Computation of invariant manifolds in large-scale dissipative systems.

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The invariant manifolds of a dynamical system are organizing centers which drive its behaviour around them. Therefore, their computation and the study of their dependence on the parameters of the system is necessary in order to understand its dynamics. The continuation of steady solutions with respect to parameters is now a common tool in Science and Engineering (see [1] among many others). The computation of other invariant manifolds as periodic orbits and invariant tori are not so usual, although all of them can be cast into a common framework.

Consider a system of autonomous differential equations

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

$x \in \mathcal{U} \subset \mathbb{R}^n$, depending, for simplicity, on a single parameter $\lambda \in \mathbb{R}$. We assume that it has been obtained after the discretization of a system of parabolic partial differential equations, by means of finite differences, finite elements, or spectral methods. The computation of their fixed points, periodic orbits and invariant tori can be reduced to the calculation of fixed points of a map $G(x, \lambda)$, i.e., to the solution of an equation of the form

$$x - G(x, \lambda) = 0. \tag{2}$$

In the case of fixed points $G(x, \lambda) = \psi(T, x, \lambda)$, where $\psi(T, x, \lambda)$ is the solution of (**??**) with initial condition x at time T, and $x \in \mathbb{R}^n$. The integration time T must be adequately chosen. In the case of periodic orbits, $G(x, \lambda)$ is the Poincaré map, defined on a manifold which intersects transversally the periodic orbit, and $x \in \mathbb{R}^{n-1}$. Finally, in the case of invariant tori, $G(x, \lambda)$ is a synthesized map defined on the intersection of two manifolds which cut transversally the tori (see [2]), and $x \in \mathbb{R}^{n-2}$.

Steady solutions are usually computed by solving $f(x, \lambda) = 0$ by Newton-Krylov methods. This implies that a preconditioner for the systems with matrix $D_x f(x, \lambda)$ must be provided. This method should always be the first option to be taken into consideration. The advantage of solving (**??**) appears when there is no effective preconditioner at hand. If the initial system (**??**) is dissipative, the differential of $x - G(x, \lambda)$, $I - D_x G(x, \lambda)$, has all its eigenvalues clustered around $+1$, and therefore no preconditioner will be usually required for the linear solvers. This is what also happens in the computation of periodic orbits (see [3]) and tori. The time evolution drives the system to a low-dimensional inertial manifold where the dynamics take place, damping the rest of the components.

The application of Newton-Krylov methods to (**??**) implies the computation, during the linear solvers inner loop, of the action of $D_x G(x, \lambda)$ on vectors v. These products can be obtained by the integration of the variational equations

$$\dot{y} = D_x f(x, \lambda) y. \tag{3}$$

If $\phi(t, x, y, \lambda)$ is its solution with initial condition y, then $D_x G(x, \lambda)v = \phi(T, v, x, \lambda)$ in the case of fixed points. For the expression of the differential of the Poincaré map which is needed in the two other cases see [4].

If the invariant object is stable or only weakly unstable the Picard iterations $x^{k+1} = G(x^k, \lambda)$ can be accelerated and stabilized by using several techniques. This can be enough to unfold an important portion of the bifurcation diagram of the system. When the solutions become more unstable the application of Newton-Krylov or Newton-Picard [5] methods is mandatory.

Although the linear systems with matrix $I - D_x G(x, \lambda)$ will not normally need preconditioning, it is possible to accelerate the convergence of the linear solvers by using the information of the stability of nearby solutions, previously calculated during the continuation process [6]. This is specially useful if multiple shooting is employed.

Two examples of application of these techniques to fluid dynamics problems will be shown. The first corresponds to the thermal convection of a binary fluid in a two-dimensional rectangular box. In this case branches of fixed points, periodic orbits and invariant tori have been calculated. In the second, branches of periodic orbits (waves) have been computed for the three-dimensional thermal convection of a pure fluid in a rotating spherical shell.

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