

Selected Publications through 2007

Yannis G. Kevrekidis

2007
"Coarse-Grained Analysis of Stochasticity-Induced Switching between Collective Motion States." <i>Proc. Nat. Acad. Sci. U.S.A.</i> , 104 , 5931, 2007 [with A. Kolpas and J. Moehlis].
"Slow Observables of Singularly Perturbed Differential Equations." <i>Nonlinearity</i> , 20 , 2463, 2007 [with Z. Artstein, M. Slemrod, and E.S. Titi].
"Coarse-Grained Dynamics of an Activity Bump in a Neural Field Model." <i>Nonlinearity</i> , 20 , 2127, 2007 [with C.R. Laing and T.A. Frewen].
"Bistability and Oscillations in the Huang-Ferrell Model of MAPK Signaling." <i>PLoS. Comp. Biol.</i> , 3 , 1819, 2007 [with L. Qiao, R.B. Nachbar, and S.Y. Shvartsman].
"An Equation-Free Approach to Analyzing Heterogeneous Cell Population Dynamics." <i>J. Math. Biol.</i> , 55 , 331, 2007 [with K.A. Bold, Y. Zou, and M.A. Henson].
"Reduced Computations for Nematic Liquid Crystals: A Time-Stepper Approach for Systems with Continuous Symmetries." <i>J. Non-Newtonian Fluid Mech.</i> , 146 , 51, 2007 [with C. Siettos and L. Russo].
"Deciding the Nature of the Coarse Equation through Microscopic Simulations: The Baby-Bathwater Scheme." <i>SIAM Review</i> , 49 , 469, 2007 [with J. Li, P.G. Kevrekidis, and C.W. Gear].
"Projective and Coarse Projective Integration for Problems with Continuous Symmetries." <i>J. Comp. Phys.</i> , 225 , 382, 2007 [with M.E. Kavousanakis, R. Erban, A.G. Boudouvis, and C.W. Gear].
"Reaction Dynamics in a Parallel Flow Channel PEM Fuel Cell." <i>J. Electrochem. Soc.</i> , 154 , B835, 2007 [J. Benziger, J.E. Chia, and E. Kimball].
"The Effect of Co-Adsorbed Oxygen on the Adsorption and Diffusion of Potassium on Rh(110): A First-Principles Study." <i>J. Phys. Chem. C</i> , 111 , 7446, 2007 [with Y. Xu, H. Marbach, R. Imbihl, and M. Mavrikakis].
"Acceleration Method for Coarse-Grained Numerical Solution to the Boltzmann Equation." <i>J. Fluids. Eng.</i> , 129 , 908, 2007 [with H.A. Al-Mohssen, and N.G. Hadjiconstantinou].
"General Tooth Boundary Conditions for Equation Free Modeling." <i>SIAM J. Sci. Comp.</i> , 29 , 1495, 2007 [with A.J. Roberts].
"A Computer-Assisted Study of Global Dynamic Transitions for a Non-Invertible System." <i>Int. J. Bifurc. Chaos.</i> , 17 , 1305, 2007 [with R.A. Adomaitis and R. de la Llave].

