A Case Study on Visualization for Boundary Value Problems

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Abstract

In this paper we present a method, and a software based on this method, making highly inter-active visualization possible for computational results on nonlinear BVPs associated with ODEs. The program PCR relies partly on computer graphics tools and partly on real-time computations, the combination of which not only helps the understanding of complex problems, it also permits the reduction of stored data by orders of magnitude. The method has been implemented on PCs (running on DOS) and on the Application Visualization System (AVS) for UNIX machines, this paper provides a brief introduction to the latter version besides describing the mathematical background of the method.

1 Introduction

This paper is intended to describe a method, and a software based on this method, which may be very helpful when presenting, storing or trying to understand computational results on nonlinear boundary-value problems (BVPs) associated with ordinary differential equations (ODEs). Such BVPs occur in various fields of applied mathematics: in mechanics, in particular in rod theory and also in structural engineering, also in robotics, finding optimal paths for a device. There are standard codes available (for example AUTO[Doedel 1986]) solving such BVPs, however, the problem is often that the huge data files created by such a software are hard to store and even much harder to understand. The best tool to visualize such data are bifurcation diagrams which serve as "charts", interpreted in some parameter space. Such bifurcation diagrams can be extremely complicated, and relating them to the physical behaviour of the system is a very hard task. Our method is based on the construction of a very special bifurcation diagram, which enables the user to identify instantaneously the physical configurations corresponding to the points of the diagram. In our software PCR this is realized simply by clicking with the mouse on the desired point; in the adjacent window the corresponding physical configuration would show up immediately. This kind of special diagram also helps to shrink the size of the stored data radically, in some cases by several orders of magnitude.

We will sketch the history of our research program in section 2, then outline briefly the underlying deep, but well-known and non-technical ideas from the theory of ODEs and dynamical systems in Section 3. Athough these ideas might seem simple, it is non-trivial to apply them to particular problems and even less so to build a code which realizes them in an interactive way. The code PCR has been implemented on Personal Computers running DOS, using Microsoft QuickBasic 4.5 and on UNIX workstations, using the Application Visualization System (AVS)[1992].

2 Motivation and background

This research was motivated by a project of Li and Maddocks [1994]: They constructed a mathematical model for DNA molecules (a homogeneous, elastic ring with circular cross section) and did extensive analytical and numerical studies on this model. The numerical investigations were carried out with AUTO [Doedel, 1986], a continuation code for BVPs associated with ODEs. The data produced by AUTO exceeded 1.5 Gbytes, also, the produced bifurcation diagrams were extremely difficult to relate to the physical behavior of the ring. There were several conjectures related to the computation results, however, it was nearly impossible to check them "visually", due to the large amount of stored data and also because points on the bifurcation diagram could not be identified with phyisical configurations. At this stage we started to build a visualization tool which would permit to reduce the size of the stored data and also link the bifurcation diagram to the physical configurations in an inter-active way. Our goal was to build a general visualization tool, adaptable to any BVP associated with ODEs. We used ideas published earlier by Domokos [1994]. As a result, the package PCR was produced, running both on Personal Computers and also on UNIX workstations. PCR helped to reduce the data size by a factor over 1000, it proved to be also very helpful in analyzing the dataset. We will indicate the application of PCR to the problem of Li and Maddocks [1994] in section 5.

3 Mathematical background, formulation of results

Results in bifurcation problems are usually presented in the form of bifurcation diagrams. We are not aware of any general definition for "bifurcation diagram", in fact, depending on what purpose we have in mind, we may design rather different kinds of bifurcation diagrams. As examples we mention the widely applied method of using Fourier coefficients as coordinates. Our present goal when designing bifurcation diagrams is threefold:

1./ To create diagrams which are topologically correct, i.e. *one* point of the diagram corresponds to *one* solution of the BVP and vice versa, also that the mapping is continuous.
2./ To create diagrams from which the physical configurations of the BVP can be easily reconstructed.
3./ To minimize the amount of stored data.
All three of the above criteria are met by the set of coordinates ("global coordinates") to be described below.

Global coordinates can be created for explicit ODEs satisfying the Lifschitz-condition, i.e. for ODEs which meet the requirements of the Uniqueness Theorem [Bieberbach, 1923]. Nearly all applications in mechanics are "well-behaved" and fall into this category.(For a rare exceptions see [Domokos 1993].) For such well-behaved ODEs a semi-infinite trajectory is completely and uniquely determined by the initial conditions. For example, consider a linearly elastic cantilever beam, clamped at the left end and free at the right end subjected to the compressive force P (Fig.1).

