Math. Forschungsinstitut
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MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Tagungsbericht 3/1993

Computational Methods for Nonlinear Phenomena

10.1. bis 16.1.1993

Die Tagung fand unter der Leitung der Herren Tassilo Küpper (Köln), Hubert Schwetlick (Halle), Rüdiger Seydel (Ulm) und Hans Troger (Wien) statt.

Mathematiker, Ingenieure und Physiker aus Belgien, Deutschland, England, Österreich, Rußland, Schweiz und U.S.A. waren der Einladung gefolgt. Es wurden insgesamt 27 Vorträge gehalten, ergänzt durch einen Abendvortrag.

Im Mittelpunkt des Interesses standen numerische und analytische Methoden zur Untersuchung nichtlinearer Phänomene, doch waren auch die Anwendungen von großer Bedeutung bei dieser Tagung. So berichteten und diskutierten die Teilnehmer über nichtlineare Probleme aus der Technik, der Physik und der Biologie. Außerdem wurde Software für Verzweigungsprobleme vorgestellt und in einem Abendvortrag eine Übersicht über Hamilton'sche Störungstheorie gegeben.

Das Programm war so gestaltet, daß es anregende Diskussionen und persönliche Gespräche zuließ. Die angenehme Oberwolfach-Atmosphäre und die vorbildliche Organisation des Instituts trugen wesentlich zum Gelingen der Tagung bei.

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Vortragsauszüge

WOLF-JÜRGEN BEYN:

Numerical approximation of connecting orbits

We consider the numerical computation of orbits which connect steady states or periodic orbits in a parameter dependent dynamical system. Such problems typically arise when determining the shape and speed of travelling waves in parabolic systems.

Connecting orbits satisfy a boundary value problem on the real line. We analyze the error caused by truncation to a finite interval and by the choice of boundary conditions.

More specifially, we consider orbits connecting a steady state to a periodic orbit. It will be shown that a crucial role is played by the property of 'asymptotic phase' and by the corresponding foliations of stable and unstable manifolds.

HANS BRAUCHLI:

Bifurcation of the configuration manifold illustrated by the example of the multiply hinged arch

The plane five-hinged arch is a simple mechanism with two degrees of freedom. Depending on the distance of the two base joints, its configuration space is a sphere or a closed surface of genus four. Near the critical parameter value, strong singularities of the curvature occur. The orbits are deflected by an angle depending on the discrete curvature.

FRIEDRICH H. BUSSE:

Numerical analysis of tertiary and quarternary solutions and their stability in cases of fluid flows in plane layers

Some fluid systems with a high degree of symmetry reach a turbulent state of motions through a sequence of supercritical bifurcations. Rayleigh-Bénard convection in a layer heated from below and the Taylor-Couette system are the prime examples. The basic state is typically replaced by by roll-like motions representing the secondary state. The remaining symmetries of the motions are broken in a number of different ways as transitions to tertiary and quarternary states occur. The Galerkin method for solving the basic equations of motion provides a convenient way to incorporate all symmetry properties of the fluid flow and to facilitate the analysis of its stability. Thermal convection with and without a mean shear provides numerous examples. Universal tertiary states such as wavy rolls will be discussed in detail and their occurence in different experimental settings will be described.

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MICHAEL DELLNITZ

Computational Methods for Symmetry Creation

We consider Dynamical Systems which possess symmetry – PDEs on the line with periodic boundary conditions, for instance. An attractor of such a system might have less symmetry than the full symmetry of the problem. In this case there always exist several attractors which are related by symmetry transformations and, varying a parameter, it might happen that those conjugate attractors collide. Then the resulting attractor has more symmetry and this phenomenon is called *Symmetry Creation*. During the last two years Symmetry Creation has frequently been found in the numerical simulation of several PDEs (eg. in the Ginzburg-Landau equation or in the Kuramoto-Sivashinsky equation). It has also been observed in physical experiments like the Taylor-Couette apparatus or the Faraday experiment. Based on the Karhunen-Loève decomposition we will present a numerical method for the detection of Symmetry Creation in Dynamical Systems.