<p>"Coarse-Grained Computations of Demixing in Dense Gas-Fluidized Beds." <i>Phys. Rev. E</i>, 75, 051309, 2007 [with S.J. Moon and S. Sundaresan].</p>
<p>"Dynamics of Polydisperse Irreversible Adsorption: A Pharmacological Example." <i>Math. Mod. Math. Appl. Sci.</i>, 17, 759, 2007 [with R. Erban, J. Chapman, K.D. Fisher, and L.W. Seymour].</p>
<p>"Coarse Molecular-Dynamics Analysis of Stress-Induced Structural Transitions in Crystals." <i>Appl. Phys. Lett.</i>, 90, 171910, 2007 [with M.A. Amat and D. Maroudas].</p>
<p>"Gyration-Radius Dynamics in Structural Transitions of Atomic Clusters." <i>J. Chem. Phys.</i>, 126, 124102, 2007 [with T. Yanao, W.S. Koon, and J.E. Marsden].</p>
<p>"Variable-Free Exploration of Stochastic Models: A Gene Regulatory Network Example." <i>J. Chem. Phys.</i>, 126, 155103, 2007 [with R. Erban, T.A. Frewen, X.A. Wang, T.C. Elston, R. Coifman, and B. Nadler].</p>
<p>"Heterogeneous Animal Group Models and their Group-Level Alignment Dynamics: An Equation-Free Approach." <i>J. Theor. Biol.</i>, 246, 100, 2007 [with S.J. Moon, B. Nabet, N.E. Leonard, and S.A. Levin].</p>
<p>"Condition Estimates for Pseudo-Arclength Continuation." <i>SINUM</i>, 45, 263, 2007 [with K.I. Dickson, C.T. Kelley, and I.C.F. Ipsen].</p>
<p>"Variance Reduction for the Equation-Free Simulation of Multiscale Stochastic Systems." <i>SIAM MMS.</i>, 6, 70, 2007 [with A. Papavasiliou].</p>
<p>"Ignition and Front Propagation in Polymer Electrolyte Membrane Fuel Cells." <i>J. Phys. Chem. C</i>, 111, 2330, 2007 [with J.B. Benziger, E.S. Chia, and Y. De Decker].</p>
<p>"Template-Based Stabilization of Relative Equilibria in Systems with Continuous Symmetry." <i>J. Nonlinear Sci.</i>, 17, 109, 2007 [with S. Ahuja and C.W. Rowley].</p>
<p>2006</p>
<p>"Strong Convergence of Projective Integration Schemes for Singularly Perturbed Stochastic Differential Systems." <i>Comm. Math. Sci.</i>, 4, 707, 2006 [D. Givon and R. Kupferman].</p>
<p>"Spatially Distributed Stochastic Systems: Equation-Free and Equation-Assisted Bifurcation Analysis." <i>J. Chem. Phys.</i>, 125, 204108, 2006 [with L. Qiao, R. Erban, and C.T. Kelley].</p>
<p>"The STR-PEM Fuel Cell as a Reactor Building Block." <i>AIChE J.</i>, 52, 3902, 2006 [with E. Chia and J.B. Benziger].</p>
<p>"Equation-Free Particle-Based Computations: Coarse Projective Integration and Coarse Dynamic Renormalization in 2D." <i>Ind. Eng. Chem.</i>, 45, 7002, 2006 [with Y. Zou and R. Ghanem].</p>
<p>"Particle Simulation of Vibrated Gas-Fluidized Beds of Cohesive Fine Powders." <i>Ind. Eng. Chem.</i>, 45, 6966, 2006 [with S.-J. Moon and S. Sundaresan].</p>

