Short Course on Numerical Bifurcation and Center Manifold Analysis in Partial Differential Equations

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October 12, 2001

1 A Short Summary

The announced Short Course presents the main ideas of some chapters of my book (in preparation) with a similar title. So I start with a short summary and a list of the chapters planned in this book. Finally, I give contents for those chapters presented during the short course, and, in footnote style, for those chapters available as reading material in a nearly final version.

Since the general cases are much too technical for this short course, I essentially restrict the presentation to the simple model problem

$$-\Delta u + \lambda f(u) = 0 \text{ in } \Omega,\ u|_{\partial\Omega} = 0. \tag{1}$$

The general cases are presented in the available chapters of the book.

2 Main Goals and Outline of the Book

The main goal of this book is to explore numerics and theory of reduction techniques for large dynamical systems, in particular, partial differential equations. Their space discretization yields large systems . The questions of convergence of the discretized to the original dynamical system is the core of this presentation.

We are interested in the underlying low dimensional models of complicated nonlinear behavior in differential equations, e.g., local bifurcations of stationary solutions and periodic orbits, their local dynamics via center manifolds. Some aspects of global bifurcation as homo-clinic orbits are studied as well. A quantitative and qualitative description of nonlinear dynamics for many systems is available merely via numerical methods. However, since nonlinear systems are sensitive to small perturbations at bifurcation points, discretizations of differential equations may destroy the bifurcation scenario.

The book is aimed for graduate students and scientists who want to study and analyze numerically bifurcations of differential equations in mathematics, science and engineering. It consists mainly of five parts and appendices: I:INTRODUCTION INTO BIFURCATION gives examples, motivations and basic numerical results. II:ELLIPTIC OPERATORS AND DISCRETIZATION METHODS introduces general elliptic operators and the important discretizations from finite difference to wavelet methods with convergence proofs for nonlinear problems including bifurcation; III: NUMERICAL LIAPUNOV SCHMIDT METHODS reduces stationary and Hopf bifurcation problems to a system of algebraic equations. IV:NUMERICAL CENTER MANIFOLD METHODS study local dynamics near stationary solutions and periodic orbits via low dimensional reduced systems V:NUMERICAL HOMO-CLINIC ORBITS and Lin method analyze dynamics and long time behavior induced by global bifurcations, e.g. homo-clinic orbits. There are still a lot of open questions w.r.t. the last part. So it is not yet possible to give the same type of precise convergence results as for discretization of Liapunov-Schmidt and center manifold methods. VI: APPENDIX presents a C++ programme for path following and studies of singularities for general classes of operator equations, discretizations, linear and nonlinear solvers and the necessary tools from Functional Analysis and Calculus in Banach spaces.

The numerical realization of these reduction techniques for partial differential equations is the central point of all these discussions. To reach this goal, numerical methods for partial differential equations are studied. We discuss the actual discretization methods as difference, finite element, spectral and wavelet methods. We generalize the usual concepts of stability, consistency and convergence of discrete problems and appropriate pairs of projection operators. The basic tools are approximation theory and a combination of monotone operators and their compact perturbations allowing two benefits: We obtain, for elliptic and parabolic operators, including the Navier-Stokes equations, partially new space discretization methods, e.g., collocation methods on non degenerate subdivisions, and new convergence results for wavelet methods. We reach our goal to ensure convergence of approximate bifurcation scenarios and their dynamics. It is well known that equi variance has a significant impact on bifurcation and the dynamics. So we include two chapters for the numerical realization of finite and infinite groups. Various solution techniques for large sparse systems are modified and incorporated into the context of bifurcation analysis. Moreover, we formulate the theoretical reduction techniques in such a way that a numerical implementation follows directly and efficiently.

In fact, numerical analysis penetrates the whole text and is the essential ingredient of the book. Symmetry and normal form theory are exploited, aiming for efficient numerical algorithms. Furthermore, we discuss utilization of computer algebraic techniques in a study of Hopf bifurcation. We include several case studies on reaction-diffusion equations and biological problems at different levels to illustrate the reduction techniques and analysis of bifurcation scenarios, and their numerical implementations.

