EXPLORING BORDERS OF CHAOS

PROF. DR. YURI KUZNETSOV
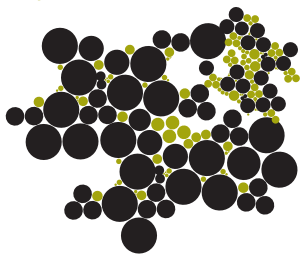
UNIVERSITY OF TWENTE.

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EXPLORING BORDERS OF CHAOS

INAUGURAL LECTURE GIVEN
TO MARK THE ASSUMPTION
OF THE POSITION AS PROFESSOR OF

NUMERICAL BIFURCATION METHODS

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BY

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INTRODUCTION

MIJNHEER DE RECTOR MAGNIFICUS, GEACHTE DAMES EN HEREN

In my lecture, I will try to reflect on the history and current state of art of my research field, discuss its role in the mathematical modeling in various branches of modern Science, and sketch some implications of recent trends for research, software development, and education.

This lecture is about mathematical tools to study deterministic processes. What is a deterministic process? The progress of Science is to big extent marked by our increasing ability to predict future states of various systems. This is based on describing system states by elements of some set X so that at a moment t of time the system is in the state $x(t) \in X$. The set X is called the phase space of the system. The behavior of the system is a deterministic process if $x(t)$ is fully determined by $x(0)$, i.e. there is a family $\{\phi^t\}_{t \geq 0}$ of maps $\phi^t : X \to X$, such that

$$x(t) = \phi^t(x(0)).$$

The map ϕ^t is called the evolution operator of the system. It is postulated that ϕ^0 is the identity map. It is further assumed that the evolution from the state $x(t)$ to the state $x(t+s)$ depends only on the time difference s and not on the moment t itself, so that $x(t+s) = \phi^s(x(t))$ implying $\phi^{t+s} = \phi^t \circ \phi^s$. The last property means that the system is autonomous, i.e. its structural properties do not change with time. The image in X of the domain of definition of the map $t \mapsto x(t)$ is called the orbit (see Figure 1).
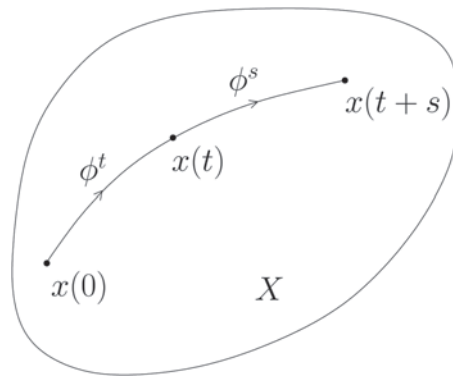
Figure 1:   An orbit of a dynamical system.

Collecting all introduced ingredients, i.e. time, phase space, and the evolution operator, we come to the notion of a *dynamical system* that is a mathematical model of a deterministic process. Marquis P.S. de Laplace suggested that the evolution of the whole Universe is a deterministic process:

We may regard the present state of the universe as the effect of its past and the cause of its future. An intellect which at a certain moment would know all forces that set nature in motion, and all positions of all items of which nature is composed, if this intellect were also vast enough to submit these data to analysis, it would embrace in a single formula the movements of the greatest bodies of the universe and those of the tiniest atom; for such an intellect nothing would be uncertain and the future just like the past would be present before its eyes.

—P.S. de Laplace, A Philosophical Essay on Probabilities

Of course, de Laplace had in mind a classical mechanical system and already this made his vision unrealistic from our point of view. However, a significant progress in various fields of Science was achieved by modeling of certain subsystems of the universe by dynamical systems

and studying how their evolution depends on parameters describing their internal properties and time-independent interactions with the external world. Such models employed various phase spaces X, ranging from the set of real numbers (when abundance of a certain substance as function of time was studied) to an infinite-dimensional projective complex space (when the evolution of the state of an isolated quantum system between observations is analyzed). Note that mean fields or probabilistic distributions appearing in statistical description of large systems often evolve deterministically. We shall see later that the relationship between determinism and predictability is much more nontrivial than it might look.

We will first focus on a special situation when the phase space X is the set of all n-tuples $\mathbf{R}^n$, time t is continuous, and the evolution operator is implicitly defined by the solutions of a system of ordinary differential equations (ODEs)

$$\dot{x}(t) = f(x(t)), \quad f : \mathbf{R}^n \to \mathbf{R}^n,$$

where f is a smooth vector field. By a tradition going back to Sir I. Newton, the dot denotes the derivative w.r.t. time t. Dynamical systems of this type appear in many applications, since contributions from various effects on each $\dot{x}_k$ are often additive, which simplifies the derivation of models. As a typical example, we can consider the *Brusselator*, a hypothetical homogeneous chemical system composed of substances X,B,D,E, that react according to the following irreversible stages:

$$A \to X$$
$$B + X \to Y + D$$
$$2X + Y \to 3X$$
$$X \to E$$
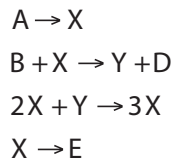
The law of mass action leads under certain assumptions to the following system of two differential equations

$$\begin{cases} \dot{x} = a - (b+1)x + x^2 y, \\ \dot{y} = bx - x^2 y, \end{cases} \tag{1}$$

where (x,y) are scaled concentrations of X and Y respectively.

ODEs also appear in the analysis of distributed dynamical systems when X is a function space that has an invariant finite-dimensional manifold, e.g. a surface composed of orbits, on which (local) coordinates x_i can be introduced. There is yet another manner in which ODEs appear: As differential equations describing profiles of planar travelling waves in partial differential equations (PDEs) modeling some distributed dynamical systems.

J. Liouville proved in the 1840s that many ODEs cannot be solved in explicit form. For example, the y-component of the solution of the following simple system

$$\begin{cases} \dot{x} = 1, \\ \dot{y} = -x + y^2, \end{cases} \tag{2}$$

(that is equivalent to the single Bernoulli equation $y' = y^2 - x$) cannot be expressed as a finite combination of elementary functions of t or algebraic functions and integrals of such functions. The reason for this difficulty is the nonlinearity of the system. Actually, very few nonlinear ODEs can be solved explicitly.
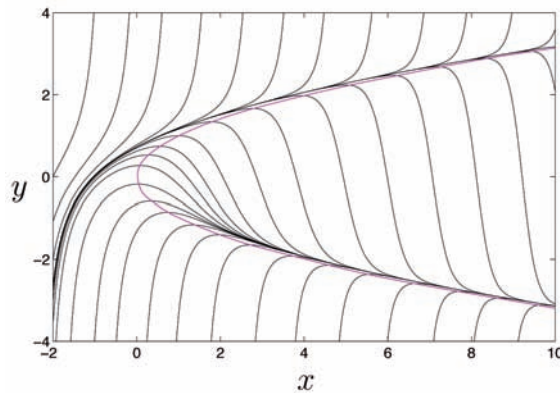
Figure 2:   The phase portrait of the Bernoulli system (2).