<p>"Coarse Molecular-Dynamics Determination of the Onset of Structural Transitions: Melting of Crystalline Solids." <i>Phys. Rev. B</i>, 74, 132201, 2006 [with M. Amat and D. Maroudas].</p>
<p>"An Equation-Free Approach to Coupled Oscillator Dynamics: The Kuramoto Model Example." <i>Int. J. Bifurc. Chaos</i>, 16, 2043-2052, 2006 [with S.-J. Moon].</p>
<p>"An Equation-Free Approach to Nonlinear Control: Feedback Linearization with Pole-Placement." <i>Int. J. Bifurc. Chaos</i>, 16, 2029, 2006 [with C.I. Siettos and N. Kazantzis].</p>
<p>"Compaction and Dilation Rate Dependence of Stresses in Gas-Fluidized Beds." <i>Phys. Fluids</i>, 18, 083304, 2006 [with S.J. Moon and S. Sundaresan].</p>
<p>"A Systems-Based Approach to Multiscale Computation: Equation-Free Detection of Coarse-Grained Bifurcations." <i>Comp. Chem. Eng.</i>, 30, 1632, 2006 [with C. Siettos and R. Rico-Martinez].</p>
<p>"Equation-Free Dynamic Renormalization in a Glassy Compaction Model." <i>Phys. Rev. E</i>, 74, 016702, 2006 [with L. Chen and P.G. Kevrekidis].</p>
<p>"The Moment Map: Nonlinear Dynamics of Density Evolution via a Few Moments." <i>SIADS</i>, 5, 403, 2006 [with D. Barkley, and A.M. Stuart].</p>
<p>"Diffusion Maps, Spectral Clustering and the Reaction Coordinates of Dynamical Systems." <i>Appl. Comp. Harm. Anal.</i>, 21, 113, 2006 [with B. Nadler, S. Lafon, and R.C. Coifman].</p>
<p>"Experimental Study of a Neimark-Sacker Bifurcation in Axially Forced Taylor-Couette Flow." <i>J. Fluid. Mech.</i> 558, 1, 2006 [with M. Sinha and A.J. Smits].</p>
<p>"Multiscale Analysis of Re-Entrant Production Lines: An Equation-Free Approach." <i>Physica A</i>, 363, 1, 2006 [with Y. Zou and D. Armbruster].</p>
<p>"Oxidation of Aliphatic and Aromatic Sulfides Using Sulfuric Acid." <i>Ind. Eng. Chem. Res.</i>, 45, 518, 2006 [with J. Nehlsen and J.B. Benziger].</p>
<p>"Guiding Chemical Pulses through Geometry: Y Junctions." <i>Phys. Rev. E</i>, 73, 036219, 2006 [L. Qiao, C. Punckt, and H.H. Rotermund].</p>
<p>"Geometry-Induced Pulse Instability in Microdesigned Catalysts: The Effect of Boundary Curvature." <i>Phys. Rev. E</i>, 73, 036217, 2006 [L. Qiao, C. Punckt, and H.H. Rotermund].</p>
<p>"An Equation-Free Approach to Coupled Oscillator Dynamics." <i>Phys. Rev. Lett.</i>, 96, 144101, 2006 [S.-J. Moon and R. Ghanem].</p>
<p>"The Power Performance Curve for Engineering Analysis of Fuel Cells." <i>J. Power Sources</i>, 155, 272, 2006 [J.B. Benziger, B. Satterfield, W.H.J. Hogarth, and J.P. Nehlsen]</p>
<p>"Gene Regulatory Networks: A Coarse-Grained, Equation-Free Approach to Multiscale Computation." <i>J. Chem. Phys.</i>, 124, 084106, 2006 [R. Erban, D. Adalsteinsson, and T.C. Elston].</p>
<p>"Equation-Free Dynamic Renormalization of a KPZ-type Equation." <i>Phys. Rev. E.</i>, 73, 036703, 2006 [with D.A. Kessler and L. Chen].</p>

<p>"An Equation-Free Computational Approach for Extracting Population-Level Behavior from Individual-Based Models of Biological Dispersal." <i>Physica D</i>, 215, 1, 2006 [R. Erban and H.G. Othmer].</p>
<p>"Patch Dynamics with Buffers for Homogenization Problems." <i>J. Comp. Phys.</i>, 213, 264, 2006 [G. Samaey and D. Roose].</p>
<p>"Equation-Free, Coarse Grained Computational Optimization Using Time-Steppers." <i>Chem. Eng. Sci.</i>, 61, 779, 2006 [A. Bindal, M.G. Ierapetritou, S. Balakrishnan, A. Armaou, and A.G. Makeev].</p>
<p>2005</p>
<p>"Equation-Free Dynamic Renormalization: Self-Similarity in Multidimensional Particle System Dynamics." <i>Phys. Rev. E</i>, 72, 046702, 2005 [with Y. Zou and R. Ghanem].</p>
<p>"Constraint-Defined Manifolds: A Legacy-Code Approach to Low-Dimensional Computations." <i>J. Sci. Comp.</i>, 25, 17, 2005 [with C.W. Gear].</p>
<p>"Coarse-Grained Numerical Bifurcation Analysis of Lattice Boltzmann Models." <i>Physica D</i>, 210, 58, 2005 [with P. van Leemput and K.W.A. Lust].</p>
<p>"Geometric Diffusions for the Analysis of Data From Sensor Networks." <i>Curr. Opin. Neurobiol.</i>, 15, 576, 2005 [with R.R. Coifman, M. Maggioni, and S.W. Zucker].</p>
<p>"Projecting on a Slow Manifold: Singularly Perturbed Systems and Legacy Codes." <i>SIADS</i>, 4, 711, 2005 [with C.W. Gear, T.J. Kaper, and A. Zagaris].</p>
<p>"Equation-Free Optimal Switching Policies for Bistable Reacting Systems Using Coarse Time-Steppers." <i>Int. J. R.N.C.</i>, 15, 713, 2005 [with A. Armaou].</p>
<p>"Equation-Free, Multiscale Computation for Unsteady Random Diffusion." <i>SIAM MMS</i>, 4, 915, 2005 [with D. Xiu].</p>
<p>"Coarse Nonlinear Dynamics of Filling-Emptying Transitions: Water in Carbon Nanotubes." <i>Phys. Rev. Lett.</i>, 95, 130603, 2005 [with S. Sriraman and G. Hummer].</p>
<p>"Core Collapse via Coarse Dynamic Renormalization." <i>Phys. Rev. Lett.</i>, 95, 081102, 2005 [with A. Szell and D. Merritt].</p>
<p>"Optical Imaging and Control of Genetically Designated Neurons in Functional Circuits." <i>Ann. Rev. Neurosci.</i>, 28, 533, 2005 [with G. Miesenboeck].</p>
<p>"Equation-Free/Galerkin-Free POD-Assisted Computation of Incompressible Flows." <i>J. Comp. Phys.</i>, 207, 568, 2005 [with S. Sirisup, D. Xiu, and G.E. Karniadakis].</p>
<p>"A Parrinello-Rahman Approach to Vortex Lattices." <i>Phys. Lett. A.</i>, 341, 128, 2005 [with R. Carretero-Gonzalez, P.G. Kevrekidis, D. Maroudas, and D.J. Frantzeskakis].</p>
<p>"Application of Coarse Integration to Bacterial Chemotaxis." <i>SIAM MMS</i>, 4, 307, 2005 [with S. Setayeshgar, C.W. Gear, and H.G. Othmer].</p>
<p>"The Gap-Tooth Scheme for Homogenization Problems." <i>SIAM MMS</i>, 4, 278, 2005 [with G. Samaey and D. Roose].</p>

