# CONTINUATION OF PERIODIC ORBITS IN LARGE-SCALE DISSIPATIVE SYSTEMS

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We present a numerical algorithm for the continuation of periodic orbits of high-dimensional dissipative dynamical systems. It is based on single shooting and Newton-Krylov methods. A non-trivial fluid dynamics problem, which after a pseudo-spectral discretization gives rise to a system of dimension $O(10^4)$, has been used as test. The efficiency of the algorithm, which allows the unfolding of a complex bifurcation diagram of periodic orbits, shows the suitability of the method for large-scale nonlinear dissipative partial differential equations.

## 1. Introduction

Many researchers have benefited from the availability of continuation and bifurcation packages such as AUTO[1] to compute fixed points, periodic orbits and other invariant manifolds of dynamical systems. Due to the small size of the systems they are designed for, they implement direct solvers for the linear problems involved in the computations. The extension to high-dimensional problems is not straightforward; the main obstacle being the computational cost of the linear algebra. The development of modern techniques, many of them based on Krylov or Arnoldi methods, allow the study of large systems such as those in computational fluid dynamics. In particular, continuations of periodic orbits in large-scale dissipative systems have been performed in a few problems[2,3] of moderate dimension. These studies use the Newton-Picard[2] algorithm. In this work, we present an alternative to that method. We apply Newton-Krylov techniques to obtain the fixed points of a Poincaré map. Because of the dissipative nature of the problems the method is addressed to, their Floquet multipliers are clustered around the origin. This is the reason why the convergence of the iterative methods we employ is fast.

## 2. Continuation method for periodic orbits

Consider a finite dimensional dynamical system with governing equations

$$\dot{x} = f(x, \lambda), \tag{1}$$

with $(x, \lambda) \in \mathcal{U} \subset \mathbb{R}^n \times \mathbb{R}$, and where $\lambda$ is a parameter on which the problem depends.

Periodic orbits of (1) are obtained as fixed points of a Poincaré map. After an hyperplane $\Sigma$, defined as $g(x) = \omega_\sigma^\top (x - x_\sigma) = 0$ is selected, the Poincaré map, $P : \mathcal{V} \subset \Sigma \to \Sigma$, is defined as $P(x, \lambda) = \varphi(t(x), x, \lambda)$ where $x \in \mathcal{V}$, $\varphi(t, x, \lambda)$ is the solution of $\dot{x} = f(x, \lambda)$ with initial condition $x = \varphi(0, x, \lambda)$, and $t(x)$ verifies $t(x) > 0$, $\varphi(t(x), x, \lambda) \in \Sigma$. The periodic orbits are then given by

$$x - P(x, \lambda) = 0, \quad x \in \Sigma. \tag{2}$$

Predictor-corrector parameter and pseudo-arclength continuation methods are used to study the dependence of the solutions of (2) on the parameter $\lambda$. Second degree polynomial extrapolation is used as predictor and Newton's method as corrector. Both methods admit an unified formulation by adding a normalizing equation

$$n(x, \lambda) \equiv \theta \omega_x^\top (x - x_0) + (1 - \theta)\omega_\lambda (\lambda - \lambda_0) = 0, \tag{3}$$

$(x_0, \lambda_0)$ being the predicted point along the curve of solutions. In the case of pseudo-arclength continuation $(\omega_x, \omega_\lambda)$ is an approximation to the tangent to the curve of solutions $(x(s), \lambda(s))$ at $(x_0, \lambda_0)$, which can also be obtained by extrapolation, and $0 \leq \theta \leq 1$ is a parameter that controls the relative weight of $x$ and $\lambda$ in the normalizing equation. For parameter continuation $\theta = 0$ and $\omega_\lambda$ a non-zero arbitrary constant.

The system that determines a unique solution is then

$$x - P(x, \lambda) = 0, \quad n(x, \lambda) = 0, \quad x \in \Sigma, \tag{4}$$

and the linear system to be solved at each Newton's iteration, $(x^{i+1}, \lambda^{i+1}) = (x^i, \lambda^i) + (\Delta x^i, \Delta\lambda^i)$, is

$$\begin{pmatrix} I - D_x P(x^i,\lambda^i) & -D_\lambda P(x^i,\lambda^i) \\ \theta\omega_x^\top & (1-\theta)\omega_\lambda \end{pmatrix} \begin{pmatrix} \Delta x^i \\ \Delta\lambda^i \end{pmatrix} = \begin{pmatrix} -x^i + P(x^i,\lambda^i) \\ -n(x^i,\lambda^i) \end{pmatrix}. \quad (5)$$