DIETRICH FLOCKERZI:

Invariant Manifolds in Control Theory

We present some examples how the theory of invariant manifolds has recently been used in the study of affine nonlinear control problems. First we investigate the problem of local asymptotic stabilization for systems having a well-defined relative degree. Secondly we deal with local qualitative control problems including various classical control problems. Finally, for systems with disturbances, we investigate the error feedback regulator problem and present a state space approach to nonlinear H_∞-control.

FOTIOS GIANNAKOPOULOS:

Bifurcation Phenomena in a Model for Neural Dynamics

We present a mathematical model which describes the dynamics of a simple neural net consisting of an excitatory and an inhibitory neuron. The mathematical model is a system of two nonlinear differential equations. We show that the system possesses characteristical nonlinear properties such as hysteresis and bifurcation of periodic solutions. Examples of hysteresis and Hopf curves are given.

ANDREAS GRIEWANK:

Derivative Convergence for Iterative Equation Solvers

When nonlinear equation solvers are applied to parameter dependent problems their iterates can be interpreted as functions of these variable parameters. If they exist the derivatives of these iterated functions can be recursively evaluated by the forward mode of automatic differentiation. Then one may ask whether and how fast these derivative values converge to the derivative of the implicit solution function, which may be needed for parameter identification, sensitivity studies, or design optimization.
It is shown here that derivative convergence is achieved with an R-linear rate for a large class of secant updating methods, whose iterates converge Q-superlinearly. For a wider

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class of multi-step contractions we obtain R-linear convergence of a simplified derivative updating scheme, which is more economical and can be easily generalized to second higher derivatives. We also formulate a constructive criterion for derivative convergence based on the implicit function thoerem. All theoretical results are confirmed by numerical experiments on small test examples.

ANNEGRET HOY:

A New Principle for Constructing Tensor Methods

Tensor methods converge local superlinearly towards regular as well as singular solutions of nonlinear equations. This property makes them attractive for solving nonlinear equations. The new construction principle leads to a special tensor method which is characterized by the following features:

- local cubic convergence towards regular solutions
- local superlinear convergence with Q-order 1.5 towards regular singularities
- use of second order directional derivatives which keep computational costs at a low level.

This set of useful features can be viewed as a further development of the methods due to Schnabel/Frank and Griewank, respectively.
Interesting points for further discussion may be: irregular singularities and variants for globalization.

VLADIMÍR JANOVSKÝ (joint work with V. Seige):

Qualitative Analysis of Newton Iterations for Imperfect Bifurcation Singularities

A simple bifurcation point of a parameter-dependent mapping F is considered. Given a small perturbation of F, the bifurcation point may degenerate into a pair of limit points. In this situation, the performance of Newton methods for finding the limit points is studied. The prior objective of the analysis are qualitative properties of the basins of attraction. Center Manifold-like Theorem for the continuous version of the method (Newton flow) is proved. Normal form of Newton flow on the center manifold is derived and analysed. Presented numerical experiments support the conjecture that important properties of Newton flow are also shared by Newton iterations.

HANS G. KAPER:

Computational Methods for the Ginzburg-Landau Equation and Flux Vortex Behavior in High-temperature Superconductors

The High-Performance Computing and Communications (HPCC) program at Argonne is focused on applications of massively parallel architectures in several scientific disciplines. One of the areas of interest is materials science, where the laboratory has an extensive research program in high-T_C superconductivity. In the context of the HPCC program, we are responsible for large-scale numerical simulations of flux vortex behavior in the

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presence of impurities. This behavior can be modeled at various levels; for example, one can study the nonlinear Ginzburg-Landau equation for the order parameter in the presence of a magnetic field and show how vortices are formed as the result of bifurcations, or one can study vortices directly as interacting elastic filaments in a random medium. Both approaches are included in our research program, which addresses analytical as well as computational aspects of the problem and is done in close collaboration with researchers at the laboratory and universities. I will present some recent results of this work in my talk.

