Final Report
(Funding Period 2005–2010)

Department of Energy Awards 97891/97888/97889

Konstantin Mischaikow, Rutgers University/Georgia Institute of Technology
Michael Schatz, Georgia Institute of Technology
William Kalies, Florida Atlantic University
Thomas Wanner, George Mason University

Personnel Supported:
In accordance with the proposal, the following faculty and students received financial support.

• Faculty
  – Konstantin Mischaikow, Mathematics, Georgia Institute of Technology and Mathematics and BioMaPS, Rutgers University
  – Michael Schatz, Physics, Georgia Institute of Technology
  – William Kalies, Mathematics, Florida Atlantic University
  – Thomas Wanner, Mathematics, George Mason University

• Students
  – Hyunju Ban, Ph.D. student, Mathematics, Florida Atlantic Univ.
    * Received Ph.D. Fall 2006
    * Thesis Title: Computing Global Decompositions of Dynamical Systems
  – Jean-Philippe Lessard, Ph.D. student, Mathematics, Georgia Tech.
    * Received Ph.D. Fall 2007
    * Thesis Title: Validated Continuation for Infinite Dimensional Problems
  – Tina Hartley, Ph.D. student, Mathematics, George Mason Univ.
    * Received Ph.D. Summer 2008
    * Thesis Title: An Analysis of Phase Separation Processes for Stochastic and Non-local Extensions of the Classical Phase-Field Model
  – Mark Wess, Ph.D. student, Mathematics, Florida Atlantic Univ.
    * Received Ph.D. Fall 2008
    * Thesis Title: Computing Topological Dynamics from Time Series
  – Andrew Corrigan, Ph.D. student, Comp. Data Sciences, George Mason Univ.
    * Received Ph.D. Summer 2009
    * Thesis Title: Kernel-Based Meshless Methods
Hüseyin Kurtuldu, Ph.D. student, Physics, Georgia Tech.
  * Received Ph.D. Summer 2010
  * Thesis Title: New methods of characterizing spatio-temporal patterns in laboratory experiments

Vidit Nanda, Ph.D. student, Mathematics, Georgia Tech., currently Ph.D. student, Mathematics, Rutgers Univ.

Marcus Fontaine, Ph.D. student, Mathematics, Florida Atlantic Univ.

Alex Opritsa, undergraduate student, Mathematics, Florida Atlantic Univ.

Scott Cochran, Ph.D. student, Mathematics, George Mason Univ.

Hanein Edrees, undergraduate student, Mathematics, George Mason Univ.

Papers:

  - Appeared


• **Accepted**


3


• Submitted


• In preparation

– J.-B. van den Berg, J.-P. Lessard, and K. Mischaikow, Rigorous branch following.


– K. Mischaikow and V. Nanda, Computing the homology of maps on manifolds with high confidence from dense uniform samples.


– W. Kalies, K. Mischaikow, and R. VanderVorst, Robust global decompositions of dynamical systems.

**Organization of Workshops/Special Sessions:**

• *Computational Homology and Materials Science*, Georgia Institute of Technology, Atlanta, Georgia (February 2006).
As was indicated in the proposal this grant was used to sponsor the above mentioned Workshop. Additional funding was provided by the Georgia Institute of Technology and a DARPA contract. This workshop brought together materials scientists and mathematicians to explore the use of topological methods in the analysis of materials. The speakers and contents of their talks can be found at

http://chomp.rutgers.edu/projects/

- **Computational Homology and Fluid Dynamics**, Georgia Institute of Technology, Atlanta, Georgia (March 1-3, 2007).

  This workshop, which was planned for in the original proposal, brought together a select group of physicists, applied mathematicians and engineers with an interest in characterizing quantitatively structures and dynamics of spatio-temporally chaotic and turbulent fluid flows. Additional funding for the meeting was provided by the Georgia Institute of Technology. This workshop was highly successful in drawing an internationally diverse and widely renown set of invited speakers, including a member of the National Academy of Sciences (Guenter Ahlers) and a Max Planck Institute Director (Eberhard Bodenschatz). The full list of invited speakers and the contents of their talks can be found at

  http://chomp.rutgers.edu/projects/

  All sessions of the 3 day workshop were marked by lively discussions with very active audience participation. Numerous remarks by participants on the high quality of the workshop were received by the organizers.

- **Computational Topology and Dynamics Workshop**, Montana State University, Bozeman, MT Aug. 10-12, 2008.

  This was a highly focused workshop on recent developments in the theory, algorithms, and software associated with the use of computational homology to study nonlinear dynamics. This includes the rigorous analysis of infinite dimensional systems, global dynamics of multiparameter systems, and the development of topological techniques to analyze nonlinear time series data.

- **Other**

  - W. Kalies, Co-organizer of special session on Dynamical Systems at the Fall 2009 Southeastern Sectional Meeting of the AMS. (October 2009).

