Parallel Bifurcation Analysis of Discontinuous Periodically Forced Reactors

Artur Grabski[1], Lucia Russo[2] and Gaetano Continillo[1]
[1]Department of Engineering, Università del Sannio, Benevento, Italy
[2]Department of Chemical and Food Engineering, Università di Salerno, Italy

Corresponding author, G. Continillo: continillo@unisannio.it

Introduction

Periodic forcing of chemical processes, as a means to obtain better average performance compared to steady–state operation, has been extensively addressed for a long time (starting from Bailey, 1973). For example, in the last 30 years, the real advantages of forced unsteady–state operation over conventional steady-state regimes of catalytic fixed–bed reactors have been widely supported, and processes involving reversible exothermic reactions perform better in a Reverse Flow Reactor (RFR) configuration, compared to traditional multi stage fixed–bed arrangements (e. g. Matros and Bunimovich 1996). When used for catalytic combustion, periodical inversion of the flow traps the high–temperature region in the reactor.

Rational design and operation of a RFR requires efficient prediction of the prevailing regimes and accurate detection of multistability conditions. The regime sought for these dynamically forced systems is, usually, a periodic solution with the same period of the forcing. This is considered the most reliable operation condition. However, depending on the operating or design parameters, these reactors can show a rich dynamical response. Indeed, it has been shown that multiperiodic, quasi-periodic or even chaotic regimes can be attained (e. g. Řeháček *et al* 1998). Recently, frequency locking was also detected (Mancusi *et al* 2004).

In this work we propose a new approach to a parallel continuation algorithm for periodically–forced systems with time–discontinuous forcing. The approach is based on parallelising the numerical computation of the Jacobian derivatives, that is by far the most expensive task in the analysis for such systems. The example of a Reverse Flow catalytic combustor (taken from Mancusi *et al* 2003) is presented first, then the rationale of the new approach is briefly outlined, and finally speedup results are reported regarding computation conducted on up to 8 nodes on a Linux cluster. The resulting procedure opens to detailed bifurcation analysis a class of distributed models resulting into large systems of ODEs, which could be otherwise untreatable.

Tubular catalytic reactor

The catalytic reactor was studied earlier by Mancusi *et* al (2003). The model describes the two–phase catalytic system, axial dispersion in both phases, external cooling. The dimensionless mass and heat balances, considering the first order reaction in the solid catalyst phase, are presented in Table 1. Here the quantities are: α conversion, θ temperature, Pe Peclet number, St Stanton number, β heat of reaction, γ activation energy, ξ spatial coordinate, τ time coordinate, T period of the forcing. Conventional Danckwerts boundary conditions are assumed for both phases.

Figure 1 presents the solution diagram obtained by varying the switch time (T), including stable and unstable steady states and two pitchfork bifurcation points. Starting from low values of the period, the symmetric solutions is stable (Russo *et al*., 2002) until the pitchfork

bifurcation is found. By further increasing the inversion period, a second pitchfork bifurcation is encountered and the unstable symmetric solution regains stability. The computation of this diagram takes several hours on a 1 GHz PC.

Table 1. Model equations.

$$\frac{\partial \alpha}{\partial \tau} + \left(2g(\tau) - 1\right)\frac{\partial \alpha}{\partial \xi_R} = \frac{1}{Pe_M}\frac{\partial^2 \alpha}{\partial \xi_R^{\,2}} + \phi(\alpha, \theta_S) \;,\; g(\tau) = \begin{cases} 1 & if\ \tau/T \bmod(2) < 1 \\ 0 & if\ \tau/T \bmod(2) > 1 \end{cases}$$

$$\frac{\partial \theta_G}{\partial \tau} + \left(2g(\tau) - 1\right)\frac{\partial \theta_G}{\partial \xi_R} = \frac{1}{Pe_H}\frac{\partial^2 \theta_S}{\partial \xi_R^{\,2}} + St(\theta_S - \theta_G) + \delta(\theta_H - \theta_G)$$

$$\sigma\frac{\partial \theta_S}{\partial \tau} = \frac{1}{Pe}\frac{\partial^2 \theta_S}{\partial \xi_R^{\,2}} + \phi(\alpha, \theta_S) + St(\theta_G - \theta_S) \;; \qquad \phi(\alpha, \theta_S) = Da(1-\alpha)\exp\left(\gamma\frac{\beta\theta_S}{1+\beta\theta_S}\right)$$

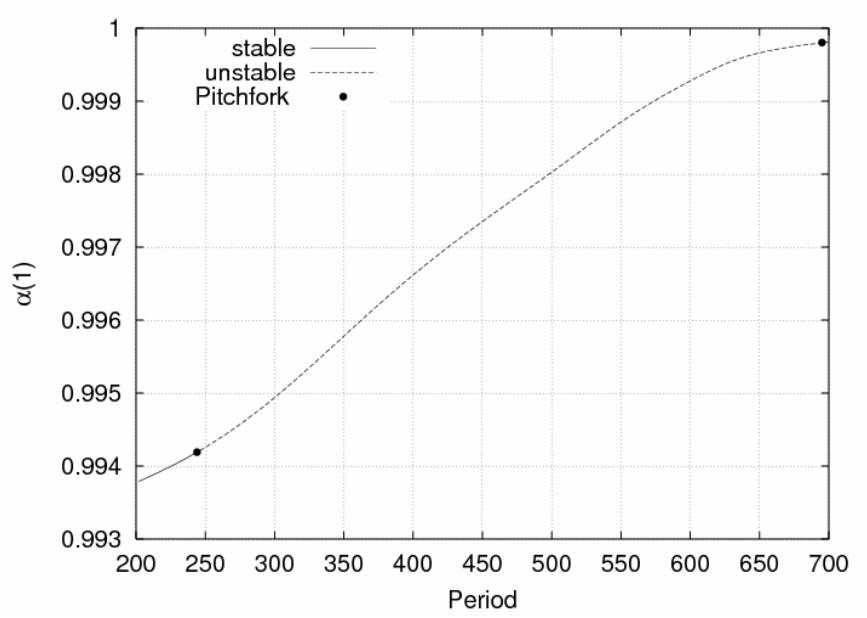

Figure 1. Solution diagram.

