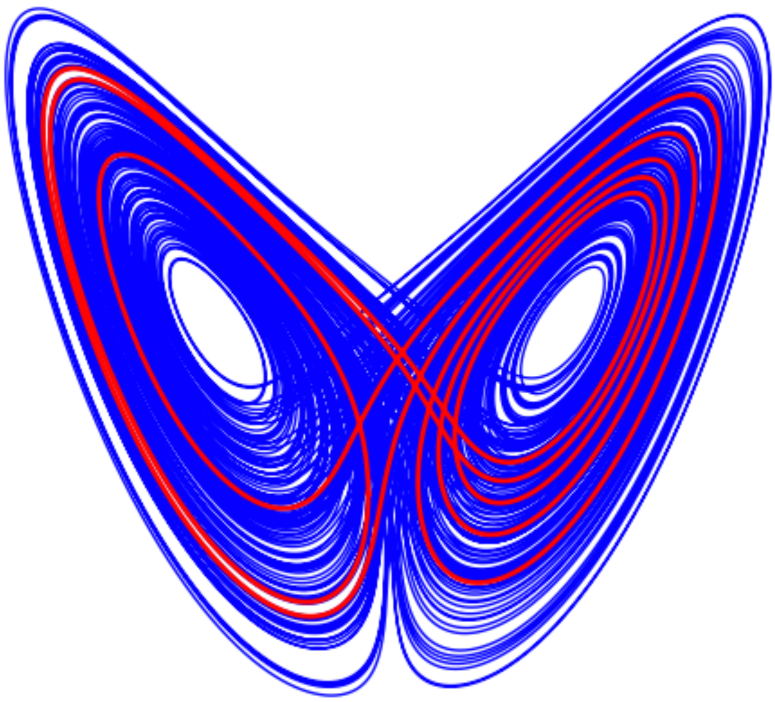
EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling



Computing Periodic Orbits of ODEs with Deflation

Bogdan Toader

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1. Project Background

This project is motivated by the need to understand specific types of plasma behaviour, like Edge Localised Modes.

This project, undertaken in collaboration with Culham Centre for Fusion Energy (CCFE), the UK's national laboratory for fusion research, is motivated by the need to understand the plasma behaviour in the process of generating fusion energy.

To get energy from fusion, gas made from a combination of deuterium and tritium (two isotopes of hydrogen) is heated to very high temperatures (100 million degrees Celsius). At this temperature, the gas becomes plasma. The plasma is confined in a toroidal reactor known as a tokamak, where it is controlled with strong magnetic fields. In this process, some physical phenomena have not been investigated from a mathematical point of view.

One such phenomenon is an edge localised mode (ELM), which is a magneto-hydrodynamic instability occurring in plasma in the high confinement regime of the tokamak. It is important to understand under what conditions these instabilities appear as they can damage the tokamak installation. A deeper understanding of the dynamics leading to an ELM would allow us to control it and to mitigate its effects.

In this project, we aim to investigate a potential cause of ELMs, by analysing the periodic solutions of the underlying mathematical model of plasma behaviour.

2. Calculating Numerical Solutions of ODEs

We investigate a numerical method for calculating periodic solutions of a reduced model for magneto-hydrodynamics.

In this report, we will combine two numerical techniques, the standard shooting method and the deflation method, to calculate multiple periodic and stationary solutions of a simplified ODE model for magneto-hydrodynamics. By incorporating our methods into a continuation framework, we will be able to compute bifurcation diagrams that describe the behaviour of the system for a given parameter configuration.

Glossary of Terms

For a system whose state at time t is given by vector $\boldsymbol{x}(t)$, and depends on a parameter λ, we define the following:

- Stationary solution: a solution whose derivative is zero. A stationary solution can be stable (if a perturbation from it approaches zero as time approaches infinity) or unstable (if a perturbation is amplified as time approaches infinity);
- Periodic solution: a solution where $\boldsymbol{x}(0) = \boldsymbol{x}(T)$ for some positive time T;
- Phase plane: a plot showing the dependence between two state variables or one state variable and its derivative
- Bifurcation point: a pair $(\boldsymbol{x}_0, r_0)$ where the number of solutions changes when r passes through r_0; a Hopf bifurcation connects stationary solutions to periodic solutions
- Bifurcation diagram: a plot showing how the solutions change as the value of the parameter r changes;
- Standard shooting method: the numerical method we use to calculate periodic solutions (described in detail later);
- Deflation: the numerical method we use to calculate multiple solutions (described in detail later);
- Continuation: the framework we use to compute the bifurcation diagram for a range of parameter values $[r_{min}, r_{max}]$.