YANNIS G. KEVREKIDIS:

Model Reduction for PDEs

We study low-dimensional dynamics and instabilities in pattern forming systems with complex geometries (e.g. transitional flows). We use techniques inspired from the theory of approximate inertial manifolds as well as image processing (Karhunen-Loéve, SVD) to obtain reduced dynamic models on which the bifurcation calculations can be performed. In particular, we introduce a combination of the two, yielding low-dimensional, approximately invariant *nonlinear* subspaces on which the long term dynamics lie. Our test examples include flows in complex geometries, reaction-diffusion and amplitude equations.

ALEXANDER KHIBNIK (joint work with Yu. Kuznetsov, V. Levitin, E. Nikolaev):

Designing Software for Bifurcation Problems: Philosophy and Practical Experience

We discuss different aspects of LOCBIF software project. The applied fields we are experienced with (ecology, biochemistry, chemistry, electrical circuits etc.) motivate the concentration on generic vector fields and diffeomorphisms with relatively low number of variables and relatively high number of parameters (3 or more). The graph of adjacency of singularities up to codimension three represent the concentrated view on that how different singularities are organized with respect to their unfoldings. In numerical approach, this graph is reformulated using the language of (scalar) test bifurcation functions. Then continuation techniques is applied, which allows us to end up with the code supporting "travelling" along a solution manifold and exploring its stratification. Computer science aspects of the project (tool for defining models, graphic user interface) are discussed as well as directions of further developments.

URS KIRCHGRABER:

Hamiltonian Perturbation Theory – from Poincaré to Nekhoroshev

The purpose of this talk is to review Hamiltonian Perturbation Theory as it evolved during the last hundred years since Poincaré's famous "Les méthodes nouvelles de la mécanique céleste" was published. The central theme dealt with is the stability of elliptic equilibria. The construction of formal integrals, Siegel's theorem on the divergence of the Birkhoff normal form, the nonexistence of integrals, a KAM-result of J. Pöschel, an example of Arnold diffusion due to R. Donady, the Zehnder-Genecaud result on the existence of infintely many

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transversal homoclinic points are described. The main emphasis is on a Nekhoroshev-type estimate of A. Giorgilli and its application to the Trojan asteroids.

PETER KUNKEL:

Test Functions and Augmented Systems

The numerical determination of singular points is commonly based on the use of appropriate augmented systems. A general rule for the construction of suitable test functions and related augmented systems is presented. The approach is based on a translation process applied to results of the so-called recognition problem in singularity theory.

HANS D. MITTELMANN:

Stable Capillary Surfaces Under Zero Gravity

Symmetric capillary surfaces in a cube are considered under zero gravity conditions. Only local minima of the total energy are computed for contact angles of 70, 50 and 40 degrees. Graphs of the energy, the area and the pressure versus the volume reveal several interesting facts. Particular attention is paid to nonlinear phenomena including hysteresis and that for angles below a bound, here 45 degrees, the liquid creeps along the edges without limit. This latter effect can be observed for arbitrarily small volumes in the case of a 40 degree contact angle. Other observations include that up to ten local minima exist for certain volumes and that the volume ranges for which various shapes are minimizing the energy depend strongly on the contact angle.

GERALD MOORE:

Computation and Parametrisation of Invariant Manifolds

The computation of invariant manifolds for the autonomous system

$$(+) \qquad \dot{\underline{u}} = \underline{F}(\underline{u}) \qquad \underline{F} : R^n \to R^n$$

is often attempted by utilising the dynamics on the manifold itself, e.g. a Poincaré map. We would prefer to view the problem geometrically and divorce the computation from these dynamics.

If $\mathcal{M}$ is a k-dimensional C^1 sub-manifold of R^n then $\mathcal{M}$ is invariant for (+) if

$$P_{T_x\mathcal{M}}^{\perp}\underline{F}(\underline{x}) = \underline{0} \quad \forall \underline{x} \in \mathcal{M}$$

($T_x\mathcal{M}$ being the k-dimensional tangent space of M at $\underline{x}$ and P_S the othogonal projection onto a subspace S of R^n), which provides $n-k$ equations at each point of $\mathcal{M}$. The remaining equations necessary represent a choice of parametrisation of $\mathcal{M}$. For example, in the common continuation framework where a nearby manifold $\mathcal{M}'$ is already known, this can completely provide the parametrisation, i.e. the additional k equations may be taken as

$$P_{T_{x^0}\mathcal{M}'}(\underline{x} - \underline{x}^0) = \underline{0} \qquad \forall \underline{x}^0 \in \mathcal{M}'.$$

