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Numerical Analysis of Higher-Order Singularities in Complex Chemical Process Models in ProMoT

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Abstract

In this contribution, a tool is presented that allows the continuation of singularities of higher codimension also for complex chemical process models. The tool is an extension of the process-modelling tool ProMoT. It allows creating analytically augmented systems for singularity points with currently codimension up to 2. Required higher order directional derivatives up to the third order are obtained analytically via an interface to the computer algebra system Maxima.

Keywords: nonlinear analysis, singularity theory, bifurcation, augmented system.

1. Introduction

Chemical production processes often show a strongly nonlinear behaviour. Understanding, controlling, or even exploiting this behaviour can improve the productivity and safety of a process. Numerical singularity analysis has become a well-established mathematical tool for the nonlinear analysis of process models. One objective of singularity analysis is to find the singular point with highest possible order, the so-called organizing centre, because in the neighbourhood of the organizing centre the system shows all possible types of qualitative steady state behaviour. Therefore, knowledge about the most degenerate points can be considered as a full description of the qualitative system dynamics. Nowadays a lot of different tools for bifurcation analysis exist, such as AUTO (Doedel et al., 2002), CONTENT (Kuznetsov and Levitin, 1997), Diva (Häfele et al., 2003), etc. But these tools only offer continuation methods for low order singularities such as limit points and cusps. In literature also some tools can be found, which allow to find singular points of higher order, for example in Govaerts (1997) and Gehrke and Marquardt (1997). However, these tools are applicable only to systems of low order and low complexity.

In this contribution the development of a new general-purpose singularity analysis tool is reported. It is applicable to complex chemical engineering process models, and allows automatic generation of augmented systems for degenerate singularities. The

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user is able to use this tool without detailed knowledge of singularity theory, and without having to change his or her model.
The tool is based on the process-modelling tool ProMoT that serves as a model generation engine. ProMoT is used to create models and to generate compilable source code of the model and of additional equations defining the singularity conditions. The required symbolic derivatives are obtained via a link to the computer algebra system Maxima.
Some basic facts from singularity theory are stated in the second section of this contribution. The third section describes the predictor-corrector continuation methods that are used for computing the solution manifolds of the nonlinear systems. The last two sections treat the implementation of the tool and the application of the singularity theory approach to a fuel cell model.

2. Some facts from singularity theory

Singular analysis of a system $F(\underline{x},\lambda)=\underline{0}$ ($F: R^N \times R \to R^N$, $\underline{x} \in R^N$, $\lambda \in R$) allows finding the most degenerate point in the parameter space. In neighbourhood of such a point, all possible types qualitative nonlinear behaviour can be found. In this sense, the most degenerate singular point gives a global description of the qualitative system dynamics.