J.H. Poincaré laid in the 1880s foundations of a qualitative (geometric) analysis of ODEs that allows one to establish properties of the collection of all orbits of an ODE system (called phase portrait) even if its explicit general solution is unavailable. For example, Figure 2 shows the phase portrait of system (2). Its qualitative features are easily predictable by noticing that the corresponding vector field is horizontal along parabola $x = y^2$.

The simplest interesting orbits of ODE systems are *equilibria* and *cycles* corresponding to stationary and periodic processes, respectively. Other important types of orbits are *homoclinic* and *heteroclinic* orbits that connect (possibly to themselves) equilibria and cycles. J.H. Poincaré and I.O. Bendixson proved that a bounded orbit of a planar ODE (with $n = 2$) can either approach an equilibrium, or a cycle, or a singular cycle composed of homo- and heteroclinic orbits to equilibria. Poincaré also recognized in the 1890s that a multidimensional ODE system (with $n \geq 3$) can have infinite number of isolated periodic orbits and an individual orbit can indefinitely wander between these cycles as $t \to \pm\infty$, without approaching any of them. This occurs, for example, near a homocinic orbit to a cycle, when the surface composed of all

orbits approaching the cycle as $t \to +\infty$ intersects transversally the surface composed of all orbits approaching the same cycle as $t \to -\infty$. It seems, however, that he expected such a complicated phenomenon (that we now call the Poincaré homoclinic structure) to occur only in very special dynamical systems from Classical Mechanics, which preserve energy and phase volume, and for which the presence of this structure implies nonintegrability. It is also remarkable that he gave up to sketch a cross-section of the homoclinic structure. The analysis of orbits near the Poincaré homoclinic structure was continued by G.D. Birkhoff in the 1930s and finished by S. Smale, Ju.I. Neimark and L.P. Shilnikov in the 1960s.

One of the major discoveries in the mathematics of the 20th century was that generic dissipative ODE systems can exhibit a robust complicated behavior that has many features of a random process but is nevertheless deterministic. Moreover, chaotic motions can be confined to an attracting set in the phase space that is bounded and has a fractal structure. These invariant sets were called strange attractors by D.P. Ruelle and F. Takens in 1971. It has been noticed by E.N. Lorenz in 1963 that the deterministic nature of such processes does not mean their practical predictability: A slightest difference in initial data leads to very different solutions.

Figure 3 shows a strange attractor in the *Rössler prototype system*

$$\begin{cases} \dot{x}_1 = -x_2 - x_3, \\ \dot{x}_2 = x_1 + Ax_2, \\ \dot{x}_3 = Bx_1 - Cx_3 + x_1x_3, \end{cases} \tag{3}$$
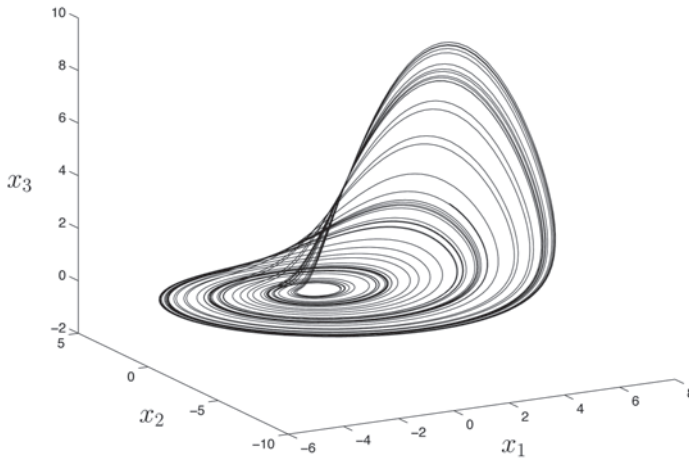
with $A = 0.36, B = C = 0.4$.

Figure 3:   *A strange attractor in the Rössler system (3).*

J.H. Poincaré also introduced the notion of *bifurcation*, i.e. the qualitative change of the phase portrait of a dynamical system when parameters of the system are slightly changed. He also prepared all necessary tools to study one of the simplest - and thus often occurring in applications – bifurcation, namely, the birth of a limit cycle from an equilibrium when it changes stability in an oscillatory manner. While Poincaré focused on the changes of special orbits (e.g. cycles), it was A.A. Andronov who started in the 1920s to consider bifurcations of the whole phase portrait. Figure 4 shows this phenomenon (called the *Andronov-Hopf bifurcation*) in the Brusselator model (1). Given value a, it happens when the parameter b crosses the critical value $b_0 = 1 + a^2$. For $b < b_0$ there exists a stable equilibrium that becomes unstable for $b > b_0$ when limit cycle is born.
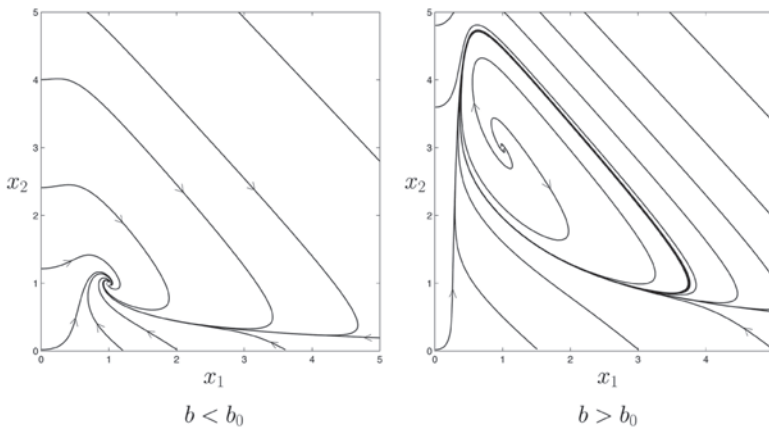
Figure 4:   Andronov-Hopf bifurcation in the Brusselator model (1).

S. Smale proved in the 1960s that a generic dissipative system can have an infinite number of limit cycles and that the set of the bifurcation parameter values of a generic parameter-dependent system can be very complicated, in fact fractal. Actually, he constructed a multidimensional system such that all its small perturbations are not structurally stable, i.e. their phase portrait changes qualitatively under proper further parameter variations. This led usually optimistic V.I. Arnold to very pessimistic conclusions in 1978:

For the qualitative theory of differential equations this result has approximately the same significance as Liouville's theorem on the impossibility of solving differential equations by quadrature for the integration theory of differential equations. It shows that the problem of the complete topological classification of differential equations with high-dimensional phase space is hopeless, even if restricted to generic equations and nondegenerate cases.

Most differential equations admit neither exact analytic solution nor a reasonably complete qualitative analysis.

—V.I. Arnold, Geometrical Methods in the Theory of Ordinary Differential Equations

Figure 5 illustrates complexity of bifurcation sets by presenting a partial bifurcation set of a system of three ODEs that describe behavior of a tritrophic food chain composed of a logistic prey, a Holling type II predator, and a Holling type II top-predator, with population densities x_1, x_2, and x_3, respectively. The corresponding nonlinear ODE system is one of the most studied models in Theoretical Biology [Kuznetsov & Rinaldi, 1996]. It depends on several parameters that determine intra- and interspecies interactions.

