

## **LIST OF PUBLICATIONS (2002-2022)**

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

The most important and representative interdisciplinary journal publications in my main research field „Mathematical Modeling in Natural Science“:

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)

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)

Engelhart, M., Lebiedz, 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)

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 Journals, Proceedings, Monographs**

1. Kestenbaum, H., Lange de Oliveira, A., Schmidt, W., Schüth, F., Ehrfeld, W., Gebauer, K., Löwe, H., Richter, T., Lebiedz, 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. Lebiedz, D., Züchner, H., Gutfleisch, O. A secondary ion mass spectrometry study of hydrogen interaction with  $\text{Nd}_2(\text{Fe/Co})_{14}\text{B}$ . *J. Alloy Compd.* 356-357, 679 (2003)
3. 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), selected for online-publication in *Virtual Journal of Biological Physics Research* 6(10) (2003)
4. 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)
5. Lebiedz, D. Computing minimal entropy production trajectories: An approach to model reduction in chemical kinetics. *J. Chem. Phys.* 120, 6890 (2004)
6. Lebiedz, D., Züchner, H., Gutfleisch, O. Hydrogen-induced effects in alloys of type  $\text{Nd}_2(\text{Fe/Co})_{14}\text{B}$  studied by X-ray photoelectron spectroscopy. *Chem. Mater.* 16, 3098 (2004)
7. Lebiedz, 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)
8. Lebiedz, 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)
9. Lebiedz, D., Maurer, H. External optimal control of self-organisation dynamics in a chemotaxis reaction diffusion system. *Syst. Biol. (Stevenage)* 1, 222 (2004)
10. Inderwildi, O.R., Lebiedz, 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)
11. Zobeley, J., Lebiedz, D., Kammerer, J., Ishmurzin, A., Kummer, U. A new time-dependent complexity reduction method for biochemical systems. *Trans. Comput. Syst. Biol.* 1, 90 (2005)
12. Inderwildi, O.R., Lebiedz, 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)
13. Lebiedz, 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)
14. Inderwildi, O.R., Lebiedz, 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)
15. Brandt-Pollmann, U., Lebiedz, 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)
16. Lebiedz, D., Sager, S., Bock, H.G., Lebiedz, 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)
17. Lebiedz, 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)

18. Lebiedz, 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)
19. Inderwildi, O.R., Lebiedz, D., Deutschmann, O., Warnatz, J. Influence of coadsorbates on the NO dissociation on a rhodium(311) surface. *ChemPhysChem* 6, 2513 (2005)
20. Su, Q., Inderwildi, O.R., Deutschmann, O., Warnatz, J., Lebiedz, D. A transient modeling and simulation study of catalytic NO<sub>x</sub> decomposition over Rhodium. *JSAE Technical paper* 20056117-115 (2005)
21. Shaik, O.S., Kammerer, J., Gorecki, J., Lebiedz, 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)
22. 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)
23. 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)
24. 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)*
25. Hoffman, K., Lebiedz, D., Maurer, H., Pesch, H.J. Simulation and optimal control of 2-D chemotactic processes via nonlinear programming. *Proceedings of EUCCO, Montpellier, France (2007)*
26. Reinhardt, V., Winckler, M., Warnatz, J., Lebiedz, D. Kinetic mechanism reduction by trajectory-based optimization methods. In *Proceedings of the European Combustion Meeting (2007)*
27. Sager, S., Brandt-Pollmann, U., Diehl, M., Lebiedz, 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)
28. Slaby, O., Sager, S., Shaik, O. S., Kummer, U., Lebiedz, D. Optimal control of self-organized dynamics in cellular signal transduction. *Math. Comput. Mod. Dyn.* 13, 487 (2007)
29. Siehr, J., Mommer, M. S., Slaby, O., Lebiedz, D. Targeting characteristic wave properties in reaction diffusion systems by optimization of external forcing. *Phys. Rev. E* 76, 056211 (2007)
30. Shaik, O. S., Sager, S., Slaby, O., Lebiedz, D. Phase tracking and restoration of circadian rhythms by model-based optimal control. *IET Syst. Biol.* 2, 16 (2008)
31. Reinhardt, V., Winckler, M., Lebiedz, D. Approximation of slow attracting manifolds in chemical kinetics by trajectory-based optimization approaches. *J. Phys. Chem. A*, 28, 1712 (2008)
32. Schulmeister, S., Ruttorf, M., Thiem, S., Kentner, D., Lebiedz, D., Sourjik, V. Protein exchange dynamics at chemoreceptor clusters in *Escherichia coli*. *Proc. Natl. Acad. Sci. USA* 105, 6403 (2008)
33. Vladimirov, N., Løvdok, L., Lebiedz, D., Sourjik, V. Dependence of bacterial chemotaxis on gradient shape and adaptation rate. *PloS Comput. Biol.* 4: e1000242 (2008)
34. 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)