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It is often better, however, to impose at least part of the parametrisation directly.

i) For periodic solutions, $\mathcal{M}$ is an embedding of S^1 in R^n and we choose the canonical arc-length parametrisation. $\mathcal{M}'$ only enters via a single phase condition. The final BVP to be solved is analogous to the usual time parametrisation but with vector field $\underline{F}/\|\underline{F}\|$ and parameter L (length of curve) rather than period.

ii) For homoclinic/heteroclinic orbits, $\mathcal{M}$ is an embedding of $(0,1)$ in R^n and we again choose arc-lenght parametrisation. $\mathcal{M}'$ now plays no role. The final BVP is over $(0,1)$ with singularities at the endpoints rather than over $(-\infty,\infty)$ as with time parametrisation.

iii) For invariant tori, $\mathcal{M}$ is an embedding of $S^1 \times S^1$ in R^n. Parametrisations defined by conditions on the first fundamental form, e.g. orthogonality constant surface area, are being investigated.

iv) With stable/unstable manifolds of fixed points, we end up with a quasi-linear hyperbolic system extending out from the singular fixed point. In this case an adaptively changing parametrisation is indicated.

FRIEDRICH PFEIFFER:

Dynamical Systems with Impulsive and Frictional Contacts

Unilateral contact constraints in dynamical systems with impacts and stick-slip-phenomena arise from kinematical magnitudes like relative distance and relative velocity. The end of the contact event is indicated by normal contact forces and tangential constraint forces, respectively. Constraints and constraint forces are complementary in a sense, that either relative kinematics in contact is zero and the corresponding constraint forces are not zero, or vice versa. This property can be used to solve for multibody systems with many contacts the formal uniqueness problem by the complementarity procedure from optimization theory. The structure variant character of such systems affords a thourough interpolation of indicators and constraints. Some practical examples demonstrate the technical relevancy of the theory.

GERD PÖNISCH:

Direct Methods for Computing Bifurcation Points

A nonlinear system of n algebraic equations of the form $F(y,\lambda,\alpha) = 0$ depending on n state variables y, the control parameter λ and l unfolding parameters α is considered. It is assumed that there exist simple singular solution points (y^*,λ^*,α^*) at which the Jacobian $\partial_y F(y^*,\lambda^*,\alpha^*)$ has rank $n-1$. Simple singular points (y^*,λ^*,α^*) of this kind are for example turning points, simple bifurcation points, hysteresis points, pitchfork bifurcation points etc. They can be characterized by appending the original problem $F(y,\lambda,\alpha) = 0$ by $l+1$ equations $f(y,\lambda,\alpha) = 0$ such that (y^*,λ^*,α^*) is a regular solution of the combined system. For simple singular points with codimension ≤ 2 we constructed robust functions f_i that can be evaluated and differentiated cheaply. By exploiting the special structure of the defining equations $f_i(y,\lambda,\alpha) = 0$ we developed Newton-type methods for computing

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the desired simple singular point $(y^*, \lambda^*, \alpha^*)$. In this way Q-quadratically convergent methods are obtained whose efficiency is demonstrated by a numerical example.

G.W. REDDIEN:

On the Reduced Basis Method

The reduced basis method can be used to reduce the size of approximating systems without significantly increasing the error inherent in the underlying discretization. Given a system of equations $F(z) = 0, F : R^{m+d} \to R^m$, the reduced basis method solves $PF(x_0 + V_d\tau - V_R y) = 0$ where $P^2 = P$ and $V_d \oplus V_R$ is a subspace of a regular splitting $V_d \oplus V$ of R^{m+d}. A method is given for constructing projections that minimize constants in standard error estimates and make the method more robust. It is shown how to select P to achieve additional accuracy in the parameter τ at simple turning points.