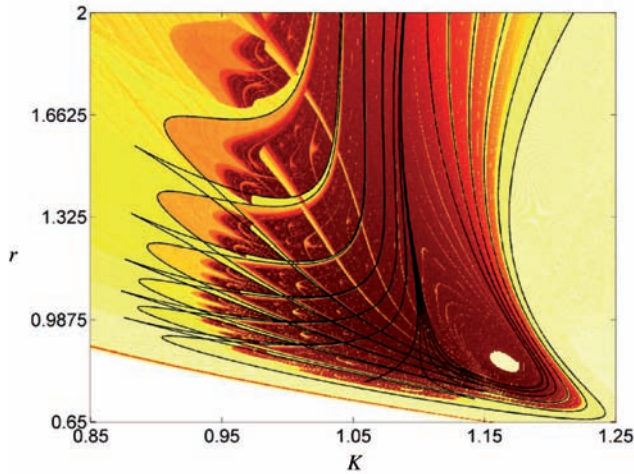*Figure 5:   The partial bifurcation set of the ecological model (4).*

In the properly rescaled variables, the system looks as follows:

$$
\begin{cases}
\dot{x}_1 = x_1\left[r\left(1-\dfrac{x_1}{K}\right)-\dfrac{a_1 x_2}{1+b_1 x_1}\right], \\[2mm]
\dot{x}_2 = x_2\left[\dfrac{a_1 x_1}{1+b_1 x_1}-\dfrac{a_2 x_3}{1+b_2 x_2}-d_1\right], \\[2mm]
\dot{x}_3 = x_3\left[\dfrac{a_2 x_2}{1+b_2 x_2}-d_2\right].
\end{cases}
\tag{4}
$$

The bifurcation set in the (K, r) -plane in Figure 5 [Kuznetsov, De Feo, & Rinaldi, 2001] is constructed for

$$a_1 = 5, \, a_2 = 0.1, \, b_1 = 3, \, b_2 = 2, \, d_1 = 0.4, \, d_2 = 0.01,$$

and the darkness levels on it correspond to more and more complicated cycles with the increasing number of the prey-predator oscillations per period.

Thus, the dynamical systems theory has provided scientists with a universal language to describe and study various deterministic processes, identified simplest asymptotic regimes and bifurcations, but found principle obstacles to the complete bifurcation analysis of dynamical systems.

NUMERICAL ANALYSIS OF ORDNARY DIFFERENTIAL EQUATIONS

Further progress in the theory of dynamical systems, as well as its application to realistic models from various scientific disciplines, would have been impossible without computers. Given a system of smooth ODEs depending on parameters,

$$\dot{x} = f(x, \alpha), \quad f : \mathbf{R}^n \times \mathbf{R}^m \to \mathbf{R}^n, \tag{5}$$

our ultimate goal would be to construct its *bifurcation diagram* (i.e., to obtain its bifurcation set in the parameter space $\mathbf{R}^m$ and to provide all qualitatively different phase portraits in its phase space $\mathbf{R}^n$, as well as to describe how these portraits bifurcate under parameter variations). As we have seen above, this task might be impossible since the bifurcation set can have infinite number of complex-shaped regions. However, even a partial knowledge of the bifurcation set (as in Figure 5) and corresponding phase portraits can provide important information on the behavior of the model. One might thus try to *explore the borders of chaos*, i.e. delimit them in the parameter space and explain which bifurcation scenarios lead to complicated dynamics. In Figure 5, the chaotic domain is visibly delimited by several black curves, on which bifurcations of cycles occur and which can be computed by numerical methods discussed below. Actually, the system (4) also has a Poincaré homoclinic structure associated to a cycle and other homoclinic and heteroclinic orbits.

Fortunately, bifurcation diagrams are not entirely irregular but include canonical building blocks, common for all generic systems. All generic bifurcations of equilibria and limit cycles in multi-dimensional

ODEs, as well as many bifurcations of connecting orbits in one- and two-parameter systems (e.g., with $m = 1, 2$) have been studied theoretically. Here major contributions have been made by A.A. Andronov and other members of the Nizhny Novgorod (Gorky) school, including E.A. Leontovich, N.N. Bautin, Ju.I. Neimark, and L.P. Shilnikov. Particularly fruitful period in the development of the bifurcation theory started in the 1970s, when ideas and methods from the theory of singularities of differentiable functions (e.g., normal forms, codimension, versal deformations, etc.) have been applied to study bifurcations of phase portraits of dynamical systems by R.F. Thom, V.I. Arnold, F. Takens, and others.

Bifurcations can be classified by their *codimension*, i.e. the minimal number of parameters needed to be tuned in order to encounter this bifurcation in a generic ODE system. Thus, bifurcations of codim 1 occur at isolated parameter values in ODEs depending on one parameter and on curves in the two-parameter ODEs, bifurcations of codim 2 occur at isolated points in the parameter plane of ODEs with two parameters, etc. The Andronov-Hopf bifurcation has codim 1. Sometimes, it is possible to construct and study simple canonical ODE systems that capture (at least some) key features of bifurcation diagrams of generic systems near critical equilibrium points for nearby parameter values. For example, in generic planar systems depending on one parameter, the Andronov-Hopf bifurcation happens qualitatively in the same way as in the Poincaré normal form

$$\begin{cases} \dot{x}_1 = \alpha_1 x_1 - x_2 + l_1 x_1 (x_1^2 + x_2^2), \\ \dot{x}_2 = x_1 + \alpha_1 x_2 + l_1 x_2 (x_1^2 + x_2^2), \end{cases} \tag{6}$$

at $\alpha_1 = 0$ with $l_1 \neq 0$. The sign of the normal form coefficient l_1 determines whether the bifurcation is sub- or super-critical. If the system depends on two parameters, this bifurcation occurs when one crosses a curve in

the parameter plane. At isolated points of this curve, the normal form coefficient l_1 may vanish, which leads to a codim 2 bifurcation, called the *Bautin bifurcation*. Its normal form includes the 5th order terms,

$$
\begin{cases}
\dot{x}_1 = \alpha_1 x_1 - x_2 + \alpha_2 x_1 (x_1^2 + x_2^2) + l_2 x_1 (x_1^2 + x_2^2)^2, \\
\dot{x}_2 = x_1 + \alpha_1 x_2 + \alpha_2 x_2 (x_1^2 + x_2^2) + l_2 x_2 (x_1^2 + x_2^2)^2,
\end{cases}
\tag{7}
$$

and depends on two parameters. The bifurcation set of this normal form on the (α_1, α_2) -plane includes the Andronov-Hopf bifurcation line $\alpha_1 = 0$ on which a cycle is born (sub- or supercritically), as well as the half-parabola

$$
\alpha_1 = \frac{\alpha_2^2}{4l_2}
$$

for α_2 satisfying $l_2 \alpha_2 < 0$, on which two cycles of opposite stability collide and disappear in what is called the *fold bifurcation* of cycles. This is the simplest example, when an equilibrium bifurcation of codim 2 involves a global bifurcation of codim 1. This example shows that codim 2 points serve as *organizing centers* for planar bifurcation diagrams. Their detection and computation of the relevant normal form coefficients allow us to predict local bifurcation diagrams near such points in concrete ODE models. The normal forms determine which bifurcation curves of codim 1 meet at codim 2 organizing centers. Finally remark, that near each equilibrium bifurcation, all interesting dynamics happen on an invariant manifold of a relatively low dimension (determined by the number of critical eigenvalues on the imaginary axis), where the normal form has to be computed. In the simplest cases, all other orbits rapidly converge towards this *center manifold*.