<p>"Coarse Master Equation from Bayesian Analysis of Replica Molecular Dynamic Simulations." <i>J. Phys. Chem.</i>, 109, 6479, 2005 [with S. Sriraman and G. Hummer].</p>
<p>"The Dynamic Response of PEM Fuel Cells to Changes in Load." <i>Chem. Eng. Sci.</i>, 60, 1743, 2005 [with J. Benziger, E. Chia and J.F. Moxley].</p>
<p>"An Equation-Free, Multiscale Approach to Uncertainty Quantification." <i>IEEE Comp. Sci. Eng.</i>, 7, 16, 2005 [D. Xiu, and R. Ghanem].</p>
<p>"Effective Equations for Discrete Systems: A Time Stepper Based Approach." <i>Int. J. Bifurcations Chaos.</i>, 15, 975, 2005 [with J. Moeller, O. Runborg, P.G. Kevrekidis, and K. Lust].</p>
<p>"Coarse-Grained Kinetic Computations for Rare Events: Application to Micelle Formation." <i>J. Chem. Phys.</i>, 122, 044908, 2005 [with D.I. Kopelevich and A.Z. Panagiotopoulos].</p>
<p>"Coarse-Grained Computations for a Micellar System." <i>J. Chem. Phys.</i>, 122, 044907, 2005 [with D.I. Kopelevich and A.Z. Panagiotopoulos].</p>
<p>2004</p>
<p>"Coarse Multiscale Computation." <i>Abstr. Papers Amer. Chem. Soc.</i>, 225, U704, 2004 [with D.I. Kopelevich and A.Z. Panagiotopoulos].</p>
<p>"A Process for the Removal of Thiols from a Hydrocarbon Stream by a Heterogeneous Reaction with Lead Oxide." <i>Energy & Fuels</i>, 18, 721, 2004 [with J.P. Nehlsen and J.B. Benziger].</p>
<p>"Bifurcation Analysis of Nonlinear Reaction-Diffusion Problems Using Wavelet-Based Reduction Techniques." <i>Comp. & Chem. Eng.</i>, 28, 557, 2004 [with J. Krishnan and O. Runborg].</p>
<p>"Vortices in Bose-Einstein Condensates: Some Recent Developments." <i>Modern Phys. Lett. B</i>, 18, 1481, 2004 [with P.G. Kevrekidis, R. Carretero-Gonzalez, and D.J. Frantzeskakis].</p>
<p>"Water Balance and Multiplicity in a Polymer Electrolyte Membrane Fuel Cell." <i>AIChE J.</i>, 50, 2320, 2004 [with E-S.J. Chia and J.B. Benziger].</p>
<p>"Optimal Sensor Location and Reduced Order Observer Design for Distributed Process Systems." <i>Comp. Chem. Eng.</i>, 28, 27, 2004 [with A.A. Alonso, J.R. Banga, and C.E. Frouzakis].</p>
<p>"Time-Steppers and Coarse Control of Microscopic Distributed Processes." <i>Int. J. Robust and Nonlinear Control</i>, 14, 89, 2004. [with A. Armaou and C.I. Siettos].</p>
<p>"Distributed Nonlinear Control of Diffusion-Reaction Processes." <i>Int. J. Robust and Nonlinear Control</i>, 14, 133, 2004 [with S. Djuljevic and P.D. Christofides].</p>
<p>"Computing in the Past with Forward Integration." <i>Phys. Lett. A</i>, 321, 335, 2004 [with C.W. Gear].</p>
<p>"Application of Wavelet-Based Reduction Techniques to Nonlinear Reaction-Transport Problems." <i>Comp. Chem. Eng.</i>, 28, 557, 2004 [with J. Krishnan and O. Runborg].</p>