DIRK ROOSE:

Scientific Software Aspects in Bifurcation Analysis

In the first part of the talk, the correct status of software for bifurcation analysis is briefly reviewed. Attention is paid to the requirements for a (standard) interactive environment and for reliable numerical algorithms.
In the second part, an algorithm is presented for determining the steplength used in a continuation procedure. The algorithm takes into account the behaviour of test functions for bifurcations in order to increase the robustness of continuation w.r.t. undesired branch switching. This approach also reduces the possibility to overlook important bifurcations.

JÜRGEN SCHEURLE (joint work with B. Fiedler):

Discretization of Autonomous Equations and Homoclinic Orbits

One-step discretizations of order p and step size ε of autonomous ordinary differential equations $\dot{x} = f(\lambda, x)$ can be viewed as time - ε maps of rapidly forced, non-autonomous equations

$$\dot{x} = f(\lambda, x) + \varepsilon^p g(\varepsilon, \lambda, \frac{t}{\varepsilon}, x), \quad x \in \mathbb{R}^n, \ \lambda \in \mathbb{R}, \quad \text{"}\cdot\text{"} = \frac{d}{dt},$$

where g has period 1 in t/ε. We study the behaviour of a homoclinic orbit $\Gamma = \Gamma(t), \varepsilon = 0, \lambda = 0 (t \in \mathbb{R})$ under discretization. Under generic assumptions, Γ turns out to break, and the perturbed stable and unstable invariant manifolds intersect each other transversally for small positive ε which implies chaotic behaviour. However, the transversality effects are estimated from above to be exponentially small in ε. For example, the length $l(\varepsilon)$ of the parameter interval of λ-values for which the intersection of the local invariant manifolds is non-empty can be estimated by

$$l(\varepsilon) \leq Ce^{-2\pi\eta/\varepsilon}$$

where C, η are positive constants. The factor η is related to the minimal distance from the real axis of the poles of $\Gamma(t)$ in the complex t-plane.

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Our results are visualized by high precision numerical experiments. The experiments show that, due to exponential smallness, homoclinic transversality becomes practically invisible under normal circumstances, already for only moderately small step size.

HUBERT SCHWETLICK (joint work with E.L. Allgower):

Stable Computation of Simple Bifurcation Points and Emanating Branches

For determining simple bifurcation of nonlinear systems $F(y) = F(x, \lambda) = 0$, an extended system $F(y + \mu d) = 0$, $w^{iT} v^i(y) = 0$, $(i = 1, 2)$ is used where

$$v^i(y) := B_i(y)^{-1} e^{n+1}, \quad B_i(y) := \begin{bmatrix} \partial F(y) & + & d^i w^{iT} \\ & r^{iT} & \end{bmatrix}.$$

This is a generalization of Pönisch's [85] system where only row replacements in ∂F are used. The general rank-1-regularization used here allows to choose the parameters $\{d, d^i, r^i, w^i\}$ such that a bound of $\|B_i^{-1}\|$ is small (which increases robustness), that $B_2 - B_1$ has rank 1 (which saves computational costs), and that also simple bifurcation points which are turning points with respect to e^{n+1} (i.e. where $\ker \partial F(y') \perp e^{n+1}$ holds) can be computed. An implementation is described which, from the viewpoint of computational costs, is comparable to Janovsky's [89] modification of Pönisch's method. Moreover, the quantities computed during the iteration allow to determine the tangents of the branches emanating at the bifurcation point.

PETER SZMOLYAN:

Bifurcations in Singularly Pertubed Problems

In this talk we consider singularly pertubed ordinary differential equations of the form:

$$(1) \qquad \begin{aligned} \dot{x} &= f(x, y, \varepsilon, \mu) \\ \varepsilon \dot{y} &= g(x, y, \varepsilon, \mu) \end{aligned} \qquad x \in \mathbb{R}^n,\ y \in \mathbb{R}^K,\ \mu \in \mathbb{R}^P,\ 0 < \varepsilon \ll 1$$

We demonstrate how Fenichel's invariant manifold theory (3DE79) for problem (1) can be used to understand certain global aspects of the problem. In particular we show that the existence of transversal singular ($\varepsilon = 0$) heteroclinic and homoclinic orbits implies the existence of these orbits for small positive values of ε. The method is applied to the travelling wave problem of the Fitzhugh-Nagumo equations. As a second application we briefly discuss the bifurcation of heteroclinic orbits in the problem of viscous profiles for magnetohydrodynamic shock waves (joint work with H. Freistühler, RWTH). We present some open questions which could be investigated numerically.