Already for planar ODEs, we have to rely on a computer to obtain information on the structure of the bifurcation set. This is particularly

true for bifurcations of cycles and connecting orbits, but even the analysis of equilibria in multidimensional ODEs is practically impossible without numerical calculations.

Let us start with the problem of the computation of the normal form coefficients for local bifurcations. If the bifurcation parameter values and the equilibrium are known exactly, then one could try to transform a given system to its normal form up to a certain order *symbolically*, either by hand or using computer algebra software. This, however, is rarely the case for realistic models, where the bifurcation parameter values and the critical equilibria are known only approximately, from numerical calculations explained below. The situation is even more hopeless for bifurcations of periodic orbits, which are practically never known analytically. Moreover, to analyze bifurcations of cycles, one would apparently need to transform the corresponding Poincaré map to its normal form, while this map and its derivatives are only available numerically. Fortunately, based on works by P.H. Coullet & E.A. Spiegel and G. Iooss published in the 1980s, special methods (that use *Fredholm solvability* conditions applied to homological equations) have been recently developed for codim 1 and 2 bifurcations of equilibria and cycles [Kuznetsov, 1999; Kuznetsov, Govaerts, Doedel, & Dhooge, 2005]. These methods are suitable for the numerical evaluation of the normal form coefficients. Moreover, they allow to completely avoid the numerical computation of the Poincaré map and its derivatives while computing the coefficients of the periodic normal forms for local bifurcations of cycles.

Numerical computation of either an equilibrium or a cycle (as well as their bifurcations), or a connecting orbit, can be reduced to the *continuation of a curve* in some space $\mathbf{R}^N$. The simplest example is the computation of a branch of equilibrium points of an ODE system depending on one parameter. This branch is by definition a connected set of solutions to the system of n equations $F(u) \equiv f(x, \alpha) = 0$ with

$N = n + 1$ variables $u = (x, \alpha) \in \mathbf{R}^N$, i.e. an implicitly defined curve. There exist standard predictor-corrector methods to approximate such curves, e.g. the *pseudoarclength continuation*, where prediction is the tangential and the correction is done by Newton iterations in the orthogonal plane to the prediction vector. A more difficult problem is how to reduce the continuation of a cycle to a finite-dimensional problem $F(u) = 0$. Here two different approaches are possible: Computing cycles as fixed points of the evolution operator $\phi_\alpha^{T_0}$ corresponding to (5), where T_0 is the (unknown) period of the cycle, or formulate a boundary-value problem for the corresponding periodic solution $x(t)$. In the first method (that essentially is based on the Poincaré map), the continuation of a cycle is performed as that of a solution $u = (x, T_0, \alpha) \in \mathbf{R}^{n+2}$ to the system of $n + 1$ equations

$$\begin{cases} \phi_\alpha^{T_0}(x) - x = 0, \\ \qquad \Psi(x) = 0, \end{cases} \tag{8}$$

where the second equation is a phase condition selecting a base point on the cycle. In the second method, one introduces the boundary-value problem (BVP)

$$\begin{cases} \dot{\xi}(\tau) - T_0 f(\xi(\tau), \alpha) = 0, \\ \qquad \xi(0) - \xi(1) = 0, \\ \qquad \qquad \Psi[\xi] = 0, \end{cases} \tag{9}$$

in which the last equation is again a phase condition that selects one periodic solution among a continuum of solutions that differ by a phase shift. This boundary-value problem has still to be discretized to obtain a finite-dimensional continuation problem for (approximation data for) $\xi(\tau)$, T_0, and α. Note that the true periodic solution of the original ODEs is

$$x(t) = \xi\left(\frac{t}{T_0}\right).$$

The most popular discretization method is the piecewise-polynomial approximation with orthogonal collocation. Together with the pseudo-arclength continuation, it was introduced in the 1980s into the numerica bifurcation analysis of cycles by H.B. Keller and E.J. Doedel and implemented in one of the most efficient continuation codes - AUTO. The BVP method is believed to work better for ODEs with slow-fast solutions.

To compute a bifurcation curve for an equilibrium or a cycle in two-parameter ODEs (5), we have to construct a defining system to which the continuation algorithm can be applied. Such a defining system should in any case contain the defining system for the equilibrium or a cycle in question, as well as some equations determining the bifurcation. Again two approaches are possible: Either we add to the basic system the minimally required number of equations (equal to the codimension of the bifurcation), or allow one to add more equations for some auxiliary quantities describing the critical situation. For example, to characterize an equilibrium with a zero eigenvalue of the Jacobian matrix, we can add either one equation for its determinant to vanish,

$$\begin{cases} f(x,\alpha) = 0, \\ \det f_x(x,\alpha) = 0, \end{cases} \tag{10}$$

or a system of equations for its normalized null-vector,

$$\begin{cases} f(x,\alpha) = 0, \\ f_x(x,\alpha)v = 0, \\ \langle v,w \rangle - 1 = 0, \end{cases} \tag{11}$$

where w is any vector not orthogonal to the null-space of $f_x(x,\alpha)$. The defining system (10) is called the *minimally augmented*, while the system (11) is the (*maximally) augmented* defining one. Clearly, the minimally augmented systems are smaller. Moreover, there is a clever method to avoid computation of the determinants: We can express a condition for a rank drop of a big matrix via the same rank drop of a smaller matrix that is computable by solving an auxiliary linear *bordered system*. In the above case, one can substitute the equation det $\det f_x(x,\alpha) = 0$ in (10) by the equation $g(x,\alpha) = 0$, where the scalar function g is to be obtained by solving

$$\begin{pmatrix} f_x(x,\alpha) & u \\ w^T & 0 \end{pmatrix} \begin{pmatrix} v \\ g \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{12}$$

where the bordering vectors w and u are selected to make the matrix of this system nonsingular. If $g = 0$, then v satisfies (11), implying that $f_x(x,\alpha)$ is singular and its determinant vanishes. There is also an efficient way to compute the derivatives of g w.r.t. x and α. This *bordering technique* goes back to a work by A. Griewank and G. Reddin of 1984 and is fully developed by W.-J. Beyn and W. Govaerts in the 1990s. It is standard nowadays, also for bifurcations of limit cycles [Doedel, Govaerts, & Kuznetsov, 2003]. Moreover, auxiliary data obtained during the continuation can be effectively reused in the computation of the normal form coefficients for the corresponding bifurcations.