<p>"Remarks on a Smoluchowski Equation." <i>Discrete and Continuous Dynamical Systems</i>, 111, 101, 2004 [with P. Constantin and E.S. Titi].</p>
<p>"Coarse Bifurcation Diagrams via Microscopic Simulators: a State-Feedback Control-Based Approach." <i>Int. J. Bif. Chaos.</i>, 141, 207, 2004 [with C.I. Siettos and D. Maroudas].</p>
<p>"Apparent Hysteresis in a Driven System with Self-Organized Drag." <i>Phys. Rev. Lett.</i>, 9216, 160603, 2004 [with M. Haataja and D. Srolovitz].</p>
<p>"Coarse Projective kMC Integration: Forward/Reverse Initial and Boundary Value Problems." <i>J. Comp. Phys.</i>, 1962, 474, 2004 [with R. Rico-Martinez and C.W. Gear].</p>
<p>"Equation-Free Multiscale Computations for a Lattice-Gas Model: Coarse-Grained Bifurcation Analysis of the NO+CO Reaction on Pt100." <i>Chem. Eng. Sci.</i>, 598, 1733, 2004 [with A.G. Makeev].</p>
<p>"Coarse Bifurcation Studies of Bubble Flow Lattice Boltzmann Simulations." <i>Chem. Eng. Sci.</i>, 59, 2357, 2004 [with C. Theodoropoulos, K. Sankaranarayanan, and S. Sundaresan].</p>
<p>"Equation-Free: The Computer-Assisted Analysis of Complex Multiscale Systems." <i>AIChE J.</i>, 507, 1346, 2004 [with C.W. Gear and G. Hummer].</p>
<p>"Optimal Sensor Placement for State Re-construction of Distributed Process Systems." <i>AIChE J.</i>, 507, 1438, 2004 [with A.A. Alonso and C.E. Frouzakis].</p>
<p>"The Stirred Tank Reactor Polymer Electrolyte Membrane Fuel Cell." <i>AIChE J.</i>, 50, 1889, 2004 [with J.B. Benziger, E-S.J. Chia, E. Karnas, J. Moxley, and C. Teuscher].</p>
<p>"Dragging Bistable Fronts." <i>Physica Scripta</i>, 69, 451, 2004 [with P.G. Kevrekidis, B.A. Malomed, H.E. Nistazakis, and D.J. Frantzeskakis].</p>
<p>"From Molecular Dynamics to Coarse Self-Similar Solutions: A Simple Example Using Equation-Free Computation." <i>JNNFM</i>, 120, 215, 2004 [with L. Chen, P.G. Debenedetti, and C.W. Gear].</p>
<p>"Steady State Multiplicity in a Polymer Electrolyte Membrane Fuel Cell." <i>AIChE J.</i>, 509, 2320, 2004. [with E-S.J. Chia and J.B. Benziger].</p>
<p>"Equation-Free Modeling of Evolving Diseases: Coarse-Grained Computations with Individual-Based Models." <i>Proc. Roy. Soc. London</i>, 4602050, 27621, 2004 [with J. Cisternas, C.W. Gear, and S. Levin].</p>
<p>"Asymptotic States of a Smoluchowski Equation." <i>Arch. Rat. Mech. Anal.</i>, 174, 365, 2004 [with P. Constantin and E.S. Titi].</p>
<p>"Vortices in Bose-Einstein Condensates: Some Recent Developments." <i>Mod. Phys. Lett. B</i>, 18, 1481, 2004 [with P.G. Kevrekidis, M. Garretero-Gonzalez, and D.J. Frantzeskakis].</p>
<p>"Nonlinear Dynamics Analysis Through Molecular Dynamics Simulations." In <i>Multiscale Modeling and Simulation</i>, S. Attinger and P. Koumoutsakos, eds., Lecture Notes in Computational Science and Engineering, 39, Springer Verlag, p. 69, 2004 [with J. Li and S. Yip].</p>

