

LIST OF PUBLICATIONS (2002-2019)

(see also <http://scholar.google.de>)

Most important interdisciplinary publications in the research field „Mathematical methods in Natural Science“:

Lebiedz, D., Brandt-Pollmann, U. Manipulation of self-aggregation patterns and waves in a reaction-diffusion-system by optimal boundary control strategies. *Phys. Rev. Lett.* 91, 208301 (2003)

Lebiedz, D. Computing minimal entropy production trajectories: An approach to model reduction in chemical kinetics. *J. Chem. Phys.* 120, 6890 (2004)

Vladimirov, N., Løvdok, L., Lebiedz, D., Sourjik, V. Dependence of bacterial chemotaxis on gradient shape and adaptation rate. *PLoS Comput. Biol.* 4, e1000242 (2008)

Skanda, D., Lebiedz, D. An optimal experimental design approach to model discrimination in dynamic biochemical systems. *Bioinformatics* 26, 939 (2010)

Lebiedz, D., Siehr, J. Unger, J. A Variational principle for computing slow invariant manifolds in dissipative dynamical systems. *SIAM J. Sci. Comput.* 33, 703 (2011)

Skanda, D., Lebiedz, D. A robust optimization approach to experimental design for model discrimination of dynamical systems. *Math. Prog.* 141, 405 (2013)

Heiter, P., Lebiedz, D. Towards differential geometric characterization of slow invariant manifolds in extended phase space: Sectional curvature and flow invariance. *SIAM J. Appl. Dyn. Syst.* 17, 732 (2018)

Diploma Theses, PhD Thesis, Habilitation Thesis

Isolierung der Promotorregion und der Splice-Varianten des monozytären cysteinreichen Scavengerrezeptors CD163 (RM3/1), Diploma Thesis Biochemistry, University of Münster, 1998

Wasserstoffinduzierte Effekte im System $\text{Nd}_2(\text{Fe/Co})_{14}\text{B}$, Eine SIMS- und XPS-Studie, PhD Thesis Physical Chemistry, University of Münster, 2001

Numerische Simulation und Optimale Steuerung parabolischer Differentialgleichungen in Chemotaxis-Modellen, Diploma Thesis Applied Mathematics, University of Münster, 2002

Optimal Control, Model- and Complexity-Reduction of Self-Organized Chemical and Biochemical Systems: A Scientific Computing Approach, Habilitation Thesis, University of Heidelberg, 2006