Mathematical Model

We analyse a system ordinary differential equations (ODEs) of a conducting fluid in the presence of a magnetic field for a layer of fluid confined between two fixed horizontal planes. This model preserves the qualitative behaviour of more realistic magneto-hydrodynamics partial differential equation (PDE) models and it is a simple enough model to which we can apply our method without worrying about issues related to solving large-scale systems of PDEs.

The unknowns in our model are the amplitudes of the velocity of the fluid, the temperature, and the magnetic field. We visualise the results by looking primarily at the amplitude of the velocity, denoted by $a(t)$.

The system has five parameters, but the parameter of the system that we focus on is related to the Rayleigh number, which is the ratio between heat transfer by convection and heat transfer by conduction. We denote this parameter by r.

Our aim is to calculate all the periodic and stationary solutions of this system for a range of values of the parameter r. It is a nonlinear system and finding its solutions cannot be done analytically, so we combine two numerical methods (standard shooting and deflation) for calculating all the solutions for a given value of r. We then repeat this process for each value of r in the required range.

Shooting methods involve varying (artificial) parameters in order to satisfy the boundary conditions.

Standard Shooting

The method we use for calculating the periodic solutions of the system for a given parameter value is called the **standard shooting method**.

This method applies a root finding algorithm (called the Newton's method) to the residual R defined as:

$$R(\boldsymbol{x}(0), T) = \boldsymbol{x}(0) - \boldsymbol{x}(T)$$

The solutions that Newton's method finds are the starting point of the periodic solution, $\boldsymbol{x}(0)$, and the period T of the solution. This is an iterative process, meaning that it starts from an initial guess of the state and period and it finds successive approximations to the real solutions until a certain convergence is reached:

$$|\boldsymbol{x}(0) - \boldsymbol{x}(T)| < \epsilon.$$

At each iteration, we solve a linear system whose the matrix relates small changes in the starting state $\boldsymbol{x}(0)$ and the period T of the periodic orbit to the resulting change in the residual. This matrix is called the Jacobian. Calculating it is the main challenge of the standard shooting method, as it can become quite computationally intensive for large-scale systems.

Using deflation for calculating multiple periodic solution is the novel aspect of our approach.

Deflation

The novel part of our approach is incorporating **deflation**, a technique used to calculate multiple solutions of the system (periodic or stationary) for a given parameter configuration.

We will introduce the idea of deflation using an example of polynomial root finding. Let us assume we want to find the roots of the polynomial

$$p(x) = x^2 - 1.$$

In most real-world applications, finding the solution of an equation analytically is not an option, so we need to use a numeric approach. We apply, for example, Newton's method, to find one solution, $x_1 = 1$. Running the algorithm again on the same problem will give the same solution; the key concept in deflation is to modify the polynomial slightly in order to be able to find a new solution using the same method. The new polynomial, $q(x)$, has to satisfy two properties:

1. q has the same solutions as p except the one we have just found (x_1).
2. Our root finding algorithm cannot give x_1 as a solution to q.

Deflation involves removing previously found solutions so that new solutions can be found.

We obtain a polynomial q that satisfies these two properties if we multiply p by $\frac{1}{x-1}$:

$$q(x) = \frac{x^2 - 1}{x - 1}.$$

We say that the solution x_1 has been deflated. Applying the root finding algorithm to $q(x)$ gives the second solution, $x_2 = -1$.

When applying deflation to systems of ODEs or PDEs for finding not only stationary, but also periodic solutions, the term used to deflate solutions of such systems is adapted accordingly, as we work with functions rather than numbers.

3. Results: Bifurcation Diagram

We are interested in the behaviour of our system as we change the parameter r. In order to plot the bifurcation diagram, we need to choose a scalar value $[a]$ that reflects the state of the system, and we choose it to be the maximum amplitude of the velocity of the fluid. Note that for a stationary solution, $a(t)$ is constant for all values of t. We remind the reader that the parameter r is a modified Rayleigh number. We compute the bifurcation diagram for $r \in [1,4]$ and show it in Figure 1.

