

Applied Mathematical Sciences

Àlex Haro
Marta Canadell
Jordi-Lluís Figueras
Alejandro Luque
Josep-Maria Mondelo

The Parameterization Method for Invariant Manifolds

From Rigorous Results to Effective
Computations



Springer

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Computations

Àlex Haro
Barcelona Graduate School of Mathematics
Departament de Matemàtiques i Informàtica
Universitat de Barcelona
Barcelona, Spain

Jordi-Lluís Figueras
Department of Mathematics
Uppsala University
Uppsala, Sweden

Josep-Maria Mondelo
Institut d'Estudis Espacials de Catalunya,
and Barcelona Graduate School
of Mathematics
Departament de Matemàtiques
Universitat Autònoma de Barcelona
Bellaterra, Spain

Marta Canadell
Institute for Computational
and Experimental Research
in Mathematics
Brown University
Providence, USA

Alejandro Luque
Instituto de Ciencias Matemáticas
Consejo Superior de Investigaciones
Científicas
Madrid, Spain

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Editors

S.S. Antman, Institute for Physical Science and Technology, University of Maryland, College Park, MD, USA

ssa@math.umd.edu

Leslie Greengard, Courant Institute of Mathematical Sciences, New York University, New York, NY, USA

Greengard@cims.nyu.edu

P.J. Holmes, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, USA

pholmes@math.princeton.edu

Advisors

J. Bell, Lawrence Berkeley National Lab, Center for Computational Sciences and Engineering, Berkeley, CA, USA

P. Constantin, Department of Mathematics, Princeton University, Princeton, NJ, USA

J. Keller, Department of Mathematics, Stanford University, Stanford, CA, USA

R. Kohn, Courant Institute of Mathematical Sciences, New York University, New York, USA

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Preface

Poincaré's program for the global analysis of a dynamical system starts by considering simple solutions, such as equilibria and periodic orbits, together with their corresponding asymptotic solutions in forward and backward time. Geometrically speaking, these solutions correspond to invariant objects that form the skeleton of the dynamics in phase space. After the middle of the twentieth century, they were joined by a plethora of other invariant objects, such as hyperbolic sets, attractors, quasi-periodic orbits and normally hyperbolic invariant manifolds. All these landmarks were used to perform qualitative sketches to organize the long-term behavior of the system. With the advent of the age of computers, this qualitative approach started to be more quantitative, as researchers started to develop algorithms for effectively computing these invariant objects. Hence, it is not surprising that the last 30 years have witnessed a strong interest in the development of methods for their computation, spreading the range of applications and fostering the collaboration with other scientists and engineers. Meanwhile, the complexity of problems and applications has increased rapidly, thus motivating new research in the development of mathematical methods, computational algorithms and software implementations. Also, the interactions between these aspects have given rise to mutual refinements.

With the dawn of the twenty-first century, the parameterization method has emerged as a novel method that has promoted new developments in the theory and computation of invariant manifolds. It is a new point of view in which parameterizations of invariant manifolds are obtained through an analysis (which can be function-theoretical or numerical) of their invariance equations that takes advantage of the geometric structures of the problem under study. By its very nature, the parameterization method has led to a considerable synergy between rigorous mathematics and numerical computations. Of course, the methodology is not isolated and has received inspiration from many other approaches in each of the contexts it has been applied. Although traces of the method go back to Poincaré and particular formulations had been used in the literature, the systematic application of the method is relatively recent. The foundational papers of the parameterization method [CFdlL03a, CFdlL03b, CFdlL05] dealt with rigorous results on invariant manifolds

of fixed points of maps (some partial rigorous and numerical results had already appeared in [CF94, FR81, dIL97, Sim90]). The paper [dILGJV05] provided rigorous results on KAM theory without using classical angle-action coordinates (see some precedents in [dIL01]). The series of papers [HdIL06c, HdIL06b, HdIL07] considered invariant tori and whiskers of quasi-periodically forced systems, covering from rigorous results, numerical algorithms, and implementations in actual examples. Since then, the range of applications of the parameterization method has been continuously growing.