Publications in Peer-Reviewed Journals

1. Kestenbaum, H., Lange de Oliveira, A., Schmidt, W., Schüth, F., Ehrfeld, W., Gebauer, K., Löwe, H., Richter, T., Lebiez, D., Untiedt, I., Züchner, H. Silver catalysed oxidation of ethylene to ethylene oxide in a microreaction system. *Ind. Eng. Chem. Res.* 41, 710 (2002)
2. Lebiez, D., Züchner, H., Gutfleisch, O. A secondary ion mass spectrometry study of hydrogen interaction with $\text{Nd}_2(\text{Fe}/\text{Co})_{14}\text{B}$. *J. Alloy Compd.* 356-357, 679 (2003)
3. Lebiez, D., Brandt-Pollmann, U. Manipulation of self-aggregation patterns and waves in a reaction-diffusion-system by optimal boundary control strategies. *Phys. Rev. Lett.* 91, 208301 (2003), selected for online-publication in *Virtual Journal of Biological Physics Research* 6(10) (2003)
4. Lebiez, D. Computing minimal entropy production trajectories: An approach to model reduction in chemical kinetics. *J. Chem. Phys.* 120, 6890 (2004)
5. Lebiez, D., Züchner, H., Gutfleisch, O. Hydrogen-induced effects in alloys of type $\text{Nd}_2(\text{Fe}/\text{Co})_{14}\text{B}$ studied by X-ray photoelectron spectroscopy. *Chem. Mater.* 16, 3098 (2004)
6. Lebiez, D., Brandt-Pollmann, U. Dynamic control and information processing in chemical reaction systems by tuning self-organization behavior. *Chaos* 14, 611 (2004), selected for online-publication in *Virtual Journal of Biological Physics Research* 8(5) (2004)
7. Lebiez, D., Brandt-Pollmann, U. Manipulation of surface reaction dynamics by global pressure and local temperature control: A model study. *Phys. Rev. E* 70, 051609 (2004)
8. Lebiez, D., Maurer, H. External optimal control of self-organisation dynamics in a chemotaxis reaction diffusion system. *Syst. Biol. (Stevenage)* 1, 222 (2004)
9. Inderwildi, O.R., Lebiez, D., Deutschmann, O., Warnatz, J. Coverage dependence of oxygen decomposition and surface diffusion on rhodium (111): A DFT study. *J. Chem. Phys.* 122, 034710 (2005)
10. Zobeley, J., Lebiez, D., Kammerer, J., Ishmurzin, A., Kummer, U. A new time-dependent complexity reduction method for biochemical systems. *Trans. Comput. Syst. Biol.* 1, 90 (2005)
11. Inderwildi, O.R., Lebiez, D., Deutschmann, O., Warnatz, J. Influence of initial oxygen coverage and magnetic moment on the NO decomposition on rhodium (111). *J. Chem. Phys.* 122, 15470 (2005)
12. Lebiez, D., Brandt-Pollmann, U. Specific external forcing of spatiotemporal dynamics in reaction-diffusion systems. *Chaos* 15, 023901 (2005), selected for online-publication in *Virtual Journal of Biological Physics Research* 9(7) (2005)
13. Inderwildi, O.R., Lebiez, D., Warnatz, J. Linear relationships between activation energies and reaction energies for coverage-dependent dissociation reactions on rhodium surfaces. *Phys. Chem. Chem. Phys.* 7, 2552 (2005)
14. Brandt-Pollmann, U., Lebiez, D., Diehl, M., Sager, S., Schlöder, J.P. Real-time nonlinear feedback control of pattern formation in (bio)chemical reaction-diffusion processes: A model study. *Chaos* 15, 033901 (2005), selected for online-publication in *Virtual Journal of Biological Physics Research* 10(2) (2005)
15. Lebiez, D., Sager, S., Bock, H.G., Lebiez, P. Annihilation of limit-cycle oscillations by identification of critical perturbing stimuli via mixed-integer optimal control. *Phys. Rev. Lett.* 95, 108303 (2005), selected for online-publication in *Virtual Journal of Biological Physics Research* 10(6) (2005)
16. Lebiez, D. Exploiting optimal control for target-oriented manipulation of (bio)chemical systems: a model-based approach to specific modification of self-organized dynamics. *Int. J. Mod. Phys. B* 19, 3763 (2005), invited review paper
17. Lebiez, D., Kammerer, J., Brandt-Pollmann, U. Automatic network coupling analysis for dynamical systems based on detailed kinetic models. *Phys. Rev. E* 72, 041911 (2005), selected for online-publication in *Virtual Journal of Biological Physics Research* 10(8) (2006)
18. Inderwildi, O.R., Lebiez, D., Deutschmann, O., Warnatz, J. Influence of coadsorbates on the NO dissociation on a rhodium(311) surface. *ChemPhysChem* 6, 2513 (2005)