  - W. Kalies and T. Wanner, Organizer of a minisymposium on *Computational Topology and Dynamics*, ICIAM 07: 6th International Congress on Industrial and Applied Mathematics, Zürich, Switzerland (July 2007).

  - K. Mischaikow, Co-Organizer of a minisymposium on *Dynamics of Gene Regulation*, ICIAM 07: 6th International Congress on Industrial and Applied Mathematics, Zürich, Switzerland (July 2007).

– M. Schatz, Organizer/Chair of focus session entitled *Characterization of Spatiotemporal Complexity in Fluids and Materials*, March Meeting of the American Physical Society, Denver, CO (March 2007).

  * This focus session provided an opportunity to communicate the ideas of homology applied to physical problems to the broad community of physicists that attend this primary international meeting of the American Physical Society.


– K. Mischaikow, Co-organizer of a conference on *Dynamics, Topology and Computations*, Mathematical Research and Conference Center, Bedlewo, Poland, June, 4-10, 2006.


**Talks:**

• W. Kalies


  – 2009 Invited talk: Computational dynamics from a topological viewpoint, IMA New Directions Short Course: Applied Algebraic Topology, Minneapolis, MN.

  – 2009 Minisymposium talk: Dimension Reduction and Topological Analysis of Attractors, SIAM Conference on Applications of Dynamical Systems, Snowbird, UT.


  – 2008 Contributed talk: Multivalued maps for time series, Workshop on Computational Topology and Dynamics, MSU, Bozeman, MT.

  – 2008 Minisymposium talk: Building databases for global dynamics of multiparameter systems, Foundations of Computational Mathematics ’08, Hong Kong.

  – 2007 Invited talk: Computational dynamics from a topological point of view, CSUMS lecture at College of William and Mary, Williamsburg, VA.


  – 2007 Colloquium talk: Building a Database for Global Dynamics of Multiparameter Systems, Mathematics Colloquium, Vrije University, Amsterdam, the Netherlands.
2007 Invited talk: Introduction to homology, Computational Homology and Fluid Dynamics Workshop, Atlanta, GA.

2007 Invited talk: Computing Global Decompositions of Dynamical Systems, Workshop on Topological and Computational Approaches to Dynamical Systems and Applications, Ryukoku University, Kyoto, Japan.

2006 Invited talk: Computing Global Decompositions of Dynamical Systems, Dynamical and Control Seminar, Rutgers University.


2006 Plenary talk: A computational approach to Conley’s decomposition theorem, Conference on Dynamics, Topology, and Computation, Bedlewo, Poland

2006 Invited talk: Computing recurrence in dynamics, Nowy Sacz, Poland

2006 Invited talk: Computational dynamics via combinatorial approximation and Conley theory, Workshop on Computational and Topological Aspects of Dynamics, Lorentz Center, Leiden Universiteit, the Netherlands.

2006 Invited talk: Computational dynamics via combinatorial approximation and the Conley index, Seminars on Nonlinear Dynamics of Natural Systems, Vrije Universiteit, the Netherlands.

2006 Invited talk: Introduction to homology, Computational Homology and Material Science Workshop, Atlanta, GA.

2006 Colloquium talk: An algorithmic approach to Conley’s decomposition theorem, Georgia Institute of Technology, Atlanta, GA.

K. Mischaikow


Homology of Random Fields, Colloquium, University of Sherbrooke, Sherbrooke, Canada, Feb. 2008.

Building a data-base for the global dynamics of multi-parameter systems, Invited Speaker, ICMC Summer Meeting on Differential Equations, Sao Carlos, Brazil, Jan. 2008.


– Homology: a tool for understanding high dimensional data sets, Invited Speaker, Columbia University Medical Center, July 2007.


– Computational Homology, Invited Speaker, APS meeting, Denver, March 2007

– Building a Data Base for the Global Dynamics of Multi-Parameter Systems, Invited talk, Workshop on Topological and Computational Approaches to Dynamical Systems and Applications, Ryukoku University, Kyoto, Japan.

– Rigorous Numerics via Algebraic Topology, Invited talk, Faculty Research Perspectives, Rutgers University, Feb. 2007.

– Building a Database of Dynamical Systems, Experimental Math Seminar, Invited talk, Rutgers University, December 2006.


- Applications to Dynamical Systems, Topology and its Applications, IMA PI Summer Program for Graduate Students, July 10-15, Mississippi State University.
- Computational Homology, Invited talk, Nowy Sacz, Poland June 2, 2006.
- Topological approach to fast-slow systems, Invited talk, Jagiellonian University, Krakow, June 1, 2006.
- Computational Homology in Nonlinear Dynamics, plenary speaker, ICMC Summer Meeting in Differential Equations, Sao Carlos, Brazil, Feb 20-22, 2006.

