On the use of Reduced Order Models in Bifurcation Analysis of Distributed Parameter Systems

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Abstract

Bifurcation theory provides a powerful tool for analyzing the nonlinear dynamic behavior of process systems. However, although the theory in principle applies to lumped as well as distributed parameter processes, it is in practice necessary to reduce the order of distributed (PDE) models prior to application of the theory. In this paper we consider the problem of determining an appropriate model reduction method for this task. We first show that simply applying some *ad hoc* discretization method, such as finite differences or finite elements, can result in spurious bifurcations and erroneous predictions of stability. To avoid this problem we propose a method for estimating the error introduced by the model reduction. Apart from simply providing a label of confidence in the obtained results, the estimated error can be used to improve the model reduction. We here propose a method based on moving the discretization mesh such as to spatially equidistribute the total error. The method is applied to the analysis of a heat-integrated fixed bed reactor.

1 Introduction

The problem we consider in this paper is the determination of the possible stationary dynamic behaviors of a given distributed parameter dynamic system described by a set of 1-D partial differential equations, here written on the explicit 2nd order form

$$u_t = F(t, x, u, u_x, u_{xx}, p) \tag{1}$$

with appropriate initial and boundary values. The independent variables t and x denote time and position, respectively, and p is a set of system parameters. Extension to higher dimensional systems is relatively straightforward, but we restrict ourselves to 1-D models here in order to keep the exposition at a reasonable level.

By applying a homotopy method combined with continuation and bifurcation analysis, it is possible to trace out all possible behaviors of the system (1). *Homotopy methods* are used to determine all possible steady-state solutions for a given value of the parameters p. Starting at these steady-states, *continuation* can then be used to trace out the branches of steady states as a function of the parameters p. *Bifurcation analysis* implies monitoring the eigenvalues of the linearized model along the branches of steady-states, and determining those points where eigenvalues cross the imaginary axis. Such points are called bifurcation points, and bifurcation theory ensures that around such points a system locally has more than one stationary solution. Two commonly encountered types of bifurcations

are Saddle-Node bifurcations (SN), in which a single real eigenvalue crosses the imaginary axis, and Hopf points (HB), in which a complex conjugate pair of eigenvalues cross. Around a Saddle-Node point the system possesses multiple steady-states and around a Hopf point the system possesses a limit cycle coexisting with a steady-state. When Hopf points are encountered, the resulting limit cycles can be traced as a function of the parameters p using continuation and bifurcation analysis as outlined for steady-states above. For an introduction to numerical continuation and bifurcation analysis, see e.g., Seydel (1994).

The analysis method as outlined above is quite standard for the case of finite dimensional systems, i.e., systems described by ordinary differential equations (ODE). Powerful software available for this task include for instance AUTO (Doedel, 1997). For the case of PDEs, however, the problem is somewhat more involved. First, steady-states can be solved without lumping (discretization) by simply solving the boundary value ODE problems resulting when $u_t = 0$ in (1). Similarly, the eigenvalues of steady-state solutions can in principle be computed by linearizing the corresponding PDE and solving the eigenvalue problem. However, due to the existence of, in general, a countable infinity of eigenvalues it is not trivial to determine a bifurcation point. Rather, bifurcation points is best determined by an inverse problem formulation in which some eigenvalue(s) are forced to exist on the imaginary axis, and the eigenvalue problem is solved with respect to the corresponding parameters p. Finally, in order to trace out limit cycles, and determine their bifurcations, it is in general required to apply some form of model reduction of the PDE, so as to obtain a finite set of ODEs. Because of the heavy computational burden associated with continuation and bifurcation analysis of limit cycles, it is usually required that the reduced order model is of relatively low order. For instance, with AUTO, a typical practical limit is models of orders around 50-60.

In practice, when performing bifurcation analysis of distributed parameter processes, model reduction is usually applied prior to performing bifurcation analysis of steady-states as well as limit cycles. Usually some *ad hoc* method, such as finite differences, orthogonal collocation or finite elements, is used for the discretization, or model reduction. In most cases also the order of the reduced model is chosen more or less *ad hoc*. The problem with this approach, however, is that it is difficult to determine to what extent the obtained results can be attributed to the underlying PDE.