19. Su, Q., Inderwildi, O.R., Deutschmann, O, Warnatz, J., Lebiecz, D. A transient modeling and simulation study of catalytic NO_x decomposition over Rhodium. JSAE Technical paper 20056117-115 (2005)
20. Shaik, O.S., Kammerer, J., Gorecki, J., Lebiecz, D. Derivation of a quantitative minimal model from a detailed elementary-step mechanism supported by mathematical coupling analysis. J. Chem. Phys. 123, 324103 (2005), selected for online-publication in Virtual Journal of Biological Physics Research 11(1) (2006)
21. Sager, S., Brandt-Pollmann, U., Diehl, M., Lebiecz, D., Bock, H.G. Exploiting system homogeneities in large scale optimal control problems for speedup of multiple shooting based SQP methods. Comp. Chem. Engin. 31, 1181 (2007)
22. Slaby, O., Sager, S., Shaik, O. S., Kummer, U., Lebiecz, D. Optimal control of self-organized dynamics in cellular signal transduction. Math. Comput. Mod. Dyn. 13, 487 (2007)
23. Siehr, J., Mommer, M. S., Slaby, O., Lebiecz, D. Targeting characteristic wave properties in reaction diffusion systems by optimization of external forcing. Phys. Rev. E 76, 056211 (2007)
24. Shaik, O. S., Sager, S., Slaby, O., Lebiecz, D. Phase tracking and restoration of circadian rhythms by model-based optimal control. IET Syst. Biol. 2, 16 (2008)
25. Reinhardt, V., Winckler, M., Lebiecz, D. Approximation of slow attracting manifolds in chemical kinetics by trajectory-based optimization approaches. J. Phys. Chem. A, 28, 1712 (2008)
26. Schulmeister, S., Ruttorf, M., Thiem, S., Kentner, D., Lebiecz, D., Sourjik, V. Protein exchange dynamics at chemoreceptor clusters in *Escherichia coli*. Proc. Natl. Acad. Sci. USA 105, 6403 (2008)
27. Vladimirov, N., Løvdok, L., Lebiecz, D., Sourjik, V. Dependence of bacterial chemotaxis on gradient shape and adaptation rate. PloS Comput. Biol. 4: e1000242 (2008)
28. Kasenda, B., Rehberg, M., Franzem, M., Fritsch, K., Markert, A., Finke, J., Lebiecz, D., Illerhaus, G. Mathematical Modeling in Optimizing Methotrexate-Based Chemotherapy. Blood 114, 4766 (2009)
29. Slaby, O., Lebiecz, D. Oscillatory NAD(P)H waves and calcium oscillations in neutrophils ? A modeling study of feasibility. Biophys. J. 96, 417 (2009)
30. Mommer, M. S., Lebiecz, D. Modeling subdiffusion using reaction diffusion systems. SIAM J. Appl. Math. 70, 112 (2009)
31. Hallett, M. B., Lebiecz, D., Mommer, M. S., Reble, C., Saltmarsh, E. J. Fantastic Ca²⁺ "z-waves" fade out quietly. Cell Calcium 46, 85 (2009)
32. Løvdok, L., Bentele, K., Vladimirov, N., Müller, A., Pop, F., Lebiecz, D., Kollmann, M., Sourjik, V. Role of Translational Coupling in Robustness of Bacterial Chemotaxis Pathway. PloS Biology 7, e1000171 (2009)
33. Kasenda, B., Rehberg, M., Franzem, M, Fritsch, K., Markert, A., Finke, J. Haug, S., Lebiecz, D. Illerhaus, G. Development of a semi-quantitative mathematical model to optimize methotrexate-based chemotherapy. Onkologie 32, 113 (2009)
34. Vladimirov, N., Lebiecz, D., Sourjik, V. Predicted auxiliary navigation mechanism of peritrichously flagellated chemotactic bacteria. PloS Comput. Biol. 6, e1000717 (2010)
35. Skanda, D., Lebiecz, D. An optimal experimental design approach to model discrimination in dynamic biochemical systems. Bioinformatics 26, 939 (2010)
36. Lebiecz, D. Entropy-related extremum principles for model reduction of dissipative dynamical systems. Entropy 212, 706 (2010)
37. Lebiecz, D., Reinhardt, V., Siehr, J. Minimal curvature trajectories: Riemannian geometry concepts for slow manifold computation in chemical kinetics. J. Comput. Phys. 229, 6512 (2010)
38. Engelhart, M., Lebiecz, D., Sager, S. Optimal control of selected chemotherapy ODE models: A view on the potential of optimal schedules and choice of objective function. Math. Biosci. 229, 123 (2011)