- M. Schatz

  - Using homology to characterize laboratory fluid flows, Invited talk, Workshop on Topology: Identifying Order in Complex Systems, Rutgers University, March 2009.
  - Reducing the dimensionality of spatio-temporal data in Rayleigh-Bénard convection using homology and Karhunen-Loève decomposition, Contributed talk, APS/Division of Fluid Dynamics Meeting, San Antonio, TX, Nov. 2008
  - Using homology to characterize spatiotemporal dynamics, Seminar, Institute of Mathematical Sciences, Chennai, India (Jan 2008).
  - 3D space-time topology in Rayleigh-Bénard convection, Contributed talk, American Physical Society Fluid Dynamics Meeting, Salt Lake City, UT (Nov. 2007).
– Computational Homology in Rayleigh-Benard convection, Contributed talk, Workshop on Computational Homology and Materials Science, Atlanta, Georgia (March 2007).


– Homological Characterization of Patterns, IGERT seminar, Northwestern University, Mar. 2006.


– T. Wanner

– “Dynamics and morphology of phase separation”. SIAM-GMU Faculty Research Symposium, Fairfax, Virginia (November 6, 2009).


– “The dynamics of nucleation in stochastic Cahn-Morral systems”. Jagiellonian University, Krakow, Poland (October 13, 2009).

– “Homology of complicated and random evolving patterns”. Sandia CSRI Workshop on Combinatorial Algebraic Topology, Santa Fe, New Mexico (August 29, 2009).

– “The Dynamics of Nucleation in Stochastic Cahn-Morral Systems”. International Conference on Random Dynamical Systems, Chern Institute of Mathematics, Tianjin, China (June 8, 2009).


– “Spinodal decomposition: Complex patterns and topology”. Soft Matter Laboratory, Yale University, New Haven, Connecticut (February 24, 2009).

– “Determining the topology of random evolving patterns from discretizations”. LCDS Seminar, Brown University, Providence, Rhode Island (February 23, 2009).

– “Homological analysis of complicated random patterns”. Applied Dynamics Seminar, University of Maryland, College Park, Maryland (February 14, 2008).
– “Topological quantification of complex microstructures”. US Food and Drug Administration, Silver Spring, Maryland (January 31, 2008).
– “Der Cahn-Hilliard Attraktor in zwei Raumdimensionen”. Oberseminar, Universität Augsburg, Germany (July 12, 2007).
– “Homological Characterization of Patterns”. Computational Homology and Fluid Dynamics Workshop, Atlanta, Georgia (March 1, 2007).
– “Structure of the Attractor of the Cahn-Hilliard Equation on a Square”. Seminar, Kyoto University, Kyoto, Japan (February 12, 2007).
– “Homological Analysis of Complex Transient Patterns via Discretizations”. Workshop on Topological and Computational Approaches to Dynamical Systems and Applications, Kyoto, Japan (February 9, 2007).
– “Complex Transient Patterns and their Topology”. Winter Meeting of the Canadian Mathematical Society, Toronto, Canada (December 11, 2006).
– “Probabilistic and Numerical Validation of Homology Computations for Nodal Domains”. Dynamics and Control Seminar, Rutgers University, Piscataway, New Jersey (October 24, 2006).
– “Topological quantification of complex microstructures”. Day of Computational Mathematics, Nowy Sacz, Poland (June 2, 2006).
– “Computational homology and the evolution of complex patterns”. Graduate Seminar, George Mason University, Fairfax, Virginia (April 26, 2006).
– “Computational homology and the evolution of complex patterns”. College of William and Mary, Williamsburg, Virginia (March 24, 2006).
– “Computational homology and the evolution of complex patterns”. New Jersey Institute of Technology, Newark, New Jersey (February 24, 2006).
– “Homological characterization of patterns in phase separation”. Workshop on Computational Homology and Materials Science, Atlanta, Georgia (February 4, 2006).
– “Computational homology tutorial: Accuracy of homology computations”. Workshop on Computational Homology and Materials Science, Atlanta, Georgia (February 2, 2006).
– “On the accuracy of homology computations for nodal domains”. Georgia Institute of Technology, Atlanta, Georgia (December 1, 2005).

Work Completed during the Funding Period:
This is a collaborative project between the principal investigators. However, as is to be expected, different PIs have greater focus on different aspects of the project. Indicated below are the major directions of research which were pursued during the funding period with an indication of which PIs are most involved.