In this paper we illustrate, through a reaction-convection-diffusion problem, some potential pitfalls in employing an *ad hoc* discretization method for bifurcation analysis of distributed parameter systems. We then propose a method in which the error introduced by the discretization can be estimated and monitored. In order to reduce the model order required for a given level of accuracy, we also propose to control the discretization mesh dynamically so as to minimize the error.

2 Example Process

As an example process we will consider a reaction-convection-diffusion process, in the form of an adiabatic fixed-bed reactor in which the effluent is used to preheat the feed.

The dimensionless pseudohomogeneous model is

$$\sigma \frac{\partial \alpha}{\partial \tau} = -\frac{\partial \alpha}{\partial z} + \frac{1}{Pe_m}\frac{\partial^2 \alpha}{\partial z^2} + Da\ R(\alpha, \theta) \tag{2}$$

$$\frac{\partial \theta}{\partial \tau} = -\frac{\partial \theta}{\partial z} + \frac{1}{Pe_h}\frac{\partial^2 \theta}{\partial z^2} + Da\ R(\alpha, \theta) \tag{3}$$

where α is the conversion and θ a dimensionless temperature. The reaction term is given

by

$$R(\alpha,\theta) = (1-\alpha)^r exp\left(\gamma \frac{\beta\theta}{1+\beta\theta}\right) \tag{4}$$

The boundary conditions are

$$\alpha(0,\tau) = \frac{1}{Pe_m}\frac{\partial\alpha}{\partial z}|_{z=0}\,; \quad \theta(0,\tau) = f\theta(1,\tau) + \frac{1}{Pe_h}\frac{\partial\theta}{\partial z}|_{z=0} \tag{5}$$

$$\frac{\partial\alpha}{\partial z}|_{z=1} = 0\,; \quad \frac{\partial\theta}{\partial z}|_{z=1} = 0 \tag{6}$$

where f represents the efficiency of the effluent-feed heat-exchange. See also Jacobsen and Berezowski (1998). We will here consider the reactor behavior as a function of the Damkohler number Da (reactor size). Thus, we fix all other parameters as $\sigma = 0.001, \quad Pe_h = Pe_m = 200, \quad \gamma = 15, \quad r = 2, \quad \beta = 0.4, \quad f = 0.3$.

3 Model Reduction using Finite Elements

As stated above, the steady-state bifurcation diagram for the model (2)-(6) can in principle be determined without performing any prior model reduction, i.e., spatial discretization, of the PDE model. However, determination of the bifurcation points via the eigenvalue equations is computationally quite involved, and furthermore not the common approach to this problem. Neither are we aware of any available software packages that offers this possibility. Here we therefore adopt the typical approach, and hence choose some standard discretization method to reduce the PDEs (2)-(3) into a set of ODEs, prior to performing continuation and bifurcation analysis. For the model reduction we choose to employ orthogonal collocation on finite elements (Carey and Finlayson, 1975), and use 4 elements, each with collocation based on polynomials of order 5. This results in a model containing a total of 38 ODEs.

We employ AUTO (Doedel, 1997) for continuation and bifurcation analysis of the resulting ODE model. The continuation is in this case started at the trivial unique extinguished steady-state solution for $Da = 0$. Figure 1 shows the resulting bifurcation diagram in terms of the conversion at the outlet of the reactor as a function of the parameter Da. In the figure, solid lines denote stable steady states and dashed lines unstable steady-states. As seen from the figure, the reactor undergoes two saddle-node bifurcations (SN) and a total of ten Hopf bifurcations (HB). The periods of the limit cycles born at the Hopf points are predicted to approximately 1.0 (HB1), 0.5 (HB2), 0.33 (HB3) and 0.25 (HB4), where the time unit equals the thermal residence time in the bed. The steady-state of the reactor is found to be unstable for Da above 0.1.