Our method successfully calculates the bifurcation diagram with all the periodic and stationary solution for a specific range of the parameter.

For all values of r, we have the trivial stationary solution $a = 0$, where the fluid does not move and the heat transfer takes place in the form of conduction. At $r = 2.61$, convection sets in through a Hopf bifurcation, where two periodic solutions start to appear. These solutions start by resembling a linear oscillator (see Figure 2), but as r grows, the oscillations become more nonlinear (see Figure 3). The periodic branches continue towards previously unseen stationary branches, with which they merge at $r = 3.4$. The stationary branches start at $r = 3.5$ and have turning points at $r = 3.1$, where they change stability, from unstable to stable. This is illustrated in Figure 4, where we see that a small perturbation from a point on the unstable stationary branch causes its state to take a big jump and go to the stable stationary branch.

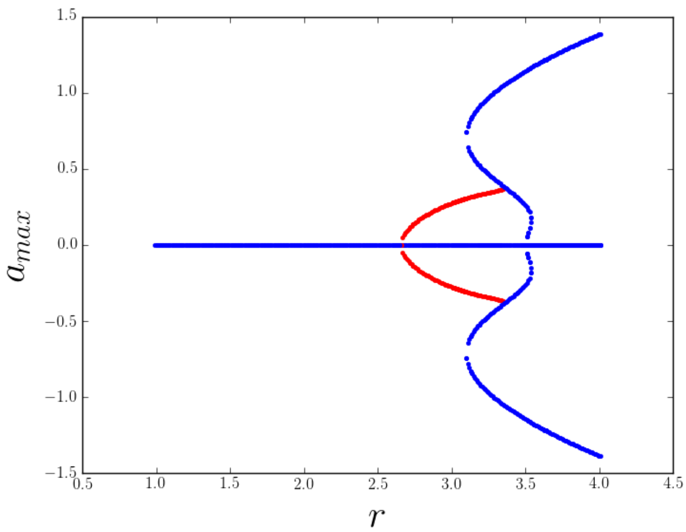

Figure 1: Bifurcation diagram for $r \in [1,4]$. Red represents periodic solutions and blue represents stationary solutions.

One thing worth mentioning is that at $r = 3.1$, by deflating all known solutions found on the previously known branches for $r < 3.1$ (the trivial stationary branch and the periodic branches), we are able to find the turning points in the new stationary branches. This means that deflation is able to find new unknown branches.

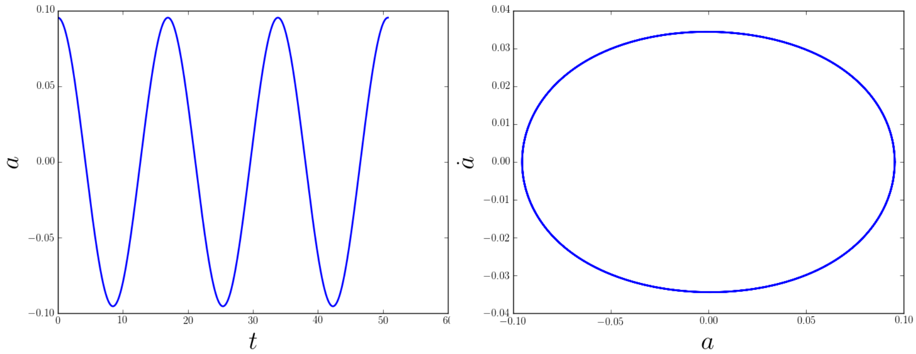

Figure 2: Periodic solution for $r = 2.7$, time series (left) and phase plane (right). The solution is similar to linear oscillation.