A remarkable property of the parameterization method is its applicability to different contexts in which other methodologies are fundamentally different. A first goal of this monograph is to provide a unified formulation of the parameterization method valid for different contexts. The specific contexts covered by this monograph are invariant manifolds associated with fixed points, invariant tori in quasi-periodically forced systems, invariant tori in Hamiltonian systems, and normally hyperbolic invariant manifolds. Although this plan may seem ambitious, our goal is not to provide a comprehensive treatment. Each of the contexts has a big amount of literature devoted to different theoretical and numerical techniques applicable. We will only cover the parameterization method, but not even in this case we will be comprehensive. For instance, the monograph is more focused in discrete than in continuous dynamical systems. Moreover, we do not cover the most recent results, because research on the parameterization method is still ongoing. This monograph complements the literature with new results, both rigorous and numerical, in contexts in which the parameterization method has already been applied. On the other hand, we also introduce normally hyperbolic invariant manifolds as a whole new context of application of the parameterization method.

The proofs done using the parameterization method involve proving convergence of iterative schemes that, by themselves, can be turned into numerical methods. This synergy between rigorous results and numerical methods is a signature of the parameterization method. A second goal of this monograph is to provide efficient and reliable algorithms for the numerical computation of invariant manifolds based on the parameterization method. Efficiency is attained through the use of the geometric structure of the problem, which leads to cancelations that simplify the structure of the functional equations to be solved at each iterative step. Reliability is a consequence of the proximity between algorithms and theory. For instance, error estimates for the approximate (numerically computed) parameterizations can be deduced easily from the invariance equations, and the non-degeneracy of the problem is usually a numerically evaluable hypothesis of the theorems that support the algorithms. In summary, we can obtain fast algorithms with low storage requirements and, more importantly, we have a notion of when they are reliable. Hence, it becomes possible to study an invariant object for parameter values very close to the one in which the object ceases to exist. These systematic studies lead to conjectures that enrich the theory.

A third objective of this monograph is to provide some methodology for computer-assisted proofs. The ability to produce theorems in a *posteriori* format is another

characteristic of the parameterization method. The rigorous numerical evaluation of the hypotheses of these theorems leads to a proof of the existence of a true invariant object near an approximate invariant one. A very convenient fact of this strategy is that the computer-assisted methodology is independent of the procedure (such as expansions, interpolation, or even hand calculations) used for the computation of the starting approximate invariant object.

A fundamental part of this monograph is a series of 12 fully detailed examples, some of which are computer-assisted proofs, that realize the three previous objectives. These examples are accompanied by some practical details of their implementation, so that the reader can either reproduce them or adapt the methodology to other problems. A public version of the software used for some of these examples is available at <http://www.maia.ub.es/dsg/param/>.

The parameterization method is unique in its ability to be applied to a problem in several stages, all mentioned in the previous paragraphs, that go from rigorous results to validated numerical results. These stages give rise to the following program: write the functional equations for the parameterization of an invariant object (the invariance equations), provide adequate functional frameworks to ensure the convergence of iterative methods for the solution of these equations, to develop numerical algorithms based on these iterative schemes, implement them in actual problems using appropriate discretizations, and rigorously validate (invoking an a posteriori theorem) the numerical results. This “from theory-to algorithms-to computations-to validations” philosophy is a driving force in this monograph.

We believe that several types of readers can benefit from this monograph. It is aimed to either applied scientists and engineers with an interest in rigorous developments or more theoretically oriented mathematicians with an interest in applications. For instance, a reader interested in the implementation of the parameterization method in applications can benefit from the detailed algorithmic descriptions of this monograph. A more mathematically oriented reader interested in KAM theory can find a complete proof of a KAM theorem in a posteriori format. The theoretical and algorithmic parts are self-contained and can be read independently.

The reader is assumed to have some familiarity with dynamical systems, more particularly with invariant manifolds and normal forms. A reader novel to dynamical system can consult introductory books such as [Arn88, BS02, Chi06, Irw01, KH95, HK03, GH90, PdM82, Rob95, Rob04]. Except for this fact, this monograph is essentially self-contained. It is divided in 5 chapters, of which the first one is an introduction and the remaining ones correspond to different contexts of application of the parameterization method. Except for notation drawn from the first chapter, Chapters 2 to 5 are independent of each other.

Chapter 1 starts by providing an overview of the literature. After that, it introduces unified formulations of the parameterization method for invariant manifolds of fixed points and for invariant tori in different contexts. These formulations are the basis of the subsequent chapters. This chapter can be considered a reading guide of the rest of the book.