The linear system (5) is solved iteratively by matrix-free methods that only require the computation of products by the matrix. We used the restarted generalized minimum residual method (GMRES). Therefore a procedure to compute products of the form $D_x P(x,\lambda)\Delta x^i$ or $D_x P(x,\lambda)\Delta x^i + D_\lambda P(x,\lambda)\Delta\lambda^i$ must be available. They can be obtained from the first variational equation

$$\dot{y} = D_x f(x,\lambda) y + D_\lambda f(x,\lambda)\mu, \quad (6)$$

with $y(0) = \Delta x^i$ and $\mu = \Delta\lambda^i$. The term $D_\lambda f(x,\lambda)\mu$ must be included in (6) only if pseudo-arclength continuation is used. Details on how to obtain the action of differential of the Poincaré map from the integration of these variational equations can be found in Ref. 4.

Once the periodic orbits have been obtained, we study their stability by computing their dominant Floquet multipliers by subspace iteration or by Arnoldi's method using the ARPACK library[5]. This needs, also, the integration of the $2n$-dimensional system (1), (6).

## 3. The test problem: thermal convection in an annulus

The method have been tested on a two-dimensional thermal convection problem of a Boussinesq fluid in an annulus with inward gravity and heated from the inside. The domain has inner and outer radii $R_i$ and $R_o$. The three non-dimensional parameters of the problem are the radius ratio, $\eta = R_i/R_o$, the Prandtl number, $\sigma = \nu/\kappa$, and the Rayleigh number, $Ra = \alpha\Delta T g d^3/\kappa\nu$, where $\nu$, $\alpha$ and $\kappa$ are the kinematical viscosity, the thermal expansion coefficient, and thermal diffusivity of the fluid respectively. $\Delta T$ is the temperature difference between both boundaries, $g$ a constant radial gravity, and $d$ the radii difference. All the results shown correspond to $\eta = 0.3$ and $\sigma = 0.025$, and $Ra$ is the moving parameter. Let $\mathbf{u}$ and $T$ be respectively the velocity and temperature fields. The conductive steady state $\mathbf{u}_c = 0$, $T_c(r) = T_i + \ln(r/R_i)/\ln\eta$ is a solution for any value of $Ra$.

The velocity field $\mathbf{u}$ is written in terms of a mean flow $f$, and a stream-function $\psi$, as $\mathbf{u} = f\hat{\mathbf{e}}_\theta + \nabla \times (\psi\hat{\mathbf{e}}_z)$. The equations for $f$, $\psi$, and the temperature perturbation, $\Theta = T - T_c$, are

$$\begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & \Delta \end{pmatrix} \partial_t \begin{pmatrix} f \\ \Theta \\ \psi \end{pmatrix} = \begin{pmatrix} \sigma\tilde{\Delta} & 0 & 0 \\ 0 & \Delta & -(r^2 \ln \eta)^{-1}\partial_\theta \\ 0 & \sigma r^{-1} Ra\, \partial_\theta & \sigma\Delta\Delta \end{pmatrix} \begin{pmatrix} f \\ \Theta \\ \psi \end{pmatrix}$$
$$+ \begin{pmatrix} P_\theta \left[\Delta\psi\partial_\theta\psi\right]/r \\ J(\psi,\Theta) - f\partial_\theta\Theta/r \\ (1-P_\theta)J(\psi,\Delta\psi) + \tilde{\Delta} f\partial_\theta\psi/r - f\partial_\theta\Delta\psi/r \end{pmatrix}, \tag{7}$$

where $\Delta = (\partial_r + 1/r)\partial_r + (1/r^2)\partial^2_{\theta\theta}$, $\tilde{\Delta} = \partial_r(\partial_r + 1/r)$, $J$ is the determinant of the corresponding Jacobian matrix in cylindrical coordinates, and $P_\theta$ is the azimuthal average operator $P_\theta g(t,r,\theta) = (2\pi)^{-1}\int_0^{2\pi} g(t,r,\theta)d\theta$. In this formulation, the no-slip and constant temperature boundary conditions become $f = \psi = \partial_r\psi = \Theta = 0$.

A simple inspection reveals that the system is $O(2)$-equivariant; $O(2)$ being generated by rotations and reflections with respect to diameters. These symmetries are responsible for the large amount of bifurcations found in the problem.