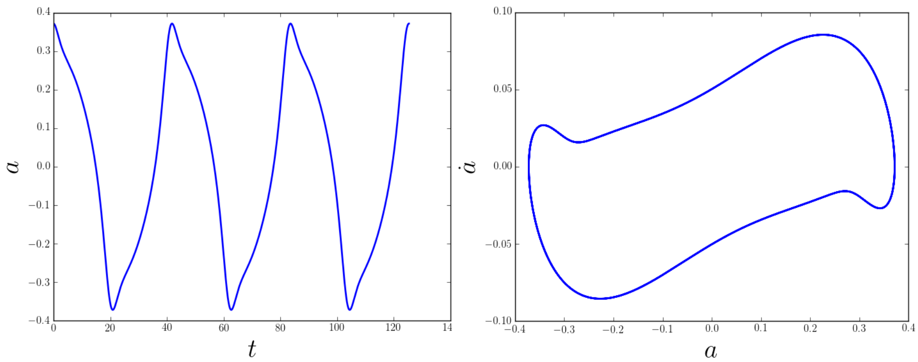

Figure 3: Periodic solution for $r = 3.36$, time series (left) and phase plane (right). The nonlinearity becomes more obvious.

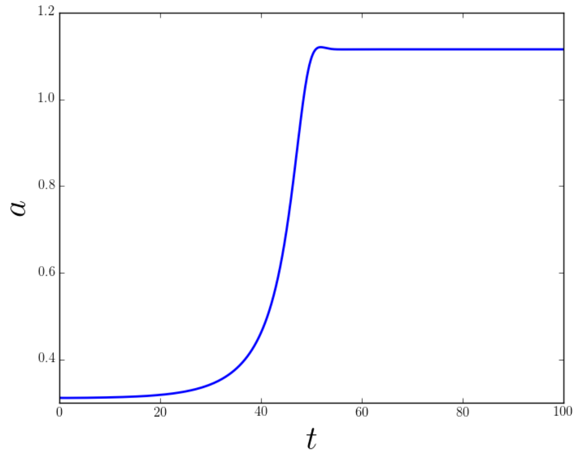

Figure 4: Stability of stationary non-trivial branch. At $r = 3.45$, there are two non-trivial stationary solutions (with positive value of a), one with $a = a_1 = 0.31$ and one with $a = a_2 = 1.11$. By starting from a perturbation near a_1 (by adding 0.001), the state of the system jumps to a_2, showing that a_1 is on an unstable branch and a_2 is on a stable branch.

4. Conclusions and Further Work

We have investigated a new way of finding multiple stationary and periodic solutions in systems of ODEs and applied it to a problem of interest to CCFE.

We have shown that deflation works beyond the stationary case and is able to find multiple periodic solutions in combination with the standard shooting method.

We combined the standard shooting method for finding periodic solutions with the deflation method for finding multiple solutions and used them in a continuation framework to obtain a complete overview of the behaviour of a system. We have shown that our method can compute bifurcation diagrams for certain parameter configurations by detecting multiple periodic solutions, which represent one of the potential explanations for the physical phenomenon of edge localised modes at the edge region of the plasma inside the tokamak.

The key benefit of our method is the use of deflation for finding multiple solutions at each iteration in the continuation algorithm. It is a simple idea but very powerful, as it can be used to detect disconnected branches in the bifurcation diagram. Its simplicity combined with the fact that the shooting method is based on Newton iterations make our method relatively easy to implement. This is important when implementing it in an existing code base, especially if there is already an implementation of Newton's method, as is the case when solving PDE systems.

Finally, there are two key extensions that could be considered. Firstly, we could apply the method in our current implementation to a strange attractor like the Lorenz system, since this is a more challenging problem. Secondly, the method should be extended to systems of PDEs. This will impose a different set of challenges, for example, related to the calculation of the Jacobian. Since the Jacobian can become very big in large-scale PDE systems, the use of matrix-free methods for calculating the Newton step in the shooting method should be investigated. Extending the method to systems of PDEs is of practical importance to CCFE (and elsewhere) and this should be the obvious step forward.

5. Potential Impact

Once the method has been demonstrated to work on a PDE, it is likely to have widespread impact on numerical work on oscillations, as there is a large community of people working on such problems. For example, The Matlab numerical bifurcation analysis tool "Matcont" had 600 downloads during one week alone.

Dr. Wayne Arter, Scientist and CCFE and industrial supervisor for this miniproject, commented: "*The work successfully demonstrated what should become a very powerful method for attacking nonlinear oscillations seen in simulations of plasma physics and other experiments.*"