• Computational Homology in Fluids: M. Schatz, K. Mischaikow. This effort focused on characterizing both the structure and dynamics of complex spatio-temporal flows that arise in thermal convection. Two major findings resulted from this work and two potentially fruitful areas for future study were identified. We briefly summarize these findings and areas below.
Major Finding 1: Detecting and Quantifying Symmetry Breaking. Homology analysis can detect sensitively the (well-known, but never before measured) breaking of Boussinesq symmetry in images of complex flow patterns from Rayleigh-Bénard convection experiments. To our knowledge, there is presently no other way to extract a measure of this symmetry breaking directly from data. Additionally, analysis of homology suggests that the boundaries that limit the lateral extent of the convecting fluid do not contribute to the symmetry breaking; i.e., the symmetry breaking is a bulk phenomenon. Moreover, our work has shown that the strength of the symmetry breaking can be quantified by an order parameter constructed from topological quantities (the Betti numbers) extracted from analysis; we have shown that this order parameter provides a characterization of symmetry breaking that is robust over a wide range of parameter that includes spatio-temporally chaotic regimes. These results suggest that homology can be used as a tool for building accurate models of complex patterns; in this case, by demanding that appropriate models should have solutions that exhibit quantitatively the same degree of symmetry breaking found by homological analysis of the experimental flows. This result is expected to be of interest to the atmospheric sciences community where the role played by the Boussinesq symmetry in modeling convective flows in the atmosphere is a subject that is still open to debate. This work is described in one paper, published in the journal *Physics of Fluids* and in one paper submitted for publication in the journal *Journal of Fluid Mechanics*.

Major Finding 2: Characterizing Convection Dynamics. Homology analysis yields an experimentally accessible measure of dynamical dimension, the number of degrees of freedom required to describe a spatio-temporally chaotic flow. Our work has shown this homology-based dimension behaves similarly to a dimension extracted using the well-known technique of Karhuenen-Lóeve decomposition (KLD) (also known in other contexts as proper orthogonal decomposition or principal components analysis). In particular, we have shown both dimensions exhibit extensivity (i.e., scale with the system size) with the same power law dependence and, remarkably, show the same (universal?) deviation from power law scaling due to finite size effects (the presence of sidewall boundaries in the experiments). The homology-based dimension possesses the practical advantage that it can often be computed much more rapidly than the KLD-based dimension. This work is described in a paper submitted for publication in the journal *Physical Review Letters*.

Future Area for Research 1: Using Homology to Connect Laboratory Experiments to Numerical Models. Our findings suggest further efforts to explore the use of homology in fluid dynamics would benefit significantly by coupling our current laboratory experiments with large scale simulation of flows with realistic boundary conditions. As a preliminary proof-of-concept we have carried out the analysis of homology at one parameter value and one aspect ratio for a short simulation (performed by Professor Mark Paul (Virginia Tech)) that matches the conditions of one of our laboratory experiments. We have found that the mean Betti numbers of the simulation and the experiment are in quantitative agreement. This result bodes well for the chances of
success for work that aims to use homology to establish detailed quantitative connections between laboratory experiments and numerical models.

– Future Area for Research 2: Computational Homology in Cardiac Dynamics. We expect the techniques developed to understand chaotic/turbulent fluid flows might be extended to other physical systems that exhibit spatio-temporal complexity. We explored this idea in a preliminary way by using homology to characterize data from both laboratory experiments and numerical simulations of arrhythmias in the heart. (The data used for these tests were obtained from experiments and simulations by Flavio Fenton (Cornell University), Stefan Luther and Eberhard Bodenschatz (Max Planck Institute for Dynamics and Self-Organization, Gottingen).) Preliminary results suggest that analysis of homology in 3D (2D spatial dimensions, 1 time dimension) is more useful than a strictly 2D spatial analysis in following tissue dynamics that changes from normal sinus rhythm to tachycardia and fibrillation.

• Microstructure Characterization: T. Wanner, K. Mischaikow. We extended our previous work on studying the time evolution of patterns associated with phase separation in conserved concentration fields. In a previously published paper we could use computational homology to quantify differences in the microstructure evolution between the deterministic and the stochastic Cahn-Hilliard model. This part of the project was aimed at extending these studies to include more sophisticated models and identify in more detail the effects of nonlocal and stochastic terms in the model.

During the first two years of the funding period, we extended previously developed code for the Cahn-Hilliard model to the three-dimensional case, and performed sample simulations for varying total mass for the deterministic Cahn-Hilliard model. These simulations indicated that different parts of the attractor for the evolution equation led to different homology signatures. While these might be due to the relatively small sample size used in the simulations, it indicates that homology can provide a measure for studying the attractor dynamics. In addition, we extended the Cahn-Hilliard code to cover the case of two-dimensional three-component alloys, and performed preliminary sample runs. The code was then extended to include periodic boundary conditions and nonlocal terms. One graduate student at George Mason University wrote a fast finite-difference semi-implicit code for simulating a phase-field model which includes both nonlocal and stochastic terms, and studied the convergence properties of the numerical scheme, particularly in the stochastic context, from a theoretical point of view.

