 u_2, \tag{1}$$
$$\frac{\partial u_2}{\partial t} = k_1 u_1 - k_2 u_2 \tag{2}$$

with $k_1, k_2 > 0$ and initial values $u_1(0) = 0.1$ and $u_2(0) = 0.9$. The exact solution reads:

$$u_1(t) = \frac{k_2}{k_1 + k_2}\left(u_1(0) + u_2(0)\right) + \frac{\exp\left(-(k_1+k_2)t\right)}{k_1 + k_2}\left(k_1 u_1(0) - k_2 u_2(0)\right), \tag{3}$$
$$u_2(t) = \frac{k_1}{k_1 + k_2}\left(u_1(0) + u_2(0)\right) - \frac{\exp\left(-(k_1+k_2)t\right)}{k_1 + k_2}\left(k_1 u_1(0) - k_2 u_2(0)\right). \tag{4}$$

after a short time the term $\exp\left(-(k_1+k_2)t\right)$ is negligible.

Some results are:



(a) *Fully Implicit:* $\Delta t = 0.01$, $k_1 = 1$, $k_2 = 100$ ***(b)*** *Fully Implicit:* $\Delta t = 0.1$, $k_1 = 1$, $k_2 = 100$

Figure 1: *Result plots for constant value of* $k_1 = 1$ *and* $k_2 = 100$*, computed with a fully implicit (*Δ*-formulation) time integration method for different time steps* $\Delta t = 0.01, 0.1[s]$.

2 Numerics

Discretized

$$\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} = -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) - k_1(u_1^{n+\theta,p+1}) + k_2(u_2^{n+\theta,p+1}) \tag{5}$$

$$\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} = -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_1(u_1^{n+\theta,p+1}) - k_2(u_2^{n+\theta,p+1}) \tag{6}$$

Linearization of $\boldsymbol{u}^{n+\theta,p+1}$:

$$\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} = -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) + \tag{7}$$

$$- k_1(u_1^{n+\theta,p} + \theta\Delta u_1^{n+1,p+1}) + k_2(u_2^{n+\theta,p} + \theta\Delta u_2^{n+1,p+1}) \tag{8}$$

$$\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} = -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + \tag{9}$$

$$+ k_1(u_1^{n+\theta,p} + \theta\Delta u_1^{n+1,p+1}) - k_2(u_2^{n+\theta,p} + \theta\Delta u_2^{n+1,p+1}) \tag{10}$$

Rearrange to $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$

$$\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} + k_1\theta\Delta u_1^{n+1,p+1} - k_2\theta\Delta u_2^{n+1,p+1} = \tag{11}$$

$$= -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) - k_1 u_1^{n+\theta,p} + k_2 u_2^{n+\theta,p} \tag{12}$$

$$\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} - k_1\theta\Delta u_1^{n+1,p+1} + k_2\theta\Delta u_2^{n+1,p+1} = \tag{13}$$

$$= -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_1 u_1^{n+\theta,p} - k_2 u_2^{n+\theta,p} \tag{14}$$

3 Numerical experiment

Data used from the values mentioned in the previous sections.

Table 1: *Stability of different time integrators for the Two-way chemical reaction.*

	Time step [s]	Runge-Kutta 4	Fully Implicit Δ-formulation
1	0.01	✓	✓
2	0.1	unstable	✓

References

Hundsdorfer, W. and J. G. Verwer (2003). *Numerical solution of Time-Dependent Advection-Diffusion-Reaction Equations*. Springer.