Since the early 1970s, many research groups started to develop numerical codes to perform bifurcation analysis of their own models, as a complement to simulations. Very few of such codes were publically available. However, in the mid 1980s the situation has changed and several groups started to offer free continuation and bifurcations software. The reasons for this shift are not fully clear. It seems that most research on bifurcation theory took place at universities or research

institutions which were expected to make their results public. Among several packages, two became widely known: AUTO86 and LINLBF, developed by E.J. Doedel at Caltec (Pasadena, CA) and A.I. Khibnik at the Research Computing Centre of the USSR Academy of Sciences (Pushchino, Moscow Region), respectively. The codes were written in FORTRAN and allowed the user to perform a similar bifurcation analysis that included the one-parameter continuation of equilibria and cycles, and detection and the two-parameter continuation of their codim 1 bifurcations. There were, however, essential differences: AUTO used maximally augmented defining systems to continue bifurcations and employed BVP methods for the cycle-related computations, while LINLBF computed bifurcations via minimally extended systems and used the numerically constructed Poincaré maps and their derivatives for cycles. LINLBF supported some three-parameter continuations and computed the normal form coefficients for codim 1 bifurcations of equilibria (i.e. saddle-node and Andronov-Hopf).

Systematic bifurcation analysis requires repeated continuation of different phase objects in free parameters, detection and analysis of their bifurcations, and branch switching based on the computation of the normal form coefficients. Such computations produce a lot of numerical data that must be analyzed and, eventually, presented in a graphical form. Thus, software for bifurcation analysis should not only be efficient numerically but should allow for interactive management and have a user-friendly graphics interface. Another motivation for the development of interactive bifurcation software came from the iterative nature of the modeling, particularly in biomedical research. Here, the dynamical models were (and are) subject to regular improvements and revisions due to accounting for new properties and mechanisms. Thus, a new model has to be quickly input into the software, studied, and the resulting bifurcation diagrams tested against reality, after which the model has to be adapted, etc. This is only possible with the interactive bifurcation programs (for a survey, see [Govaerts & Kuznetsov, 2007]).

The development of such programs is progressing rapidly. First interactive computer programs for the bifurcation analysis of ODEs appeared at the end of 1980s, when workstations and IBM-PC compatible computers became widely available at universities and civil research institutes worldwide.

By far the most popular in the West, continuation code AUTO86 already came with a simple interactive graphics program PLAUT tha allowed for a graphical representation of computed data. Subsequent versions of AUTO (94/97/2000/07p) included improved interactive data browsers and programming tools. However, the major difficulty in using all versions of AUTO is the analysis of detected bifurcation points and switching at these points to the continuation of other bifurcation curves, which requires browsing of several output files and a good understanding of their formats. No normal form coefficients were computed in the first versions of the code. AUTO used the BVP approach to the continuation of cycles and their bifurcations. For the continuation of bifurcations, maximally augmented defining systems were used.

The first user-friendly interactive program for bifurcation analysis was LOCBIF [Khibnik, Kuznetsov, Levitin, & Nikolaev, 1993] developed for PCs at the Research Computing Center of the USSR Academy of Sciences (Pushchino, Moscow Region), see Figure 6. The program was based on the code LINLBF. The software allowed for an easy switching between the computation of various curves at detected bifurcation points. The user was able to manipulate individual curves, which where stored separately in the archive.
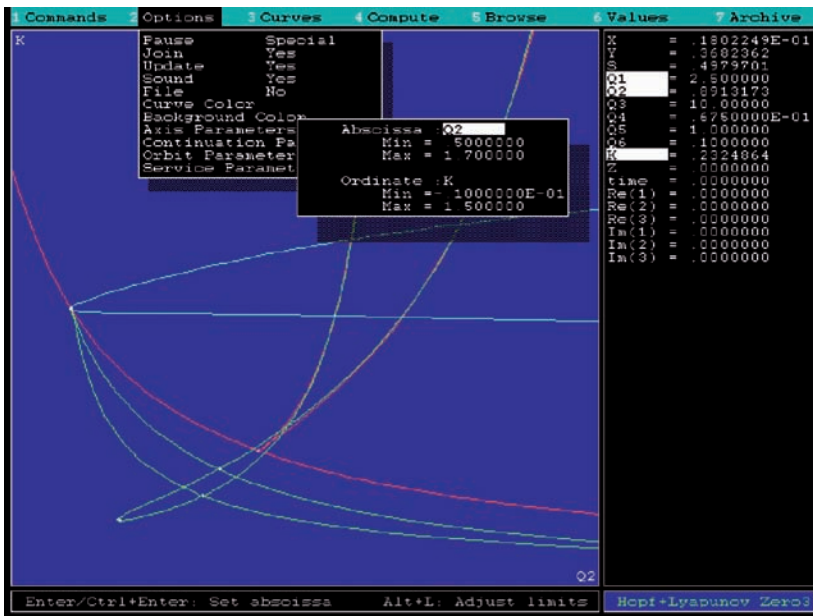
Figure 6:   LOCBIF

At about the same time, the Iron Curtain disappeared and researchers from East and West started to freely exchange results, methods, and software for the analysis of dynamical systems. At a series of international conferences (Leuven 1989; Würsburg 1990) personal contacts between different schools were established that played a crucial role in further developments. The second generation of the interactive programs for bifurcation analysis was represented by software environments which were developed by joint forces from West and East. Figure 7 shows a screen snapshot of CONTENT, the interactive software developed by Yu.A. Kuznetsov and V.V. Levitin at CWI (Amsterdam) with major contributions by W. Govaerts and E. Doedel. The software was first to run on all popular workstations under UNIX/X11 and on PCs under MS-Windows and linux. Remarkably, the portability of the user interface was achieved by employing the VIBRANT

GUI libraries developed at the National Center for Biotechnology Information (Bethesda, USA) for totally different purposes.
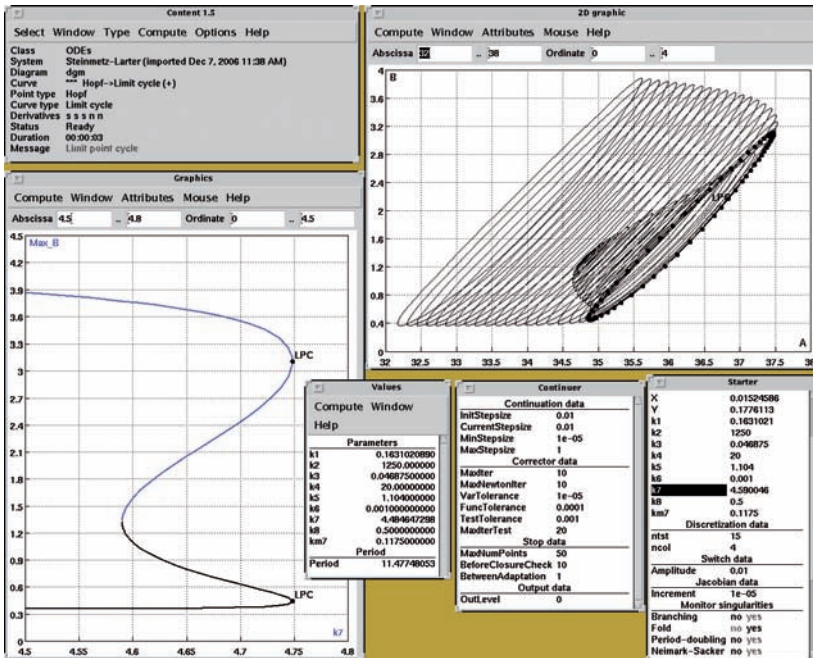