During the remaining three years of the funding period, our work on microstructure characterization in evolution equations focused on gaining a better understanding of the connections between the qualitative form of averaged Betti number evolution curves obtained from evolving complicated patterns and the basic structure of the underlying evolution equation. In this context, we concentrated on the following projects: (1) Understanding the nonmonotone complexity evolution in the classical Cahn-Hilliard models via linear behavior, (2) Studying the pattern complexity evolution in the classical phase-field model for non-isothermal phase separation, (3) Classifying the variety of phase separation phenomena that can be observed in multi-component alloys as modeled by Cahn-Morral systems.
– **Complexity Evolution via Linear Behavior:** In previous work, we had studied the classical Cahn-Hilliard equation which models phase separation in binary alloys, as well as its stochastic extension, the Cahn-Hilliard-Cook model. Our results showed that in the classical deterministic model the averaged Betti number evolution curves exhibit nonmonotone behavior during the spinodal decomposition phase, while in the stochastic model with sufficiently large noise these curves decay monotonically. Combined with experimental data for the specific case of Fe-Cr alloys, our results demonstrated that the deterministic model is inadequate for modeling the complexity evolution during spinodal decomposition. Previous theoretical work of Wanner has shown that in the deterministic Cahn-Hilliard model the dynamical behavior during the initial phase separation is dominated by linear behavior, even at distances far from the homogeneous initial state. These results rely heavily on probabilistic arguments which show that for typical solutions the influence of the nonlinearity is small. In recent work with D. Blömker (Universität Augsburg, Germany) and S. Maier-Paape (RWTH Aachen, Germany), the earlier parts of this work could be extended to the case of the stochastic Cahn-Hilliard-Cook model, yet the probabilistic techniques were not immediately applicable. Thus, our recently published results only explain the linear behavior up to moderate distances from the homogeneous state.

During the last two years, Blömker and Wanner have made considerable progress in extending the probabilistic nonlinearity estimates which makes them amenable to the stochastic partial differential equation setting. This work is still ongoing. However, even the results obtained so far show that the observed differences in the complexity evolution will be due to the differences in the deterministic and stochastic linearizations. One graduate student at George Mason University, S. Cochran, has therefore started a comprehensive study of homology evolution in the deterministic and stochastic Cahn-Hilliard models. This study is not only restricted to the Betti number evolution curves. Rather, we are determining the pattern distributions as a function of time in the space of Betti number quadruples as described above. In this way, we hope to be able to gain insight into the basic geometry of typical microstructures. Also this work is still ongoing.

– **Pattern Evolution in Stochastic and Nonlocal Phase-Field Models:** Based on the observations from the Cahn-Hilliard evolution described above, it is natural to ask how special this behavior is, and whether in systems with stronger nonlinearity influence similar behavior can be observed. As a comparison system, the graduate student T. Hartley at George Mason University has studied the classical phase-field equation, as well as recent stochastic and nonlocal extensions of this model. The phase-field equation is a natural candidate for comparison with the Cahn-Hilliard model, since its linearization exhibits qualitatively the same dispersion relation, while the nonlinearities differ.

For her thesis, Hartley has developed spectral code to solve the stochastic and nonlocal phase-field model. Most of this work was completed during the first two project years. During the third year, she performed extensive numerical simulations aimed at uncovering the effects of noise and of the nonlocal term in the system. Her simu-
lations show that despite the similarity in the dispersion relations, the nonmonotone behavior that could be seen in the deterministic Cahn-Hilliard model is no longer present — both the deterministic and the stochastic phase-field model on large domains show monotone decay. However, as the domain size decreases, the phase-field model exhibits complexity evolutions which are distinctly different from the Cahn-Hilliard case. In the latter case, even for small domains, the averaged evolution curves were qualitatively the same; in fact, they scaled as predicted by the domain size. In the phase-field model on small domains, the stochastic model begins developing a nonmonotone complexity evolution while the deterministic evolution remains monotone. This behavior is completely unexpected and we are currently studying it in more detail. First results show that indeed the nonlinearity effects in the phase-field model take hold much sooner than in the Cahn-Hilliard case, so these effects will be nonlinear. In addition, our studies show that replacing the diffusion term in the equation for the phase variable by a nonlocal term (as was originally proposed by van der Waals), can significantly change the pattern characteristics.