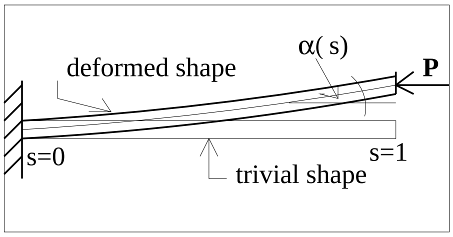

Figure 1: The cantilever beam

The ODE describing the shape of the beam in terms of the slope α as a function of the arclength s was first described by Euler:

$$\alpha'' + P\sin(\alpha) = 0. \tag{1}$$

The trajectories of this equation are uniquely determined by the three scalars $\alpha(0), \alpha'(0)$ and P (the former being "true" initial conditions, the latter one a parameter). However, not all trajectories are of interest for us, only those which meet the boundary conditions

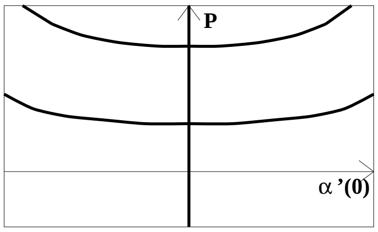

Figure 2: Segment of the global bifurcation diagram for the cantilever beam.

$$\begin{array}{lrcl} a/ & \alpha(0) & = & 0 \\ b/ & \alpha'(1) & = & 0 \end{array} \tag{2}$$

Condition (2/a) eliminates one of the "variable" initial conditions as a constant, so all trajectories which *might* meet the boundary conditions can be uniquely represented in the $[\alpha'(0), P]$ plane. This plane has property 1/, i.e. one point of the plane corresponds to one trajectory and vice versa. The scalars $\alpha'(0)$ and P are the *global coordinates* for this BVP, the plane (space) spanned by them will be called the *global representation space* of the BVP. A finite segment of the bifurcation diagram for the BVP (1-2) is illustrated in Fig.2 in the global representation space.

Based on the example of the cantilever we can now define the *global coordinates* of a two-point BVP as *those (Cauchy-type) initial conditions and parameters which are not fixed by the boundary conditions at the origin. The global representation space of the BVP is spanned by the global coordinates.* [Domokos, 1994] The bifurcation diagram in the global representation space not only has the advantage that it is topologically correct (Property 1/), it also makes the recon-

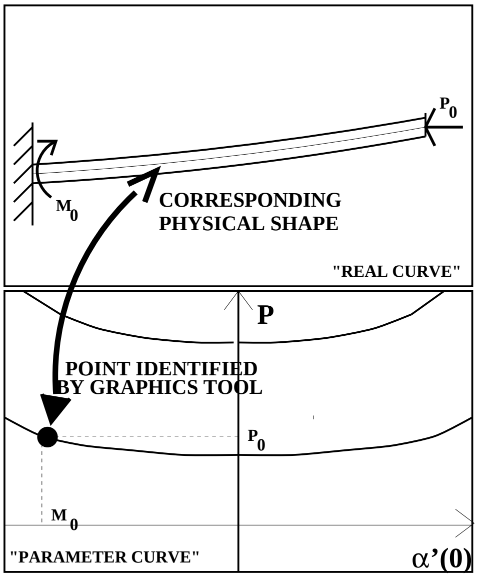

Figure 3: The double-window system of PCR

struction of physical shapes extremely simple (Property 2/). Take any point from the bifurcation diagram and add the remaining constant initial condition (in out cantilever example: $\alpha(0) = 0$) to obtain a complete set of initial conditions. Running an IVP solver with these conditions regenerates the physical shape instantly . This feature of the global bifurcation diagram dictates the basic idea of PCR: Have constantly two windows open on the screen. One window shows the bifurcation diagram (or a projection of it) and by some device we can locate points on this diagram. The other window instantly shows the corresponding physical shape. Such a configuration is shown in Fig.3:

This combination of graphics with real-time computing is the key idea of PCR.

If the dimension of the global representation space is more than 2 then we seemingly loose the topological correctness since projection to the 2D s creen may result in spurious intersection points. However, such points may be eliminated, as pointed out in the next section. We remark that the bifurcation diagram in the global representation space requires minimal data storage, thus has property 3.

4 Software implementation

The software PCR was developed based on the above described method. PCR has two implementations: a PC/DOS version, requiring 386DX/33 processor and VGA graphic screen (or up). A more sophisticated version is running on the Application Visualization System (AVS) on UNIX workstations, this latter version offers better graphics and more flexibility. In this section we describe the main features characteristic for both versions.

Our software is called PCR, which stands for: $Parameter \rightarrow Curve \leftarrow Real$. The input for the software is an $n \times m$ matrix, n (number of rows) denoting the number of data points in the global representation space, m (number of columns) denoting the dimensions of this space. As described in section 2, each of the rows contains the set of initial values which are not set constant by the boundary-conditions at the origin. The integers m and n can be arbitrary. PCR also needs an IVP solver routine for the specific BVP, there is an empty "slot" in the AVS network for that routine. After reading in the data file, PCR opens up two graphic windows,according to the setup in Figure 2. A point on the parameter curve (bifurcation diagram) can be selected by clicking with the mouse on the point. Given an n dimensional bifurcation diagram, PCR allows the user to choose any 3 dimensions and display these. In higher dimensional diagrams spurious intersection points may arise. PCR offers several tools to get rid of these points: In 4D the user may define a (nonlinear) color map according to the 4th dimension. The user can also define a 2D subspace of the m-dimensional global representation space in which a rotation can be performed, removing the spurious intersection points.