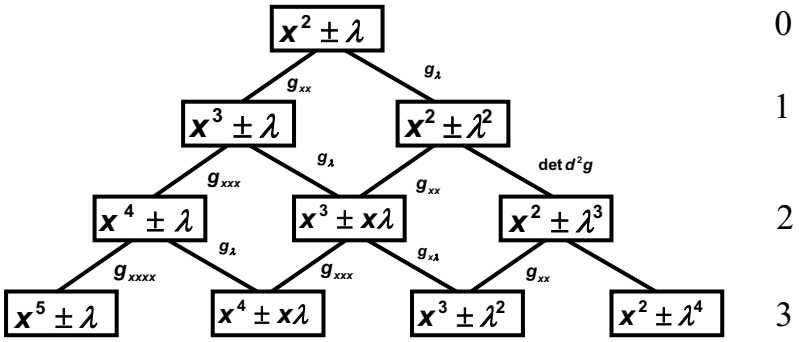

Figure 1. Normal forms hierarchy

Singularity analysis can be done with the help of the Lyapunov-Schmidt reduction as described in Golubitsky and Schaeffer (1985). The Lyapunov-Schmidt reduction allows to reduce a model to a low-order system having locally the same qualitative behaviour. For each type of bifurcation, there exists a simplest representative form, the so-called normal form, that is equivalent to a whole class of bifurcation problems. An example for a hierarchy of normal forms is presented in figure 1. It shows singularities with codimension up to 3, such as limit point, hysteresis, isola, pitchfork, etc. Derivatives of the normal form g on the edges of the graph are singularity conditions, which have to be satisfied for the given type of singularity. Because of the degeneracy of the singularity points, the computation of such points cannot be performed directly. Instead, augmented systems of equations have to be created, so that singular points of a special type are regular solutions of these systems. In this work, the regularization proposed by

Kunkel (1991) is used, which leads to a system of $3N+2$ equations for a limit point, where N is the order of the original system. Increasing the codimension of a singular point by one also requires the solution of one additional equation.

3. Numerical continuation method

For tracking solutions of underdetermined systems of the form $F(\underline{x},\lambda)=\underline{0}$ predictor-corrector continuation method can be used. Such a system is obtained from an implicit dynamical system $G(\underline{x},\dot{\underline{x}},\lambda)=\underline{0}$ ($G: R^N \times R^N \times R \to R^N$, $\dot{\underline{x}} \in R^N$) under the steady state condition $\dot{\underline{x}}=\underline{0}$. The main continuation step consists of two substeps – the corrector step and the predictor step. Below, for the extended state vector $\{\underline{x},\lambda\}$ the notation $\underline{y}$ is used.

3.1. Predictor step

Two approaches are used for the predictor step: the chord predictor and the tangent predictor (see figure 2). The chord predictor is an extrapolation of two previously computed points of the solution curve, so on step k predictor vector $\underline{T}_k$ will be $\underline{T}_k = \underline{y}_k - \underline{y}_{k-1}$. The tangent predictor can be obtained by solving the linear algebraic problem $\underline{T}_k = F_y(\underline{y}_k)^{-1} \cdot \underline{e}_n$, where $\underline{e}_n$ is a unit vector with one in the n^{th} position.

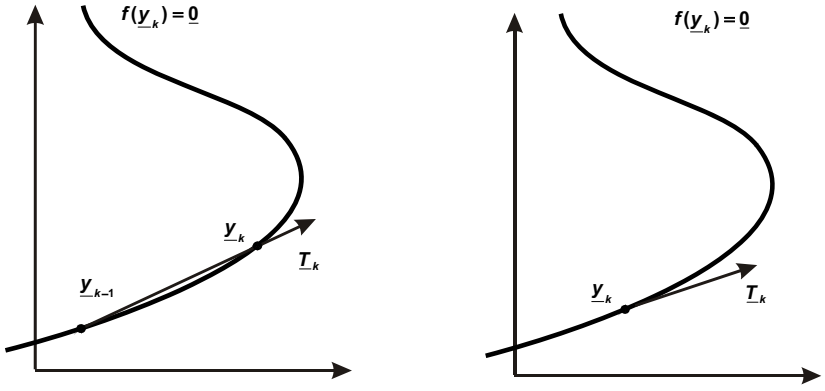

Figure 2. Chord and tangent predictors

After normalization of the predictor vector $\underline{T}_k$, the initial point $\hat{\underline{y}}_{k+1}$ for the corrector step will be equal to $\underline{y}_k + \sigma \cdot \underline{T}_k$ with a variable step size σ. The step size is increased by some predefined factor, if the Gauss-Newton method of the corrector step converges and if the amount of Newton iterations is less than a specific number. Otherwise the step size is reduced and the step is rejected.