Content of the Book:

PART I: INTRODUCTION INTO BIFURCATION

Chapter 1: Introduction + * [1]

Chapter 2: Bifurcation Problems in Differential Equations + *

Chapter 3: Continuation of Solution Branches *

Chapter 4: Numerical Computations of Bifurcation Points

Chapter 5: Bifurcation problems with symmetry *

PART II: ELLIPTIC OPERATORS AND DISCRETIZATION METHODS

Chapter 6: Elliptic Operators *

Chapter 7: Difference Methods

Chapter 8: Finite Element Methods + *

Chapter 9: Spectral Methods (*)

Chapter 10: Discretization Methods with Finite Symmetry Groups (*)

Chapter 11: Wavelet Methods

Chapter 12: Stability for General Discretization Methods + *

PART III: NUMERICAL BIFURCATION IN PARTIAL DIFFEERENTIAL EQUATIONS

Chapter 13: Liapunov Schmidt Methods + *

Chapter 14: Case Study Bifurcation for a 2d-Reaction Diffusion Equation

Chapter 15: Numerical Liapunov-Schmidt methods + (*)

Chapter 16: Case Study – Hopf Bifurcation for a 2d Brusselator

Chapter 17: Case Study – Symmetric Pattern Formation for a 3d Reaction-Diffusion Equation (*)

Chapter 18: Classification of Singularities

Chapter 19: Numerical Analysis of Imperfect Bifurcation (*)

[1] For the Chapters, marked with +, the main ideas are presented for the above special case (1) during the Short Course. The Chapters, marked with * and (*), are available in a nearly final form and present papers appeared or submitted similar to this chapter, resp. Those not included in the Short Course are listed in fotnote style below. The corresponding ps-file will be availble by end of October

Content of Chapters

PART I: INTRODUCTION INTO BIFURCATION

Chapter 1: Introduction

Exploring nonlinear phenomena in the nature has become a major subject in many fields during the last decades, from physics, chemistry, biology, engineering and social science to daily life. Mathematical models for many of these phenomena are nonlinear problems of the form

$$\frac{\partial u}{\partial t} + G(u, \lambda) = 0. \tag{2}$$

Here $G: \ X \times \mathbb{R}^p \to Y$ is a "smooth" mapping and $X, \ Y$ are Banach spaces. $\lambda \in \mathbb{R}^p$ represents various control parameters which are adjustable, e.g. Reynolds number, catalysts, temperature, density, initial or final products, etc. Normally a gradual variation of one control parameter corresponds to a unique and continuous solution curve and the linear stability theory describes well enough the state of the system. However, there exists a large number of problems for which the stability and number of solution curves changes abruptly and the structure of solution manifolds varies dramatically when a parameter passes through some critical values, e.g. buckling of a rod, onset of convection and turbulence, pattern formations in chemical and biological reactions, etc. This kind of phenomena, called *bifurcation*, describes a qualitative change in a dynamical system. In this situation the linear stability theory fails and does not give much information on the qualitative behavior of the nonlinear system. Bifurcation analysis and nonlinear stability have to be considered. Usually, this requires a combination with numerical approximations and simulations.

Basically, bifurcation theory studies how solutions of (2) and their stability and other properties change as the parameter λ varies. For two finite dimensional examples of a pitchfork bifurcation in $\mathbb{R}^2$ and a bifurcation in $\mathbb{R}^n$ with symmetric derivative we introduce the easiest case of Liapunov-Schmidt methods and indicate further reduction techniques.

Chapter 2: Bifurcation Problems in Differential Equations (with Mei)
We list practically important ordinary and partial differential equations which give rise to bifurcation. A point (u_0, λ_0) in $X \times \mathbb{R}^p$ is called a *bifurcation point* of (2) if it satisfies (usually the stationary form of) (2) and in all neighborhoods of (u_0, λ_0) the problem (2) has at least two different solution branches.