35. 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)
36. Kasenda, B., Rehberg, M., Franzem, M., Fritsch, K., Markert, A., Finke, J., Lebiedz, D., Illerhaus, G. Mathematical Modeling in Optimizing Methotrexate-Based Chemotherapy. *Blood* 114, 4766 (2009)
37. Slaby, O., Lebiedz, D. Oscillatory NAD(P)H waves and calcium oscillations in neutrophils ? A modeling study of feasibility. *Biophys. J.* 96, 417 (2009)
38. Mommer, M. S., Lebiedz, D. Modeling subdiffusion using reaction diffusion systems. *SIAM J. Appl. Math.* 70, 112 (2009)
39. Hallett, M. B., Lebiedz, D., Mommer, M. S., Reble, C., Saltmarsh, E. J. Fantastic  $Ca^{2+}$  "z-waves" fade out quietly. *Cell Calcium* 46, 85 (2009)
40. Løvdok, L., Bentele, K., Vladimirov, N., Müller, A., Pop, F., Lebiedz, D., Kollmann, M., Sourjik, V. Role of Translational Coupling in Robustness of Bacterial Chemotaxis Pathway. *PLoS Biology* 7, e1000171 (2009)
41. Kasenda, B., Rehberg, M., Franzem, M., Fritsch, K., Markert, A., Finke, J., Haug, S., Lebiedz, D., Illerhaus, G. Development of a semi-quantitative mathematical model to optimize methotrexate-based chemotherapy. *Onkologie* 32, 113 (2009)
42. Rehberg, M., Lebiedz, D. Phase tracking of circadian rhythms by model-based optimal control. *Proceedings FOSBE 2009, Denver, USA* (2009)
43. 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)
44. Vladimirov, N., Lebiedz, D., Sourjik, V. Predicted auxiliary navigation mechanism of peritrichously flagellated chemotactic bacteria. *PLoS Comput. Biol.* 6, e1000717 (2010)
45. Skanda, D., Lebiedz, D. An optimal experimental design approach to model discrimination in dynamic biochemical systems. *Bioinformatics* 26, 939 (2010)
46. Lebiedz, D. Entropy-related extremum principles for model reduction of dissipative dynamical systems. *Entropy* 212, 706 (2010)
47. Lebiedz, D., Reinhardt, V., Siehr, J. Minimal curvature trajectories: Riemannian geometry concepts for slow manifold computation in chemical kinetics. *J. Comput. Phys.* 229, 6512 (2010)
48. Engelhart, M., Lebiedz, 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)
49. 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)
50. Dedner, A., Fein, M., Klöforn, 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)
51. 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)
52. Lebiedz, D., Rehberg, M., Skanda, D. Robust optimal design of synthetic biological networks. *Methods Mol Biol.* 813, 45 (2012)
53. Stegmaier, J., Skanda, D., Lebiedz, D. Robust optimal design of experiments for model discrimination using an interactive software tool. *PLoS One* 8, e55723 (2013)
54. Skanda, D., Lebiedz, D. A robust optimization approach to experimental design for model discrimination of dynamical systems. *Math. Prog.* 141, 405 (2013)