Parallel approach

Bifurcation analysis of periodically forced dynamical systems with discontinuities, such as Reverse Flow Reactors, cannot be conducted by standard parameter continuation. Various techniques have been proposed in the literature. The most general (Mancusi *et al*, 2003) consists of studying a discrete–time system constructed by means of a suitable map (often the Poincaré map) derived from the time continuous model. This map yields the state of the system after one period of the forcing (for a RFR, this corresponds to twice the switch time). Due to the complexity of the model, the map must be computed numerically. The analysis

also requires computation of the Jacobian matrix. Obviously, the best way to operate would be to involve analytical derivatives. Unfortunately, for the model of the Reverse Flow Reactor as well as for a whole class of discontinuously forced dynamical systems, the analytical form of the flow is not available and therefore it is impossible to obtain the partial derivatives analytically. For an autonomous system, numerical computation of the partial derivatives would just imply the evaluation of the right–hand sides with perturbed values (backward and forward) of each of the n state variables. The results of these computations are used to evaluate the derivatives by means of second–order finite difference operators. For a non–analytical Poincaré map, the computation of the right–hand side requires two time integrations over the period of forcing, with perturbed initial conditions for each of the n state variables and each of the n ODEs. For such systems, the numerical computation of the Jacobian alone takes an overwhelming fraction of CPU time, close to 100% of the total time required. This huge computational load poses serious limitations on the feasibility of a comprehensive bifurcation analysis.

A significant improvement can be achieved by running these computations in parallel. Since these simulations are independent, they can be run on different processors. The data exchange between the processes is relatively small (only the initial conditions and the state vector at the end of the integration. Moreover, since almost 100% of the algorithm can be run in parallel, Amdahl's law indicated a very good expected speedup.

The idea was developed using the free bifurcation code AUTO97 (Doedel *et al.*, 1997) slightly modified to make use of the MPI library for parallel computing. The software run on a Linux cluster equipped with ROCKS 3.2.0 operating system and LAM-MPI 7.0.6 (Burns *et al.*, 1995). The hardware is composed by one 3.2 GHZ 1 GB RAM node as the front-end, five 1.8 GHZ 500 MB RAM nodes and one double processor 2.6 GHZ 2 GB RAM node. Table 2 reports CPU time as a function of the No. of nodes, also shown in the speedup line (Fig 2). The speedup is defined as (CPU time on one node)/(CPU time on N nodes). In Fig. 2 the theoretical speedup line is drawn by assuming that the code is 100% parallel – which is not the case. Table 2 is compatible with full parallel speedup on a code with parallel portion greater than 97% (Amdahl's law).

Table 2. CPU time consumption as a function of the number of processors.

Number of processors	Time elapsed (seconds)	Speedup
1 (serial)	38939	1.000
2	19982	1.949
4	10581	3.680
6	7406	5.278
8	5809	6.703

The details of the programming approach and the relevant software (parallel versions of AUTO97 and 2000) are to be published.

Future developments

As shown, the proposed algorithm provides almost linear speedup for up to 8 processors. It would be interesting to test its performance on a larger scale cluster. Meanwhile, two–

parameter continuation of branches stemming from Neimark-Sacker bifurcations and also of folds of periodic solutions for the RFR is being conducted.

The relevant software tools are under further development: particularly, optimisation for heterogeneous clusters and dynamic job allocation on the participating nodes (like peer-to-peer networks) are under study. A corresponding add-on to the current distribution of AUTO will be made freely available to the public after proper testing.

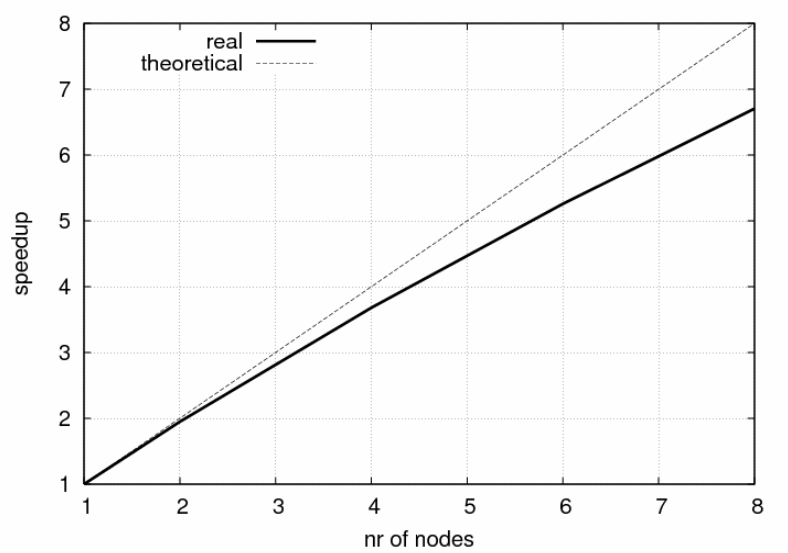

Figure 2. Speedup of parallel continuation of diagram 1

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