Figure 7:   CONTENT

CONTENT supported the continuation of equilibria and their bifurcations of codim ≤ 3 with both minimal and various augmented defining systems [Govaerts, Kuznetsov, & Sijnave, 2000]. For the continuation of cycles, the BVP methods were used. For the first time, CONTENT supported the normal form computations for many equilibrium bifurcations. The software provided extensive storage, export and import facilities for computed curves and bifurcation diagrams in numerical and picture formats. Switching between various bifurcating objects at special points was easy and flexible in CONTENT, that is still in use at hundreds of institutions all over the world.
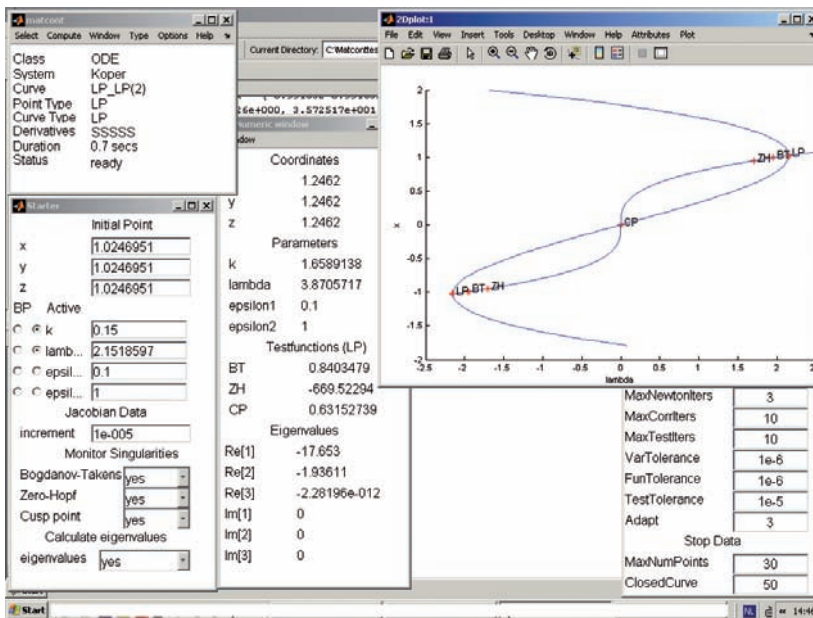
Figure 8:   MATCONT

The latest bifurcation software MATCONT (see Figure 8) belongs to the third generation of the interactive tools and is a product of the longterm scientific collaboration with W. Govaerts [Dhooge, Govaerts, & Kuznetsov, 2003; Dhooge, Govaerts, Kuznetsov, Meijer, & Sautois, 2008]. This software inherited the best features of CONTENT and AUTO. In particular, most efficient minimally augmented defining systems based on the bordering method in combination with the BVP approach to cycles were proposed and implemented in MATCONT [Doedel, Govaerts, & Kuznetsov, 2003]. The software supports the continuation of equilibria and cycles and all their codim 1 bifurcations [Beyn, Champneys, Doedel, Govaerts, Kuznetsov, & Sandstede, 2002] together with all appropriate branch switching [Kuznetsov, Meijer, Govaerts, & Sautois, 2008]. The software computes the normal form coefficients for the bifurcations of codim ≤ 2 of equilibria [Kuznetsov,

1999] and cycles [Kuznetsov, Govaerts, Doedel, & Dhooge, 2005],
as well as the interactive initialization and continuation of codim
1 homoclinic orbits with detection of many codim 2 homoclinic
bifurcations (first tested in AUTO97) [De Witte, Govaerts, Kuznetsov, &
Friedman, 2012]. This allows for a rather complete bifurcation analysis
of the two-parameter ODEs. Moreover, the MATLAB platform selected
for the development of MATCONT solved many compatibility problems
and made MATCONT to large extent a machine-independent tool.

TRENDS AND VISIONS

What are the perspectives of the numerical bifurcation analysis of dynamical systems ? Which new methods and tools should we expect? How should we teach bifurcation theory ? In which way should the development of the bifurcation software be organized ?

If we have in mind software for generic ODE systems, then it seems possible to achieve in the nearest future the long-standing goal to fully support the two-parameter analysis of equilibria, cycles, and homoclinic orbits to equilibria. For that, we have to develop and implement the branch switching to relevant homoclinic orbits at codim 2 equilibrium and homo- /hetero-clinic bifurcations. The numerical methods to start the continuation of homoclinic orbits from codim 2 equilibrium bifurcations are under development, while those for switching at the global codim 2 bifurcations are poorly understood and require more analytical work. The computation of orbits connecting equilibria to cycles and cycles to cycles also requires additional work. The corresponding defining systems are known for the three-dimensional cases [Doedel, Kooi, van Voorn, & Kuznetsov, 2008 and 2009] but no robust methods exist for $n > 3$, particularly for the initialization. There are more open questions regarding the computation of two-dimensional invariant manifolds of equilibria and cycles, where the BVP-approach has been recently successfully applied but not yet implemented into any standard software. There are still no robust methods to continue invariant tori, since they have an intrinsic tendency to lose smoothness.

It should be noted that advances in the bifurcation theory of dynamical systems and in the software development are nontrivially connected. To begin with, the progress in the theoretical analysis of bifurcations allows for the development of new numerical tools for detection and analysis of these bifurcations in concrete ODE models.