39. Lebiedz, D., Siehr, J. Unger, J. A Variational principle for computing slow invariant manifolds in dissipative dynamical systems. *SIAM J. Sci. Comput.* 33, 703 (2011)
40. Kasenda, B., Rehberg, M., Thürmann P., Franzem, M., Veelken, H., Fritsch, K., Schorb, E., Finke, J., Lebiedz, D., Illerhaus, G. The prognostic value of serum methotrexate area under curve in elderly primary CNS lymphoma patients. *Ann. Hematol.* 91, 1257 (2012)
41. Lebiedz, D., Rehberg, M., Skanda, D. Robust optimal design of synthetic biological networks. *Methods Mol Biol.* 813, 45 (2012)
42. Stegmaier, J. Skanda, D., Lebiedz, D. Robust optimal design of experiments for model discrimination using an interactive software tool. *PloS One* 8, e55723 (2013)
43. Skanda, D., Lebiedz, D. A robust optimization approach to experimental design for model discrimination of dynamical systems. *Math. Prog.* 141, 405 (2013)
44. Lebiedz, D., Siehr, J. A continuation method for the efficient solution of parametric optimization problems in kinetic model reduction. *SIAM J. Sci. Comput.* 35, A1584-A1603 (2013)
45. Kaese S, Everding S, Bohn A, Holz E, Lieder F, Baumgart P, Lebiedz D, Fischer D, Waltenberger J, Lebiedz P. Efficacy, adverse events and outcome of pre-hospital systemic thrombolysis in out-of-hospital cardiac arrest. *European Heart Journal Supplements* 1 (S2), 130 (2013)
46. Lebiedz, D., Siehr, J. An optimization approach to kinetic model reduction for combustion chemistry. *Flow, Turbulence and Combustion* 92(4), 885 (2014)
47. Lebiedz, D., Unger, J. On unifying concepts for trajectory-based slow invariant attracting manifold computation in kinetic multi-scale models. *Math. Comp. Model. Dyn.* 22, 87 (2016)
48. Heiter, P., Lebiedz, D. Towards differential geometric characterization of slow invariant manifolds in extended phase space: Sectional curvature and flow invariance. *SIAM J. Appl. Dyn. Syst.* 17, 732 (2018)
49. Heitel, M., Verschueren, R., Diehl, M., Lebiedz, D. Considering slow manifold based model reduction for multiscale chemical optimal control problems. (submitted to OCAM)
50. Heitel, M., Lebiedz, D. A view on analytical and topological properties of separatrices in 1-D holomorphic dynamical systems and complex-time Newton flows. (submitted to Nonlinearity)
51. Lebiedz, D., Poppe, J. Towards differential geometric characterization of slow invariant manifolds in extended phase space II: Geodesic stretching. (submitted to SIADS)
52. Dietrich, J., Lebiedz, D. A spectral view on slow invariant manifolds in complex time dynamical systems. (to be submitted to PRL)