Chapter 2 discusses computational aspects of invariant manifolds of vector fields at fixed points. It is focused on algorithms and implementations, since the theory of invariant manifolds of fixed points is well established. There are many classical textbooks including the main results of the theory, to which the trilogy [CFdlL03a, CFdlL03b, CFdlL05] adds the rigorous results of the parameterization method. The goal is to provide algorithms for the computation of semi-local expansions, based on the algebraic manipulation of power series and novel automatic differentiation techniques. The detailed examples of this chapter are the 2D stable manifold of the origin of the Lorenz system, the 4D center manifold of a collinear point of the Restricted Three-Body Problem, and a 6D partial normal form in the same problem that allows the generation of Conley's transit and non-transit trajectories associated with any object of the center manifold.

Chapter 3 revisits the papers [HdlL06c, HdlL06b, HdlL07, FH12]. First, it provides a full proof of a Kantorovich-like theorem for invariant tori in discrete quasi-periodic systems. The proof of this theorem leads to several algorithms for the computation of invariant tori in this context that are also detailed. Next, we explain a computer-assisted methodology for the validation of numerical results based on the previous a posteriori theorem. The chapter ends with three examples: validation of saddle invariant tori on the verge of breakdown, computation of a rigorous upper bound of the measure of Cantor-like spectra of a discrete Schrödinger operator, and validation of an attracting torus that by direct double precision seems to be a strange nonchaotic attractor.

Chapter 4 is devoted to the parameterization method in KAM theory, also referred to as KAM theory without action-angle coordinates. It adds a more geometrical perspective to the original paper [dlLGJV05] in the spirit of [GHdlL14]. More broad views on KAM theory can be found in [BHS96, dlL01], which include many references to the extensive literature. The chapter states and proves a KAM theorem in a posteriori format, with explicit bounds suitable to be applied in an effective and quantitative way. The proof is quite technical, but the reader can skip it without losing the flavor of the application of the method. We have included full descriptions of the derived algorithms and applications to the examples that follow, which are application of the theorem (by hand calculations) to obtain persistence of the golden invariant curve for tiny values of the parameter of the standard map, numerical continuation of this same curve up to values close to breakdown, and computation of 2D tori in the Froeschlé map.

Chapter 5 presents some ideas of normally hyperbolic manifold theory, focusing on the algorithmic application of the parameterization method in such context (the classical theory can be found in [HPS77, Fen72], and a more recent account in [Wig94]). This new method is applied to the following examples: computation of an attracting invariant curve in a 2D Fattened Arnold family, computation of a saddle invariant curve in a 3D Fattened Arnold family, and the computation of a 2D normally hyperbolic invariant cylinder in the Froeschlé map.

Along the monograph, we cover all the aspects of the “from theory-to algorithms-to computations-to validations” program, although not all the aspects are covered in

each chapter. Chapter 2 focuses on algorithmic and practical issues on the computation of invariant manifolds of fixed points. Chapter 3 covers the full program for a particular case (invariant tori in quasi-periodic systems). Chapter 4 is close to that, since it covers the first three aspects, and the KAM theorem stated there is ready to be used in computer-assisted proofs. Chapter 5 covers new research on the parameterization method for normally hyperbolic invariant manifolds, in particular on development of numerical algorithms. We emphasize these and other novelties in Chapter 1.

We finish this preface paraphrasing the following inspiring words in the review [CDD⁺91], written by S. Coffey, A. Deprit, E. Deprit, L. Healy, and B. R. Miller more than 20 years ago: *“The discipline (of nonlinear dynamics) instead must try with tenacity to keep pace with computational technology and make room for its innovations the same way. The challenge thus is endless, for each generation of mathematical physicist needs to keep abreast of techniques relentlessly emerging from the engineering shops.”* And techniques emerge not only from the engineering shops but also from the rigorous results in mathematical papers. Hence, researchers benefit from the combination and feedback between theorems, algorithms, and numerical experiments that often spur conjectures that motivate further research. The parameterization method is one of the emerging techniques in the area of dynamical systems. The research is on the way, and there is still much to come.

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Providence, RI, USA
Uppsala, Sweden
Madrid, Spain
Bellaterra, Spain
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Àlex Haro
Marta Canadell
Jordi-Lluís Figueras
Alejandro Luque
Josep-Maria Mondelo

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Chapter 1

An Overview of the Parameterization Method for Invariant Manifolds

Àlex Haro

The parameterization method is an important tool in the theory of invariant manifolds, in the design of efficient algorithms of computation, and in the development of computer assisted proofs. It can be applied to different kinds of invariant manifolds in different contexts of dynamical systems. In spite of this diversity, there is a core of ideas common to all of them.