By the way, actual implementation of new theoretical methods is the ultimate check for their correctness: In numerous cases such implementation revealed serious errors in the theoretical constructions. Actually, the modern theory of dynamical systems has an essential *experimental component* since many parameter-dependent normal forms can be derived analytically but cannot be studied without computer assistance (from symbolic manipulation and extensive simulations to numerical continuation and normalization). Probably, the most famous example is the study of the approximating normal form for the Neimark-Sacker bifurcation of cycles with resonance 1:4, where various analytical results by V.I. Arnold and A.I. Neishtadt were complemented by the numerical bifurcation analysis first performed by A.I. Khibnik and F.S. Berezovskaya at the Research Computing Center of the USSR Academy of Sciences in Pushchino and later extended by B. Krauskopf at Groningen. There are many other problems in the bifurcation theory, where an initial breakthrough could only be achieved via serious computations, e.g. [Kuznetsov & Meijer, 2006; Gonchenko, Kuznetsov, & Meijer, 2005]. A challenging example is the long-standing problem of the accumulation of 1:2 resonances that we discovered in 1991 by studying models of seasonally forced food chains [Kuznetsov, Muratori, & Rinaldi, 1992; Rinaldi, Muratori, & Kuznetsov, 1993]. Hopefully, this problem will have the fate of the *Feigenbaum universality* in the accumulation of the period-doubling bifurcations of 1D maps, that was first discovered in simple ecological models, understood with the help of nontrivial numerical computations, and finally proved with complex-analytic methods. In such computations new integration tools based on symbolic and automatic differentiation and high-precision arithmetic will be necessary to deal with exponentially small effects.

It is then obvious that numerical bifurcation analysis is situated at the interface of pure and applied mathematics, and software engineering. Meanwhile, this explains why it is so difficult to get a financial support for research in the numerical bifurcation analysis – it does not fit naturally

into the standard classification of research fields. After 1999, for some reasons, Belgian Research Foundation – Flanders (FWO) understands better than NWO and STW in The Netherlands this special position of numerical bifurcations analysis. Many important results in my research were achieved then in the close cooperation with W. Govaerts and our joint PhD students based at Gent University. On the contrary, due to absurd abolishing of departmental PhD budgets at Utrecht and other Dutch universities, we have lost many talented young people interested in the numerical bifurcation analysis who got positions elsewhere.

The special nature of the numerical bifurcation analysis also means that we should teach students to study deterministic processes in a different way, namely let them learn bifurcation theory, numerical analysis, and software in a series of interconnected courses. My book *Elements of Applied Bifurcation Theory* [Kuznetsov, 2004] (now in 3rd edition and recently translated into Chinese) is a step in this direction, together with other book projects and new courses at Bachelor and Master level. Moreover, the (PhD) students should be directly involved into further development of the standard software, since it is the best way to fully grasp the theory, understand numerical methods, and be able to develop and test them on concrete models, thus contributing to their analysis.

Another trend in the bifurcation analysis is the development of special numerical and software tools for more "exotic" dynamical systems than smooth ODEs, e.g. partial and delay differential equations, algebraic-differential equations, non-smooth differential equations, and integro-differential equations. There are many numerical studies of individual deterministic models of these classes. However, the systematic development of standard bifurcation software for most of them is still to be started. Note that the development of the standard bifurcation software for the non-smooth Filippov ODEs is ahead of that for other classes, see e.g. [Dercole & Kuznetsov,

2005; Piironinen & Kuznetsov, 2008]. Such nonsmooth ODEs naturally appear while sudying effects of the relay adaptive control on ecological systems [Dercole, Gragnani, Kuznetsov, & Rinaldi, 2003].

Biomedical applications lead to many interesting dynamical systems. For example, integro-differential equations with delays arise in the modelling of cortex on which we collaborate with the Clinical Neurophysiology group of Michel van Putten (MIRA, UT). Non-smooth delay differential equations are used at MIRA by the Biomechanical Engineering group (Bart Koopman and Herman van der Kooij) in modeling of bipedal walking. Hopefully, numerical bifurcation analysis will lead to a better understanding of dynamical phenomena in these research areas.

BIFURCATIONS IN NEUROSCIENCE

We now come to a topic that is directly related to my appointment at the Department of Applied Mathematics of the University of Twente, i.e. bifurcation analysis in the *Computational Neuroscience*.

Based on experiments in giant squid (Loligo pealei) axon, A.L. Hodgkin and A.F. Huxley built in 1952 the first quantitative model of the electric excitability of neurons. Their model described the behavior of the neural trans-membrane potential and three ionic currents (Na, K, and "leak") through the membrane. They discovered that the conductances for the currents were not constant but rather functions of the membrane potential and this voltage dependence was the key to understanding spikes. Separating slow and fast motions, it is possible to reduce the 4D Hodgkin- Huxley ODE to just a planar ODE system for the voltage and one "recovery" current. Major properties of this 2D system – particularly its "excitability" – can be captured by a very simple polynomial system proposed by R. Fitz- Hugh and J. Nagumo in beginning 1960s. If one takes into account the axon length and rescales variables, the model assumes the form of a nonlinear reaction-diffusion PDE system that describes voltage V and recovery variable W as functions of time and position along the axon:

$$
\begin{cases}
\dfrac{\partial V}{\partial t} = \dfrac{\partial^2 V}{\partial x^2} - f(V) - W, \\[2mm]
\dfrac{\partial W}{\partial t} = b(V - \gamma W),
\end{cases}
\tag{13}
$$

where $f(V) = V(V-a)(V-1)$ with $0 < a < 1$ and $b > 0, \gamma \ll 1$. Numerical bifurcation methods were actively used to study this and similar

local and distributed neural models. For example, it was recognized that the profile and the propagation speed of a travelling *nerve impulse* in (13),

$$V(t,x) = v(\xi),\ W(t,x) = w(\xi),\ \ \xi = x + ct,$$

can be computed numerically as a homoclinic solution (approaching the origin as $\xi \to \pm\infty$) and a bifurcation value of the parameter c in the corresponding ODE wave system:

$$\begin{cases} \dot{v} = u, \\ \dot{u} = cu + f(v) + w, \\ \dot{w} = \dfrac{b}{c}(v - \gamma w), \end{cases}$$

where the dots denote the derivative w.r.t. ξ. In fact, A.L. Hodgkin and A.F. Huxley found the pulse profile and speed using a hand calculator. In 1980s it was shown [Kuznetsov, 1994] that chaos related to Shilnikov's and Belyakov's saddle-focus homoclinic bifurcations is responsible for the appearance of complicated travelling waves that look like coupled impulses (see Figure 9). Special efforts have been made to develop robust numerical methods for homoclinic bifurcation analysis [Champneys, Kuznetsov, & Sandstede, 1996] and their implementation in AUTO and MATCONT.
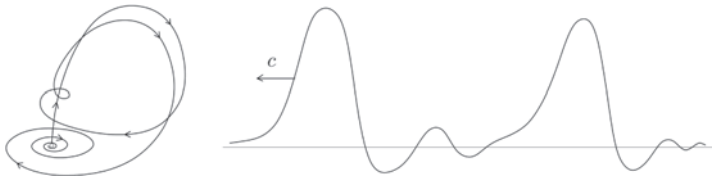

Figure 9:   Double pulse.