55. 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)
56. 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)
57. Lebiedz, D., Unger, J. A Boundary Value View on the Reverse Trajectory-Based Optimization Approach for Kinetic Model Reduction. Proceedings of 4<sup>th</sup> IWMRRF, San Francisco (2013)
58. 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)
59. Lebiedz, D., Siehr, J. An optimization approach to kinetic model reduction for combustion chemistry. *Flow, Turbulence and Combustion* 92(4), 885 (2014)
60. Lebiedz, D., Heiter, P., Unger, J. On conceptual ideas concerning slow invariant manifolds in a variational problem viewpoint. Proceedings of 5<sup>th</sup> IWMRRF, Lübbenau (2015)
61. 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)
62. Lebiedz, D. Covariant geometric characterization of slow invariant manifolds: New concepts and viewpoints. Proceedings of 6<sup>th</sup> IWMRRF, Princeton, USA (2017)
63. Heitel, M., Lebiedz, D. An online slow manifold approach for efficient optimal control of multiple time-scale kinetics. Proceedings of 6<sup>th</sup> IWMRRF, Princeton, USA (2017)
64. 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)
65. Lebiedz, D., Dietrich, J., Heitel, M. Poppe, J. Analytic continuation and differential geometry views on slow manifolds and separatrices. Proceedings of 7<sup>th</sup> IWMRRF, Trondheim, Norway (2019)
66. Poppe, J., Lebiedz, D. Stretching-based diagnostics in a differential geometry setting. Proceedings of 7<sup>th</sup> IWMRRF, Trondheim, Norway (2019)
67. Heitel, M., Lebiedz, D. Characterization of separatrices in holomorphic dynamical systems in the light of complex time. Proceedings of 7<sup>th</sup> IWMRRF, Trondheim, Norway (2019)
68. Dietrich, J., Lebiedz, D. Slow invariant manifolds of analytic dynamical systems. Proceedings of 7<sup>th</sup> IWMRRF, Trondheim, Norway (2019)
69. Lebiedz, D. Vom Zählen zum Messen: Morphologie chemisch-kinetischer Modelle *more geometrico*. In *Allgemeine Zeitschrift für Philosophie*, Beiheft „Morphologie als Paradigma in den Wissenschaften“, 309-331 (2022)
70. Lebiedz, D., Poppe, J. On differential geometric formulations of slow invariant manifold computation: Geodesic stretching and flow curvature. *Journal of Dynamical Systems and Geometric Theories* 20(1), 1-32 (2022)
71. Ginoux, J.-M., Lebiedz, D., Meucci, R., Llibre, J. Flow curvature method and energy of generalized Liénard systems. *Chaos, Solitons and Fractals* 161, 112354 (2022)
72. Baier, M., Lebiedz, D. Deep Chebyshev center-based column generation. Accepted for Proceedings of International Conference on Operations Research, Hamburg, Germany (2023)

**Preprints**

73. Heitel, M., Verschueren, R., Diehl, M., Lebiedz, D. Slow manifold based model reduction in multiscale chemical optimal control problems. arXiv:1712.01058 math.OC
74. Heitel, M., Lebiedz, D. On separatrices in 1-D holomorphic dynamical systems and complex-time Newton flows. arXiv:1911.10963 math.CV
75. Dietrich, J., Lebiedz, D. A spectral view on slow invariant manifolds in complex time kinetic systems. arXiv:1912.00748 math.ph
76. Lebiedz, D. Holomorphic Hamiltonian Xi-flow and Riemann zeros. arXiv:2006.09165 math.DS
77. Dietrich, J., Lebiedz, D. Approximating normally hyperbolic invariant manifolds by trajectory based optimization. arXiv:2210.07938 math.DS
78. Scholz, S., Berger, L., Lebiedz, D. Benchmarking of flatness-based control of the heat equation. arXiv:2307.16764 math.OC
79. Kainz, N., Lebiedz, D. Local geometry of equilibria and a Poincare-Bendixson-type theorem for holomorphic flows. arXiv:2402.07612 math.DS
80. Kainz, N., Lebiedz, D. Geometry of global sectors and basins of equilibria in holomorphic flows. To be submitted

**Other Publications and Reports (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. 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)
4. Reinhardt, V., Winckler, M., Warnatz, J., Lebiedz, D. Towards automatic reduction of kinetic mechanisms by optimization of trajectories, 21st ICDERS (2007)