We use pseudo-spectral methods to discretize (7). The fields $f$, $\psi$ and $\Theta$ are approximated by Fourier series in $\theta$ and collocation on a mesh of Gauss-Lobatto points in $r$. With the discretization we have employed the total number of unknowns is 11582. For time integration we use fourth order backward differentiation formulas (BDF) for the linear part of (7), and fourth degree extrapolation formulas for the nonlinear terms.

## 4. Results

Fig. 1(a) shows the calculated branches of periodic orbits with dominant azimuthal wave number $n = 4$. They are waves that are no longer reflection symmetric, and consequently[6] vacillate back and forth in the azimuthal direction. Information about the origin and the physical behaviour of this solutions can be found in Ref. 7. A weighted amplitude $A = \sum_{n=0}^{4} w_n|\Theta_n(r_p)|$ of the first five azimuthal modes of the temperature perturbation, at the time at which the orbit intersects $\Sigma$, versus the Rayleigh number has been plotted. In $A$, $r_p$ is a fixed radial point, and the weights, $w_n$, are selected to clearly distinguish the different branches. Solutions related by the spatial symmetries broken at the bifurcations, correspond to the same points in the diagram. The branching points have been marked with full circles (other intersections are due to the projection), the only Neimark-Sacker

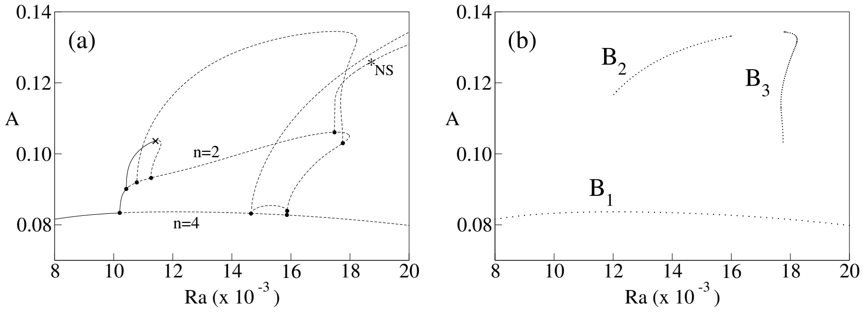


Figure 1. (a) Diagram of bifurcations of periodis orbits for the annulus problem. (b) Parts of branches of periodic orbits used to study the efficiency of the method.

bifurcation ($Ra = 18683$) found in the interval of $Ra$ considered is marked with an asterisk, and a bifurcation where two complex conjugate multipliers become real at $+1$, is indicated by a cross. A stable rotating modulated waves emerges at this point.

All the calculations described in this article were performed on a Pentium IV personal computer running at 1.8 Ghz. The average total number of GMRES iterations needed to compute the solutions along the portion of branches displayed in Fig. 1(b) have been calculated. In all the cases, the time step used was $10^{-4}$, and the stopping criterion for Newton's method was a relative difference between iterates below $10^{-7}$ and the norm of the function also below $10^{-7}$. Four cases have been considered. Branch $B_1$ was calculated by using parameter continuation and a fixed parameter step size of 200. This is a pure $n = 4$ branch, i.e., only a quarter of the unknowns are non-zero so that, in fact, a system of dimension 2942 is being solved, although we have not made use of this. For this branch the mean of the total number of GMRES iterations is 17. Branch $B_2$ was calculated with both parameter and pseudo-arclength continuation. The average number of evaluations of $DP(x, \lambda)v$ was 41 and 44 respectively. On $B_3$ there are two turning points, and it ends at a bifurcation point. The mean number of GMRES iterations increases up to 52. This branch is more expensive to compute because the solutions change significantly through the turning points. The CPU times to complete each of these calculations were 22.2, 37.5, 38.8 and 100 hours respectively. Each evaluation of $DP(x, \lambda)v$ took between 50 and 170 seconds depending on the branch considered. Therefore the CPU time to compute each periodic orbit in the diagram of Fig. 1(a) has been from ten to ninety minutes.

## 5. Conclusions

We have shown that Newton-Krylov method, applied to find fixed points of Poincaré maps of high-dimensional dissipative systems, provides an efficient, easy to implement, and robust tool to compute periodic orbits. By using Newton-Krylov method we retain the quadratical convergence of the Newton's iterations except, of course, near bifurcation points. This is important to minimize the number of evaluations of the differential of the Poincaré map, where almost all the computing time is spent.

Other invariant manifolds could also be computed by using the same ideas here described. In particular we are interested in extending these techniques to compute invariant tori for, at least, moderate-dimensional problems.

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