It is tempting to assume that the above results can be attributed to the original PDE model. However, the problem here, as in most similar problems, is that we do not have any clear idea about how well our reduced order model fits the original PDE model. In fact, it is well known from numerical analysis that discretization can introduce instability in an otherwise stable problem. Thus, it is not obvious whether the stability properties and bifurcations predicted using the discretized model should be attributed to the underlying PDE or the discretization method. Since this is essential knowledge, we should be able to somehow monitor the accuracy of our reduced order model as we perform continuation. In the next section we discuss how this can be done in a relatively simple way.

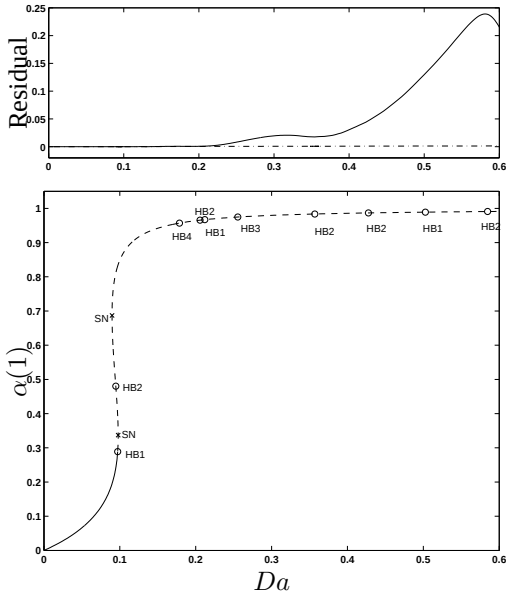

Figure 1: Bottom: steady-state bifurcation diagram for reactor with fixed mesh discretization. Outlet conversion $\alpha(1)$ as a function of the reactor size Da. Solid (dashed) lines denote stable (unstable) steady-states. Top: residuals from model reduction with fixed (solid) and moving (dashdotted) mesh.

4 Error Estimation and Control

One important motivation for choosing orthogonal collocation on finite elements for the model reduction above was, apart from its efficiency, that it is quite straightforward to calculate the residuals of the original PDEs at non-collocation points.

To discretize equation (1), introduce the notation $x_{ij}, i = 1, \cdots n, j = 1, \cdots m+2$ for the computational mesh, in which n and m denote the number of elements and their interior nodes, respectively. Apply the collocation method within each element, i.e.,

$$u_{ij}(t) \stackrel{\text{def}}{=} u(x_{ij}, t) = \sum_{p=1}^{m+2} l_{ip}(x_{ij}) u_{ip}(t) \tag{7}$$

where l_i is the $(m+1)$-th order Lagrange polynomial in element i. The elements are here connected by letting $u_{i1} = u_{i-1,m+2}$.

The approximation error within each element can now determined from residual computations, i.e., by substituting the approximate solution (7) into the original PDE (1) at selected non-collocation points. We here evaluate the residuals at the midpoints between the collocation points $\hat{x}_{ir}, r = 1, \ldots, m+1$. Define the (m+1) by (m+2) matrix $\hat{Q}_{rj} = l_{ij}(\hat{x}_{ir})$. We then have

$$\hat{u}_{ir} \stackrel{\text{def}}{=} u(\hat{x}_{ir}, t) = \sum_{j=1}^{m+2} l_{ij}(\hat{x}_{ir}) u_{ij} = \sum_{j=1}^{m+2} \hat{Q}_{rj} u_{ij}$$

Using the formulation (1), the residuals at $\hat{x}_{ir}$ can now be computed directly from values

of u_{ij} on the computational grid

$$\hat{R}_{ir} = \hat{\dot{u}}_{ir} - \hat{F}_{ir} = \sum_{j=1}^{m+2} \hat{Q}_{rj} \dot{u}_{ij} - \hat{F}_{ir}$$

where F is the RHS of the original PDE (1). An overall integral residual can now be computed, using e.g., quadrature, based on the non-collocation points. Note that the computational load involved in computing the residual this way is negligible compared to the computations involved in the continuation and eigenvalue calculations of the bifurcation analysis.

