E-10
Simulation

May 28, 2015

press release:

International call for the simulation of chemical reaction kinetics by the E-10-Simulation GmbH

Introduction:

The E-10 Simulation GmbH is about to create a new department designated for the numerical simulation of chemical reactions. In this context it is necessary to accumulate efficient simulation software in order to enter the market successfully.

Assignment: The E-10-Simulation GmbH invites all students teams (at most two students per team) to submit a simulation proposal. This proposal should include the mathematical modeling of the given problem, a choice of numerical algorithms and the evaluation of these algorithms applied to the given problem.
For more details please refer to the second page.

N. Otreal
chairman of the board
E-10-Simulation GmbH

Details of the assignment:

The goal of this assignment is the numerical simulation of the kinetics of a chemical reaction using oxyhydrogen or "Knallgas". In this reaction, a 2:1 mixture of hydrogen (H_2) and oxygen (O_2) gases ignites to create water (H_2O).
We want to model the reaction using the following chemical equations:

$$\begin{aligned}
H_2 &\xrightarrow{10^{-4}} H\cdot + H\cdot \\
H\cdot + O_2 &\xrightarrow{10^{4}} \cdot OH + \cdot O\cdot \\
\cdot O\cdot + H_2 &\xrightarrow{2\cdot 10^{-2}} \cdot OH + H\cdot \\
\cdot OH + H_2 &\xrightarrow{10^{-3}} H_2O + H\cdot \\
H\cdot + \cdot OH &\xrightarrow{10^{-3}} H_2O.
\end{aligned}$$

It can be assumed that the rate of change of the concentration of each produced substance (product) is directly proportional to the concentration of every substance participating in the reaction. The proportionality factor (the reaction speed) is given with the equations. The given time interval is $[0, 100]$ and the only substances present at the beginning are hydrogen (H_2) with a concentration of 100 and oxygen (O_2) with a concentration of 50.

The assignment can be accomplished in the following steps

- mathematical modeling of the chemical reaction using differential equations,
- choice and description of suited numerical solvers,
- implementation and comparison of the numerical solvers,
- evaluation of the results.

Submission:

Your submission should include the matlab-files as well as a presentation (pdf or powerpoint) of the results. Please save your files in a zip-file with the name "Projekt3_NAME" and send this to our consultant Christian Seifert (christian.seifert@tuhh.de) by June 17, 2015 at noon at the latest.

Scope:

The presentation should have 5 slides at most. It should include at least one slide for the modeling of the chemical reaction, one slide for the chosen numerical solvers and one slide for the comparison and evaluation of the numerical solvers. The slides will be viewed by our technical staff and should be designed in accordance to the target audience.
The matlab-code should include at least one executable file which

- adopts the numerical solvers to the problem,
- displays the numerical data, and
- plots the numerical results.