<p>"Exploration of Coarse Free Energy Surfaces Templated on Continuum Numerical Methods." In <i>Multiscale Modeling and Simulation</i>, S. Attinger and P. Koumoutsakos, eds., Lecture Notes in Computational Science and Engineering, 39, Springer Verlag, p. 81, 2004 [with D. Passerone].</p>
<p>"Damping Factors for the Gap-Tooth Scheme." In <i>Multiscale Modeling and Simulation</i>, S. Attinger and P. Koumoutsakos, eds., Lecture Notes in Computational Science and Engineering, 39, Springer Verlag, p. 93, 2004 [with G. Samaey and D. Roose].</p>
<p>2003</p>
<p>"A Comparative Study of Lattice Boltzmann and Front-Tracking Finite-Difference Methods for Bubble Simulations." <i>Int. J. Multiphase Flow</i>, 29, 109, 2003 [with K. Sankaranarayanan, S. Sundaresan, J. Lu, and G. Tryggvason].</p>
<p>"CO Oxidation on Thin Pt. Crystals: Temperature Slaving and the Derivation of Lumpedmodels." <i>J. Chem. Phys.</i>, 188, 1, 2003 [with J. Cisternas, P. Holmes, and X. Li].</p>
<p>"Nonlinear Model reduction for Dynamic Analysis of Cell Population Models." <i>Chem. Eng. Sci.</i>, 58, 429, 2003 [with Y. Zhang and M.A. Henson].</p>
<p>"Focusing Revisited: A Renormalization/Bifurcation Approach." <i>Nonlinearity</i>, 16, 497, 2003 [with C. Siettos and P.G. Kevrekidis].</p>
<p>"Adaptive Detection of Bifurcations: an Experimental Feasibility Study." <i>Physica D</i>, 176, 1, 2003 [with R. Rico-Martinez, K. Krischer, G. Flaetgen, and J.S. Anderson].</p>
<p>"Gentle Dragging of Reaction Waves." <i>Phys. Rev. Lett.</i>, 90, 018302, 2003 [with J. Wolff, A.G. Papathanasiou, H.H. Rotermund, G. Ertl, and X. Li].</p>
<p>"Buckling in Response to Applied Heat Sources." <i>Physica D</i>, 177, 71, 2003 [with J. Cisternas and P. Holmes].</p>
<p>"A Route to Computational Chaos Revisited." <i>Physica D</i>, 177, 101, 2003 [with C. E. Frouzakis and B.B. Peckham].</p>
<p>"Projective Methods for Stiff Differential Equations: Problems with Gaps in Their Eigenvalue Spectrum." <i>SIAM J. Sci. Comp.</i>, 24, 1091, 2003 [with C.W. Gear].</p>
<p>"Telescopic Projective Integrators for Stiff Differential Equations." <i>J. Comp. Phys.</i>, 187, 95, 2003 [with C.W. Gear].</p>
<p>"Coarse Brownian Dynamics for Nematic Liquid Crystals: Bifurcation, Projective Integration and Control Via Stochastic Simulation." <i>J. Chem. Phys.</i>, 11822, 10149; 2003 [with C. Siettos and M.D. Graham].</p>
<p>"Wave Initiation Through Spatiotemporally Controllable Perturbations." <i>Phys. Rev. Lett.</i>, 9014, 1483014, 2003 [with J. Wolff, A.G. Papathanasiou, H.H. Rotermund, G. Ertl, M.A. Katsoulakis, and X. Li].</p>
<p>"Local Manipulation of Catalytic Surface Reactivity.", <i>J. Catal.</i>, 216, 246, 2003 [with J. Wolff, A.G. Papathanasiou, H.H. Rotermund, G. Ertl, and X. Li].</p>