The object of this chapter is two-fold. First, to provide an overview of the history of the method together with the contents of this monograph, with some connections to the literature. Second, to describe unified frameworks for the parameterization method in several classes of problems: invariant manifolds associated with fixed points, including graph transform and normal forms, and computation of invariant tori, including invariant tori in quasi-periodically forced systems, invariant tori in Hamiltonian systems, and normally hyperbolic invariant tori. These particular contexts will be detailed in the next four chapters.

1.1 Historical Overview

The parameterization method was introduced by X. Cabré, E. Fontich and R. de la Llave [CFdIL03a, CFdIL03b] to establish existence and regularity of invariant manifolds attached to fixed points, providing also normal forms of the corresponding internal dynamics. In the excellent tutorial [CFdIL05] one can also find some historical notes. Some variants of the method go back to H. Poincaré [Poi90] and A.M. Lyapunov [Lya92], and the results have the flavor of the theory of normal forms [Mur03], in particular the Poincaré-Dulac and Sternberg theorems [Arn83, Ste57, Ste58]. The classical graph transform method, that goes back

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to Hadamard [Had01], can be seen as a particular case of the parameterization method. After all, representing (locally) a manifold as a graph is a particular *style* of parameterizing the object. The celebrated theorems of the stable manifold or the center manifold have been proved many times in the literature using the graph transform method (see, e.g., [Kel67, ST15]). In contrast with the graph transform method, the parameterization method is intended to obtain a parameterization of the invariant manifold that is adapted to its geometry (the object is not considered as a graph over a set of variables) and its dynamics (finding simple expressions for the internal dynamics). Interestingly, C. Simó already referred in [Sim90] to adapted parameterizations of invariant manifolds, meaning parameterizations for which the internal dynamics is linear; see also [Pös86]. These parameterizations are the ones that had been rigorously studied in [CF94, dIL97], and with full generality in [CFdIL03a, CFdIL03b, CFdIL05]. The parameterization method has been also applied to one-dimensional manifolds associated with parabolic directions (corresponding to an eigenvalue 1 in the case of maps) in [BFdILM07, BH08], for which the dynamics is reduced to a polynomial normal form, and the method has been generalized to higher dimensional manifolds of parabolic points for maps in [BFM15a, BFM15b]. Invariant manifolds of fixed points with both attracting and expanding directions in symplectic and volume preserving maps have been discussed in [dILMJ12]. The methodology can be applied also to invariant manifolds of periodic orbits [HdIL13, CLMJ15] or invariant tori [HdIL06c, HdIL06b], often referred to as whiskers. In fact, invariant manifolds of normally hyperbolic invariant manifolds via the parameterization method were already considered in [CFdIL03a, CFdIL03b]. An important fact of the methodology is that it leads itself to efficient implementations for computing high order numerical Taylor expansions of invariant manifolds attached to steady states, providing semi-local numerical approximations. In fact, the use of high order expansions has been part of the folklore in the literature of computations of invariant manifolds, see, e.g., [BK98, Sim90]. The parameterization method in [CFdIL03a, CFdIL03b, CFdIL05] has been applied for computing 2D stable and unstable manifolds of maps [GPH09, MJL10, MJ13], and variants of the method have been used to compute adapted normal forms around equilibria in some models from Celestial Mechanics [HMV12]. When applying the methodology to invariant manifolds of periodic orbits or invariant tori, Fourier-Taylor expansions are in order [HdIL07, HdIL13, MS14, CLMJ15].

In this monograph, we first address the computation of invariant manifolds of fixed points for vector fields. This is the subject of Chapter 2. We mainly focus on computational aspects to obtain semi-local (high order) approximations of invariant manifolds. We refer to [KOD⁺05] for a compilation of several algorithms for the globalization of stable and unstable invariant manifolds far away from the fixed point. These algorithms, that complement our approach, include: approximation by geodesic level sets [KO98], PDE discretization of the invariance equation [GV04], Doedel's boundary value problem continuation methods [DKK91, Hen02], computation of "fat" trajectories using jet transport [Hen05], and box covering of phase space [DH97]; see also the pioneering paper [JJK97]. High order expansions are adequate to describe center manifolds of fixed points in large neighborhoods [Jor99, Sim98]. They are also needed in the globalization of stable and unstable