– Phase Separation Phenomena in Multi-Component Alloys: During part of the first two project years, the graduate student A. Corrigan at George Mason University has extended the spectral Cahn-Hilliard code to the case of three-component alloys, including the physically motivated logarithmic nonlinearity. In the later part of the funding period, Corrigan completed a comprehensive first sweep of the two-dimensional parameter space of all initial concentrations of the three components which add up to one, the so-called Gibbs triangle. His simulations uncovered a variety of different phase separation phenomena. Some of these are natural extensions of binary phenomena, but others are truly new and surprising. One of the phase separation mechanisms that could be observed consists of a two-staged decomposition process: During the first stage, the major phase separates from the two minor phases in a near binary fashion, i.e., forming disconnected snake-like patterns, while the two minor phases on their joint domain simultaneously separate on a much larger spatial scale; during the second stage, the minor phase becomes quickly connected while at the same time the minor phases nucleate droplets. During this nucleation process, seemingly nonphysical annulus structures can be observed, which seem to be unstable transition states for the evolution equation and can be verified numerically, see the discussion below. Based on his simulations, we are currently working on a “map” of different phase separation kinetics based on the initial concentrations in the alloy. During the last two years of the funding period, we have initiated a more detailed study of the nucleation dynamics in the stochastic Cahn-Morral model for three-component alloys. By using our above-described method for distinguishing between droplets which nucleate at the boundary or in the interior of the considered domain, we developed a method to determine the precise size of a boundary layer, which delineates boundary effects from bulk effects in the material. This method is based on scaling techniques and is applicable even to very small domains, on which only a handful of droplets nucleate on average. We have shown that from statistical information on nucleation in such small domains, one can make precise quantitative
projections even for large domains, where the number of nucleating droplets is two orders of magnitude larger. These finding impressively justify the use of Monte-Carlo methods on fairly small domains, where at first glance boundary effects seem to dominate the nucleation behavior.

• **Probabilistic Homology Validation:** W. Kalies, T. Wanner, K. Mischaikow. Our above mentioned work on microstructure characterization is based on numerically studying the homology of certain sublevel sets of a function, whose evolution is described by deterministic or stochastic evolution equations. In practice, these sublevel sets are approximated using an underlying discretization of the considered partial differential equation. In the context of patterns associated with thermal convection, one presumes that the evolution is in principle described by a deterministic or stochastic evolution equation. The patterns are obtained by thresholding on a digital image of the experimental apparatus. Both cases raise the question of the accuracy of the resulting homology computation which we are addressing from two perspectives.

  – We have, over the course of this project, developed a probabilistic approach which gives insight into the suitability of this method in the context of random fields. In the context of periodic boundary conditions and uniform grids we obtained explicit probability estimates for the correctness of the homology computations, which in turn yield a-priori bounds for the suitability of certain grid sizes. These estimates started out as estimates for scalar homogeneous random fields, and made use of fundamentally one-dimensional techniques. Nevertheless, we were able to significantly extend our methods to also cover the case of two-dimensional random fields, for the topology of the nodal domains is significantly more complicated. Our methods are based on a mixture of excluded sign configurations, which introduce a combinatorial aspect into the problem, as well as extending results for the asymptotics of probability estimates in a singular limit.

Subsequently, we have focussed on the setting of computing the connectedness of generalized nodal sets of non-homogeneous random fields on compact intervals, i.e., nodal domains of a random field relative to a deterministic threshold function which does not have to be constant. In this case we demonstrate, not surprisingly, that using a uniform grid is far from optimal. However, we also provide a criterium for the placement of the sampling points to give what we believe are the optimal probabilities. We are also able to show that these locations do not appear to be related to the densities of the zeros of the random functions when the threshold function is chosen to be identically zero. One of the central improvements in our results is the possibility of a nonconstant threshold function. Our previous results covered only the case of centered fields which are thresholded at zero, i.e., their mean. In contrast, our new results allow for thresholding at arbitrary levels, and this opens the door for determining optimal sampling locations for randomly perturbed deterministic functions. While one would certainly expect that under small stochastic perturbations most of the topology changes will occur near the zeros of the deterministic function, our results quantify the size of the region around the zeros which is affected, and
provide the optimal sampling point locations within these regions.

Finally, the graduate student S. Cochran has started working on extending these recent results to the case of two-dimensional domains. While this work is still in progress, at the time of writing of this report he has completed the derivation of all probability expansions for the local excluded sign configurations and has begun assembling the main result, which will be the core of his Ph.D. thesis.

– In collaboration with S. Day (College of William and Mary) we have developed a computational approach which, given a cubical approximation to a nodal domain of a given function, allows one to rigorously determine if the homology has been correctly computed. This method is based on interval arithmetic computations combined with the computation of range enclosures, and it produces an adaptive cubical decomposition of the underlying base domain, such that the topology of the nodal sets in each square of the decomposition can be inferred from the signs of the function values at the corners of this square.

As a first testing ground for this newly developed code we have begun a numerical study of homology computations for nodal domains of random periodic trigonometric polynomials, which naturally arise in the study of linear stochastic evolution equations. The theoretical results described above had indicated that in order to determine the homology of nodal domains of a periodic trigonometric polynomial of degree \( N \) with high accuracy, one has to consider discretizations of size \( N^{3/2} \) in one dimension, and of size \( N^2 \) in two dimensions. Since the theoretical results only imply the sufficiency of these discretization sizes, the results from our validated computations indicate that they are also necessary. In addition, we have used our verification algorithm to study the temporal evolution of Betti number signatures in the two-dimensional Cahn-Hilliard model, thereby rigorously validating previous numerical results.

