Subproject B03

# Controlled coupling of mixed integer-continuous models with modeled uncertainties

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TRR 154
Mathematical modeling, simulation, and optimization using the example of gas networks

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## Summary


- The aim of the project is the development of a new methodology for the coupling of widely different models from different physical/mathematical domains in a network.
- Therefore, a balancing of the different errors, such as model, approximation, discretisation, and model reduction errors, as well as stochastic uncertainties, should be developed using an interpretation as the backward error.
- This poster presents a perturbation analysis for two discretizations of the Euler equations in semilinear form. In order to obtain a more accurate first order upper bound for the error in the solution due to uncertainties in the input parameters, a new componentwise condition number is derived.


## Theoretical Results

Given two nonlinear systems of equations

$$F(\boldsymbol{x};\boldsymbol{d}) = 0 \qquad \text{and} \qquad F(\tilde{\boldsymbol{x}};\tilde{\boldsymbol{d}}) = 0, \tag{1}$$

with data $\boldsymbol{d}$, its perturbed values $\tilde{\boldsymbol{d}}$, and solutions $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$. We are interested in the sensitivity of the solution $\boldsymbol{x}$ with respect to perturbations in the data $\boldsymbol{d}$. Taylor series expansion gives

$$F(\tilde{\boldsymbol{x}};\tilde{\boldsymbol{d}}) = F(\boldsymbol{x};\boldsymbol{d}) + F'_{\boldsymbol{x}}(\boldsymbol{x};\boldsymbol{d})\Delta\boldsymbol{x} + F'_{\boldsymbol{d}}(\boldsymbol{x};\boldsymbol{d})\Delta\boldsymbol{d} + O(\Delta^2)$$

$$\Leftrightarrow$$

$$\begin{aligned}
F'_{\boldsymbol{x}}(\boldsymbol{x};\boldsymbol{d})\Delta\boldsymbol{x} &= -F'_{\boldsymbol{d}}(\boldsymbol{x};\boldsymbol{d})\Delta\boldsymbol{d} + O(\Delta^2) \quad \Leftrightarrow\\
\Delta\boldsymbol{x} &= -[F'_{\boldsymbol{x}}(\boldsymbol{x};\boldsymbol{d})]^{-1}F'_{\boldsymbol{d}}(\boldsymbol{x};\boldsymbol{d})\Delta\boldsymbol{d} + O(\Delta^2) \quad \Leftrightarrow\\
D_{\boldsymbol{x}}^{-1}\Delta\boldsymbol{x} &= -D_{\boldsymbol{x}}^{-1}[F'_{\boldsymbol{x}}(\boldsymbol{x};\boldsymbol{d})]^{-1}F'_{\boldsymbol{d}}(\boldsymbol{x};\boldsymbol{d})D_{\boldsymbol{d}}D_{\boldsymbol{d}}^{-1}\Delta\boldsymbol{d} + O(\Delta^2)
\end{aligned}$$

$$\Rightarrow$$

$$\|D_{\boldsymbol{x}}^{-1}\Delta\boldsymbol{x}\|_\infty \lesssim \|D_{\boldsymbol{x}}^{-1}[F'_{\boldsymbol{x}}(\boldsymbol{x};\boldsymbol{d})]^{-1}F'_{\boldsymbol{d}}(\boldsymbol{x};\boldsymbol{d})D_{\boldsymbol{d}}\|_\infty \|D_{\boldsymbol{d}}^{-1}\Delta\boldsymbol{d}\|_\infty,$$

with $\Delta\boldsymbol{x} = \tilde{\boldsymbol{x}} - \boldsymbol{x}$, $\Delta\boldsymbol{d} = \tilde{\boldsymbol{d}} - \boldsymbol{d}$, and $\lesssim$ denoting "less than or equal to except for higher order terms". Hence, the *componentwise relative condition number* of the nonlinear system $F = 0$ in (1) is given by

$$\kappa_{\text{rel,c}}(\boldsymbol{x};\boldsymbol{d}) = \|D_{\boldsymbol{x}}^{-1}[F'_{\boldsymbol{x}}(\boldsymbol{x};\boldsymbol{d})]^{-1}F'_{\boldsymbol{d}}(\boldsymbol{x};\boldsymbol{d})D_{\boldsymbol{d}}\|_\infty. \tag{2}$$