We present an introductory study of several examples to show the qualitative difference in linear and nonlinear problems and to illustrate local and global bifurcation phenomena. Some of these examples will be used successively in the book, especially in case studies

- Breaking rod [**?**, **?**];
- Rod with axial load;
- Chladny sound figure [**?**, **?**, **?**, **?**];
- Von Kármán equations [**?**];
- Kuramoto-Sivashisky equation [**?**, **?**];
- Reaction-Diffusion equations [**?**, **?**, **?**];
- Navier-Stokes equation [**?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**].

[2]

[2]**Chapter 3: Continuation of Solution Branches (with Mei)**
We describe numerical continuation methods and the detection of singular points on the solution curves. For large systems Krylov type iteration methods are very efficient. So we discuss these types of iteration methods to solve linear problems and to determine the critical eigenvalues of the linearized operators (of the finite dimensional discretizations). Next we consider some pre-conditioning techniques which are extremely important for the good convergence of these iteration methods. Numerical results and a subsection on invariant subspaces and their efficient theoretical and practical computation conclude this Section.

- Numerical continuation methods;
- Krylov subspace;
- Pre conditioning;
- Numerical Results;
- (Invariant subspaces.)

Chapter 5: Bifurcation problems with symmetry (with Mei)
Symmetry and symmetry-breaking are features widely involved in nature and science. The

PART II: ELLIPTIC OPERATORS AND DISCRETIZATION METHODS

[3]

Chapter 8: Finite Element Methods
This is one of the standard techniques to numerically solve elliptic problems. In the usual setting mostly low oder or h, p methods are discussed and are appropriate. Since we want to apply the whole machinery to nonlinear problems including turning points, bifurcation, a.s.o., we have to allow possible high order methods as well. This enforces a careful study in particular of finite element methods with variational crimes. It is applicable to define high order collocation methods on non degenerate subdivisions of the domain.

For ODEs collocation is one of the most powerful and flexible methods. For PDEs, this seems to be a new class of discretization methods. The possible high orders are certainly attractive for singularities in nonlinear problems. However, nearly all practical questions are still open, e.g., efficient determination and solution of the underlying (non-)linear systems, operator evaluation and grid strategies. In particular we study:

- Approximation theory for Finite Elements on polygonal and curved domains with and without variational crimes;
- Conforming finite elements;
- Finite elements with variational crimes;
- Consistency and co-ercivity for variational crimes;
- Generalized Strang lemmas;

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developments of bifurcation theory with symmetries has demonstrated that highly complicated bifurcation structure can be studied systematically with group theoretic concepts. Equivariant branching lemma and bifurcation subgroups are the principle tools for simplifying bifurcation analysis. Exploiting symmetries in numerical analysis is an efficient technique to reduce computational costs and to improve condition numbers in numerical solution of linear and nonlinear problems. Group theoretic methods have been applied to develop efficient numerical schemes for both algebraic and differential equations.

We review some basic concepts in group theory and fundamental results of bifurcation theory with symmetry and their applications to numerical analysis, for examples,

- Important finite and continuous groups;
- Representation of groups and irreducibilites;
- Equivariant and symmetric operators.

[3]**Chapter 6: Elliptic Operators**
Appendix A presents Sobolev spaces relatively extensively. So, we give here the complementary features which are necessary for the context of discretization, in particular for bifurcation and dynamical properties. We study:

- Bilinear forms and induced linear operators;
- Elliptic bilinear forms;
- The Navier Stokes equation.

- Stability and convergence for general finite elements.

[4]

Chapter 12: Stability for General Discretization Methods
In the preceding chapters on difference, finite element, spectral and wavelet methods we have essentially combined approximation properties of the corresponding function spaces, the co-ercivity of bilinear forms (which is usually relatively easy to prove) and the concept of compact perturbation. These concepts allow to include

- Generalized Petrov-Galerkin methods and methods with crimes;
- Regularizing difference methods;
- Stability of generalized Petrov-Galerkin methods;
- Stability for Petrov-Galerkin methods applied to bordered systems
- Application to Navier-Stokes operator