During the final year of the funding period, T. Wanner, in collaboration with P. Dlotko, M. Mrozek (both at Jagiellonian University, Krakow, Poland) and T. Kaczynski (Université de Sherbrooke, Canada), could significantly improve the above algorithm with respect to the homology computation part. As described before, the algorithm produces a nonuniform cubical grid which allows to determine the location of the nodal domains from the signs of the function values at the vertices of the grid. Unfortunately, until recently, available codes for the computation of cubical homology required a uniform cubical complex as input. Thus, the original version of the algorithm had to extend the nonuniform cubical grid to a considerably finer uniform one, before the homology of the nodal domains could be computed. While this worked reasonably well, the limitations of this approach resulted for example in having to restrict the degree of a random trigonometric polynomial to at most \( N = 16 \). Beyond this value, memory and time restrictions made the homology computation infeasible. During the last year, we therefore adapted the recent coreduction homology algorithm to the situation of regular CW-complexes, and implemented a version for two-dimensional nonuniform cubical complexes. We have incorporated this new homology computation code into the above verification algorithm, and the results are
truly amazing. We can now easily work with random trigonometric polynomials up to degree at least $N = 33$, and the speed of the homology computations is decreased by up to four orders of magnitude.

- **Computational Homology and Dynamics:** *W. Kalies, T. Wanner, K. Mischaikow.*
Topological methods can be used to rigorously describe the dynamics of nonlinear systems. We are approaching this problem from several perspectives and through a variety of systems.

  - In collaboration with S. Day, M. Gameiro, and J.-P. Lessard we have developed a method of validated continuation that builds on traditional predictor-corrector continuation methods, but allows one to validate that the numerically computed solution approximates a true solution to the PDE within an explicit error bound. Furthermore, the cost of this new method is less than twice the cost of the traditional continuation method and hence is cheaper to employ than the standard method of using refinements to check one’s computations. We have continuously worked on improving the analytic estimates and the code to allow for general applications of this method to problems defined on multidimensional rectangular domains. In his Ph.D. thesis Lessard has applied these ideas to a wider range of problems including proving chaos for large ranges of parameter values in ODEs and studying time periodic solutions for delay differential equations. We have also developed techniques to efficiently apply these ideas to branches of equilibria.

  - We have used the validated continuation methods to continue our study of the equilibria in materials models in the context of the celebrated Cahn-Hilliard model. In addition we have begun to work towards applying these techniques to diblock copolymer systems. These latter systems are extensions of the Cahn-Hilliard model with stable solutions that represent microstructures with intriguing topological properties such as double gyroid geometries. We have also initiated a study of the dynamics of the patterns of these copolymer systems. Our contention is that computational homology can be used to effectively and efficiently quantify important features of the patterns. In this way the algebraic topology can be used to generate a nonlinear projection from the infinite dimensional phase space to a very low dimensional space that still captures essential information.

Finally, we have started complementing the numerical simulations on the evolution of Cahn-Morral systems by a study of the equilibrium structure of the three-component system in the context of nucleation. This work was performed within the framework of undergraduate research, and is in collaboration with H. Edrees, J. Price, and E. Sander (all at George Mason University). We have developed a spectral method and implemented it in the (non rigorous) path-following software package AUTO. Our results have numerically identified the transition states that can be observed during nucleation on one- and two-dimensional base domains. In particular, for the case of two-dimensional domains we could establish the occurrence of double droplets, as well as the annulus shaped transition states mentioned above which were observed during spinodal decomposition.
We have developed software for the construction of databases for the global dynamics of multiparameter nonlinear systems. It has been successfully applied to a two age class density dependent Leslie population model which has three independent parameters. This is a test model but does exhibit the crucial dynamical features and challenges that our approach is designed to identify and overcome such as multiple basins of attraction, recurrent dynamics such as periodic orbits and chaotic dynamics, nonuniform hyperbolicity and the associated bifurcations. Mathematicians have focused on bifurcation theory: how changing parameters leads to changes in structure. An example is the unfolding of a singularity theory which describes all possible structures in a small neighborhood of the singularity. Biology is characterized by robustness. The organism must function over wide ranges in parameters, sometimes orders of magnitude. The classical bifurcation theory does not address this issue. Furthermore, because of noise, bifurcations which are mathematically significant may be of no importance to the functioning of the organism. Finally, in the presence of nonuniform hyperbolicity structural stability fails to be a generic property.

The database provides a coarse description of the global dynamics over large sets of parameter values. The description is in terms of continuation classes. Two dynamical systems belong to the same continuation class if their observable dynamics at a particular level of refinement is the same. This is very different from the concept of structural stability and topological conjugacy. Two systems can be topologically conjugate and lie in different continuation classes and similarly two systems in the same continuation class can lie in different topological conjugacy classes.

In the last year of the grant, in collaboration with R. VanderVorst, we have further investigated the mathematical foundations of these global dynamical descriptions. We have developed the combinatorial theory of Morse decompositions in terms of lattices and posets. We are in the process of developing theory and algorithms for analyzing the structure of Morse decompositions over parameter space and changes due to resolution.