By computing the residual as outlined above, it is possible to monitor the accuracy of the model reduction, which in general will vary as the model parameters are varied. The residuals for the bifurcation analysis performed for the fixed bed reactor above are shown at the top of Figure 1. As seen from the figure, the residual is relatively small for small values of the parameter Da, but increases significantly for values of Da larger than 0.21. The residual computations thus indicate that the results for high Da values may be significantly affected by the model reduction.

When the residuals exceed a certain threshold value, one remedy may be to increase the order of the reduced model, e.g., by increasing the number of elements and/or the polynomial order. However, as proposed in Liu and Jacobsen (2001), one may also utilize the information contained in the residuals to adopt the mesh to the underlying PDE solution. They propose to move the mesh dynamically with the aim of spatially equidistributing the total residual. An inherent assumption is that the error is kept close to minimum by equidistributing the residual, which seems reasonable. The method is based on simple PI-control using the size of the different elements as manipulated variables, and adds a total of $n-1$ ODEs to the reduced order model, where n is the number of elements. Note that this method in general yields very different results than would be obtained by simply adapting the mesh statically to the underlying steady-state solution, as is done in most adaptive mesh methods. For details of the method, we refer to Liu and Jacobsen (2001).

Figure 2 shows the resulting steady-state bifurcation diagram for the example reactor when residual control as discussed above is employed. Note that the steady-state solutions are quite similar to those obtained with the fixed mesh in Figure 1, but that the stability properties and bifurcations differs significantly for high Da values. In particular, we now find that the reactor is stable for all Da values above 0.25. As seen from Figure 1, this is also around the region where the residual for the fixed mesh model starts to increase significantly. However, as seen from the the dash-dotted line in Figure 1, the residual for the moving mesh model is kept relatively small for all values of Da. Indeed, by computing the bifurcation points from the original PDE (using continuation of the corresponding eigenvalue problem), we find that the bifurcations and stability as predicted by the moving mesh model differs only slightly from the true values. For instance, the true region of steady-state instability is for $Da \in [0.097\ 0.026]$, while the instability region predicted with the moving mesh is $Da \in [0.098\ 0.25]$. The fixed mesh discretization, however, predicted instability for all $Da > 0.098$. From the eigenvalue calculations we also find that the original PDE model has exactly the four Hopf bifurcations predicted by the moving mesh model, and thus the fixed mesh model has a total of six spurious bifurcation points.

We finally note that the proposed method of residual monitoring and control of course also may be used for continuation and bifurcation analysis of limit cycles born at Hopf points. However, this is not included here due to space limitations.

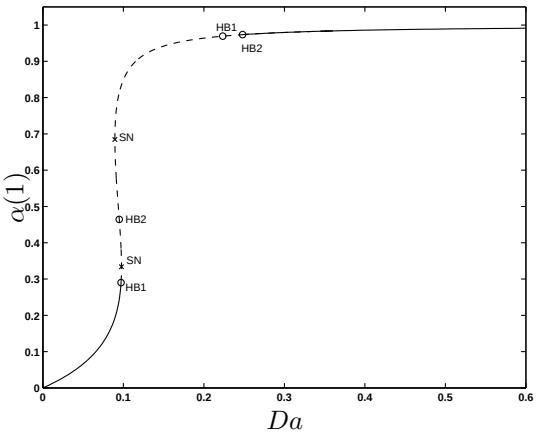

Figure 2: Bifurcation diagram for reactor with moving mesh discretization. The corresponding residuals are shown in Figure 1.

5 Conclusions

We have in this paper stressed that care should be exercised when performing bifurcation analysis based on discretized PDE models. In order to obtain a label of quality along with the results of the bifurcation analysis, we proposed a method based on orthogonal collocation on finite elements with a relatively simple evaluation of the resulting residuals. We also proposed that the residuals should be used to move the discretization mesh in order to minimize the residual. The usefulness of both the residual monitoring and control was demonstrated by application to the model of a heat integrated fixed bed reactor.

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