In reality, various individual neurons are connected into complicated networks. Since the number of neurons and synapses

in even a small piece of cortex is huge, spatial and temporal coarse graining lead to so-called neural field models in which the average membrane potential of neural populations, as opposed to individual neuronal characteristics, are studied. An example is provided by the following delayed integro-differential equation

$$\frac{\partial V}{\partial t}(t,x) = -\alpha V(t,x) + \int_{\Omega} w(x,x')f\left(V\left(t-\tau_0-\frac{|x-x'|}{c},x'\right)\right)dx', \qquad x \in \Omega, \quad (15)$$

where $V(t,x)$ is the potential at time t in position x, whose intrinsic dynamic is a decay with exponent α, while the functions w and f describe connectivity and activation in the neural tissue. The transmission delay is due to a finite propagation speed c and a constant synaptic delay τ_0. In the simplest case, the spatial domain Ω is supposed to be a finite interval, but more realistic configurations are possible. The main purpose of such models is to study collective behavior of the neurons, e.g. predict oscillations that might correspond to epilepsy and analyze their dependence on neural connections. We have recently demonstrated how to interpret this model as an abstract delay equation that defines a dynamical system on an appropriate infinite-dimensional function space X. This allowed us to apply the general machinery of the dynamical systems theory, including the center manifold reduction and normalization, and rigorously compute the normal form coefficients for Hopf and double Hopf bifurcations in this model. An example of a transient to a stable oscillatory regime is shown in Figure 10.
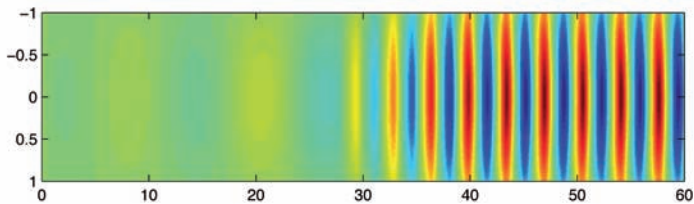

Figure 10:   A transient to oscillations.

Clearly, much extra work has to be done to bridge a huge gap between the individual neuron level and the coarse grain level of the neural field. This would lead to a better understanding how local changes in neural connectivity affect global brain oscillations, e.g. it will help us to match a neural field model for neocortex with electroencephalography (EEG) data of patients suffering from intractable focal neocortical epilepsies. Such models should generalize equation (15) and take into account known connectivities between excitatory and inhibitory cells within different layers of the cortex, as well as its inhomogeneity. This research will be conducted in close cooperation with M. van Putten (MIRA, UT).

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I thank the Executive Board of the University of Twente for the confidence expressed by my appointment. This inaugural lecture has come about because of the long cooperation between the Department of Applied Mathematics at the University of Twente (UT) and the Department of Mathematics at the Utrecht University (UU) on the analysis of delay equations and other dynamical systems. The main credit as the initiator of this collaboration has to go to Stephan van Gils (Twente), who worked hard to make a success of this endeavor. The support of the Faculty of Electrical Engineering, Mathematics and Computer Science at UT and the Faculty of Science at UU should be thankfully acknowledged.

It is my pleasure to conclude this lecture by acknowledging the many people who contributed to my development and provided friendly support to my research and teaching efforts. I am thankful to Albert Makarievich Molchanov and Aleksandr Dmitrievich Bazykin who supervised my PhD studies at the Research Computing Centre of the USSR Academy of Sciences (Pushchino, Moscow Region) in 1979-84. Being the Director of that mathematical institute at the Pushchino Biological Center, A.M. Molchanov never forced staff to work on a particular topic but allowed everyone to freely choose an interesting research problem (out of almost unlimited range) and focus on it. It was very easy to enter his office or even visit his apartment with a view on river Oka to discuss a model or some difficulties in its analysis. A.D. Bazykin, F.S. Berezovskaya, and A.I. Khibnik introduced me to the fascinating world of dynamical systems appearing in ecological modeling. A.D. Bazykin was able to predict their bifurcations almost without computations, merely by "careful observation". I learned many ideas from Emmanuil Elievich Shnol who combined a deep knowledge of abstract mathematics with a deep understanding of

numerical analysis. He has initiated the development of the standard numerical bifurcation codes in Russia. Moreover, by organizing annual Conferences in Pushchino, he was able to link the Moscow and Gorky (N. Novgorod) mathematical schools on dynamical systems. During my PhD studies in Pushchino, I had the opportunity to attend Vladimir Igorevich Arnold's seminar on differential equations at the Moscow State University and to interact with his closest associates - Ju.I. Ilyashenko, R.I. Bogdanov, A.I. Neishtadt and others. At a conference in Pushchino, I met Leonid Pavlovich Shilnikov and his coworkes from Gorky - V.V. Bykov, N.K. Gavrilov, L.A. Belyakov, V.S. Afraimovich, S.V. Gonchenko, D.V. Turaev, A.L. Shilnikov, and others. That was a start of a long and lasting friendship and cooperation.

After the collapse of the Soviet Union, I continued the development and application of numerical bifurcation methods in Italy and The Netherlands. Sergio Rinaldi (whom I first met at IIASA in Austria) invited me to work in Italy, thus starting another long-term collaboration, in this case on the analysis of ecological systems and later on their non-smooth dynamics at the Politecnico di Milano. Odo Diekmann and Jan Sanders played the crucial roles in my movement in 1992 to Amsterdam (CWI and RIACA) and eventually to Utrecht. O. Diekmann was the first who proposed to convert my brief lecture notes used in a course in Milan into the book *Elements of Applied Bifurcation Theory*, whose 1st edition appeared in Springer in 1995 and became an international success. During my work in Amsterdam, the final versions of the interactive software LOCBIF and CONTENT were released.

The Department of Mathematics of Utrecht University is since 1999 my base where advances in the numerical bifurcation theory and the development of the next generation interactive numerical bifurcation software MATCONT were booked. An informal international network was created, in which research groups of Willy Govaerts (Gent Universty), Eusebius Doedel (Caltec and Concordia, Montreal), Alan

Champneys (Bristol), Wolf-Juergen Beyn (Bielefeld) were linked in collaboration. This enormously facilitated the development of new numerical methods for the analysis of ODEs and iterated maps[1], although it might have been more rapid if more PhD students and postdocs were involved. I should also thank the coauthors with whom I worked with pleasure on at least two joint papers and who were not yet mentioned before: C. Piccardi, F. Dercole, A. Gragnani, S. Muratori, B. Sijnave, M. Friedman, M. Scheffer, P. Piiroinen, B. Kooj, B. Sandstede, M.Ya. Antonovsky, E.A. Aponina, as well as many other occasional collaborators. Special thanks to PhD students who worked under my (co-) supervision and tolerated my - at times - dictatorial style: Annick Dhooge, Hil Meijer, Taoufik Bakri, Bart Sautois, Reza Khoshsiar Ghaziani, George van Voorn, Fabio Della Rossa, and Virginie De Witte, as well as Sebastiaan Janssens.

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Ik heb gezegd.

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1 In this lecture I deliberately did not consider numerical methods and software for bifurcation analysis of iterated maps, see [Govaerts, Khoshsiar Ghaziani, Kuznetsov, & Meijer, 2007; Khoshsiar Ghaziani, Govaerts, Kuznetsov, & Meijer, 2009] and references therein.

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