3.2. Corrector step

The Gauss-Newton corrector used to find the exact solution point starting from the approximation of the predictor step. To make the underdetermined system uniquely solvable a suitable parameterization of the solution curve is required. Here local and

pseudo-arclength parameterization are used. For the local parameterization (see left in figure 3) the additional equation $u(\underline{y}) = \underline{y}^i - \underline{\hat{y}}^i_{k+1}$ is used, i.e. the state variable with index i is not varied in the corrector step. In the case of pseudo-arclength parameterization, the corrector tries to find the exact solution on a hyper-surface orthogonal to the predictor vector $\underline{T}_k$. This is defined with the help of the relation $u(\underline{y}) = (\underline{y} - \underline{y}_k, \underline{T}_k) - \sigma \cdot$

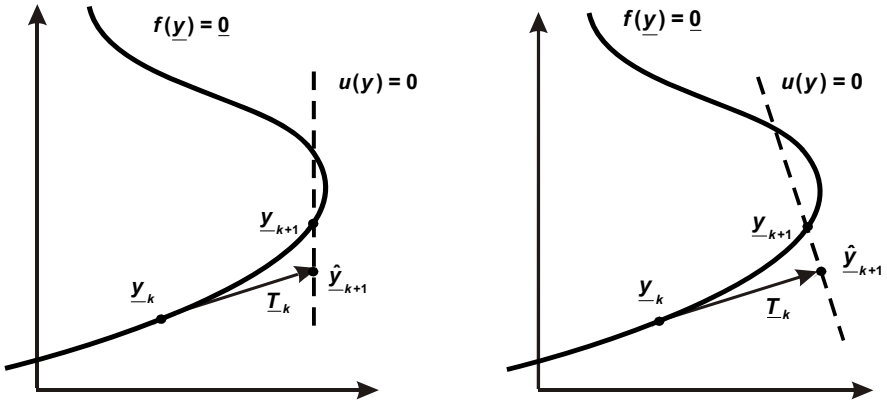

Figure 3. Local and pseudo-arclength parameterisations

4. Implementation

An implementation of the algorithms described above consists of three main steps: the generation of the augmented system of equations in symbolic form, the translation of the symbolic equations into compilable code, and the application of numerical continuation methods.

The original model equations have to be implemented in ProMoT. The generation of the augmented systems requires high order derivatives. These are obtained using symbolic differentiation methods in the computer algebra system Maxima. To this purpose, an interface between ProMoT and Maxima was created. A certain disadvantage of symbolic differentiation is currently the big size of source code for complex distributed models, which is caused by the unrolling of complex loops. However, symbolic differentiation has to be used here instead of automatic differentiation, because for the analysis of chemical process models high order derivatives in sparse matrix form are needed. To our knowledge, such derivatives cannot be provided by automatic differentiation tools like ADIFOR, ADOLC, CppAD etc. Furthermore, the Maxima based approach proposed here avoids an object oriented overloading of methods, as is used by other tools. This significantly increases the calculation speed and decreases the size of allocated memory.

The augmented system of equations is converted by ProMoT into executable code with a CAPE-ESO interface (CAPE-OPEN, 1999) that can be used for numerical analysis. The numerical continuation methods implemented in this work are based on the predictor-corrector algorithms described above. They are realized as a C++ continuation

class and are applicable to any model with a CAPE-ESO interface. The continuation methods make use of the Gauss-Newton method in the numerical library PETSc (Satish, 2004) and of the linear solver in UMFPACK (Davis, 2004). An exchange of the linear and nonlinear solvers by other methods is easily possible.

5. Application example

As an application example of the singularity analysis tool, a spatially distributed model of a high temperature fuel cell is considered. The model consists of spatially one-dimensional mass, charge and energy balances. Details of the model can be found in Mangold et al. (2004). After spatial discretization, the model consists of 201 algebraic and 200 ordinary differential equations. Figure 4 shows results of a bifurcation analysis of the model.