PART III: NUMERICAL BIFURCATION IN PARTIAL DIFFERENTIAL EQUATIONS

Chapter 13: Liapunov-Schmidt Methods
We start discussing efficient low dimensional modeling of bifurcation problems. We introduce the Liapunov-Schmidt method and its extensions. Besides the classical Liapunov-Schmidt method, we consider particularly the generalizations by Jepson/Spence and modifications. By reducing the problem to an underlying low dimensional system of algebraic equations we can often derive the bifurcation scenario directly with the established singularity theory. We discuss an iterated method for the Liapunov-Schmidt method and calculations of Taylor expansion of the reduced bifurcation equations. This allows an easy calculation

[4]**Chapter 9: Spectral Methods =Section 1,2 of Böhmer,Geiger,Rodriguez [?]** Spectral methods are particularly important if, problems equivariant w.r.t. an infinite group, have to be discretized. The approximating elements in these spectral spaces and hence the discrete approximation of these operators inherit this equi-variance Due to the high accuracy of spectral methods, applicable to only simple domains, they have been used recently in many papers to study bifurcation for operator equations. Here we present a short version of comprehensive other versions in ([**?**, **?**, **?**, **?**, **?**]).

Chapter 10: Discretization Methods with Finite Symmetry Groups: Paper Allgower,Böhmer,Georg,Miranda, [?] We have seen that symmetry imposes strong additional structure onto bifurcation phenomena. Numerically we have to distinguish between finite and infinite groups. In this chapter we study finite symmetry groups, in particular

- Symmetry in Finite Element methods;
- Equi variance of Operators;
- Twisted Reynolds projectors;
- Symmetry respecting discretizations;
- Examples of decomposition of the identity;
- Criteria for direct sum decompositions.

of the Taylor expansion of the reduced equations and its implementation. This involves the topics

- Motivating Example
- The Liapunov-Schmidt-Method
- Generalized Liapunov-Schmidt-Method
- Iterative calculations ([?, ?, ?, ?, ?]) of Taylor series of the reduced equations
- Hopf bifurcation ([?])

Chapter 15: Numerical Liapunov-Schmidt Methods
Since many elliptic equations cannot be solved directly we have to use different types of discretization methods. This is correct for problems with or without the bifurcation. The present form is based on consistent differentiability and bordered stability. Or it employs different projection operators for the pre-image and the image spaces. For many of the following discretization methods the first concept is appropriate for others, e.g., finite element methods with variational crimes, the second is required. A convergence theory covering all these different methods is developed. The discretization of Liapunov-Schmidt methods requires in particular

- General concepts of discretization methods;
- Extension operators and approximate projectors;
- Discretization near singular points;
- The numerical Liapunov Schmidt method;
- An Algorithm for numerical Liapunov Schmidt methods;
- Numerical example for stationary bifurcation;
- Example for Hopf bifurcation.

[5]

[5]**Chapter 17: Case Study – Symmetric Pattern Formation for a 3d Reaction-Diffusion Equation = Section 3,ff of Böhmer,Geiger Rodriguez**
We study stationary bifurcations of a $3d$ reaction-diffusion equation. These equations are typical models in chemical reactions, biological systems, population dynamics and nuclear reactor physics. They are of the form

$$\frac{\partial u}{\partial t} = D\Delta u + f(u, \lambda). \tag{3}$$

Here $u = (u_1, \ldots, u_k)$ represents various substances in a chemical reaction or species of a biological system; $\lambda \in \mathbb{R}^p$ is a vector of control parameters; Δ is the Laplace operator in the spatial variables and describes diffusion of different substances; the matrix $D \in \mathbb{R}^{k\times k}$ is symmetric, positive semi-definite, often diagonal and consists of diffusion constants; the mapping $f:\ \mathbb{R}^k \times \mathbb{R}^p \to \mathbb{R}^k$ is a vector of smooth functions and represents the reaction among

PART IV: NUMERICAL CENTER MANIFOLD METHODS

Chapter 21: A Numerical Center Manifold Method Reduction
Center manifold theory is essential for analyzing dynamics near local bifurcations. As the Liapunov-Schmidt reduction for stationary and Hopf bifurcations, center manifold theory is used to reduce a dynamical system near a non hyperbolic equilibrium or a periodic solution to a low-dimensional system. Furthermore, stability of solutions and local dynamics of the system can be derived from the low-dimensional system. The center manifolds were introduced in the sixties by Pliss [**?**] and Kelley [**?**]. Owing to the Lanford's contribution [**?**] this theory has been applied extensively to the study of bifurcation problems and dynamical systems, in particular, in connection with the normal form theory.