On the other hand, the *normwise relative condition number*

$$\kappa_{\text{rel,n}}(\boldsymbol{x};\boldsymbol{d}) = \frac{\|[F'_{\boldsymbol{x}}(\boldsymbol{x};\boldsymbol{d})]^{-1}F'_{\boldsymbol{d}}(\boldsymbol{x};\boldsymbol{d})\|\|\boldsymbol{d}\|}{\|\boldsymbol{x}\|}$$

is given in [1, 2]. Taking the infinity norm yields the inequality

$$\kappa_{\text{rel,c}}(\boldsymbol{x};\boldsymbol{d}) \leq \kappa_{\text{rel,n}}(\boldsymbol{x};\boldsymbol{d}),$$

due to the sub-multiplicativity of the infinity norm.

## Application to Gas Flow Simulation

A model hierarchy is used to control the different errors. As an example, we consider the Euler equations in semilinear form, given by

$$\begin{aligned}
\frac{\partial p}{\partial t} + \frac{c^2}{A}\frac{\partial q}{\partial x} &= 0,\\
\frac{\partial q}{\partial t} + A\frac{\partial p}{\partial x} &= -\frac{\lambda c^2}{2DA}\frac{q|q|}{p},
\end{aligned}$$

with *mass flow rate* $q = A\rho v$. Applying a two-point discretization in space and the implicit Euler method in time results in the nonlinear system

$$\begin{aligned}
F_1(\boldsymbol{x}^i,\boldsymbol{d}) &= \frac{1}{\tau}(x_1^i - x_1^{i-1}) + \frac{c^2}{AL}(q_s^i - x_2^i) = 0,\\
F_2(\boldsymbol{x}^i,\boldsymbol{d}) &= \frac{1}{\tau}(x_2^i - x_2^{i-1}) + \frac{A}{L}(x_1^i - p_s^i) + \frac{\lambda c^2}{2DA}\frac{x_2^i|x_2^i|}{x_1^i} = 0,
\end{aligned}$$

with $\boldsymbol{x}^i = [p_R^i, q_L^i]^T$ and $\boldsymbol{d} = [A, \lambda, D, c, p_s^i, q_s^i, x_1^{i-1}, x_2^{i-1}]^T$, called the *1S-scheme*. Using the midpoint rule in space yields the *MP-scheme*. Applying condition number (2) on these two nonlinear systems results in the following figure.

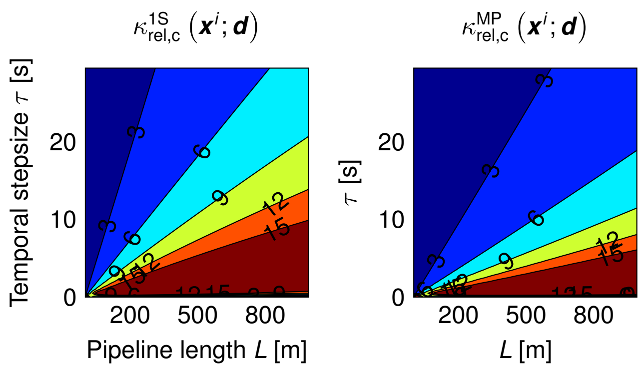


Figure 1. *Contour graphs for the condition number (2) of the 1S- and the MP-schemes as a function of L and τ.*

Using these results, a compromise between the discretization and the data uncertainty error can be made.

## References


[1] N. Higham, *Accuracy and Stability of Numerical Algorithms*, SIAM, Philadelphia, PA, second ed., 2002.

[2] H. Woźniakowski, *Numerical stability for solving nonlinear equations*, Numer. Math., 27 (1976), pp. 373–390.

[3] J. J. Stolwijk and V. Mehrmann, *Error analysis and model adaptivity for flows in gas networks*, in preparation.