ALASTAIR SPENCE:

The Detection of Hopf Bifurcations in Large Systems Arising in Fluid Mechanics

The talk is concerned with the detection of Hopf bifurcations in large finite element discretizations of the Navier-Stokes and related equations. After linearization, we need to

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find the smallest eigenvalues of a large sparse nonsymmetric block-structured eigenvalue problem.
A technique is desribed based on "preconditioning" using a generalization of the Cayley transform. and then standard iterative methods eg. Arnoldi's method.
Examples are given from four problems in fluid mechanics, viz., double-diffusive convection, flow past a cylinder, the Taylor problem, and flow over a backward-facing step.

ALOIS STEINDL:

Investigation of Codimension 2 bifurcations for a Fluid-conveying Pipe with D_N-symmetry

We consider a linearly fluid conveying viscoelastic tube which is supported by n identical springs.
If the flow rate is increased, the trivial state loses its stability. By varying the stiffness of the springs and the position of the support, we find various bifurcations of Codimension 2: Takens-Bogdanov-bifurcations, Hopf/Steady-State mode interactions and Hopf/Hopf-mode interactions.
Using equivariant bifurcation theory we investigate the bifurcating solution branches and their stability.

HANS TROGER (joint work with G. Xu, A. Steindl):

Nonlinear Stability Analysis of a Low Plateform Railway Car

To calculate the turning point of the amplitude curve of a periodic solution in R^{28} for a system of stiff nonlinear differential equations is a challenging problem. Instead of using simulation of path following methods multiparameter bifurcation theory is used to obtain from studying still the steady state the turning point of the periodic solution. The obtained results agree well with experimental results.

ANDRÉ VANDERBAUWHEDE:

Theoretical and Computational Aspects of Normal Forms

The normal form reduction of a vectorfield at one of its singularities is usually done by an order by order approach, where for each order k one looks for an appropriate transformation which simplifies as much as possible the k-th order term in the Taylor expansion of the vector field. Such an approach leads at each order to a so-called splitting problem, which in fact consists in finding an appropriate pseudo-inverse of a linear operator whose dimension increases rapidly with the dimension of the phase space and the order k. In practice this has till now put severe restrictions on normal form calculations, certainly when one wants to work symbolically, keeping the dependence on the parameters of the original vector field. In this talk we discuss an approach, based on former work of Cushman and Sanders, which seems to be able to handle these problems rather efficiently. We describe in particular a splitting algorithm which avoids the explicit calculation of inverses. We also discuss a number of other aspects of normal form calculations, some of which are still unsolved.

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BODO WERNER:

Test Function for Hopf Points

Test functions for certain bifurcation points are scalar functions being monitored during pathfollowing of parameter dependent equilibria and strictly changing sign at the bifurcation points of interest. Test functions can be used for detection, computation and path following of bifurcation points (also of higher codimension).
We present test functions for *real* and *imaginary* Hopf points with *Hopf number* ν based on bordered linear systems

$$(1) \qquad \begin{pmatrix} A^2+\nu I & Ar & r \\ l^T A & 0 & 0 \\ l^T & 0 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ \alpha(A,\nu) \\ \beta(A,\nu) \end{pmatrix} = \begin{pmatrix} 0_n \\ 1 \\ 0 \end{pmatrix}.$$

with Jacobians $A \in \mathbb{R}^{n,n}$ and certain vectors r, l defining the bordering.
Since the derivatives of the test function can be cheaply evaluated, *Hopf curves* which may smoothly connect real and imaginary Hopf points via Takens-Bogdanov points.
Examples of Hopf curves in applications (eutrophication model, 2-box-Brusselator) are given.

Berichterstatter: F. Giannakopoulos

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