We are mainly interested in applying the techniques of center manifold theory to partial differential equations and in deriving the lower dimensional underlying systems (cf. Mei [**?**]), based on detailed discussions in Carr [**?**], Iooss/Adelmeyer [**?**], Vanderbauwhede [**?**] about center manifold reduction and normal form theory for ordinary differential equations in finite dimensional spaces, and Chow/Lu [**?**], Henry [**?**] Vanderbauwhede/Iooss [**?**] for infinite dimensional systems and partial differential equations
. Similarly as in the Liapunov-Schmidt method, the center manifold and the reduced equation are explicitly available only in exceptional cases. So we calculate for general problems their Taylor expansions successively. For PDEs we have to use space (and time) discretization methods with respect to the space (and time as well) to approximate these center manifolds. Time discretizations have been studied by Lubich e.a.,[**?**, **?**]. Again stability, consistency and convergence of spatially discretized problems have to be adapted to center manifolds (cf Mei

the substances.

As a more complicated example we study a pattern formation in biology with high spherical symmetry, characterized by $l = 2, l = 3$. We have to carefully go through the different steps

- Linearized eigenvalue problem of a model problem;
- Application of the Liapunov-Schmidt reduction;
- Generic bifurcation in the $l = 2$ representation;
- Generic bifurcation in the $l = 3$ representation, where $l = 2$ and $l = 3$ refer to wave numbers in the problem.

Chapter 19: Numerical Analysis of Imperfect Bifurcation = Paper Böhmer, Janovska, Janovsky [?]
The aim in this chapter is the following: We want to re transform the bifurcation scenarios from the normal form or its unfolding of the reduced bifurcation functions to the bifurcation situation of the original operator equation. This is an astonishingly nontrivial problem and has been solved in [**?**, **?**, **?**, **?**, **?**, **?**, **?**] for stationary bifurcation of co-dimension ≤ 3 or $= 3$. We study an appropriate formulation of the bifurcation equations and the diffeomorphism with the original problem

- Computation of the differential of this diffeomorphism;
- Remarks on implementations;
- Tables necessary for practical application of these results.

[?], Böhmer/Sassmannshausen [?].
We are able to prove that by the space discretization we obtain a discrete center manifold such that the coefficients in the normal form of the discrete center manifold converge to those of the original center manifold. This implies in particular convergence of dynamical scenarios. In the Literature until now only numerical experiments for space discretized center manifolds, but no convergence results are reported. We study

- Basics for center manifolds;
- Center manifolds for simple Hopf bifurcation;
- Transformation to normal forms;
- Numerical center manifold method;
- Center manifolds for parameter dependent problems

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PART V: NUMERICAL Homoclinic Orbits

PART VI: APPENDICES

Appendix A: Functional Analysis We present the necessary basics, e.g.,

- Linear functi0onals and dual spaces;
- Linear operators and projectors;
- Linear operators in Banach spaces;
- Sobolev spaces.

Appendix B: Calculus in Banach spaces We present the necessary basics, e.g.,

- Derivatives for operators in Banach spaces;
- Integrastion and mean value theorems in Banach spaces;
- Paartial derivatives of operators;
- Higher derivatives;
- Implicitely defined operators, Newton methods;
- Taylor-formula.

Appendix C: Pathfinder, C++ program for continuation of solution curves and detecting different types of singularities

We present a C++ program in a very short version. It is aimed to allow the following: Different types of operators and discretizations, corresponding solution techniques for linear and nonlinear problems can be defined by the user or taken over from some other libraries. Then it yields a tool to compute parameter depending solution curves and the corresponding singularities. The goal is to have a programme available which is applicable to a wide class of problems, discretization methods, singularities, test functions a.s.o. with all the advantages of the C++ programming.