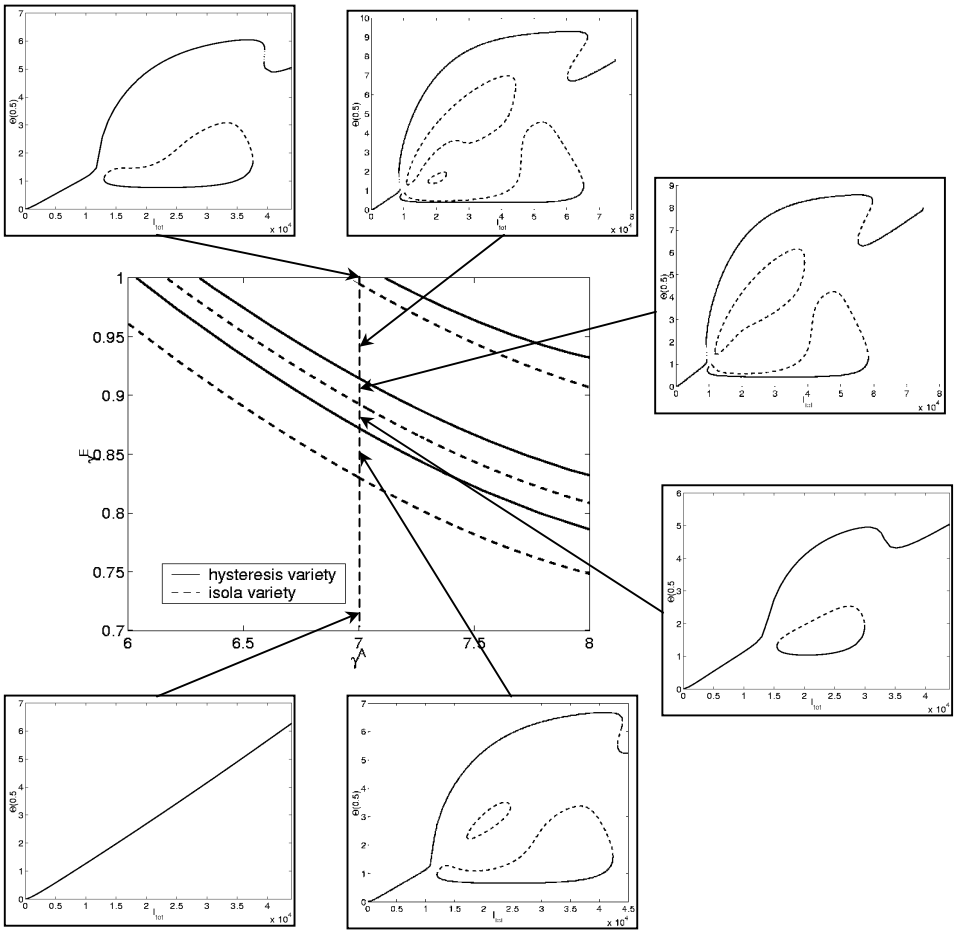

Figure 4. One-parameter continuation of steady states with continuation parameter I_{tot}

Depending on the activation energy of the electrochemical reaction and on the temperature dependence of the electrical conductivity, a wealth of nonlinear phenomena is found, including hysteresis varieties and isola varieties. The singularities are

responsible for hot spot formation in the cell. Therefore, the results of the nonlinear analysis give important hints on the process operation of a high temperature fuel cell.

6. Conclusions

In this contribution a tool for singularity analysis was developed. The tool is an extension of the process modelling tool ProMoT. It is applicable to detailed models of chemical processes, including complex plant models of high order and spatially distributed models. The tool automatically generates the augmented equation systems necessary for the computation of high order singularities using symbolic differentiation. Currently augmented systems for degenerate bifurcation up to singularity codimension two can be generated. A numerical continuation tool has been developed that proves to solve the augmented systems robustly and efficiently. The tool is embedded into the ProMoT/Diva simulation environment for the dynamical analysis of chemical engineering plants. It was applied successfully to a detailed spatially distributed model of a fuel cell.

In the future, it is planned to extend the tool to higher order real bifurcations. This involves the creation of conditions for more degenerate cusps and folds. In a next step, the analysis of complex bifurcations will be included into the tool. This requires the generation of augmented systems for Hopf and degenerate Hopf bifurcations.

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