5 Summary

In this paper we presented the theoretical basis and description of the software PCR, intended for inter-active visualization of results on BVPs. This usage of the “global coordinates” defined in section 2, offers several advantages: It minimizes the size of the stored data, it provides a topologically correct bifurcation diagram and makes the real-time reproduction of the physical configurations possible. PCR offers a variety of inter-active tools to deal with the dataset in the global representation space. Its main feature is the simultaneous viewing of the bifurcation diagram and of the physical configuration corresponding to a user-defined point on this diagram. PCR also offers several tools to understand higher-dimensional bifurcation diagrams, including colorization and rotations in the higher dimensional space.

The study of bifurcation diagrams with a tool like PCR might very often help revealing otherwise hidden features, such as connectivity of branches in the bifurcation diagram, or, realtionship between symmetries in the physical, configuration space and the global representation space, leading to deeper understanding of the problem.

In Fig. 5 we give an interesting example of application: torsional buckling of a uniform, circular rod. PCR was running on data obtained by Li and Maddocks [1994]. The global representation space is 4 dimensional in this problem and is spanned by the initial moments M_1, M_2, M_3 and the force F. Fig 4 shows the M_1, M_2, M_3 projection of this diagram and one physical configuration corresponding to the point identified on the bifurcation diagram. Without explaining it further, we would like to point out an interesting relationship between the bifurcation diagram and the physical configuration. The latter one is in unstressed state a circular ring, which has a continuous rotation symmetry group (called SO(2)). On the other hand, the bifurcation diagram reveals an 8th order discrete symmetry group generated by the three reflections to the coordinate planes (even apparent from this single picture). How this two groups relate can be explored if one is able to investigate the phyisical configurations corresponding to points which are mapped into each other by this discrete group. (This is called a group orbit.) PCR is optimally suited for such an investigation and, in fact, helped to explain the relationship between the two mentioned symmetry groups. We also remark that in this problem PCR helped to reduce the size of the data file by a factor of 100. We feel that problems of this complexity might be very hard to understand without a tool like PCR.

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References

AVS, Inc. (1992): *AVS User's Guide* Waltham, Massechusetts

Bieberbach, L. (1923): *Differentialgleichungen* Springer, Berlin

Doedel, E. (1986): *AUTO 86 user manual* Caltech,Dept. Applied Mathematics, Pasadena, California

Domokos, G., (1993): *Can strings buckle?* AMD -Vol 167 (Recent development in stability, vibration and control of structural systems) ASME 1993, Applied Mechanics Division, ISBN 0-7918-1146-8, pp 167-174

Domokos, G., (1994): *Global Description of Elastic Bars* ZAMM **74** (4) T289-T291

Li, Y and Maddocks, J.H. (1994): *On The Computation of Spatial Equili bria of Elastic Rods Including Effects of Self-Contact* submitted for publication

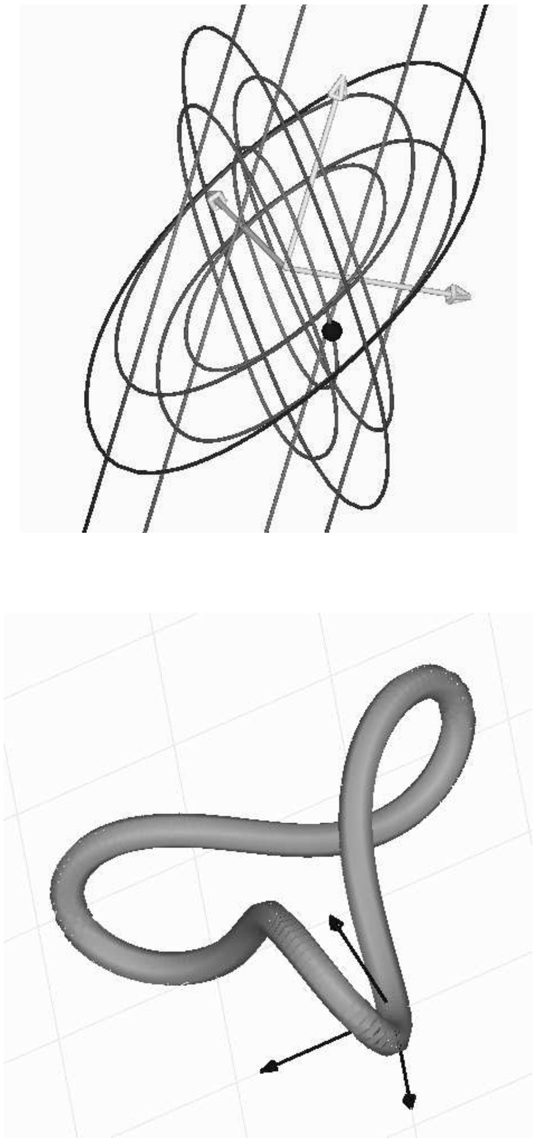

Figure 4: Bifuircation diagram and one physical configuration of ring under torsion