<p>"Bifurcation and Stability Analysis of Rotating Chemical Spirals in Circular Domains: Boundary-Induced Meandering and Stabilization." <i>Phys. Rev. E.</i>, 67, 0561267, 2003 [with M. Baer and A.K. Bangia].</p>
<p>"Coupling Fields and Underlying Space Curvature: an Augmented Lagrangian Approach." <i>Phys. Rev. E</i>, 67, 0476024, 2003 [with P.G. Kevrekidis, F.L. Williams, A.R. Bishop, and B.A. Malomed].</p>
<p>"Dark-in-Bright Solitons in Bose-Einstein Condensates with Attractive Interactions." <i>New J. Physics</i>, 5, 64.1, 2003 [with P.G. Kevrekidis, D.J. Frantzeskakis, B.A. Malomed, and A.R. Bishop].</p>
<p>"Coarse Molecular Dynamics of a Peptide Fragment: Free Energy, Kinetics and Long Time Dynamics Computations." <i>J. Chem. Phys.</i>, 11823, 10762, 2003 [with G. Hummer].</p>
<p>"Enabling Stability Analysis of Tubular Reactor Models Using PDE/PDAE Solvers." <i>Comp. Chem. Eng.</i>, 27, 951, 2003 [with E.D. Koronaki and A.G. Boudouvis].</p>
<p>"Microscopic/Stochastic Timesteppers and Coarse Control: A Kinetic Monte Carlo Example." <i>AIChE J.</i>, 497, 1922, 2003 [with C.I. Siettos, A. Armaou, and A.G. Makeev].</p>
<p>"Oscillatory Thermomechanical Instability of an Ultrathin Catalyst." <i>Science</i>, 300, 1932, 2003. [with F. Cirak, J.E. Cisternas, A.M. Cuitino, G. Ertl, P. Holmes, M. Ortiz, H.H. Rotermund, M. Schunack, and J. Wolff].</p>
<p>"Reduction and Reconstruction for Self-Similar Dynamical Systems." <i>Nonlinearity</i>, 16, 1257, 2003 [with C.W. Rowley, J.E. Marsden, and K. Lust].</p>
<p>"Deciding the Nature of the Coarse Equation through Microscopic Simulation: the Baby-Bathwater Scheme." <i>SIAM MMS</i>, 13, 391, 2003 [with J. Li, P.G. Kevrekidis, and C.W. Gear].</p>
<p>"The Gaptooth Method in Particle Simulations." <i>Phys. Lett. A</i>, 316, 190, 2003. [with C.W. Gear and J. Li].</p>
<p>"Guidance of Matter Waves Through Y-Junctions." <i>Phys. Lett. A</i>, 317, 513, 2003 [with P.G. Kevrekidis, D.J. Frantzeskakis, and G. Theocaris].</p>
<p>"An Exploding Glass?" <i>Phys. Lett. A</i>, 318, 364, 2003 [with P.G. Kevrekidis and S. Kumar].</p>
<p>"Equation-Free Coarse-Grained Multiscale Computation: Enabling Microscopic Simulators to Perform System-Level Tasks." <i>Comm. Math. Sciences</i>, 14, 715, 2003 [with C.W. Gear, J.M. Hyman, P.G. Kevrekidis, O. Runborg, and K. Theodoropoulos].</p>
<p>"Removal of Alkanethiols from a Hydro-carbon Mixture by Heterogeneous Reaction with Metal Oxides." <i>Ind. Eng. Chem.</i>, 4226, 6919, 2003. [with J.P. Nehlsen and J.B. Benziger].</p>
<p>"Enabling Dynamic Process Simulators to Perform Alternative Tasks: A Time-Stepper Based Toolkit for Computer-Aided Analysis." <i>Ind. Eng. Chem. Res.</i>, 4226, 6795, 2003 [with C.I. Siettos and C.C. Pantelides].</p>

2002

"Stability of Solitary Waves in Finite Ablowitz-Ladik Lattices." *J. Phys. A*, **35**, 1, 2002 [with P.G. Kevrekidis and B. Malomed].

"Analysis of Drag and Virtual Mass Forces in Bubbly Suspensions Using an Implicit Formulation of the Lattice Boltzmann Method." *J. Fluid Mech.*, **452**, 61, 2002 [with K. Sankaranarayanan, X. Shan, and S. Sundaresan].

"Lighting Arnold Flames: Resonance in Doubly Periodically Forced Periodic Oscillations." *Nonlinearity*, **15**, 405, 2002 [with B.B. Peckham].

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