Also in the last two years of the grant, with Ph.D. student Mark Wess, we have developed algorithms to analyze time series using computational homology via the Conley index. We are still in the early stages and are applying the methods to time series generated from a deterministic map in small dimensions, but the techniques can in principle be expanded to higher dimensions and noisy or experimental data.

Finally in the last year of the grant, we have started to apply the database techniques for global decompositions in the context of infinite-dimensional systems. Specifically, with Sarah Day and former PhD student Hyunju Ban, we are studying the Kot-Schaffer map with Ricker nonlinearity, a model for seed dispersal in plants. We have obtained rigorous numerically-computable estimates for the polynomial approximation of the Ricker nonlinearity and the Galerkin approximation of the infinite-dimensional map which allows us to make rigorous computations on a finite-dimensional approximation which also apply to the infinite-dimensional map.

- **Stress Networks in Polycrystals:** T. Wanner. Together with E. Fuller (NIST) and
D. Saylor (FDA) we have characterized stress networks in polycrystals. This part of the project is aimed at developing homological metrics which can aid in distinguishing not only microstructures, but also derived mechanical response fields.

During the funding period, we concentrated on the case of two-dimensional calcite microstructures. For different, realistic orientation distributions of the grains in the polycrystal we performed finite element simulations to obtain the stress and energy density fields in the material caused by heating. These simulations were performed using the finite element code OOF, which was developed by Edwin Fuller and others at NIST. We have found a correlation between the topology of maximal principal stress networks and the underlying grain misorientations, as well as between the elastic energy density and the grain misorientations. These results show that homology is a precise quantitative metric for the considered response fields.

We have also started analyzing three-dimensional stress data. Also in this case our results show that the homological analysis can clearly distinguish between different misorientation distributions. These results are still preliminary, since we are also analyzing the data further using methods from persistent homology to obtain more insight into the length scales involved in the stress networks, which is crucial in the three-dimensional case. These three-dimensional persistence computations have proven to be extremely time-intensive. Previously, we could perform promising preliminary simulations on a relatively small subset of the data. Only recently have we been able to obtain first complete results on a few data sets using the recent persistence code by M. Mrozek based on the homology of inclusion maps.

- **Microstructure-Controlled Drug Release: K. Mischaikow, T. Wanner.** This part of the project is concerned with the development of topological metrics in the context of controlled drug delivery systems, such as drug-eluting stents. We are particularly interested in developing metrics which can be used to link the processing stage to the resulting microstructure, and ultimately to the achieved system response in terms of drug release profiles.

For our study, we concentrated on a first basic setting: For a small number of crystal particles growing into a phase separated matrix we quantify the topological changes. This crystal growth process can take place in the context of both nucleation and spinodal decomposition, depending on the concentrations of the involved components. The underlying model for this processing stage is a coupled system of partial differential equations of Cahn-Hilliard and phase-field type, which describes the evolution of the drug, polymer, and solvent concentrations, as well as the evolution of an order parameter for distinguishing between amorphous and crystalline states. Over the course of the funding period, D. Saylor (FDA) has significantly improved his simulation code for drug-delivery problems and has provided us with first preliminary data. Our subsequent homological analysis could distinguish between different morphologies, yet a clear connection with the drug release profile could not be established.

We have therefore focused on developing topological metrics for the study of the drug release kinetics which include directional information. The drug is released only through
the “top” side of the microstructure, and this release leads to a slow directed destruction of the microstructure and subsequent release of drug from lower levels. For this, we used metrics based on persistent homology, which in turn are computed via the homology of inclusion maps, based on code by M. Mrozek. For a variety of drug microstructures, we have computed our persistence metric, and it seems to be an appropriate metric for establishing a connecting to the drug release kinetics. While this could be established on a qualitative level, we are still in the process of establishing an quantitative link. Finally, D. Saylor has recently provided the first set of experimental drug coatings, and we have begun applying the three-dimensional versions of the above metric to these data sets. At the present time, we can compare the experimental data only to two-dimensional simulation data at the corresponding parameter values. The three-dimensional simulations have been delayed due to cluster resource issues at the FDA, but we anticipate the first three-dimensional numerical results after the funding period ends.

• **Microstructure of Fuel Cells:** W. Kalies, K. Mischaikow. In collaboration with P. Voorhees (Northwestern Univ.) and M. Gameiro (Rutgers) we have been using our computational homology software to analyze the topological structure of the void, metal and ceramic components of a Solid Oxide Fuel Cell. The data was obtained by Voorhees’ lab through the use of dual-beam focused ion beam scanning electron microscopy (FIB-SEM) for making a complete 3D reconstruction. Of interest are measurements and understanding of critical microstructural features such as volume fractions and surface areas of specific phases, three-phase boundary length, and the connectivity and tortuosity of specific sub-phases.