Publications in Reviewed Proceedings and Monographs

1. Lebiedz, D., Reinhardt, V. Kammerer, J. Novel Trajectory-Based Concepts for Model and Complexity Reduction in (Bio)chemical Kinetics. p. 343 in A. Gorban et al. „Model reduction and coarse graining approaches for multi-scale phenomena. Springer (2006)
2. Lebiedz, D. Sager, S., Shaik, O. S., Slaby, O. Optimal control of self-organized dynamics in cellular signal transduction. Proceedings of the 5th Vienna Symposium on Mathematical Modeling, Vienna, Austria, 2006, Argesim Rep. 30, ISBN 3-901608-30-3 (2006)
3. Lebiedz, D., Skanda, D., Fein, M. Automatic complexity analysis and model reduction of nonlinear biochemical systems. In M. Heiner and A.M. Uhrmacher eds., “Computational Methods in Systems Biology”, Lecture Notes in Computer Science, p. 123, Volume 5307 (2008)
4. Rehberg, M., Lebiedz, D. Phase tracking of circadian rhythms by model-based optimal control. Proceedings FOSBE 2009, Denver, USA (2009)
5. Lebiedz, D. Reinhardt, V., Siehr, J. Unger, J. Geometric criteria for model reduction in chemical kinetics via optimization of trajectories. In "Coping with complexity: Model reduction and data analysis", Springer Series "Lecture Notes in Computational Science and Engineering" (2010)
6. Dedner, A., Fein, M., Klöfkorn, R., Kröner, D., Lebiedz, D., Siehr, J., Unger, J. On the computation of slow manifolds in chemical kinetics via optimization and their use as reduced models in reactive flow systems. Proceedings of the 13th International Conference on Numerical Combustion (2011)
7. Lebiedz, D., Siehr, J. Simplified reaction models for combustion in gas turbine combustion chambers. p. 161 in "Flow and Combustion in advanced gas turbine combustors", Janicka et al. eds., Springer (2013)
8. Lebiedz, D., Unger, J. A Boundary Value View on the Reverse Trajectory-Based Optimization Approach for Kinetic Model Reduction. Proceedings of 4th IWMRRF, San Francisco (2013)
9. Lebiedz, D., Heiter, P., Unger, J. On conceptual ideas concerning slow invariant manifolds in a variational problem viewpoint. Proceedings of 5th IWMRRF, Lübbenau (2015)
10. Lebiedz, D. Covariant geometric characterization of slow invariant manifolds: New concepts and viewpoints. Proceedings of 6th IWMRRF, Princeton, USA (2017)
11. Heitel, M., Lebiedz, D. An online slow manifold approach for efficient optimal control of multiple time-scale kinetics. Proceedings of 6th IWMRRF, Princeton, USA (2017)
12. Lebiedz, D., Dietrich, J., Heitel, M. Poppe, J. Analytic continuation and differential geometry views on slow manifolds and separatrices. Proceedings of 7th IWMRRF, Trondheim, Norway (2019)
13. Poppe, J., Lebiedz, D. Stretching-based diagnostics in a differential geometry setting. Proceedings of 7th IWMRRF, Trondheim, Norway (2019)
14. Heitel, M., Lebiedz, D. Characterization of separatrics in holomorphic dynamical systems in the light of complex time. Proceedings of 7th IWMRRF, Trondheim, Norway (2019)
15. Dietrich, J., Lebiedz, D. Slow invariant manifolds of analytic dynamical systems. Proceedings of 7th IWMRRF, Trondheim, Norway (2019)
16. Lebiedz, D. Vom Zählen zum Messen: Morphologie chemisch-kinetischer Modelle *more geometrico*. (2019, submitted, invited chapter in book „Morphology as a paradigm in contemporary philosophy of science“)

Publications in Proceedings, Reports and Monographs without Peer-Review

1. Ishmurzin, A., Schramm, B., Lebiedz, D., Warnatz, J. Advanced tabulation for reduced chemical reaction mechanisms. Final Report „Computational Fluid Dynamics for Combustion“, Project funded by the European Community under the ‘Competitive and Sustainable Growth’ Programme (2002)
2. Schramm, B., Ishmurzin, A., Lebiedz, D., Warnatz, J. ILDM Description of the Combustion of Large Hydrocarbons. 21. Deutscher Flammentag, VDI-Berichte 1750, 675 (2003)
3. Ishmurzin, A., Schramm, B., Lebiedz, D., Warnatz, J. Reduction of Detailed Reaction Mechanisms for Large Hydrocarbon Combustion by the ILDM method. In Proceedings of the European Combustion Meeting, Orleans (2003)
4. Reinhardt, V., Schramm, B., Lebiedz, D., Warnatz, J. ILDM Reduced Chemistry Tailored For Large Scale Reaction Mechanisms in Complex Reactive Flow Applications, 20th ICDERS (2005)
5. Inderwildi, O.R., Starukhin, D., Volpp, H.R., Lebiedz, D., Deutschmann, O., Warnatz, J. Reaction Processes on Catalytically Active Surfaces, in „Reactive Flows, Diffusion and Transport“, W. Jäger, R. Rannacher and J. Warnatz (eds.), Springer Scientific Berlin, Heidelberg, New York (2006)
6. Reinhardt, V., Winckler, M., Warnatz, J., Lebiedz, D. Towards automatic reduction of kinetic mechanisms by optimization of trajectories, 21st ICDERS (2007)
7. Reinhardt, V., Winckler, M., Warnatz, J., Lebiedz, D. Kinetic mechanism reduction by trajectory-based optimization methods, Proceedings of the European Combustion Meeting (2007)
8. Inderwildi, O.R., Lebiedz, D., Warnatz, J. Quantum Chemical Simulations in Emission Control Catalysis. In „Quantum Chemical Simulations of Surfaces and Interfaces of Materials“, V.A. Basiuk and P. Ugliengo (Eds.), American Scientific Publishers (2008)