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13. ABSTRACT (Maximum 200 words)

This project developed computational and mathematical tools, based extensively on elements of system theory, that enable microscopic/stochastic simulators to perform system-level tasks (analysis, design, control, optimization). In current engineering modeling we are often faced with situations where the system model is given at an atomistic / stochastic / agent based level, while the modeling tasks (simulation, controller design, optimization) must be performed at a much larger, macroscopic in space and time level.

The objective was to construct a bridge between existing and future microscopic simulation codes (kMC, MD, MC, BD, LB etc.) and traditional, continuum numerical analysis. To accomplish this, we traded function evaluations (in the continuum computations) for appropriately initialized "bursts" of microscopic simulations, executed over short space and time intervals, followed by post-processing based on system-identification techniques. Separation of time scales is another important ingredient of the bridge between micro-simulation and macro-modeling. We stress controller design and optimization tasks this year. We also explored how this "model on demand" approach can evolve into experimental design protocols. Several examples, from small molecule folding to complex fluid rheology and computational materials science were pursued in order to validate the approach.

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Final Report

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Abstract

This project aimed at developing computational and mathematical tools, based extensively on elements of system theory, that enable microscopic/stochastic simulators to perform system-level tasks (analysis, design, control, optimization). We stressed controller design and optimization tasks. Several examples, from small molecule folding to complex fluid rheology and computational materials science were pursued. Later important developments involved the extension of the computational technology to encompass uncertainty quantification as well as the detection of appropriate observables from data (the "variable free" component of the "equation-free" approach).

Objectives

The objective of this project was outlined in the original proposal: to enable advanced, computer-assisted analysis and design computations for complex, nonlinear, distributed (spatially varying) processes described by microscopic (atomistic, stochastic, agent-based) models. The algorithms developed as part of the project allow scientific computing tasks (like simulation, stability and bifurcation analysis, control and optimization) to be performed for problems for which the physical description is available at a "fine" microscopic or stochastic level, but the questions asked are at a macroscopic, systems level. This bridge takes the form of software "wrappers", that can be combined with state of the art microscopic simulation codes (like molecular dynamics, MD, kinetic Monte Carlo, kMC, equilibrium MC, Lattice-Boltzmann, LB, Brownian Dynamics, BD, or general agent-based, AB) simulators. It also, fortuitously, encompasses the case of large scale legacy codes, which can also be enabled by these "wrappers". System theory tools (system identification, separation of time scales) play a prominent role in this computational enabling technology.

Accomplishments

Possibly the best way to examine the accomplishments of this work is to look through the titles of publications in refereed journals (appeared, in press and submitted) that appear at the end of this final report. In the first year we performed extensive work on

the development and implementation of computational algorithms; we have also performed extensive work on the "coarse computational study" of the dynamics of a number of physical systems (based on Brownian Dynamics, on kinetic Monte Carlo, on equilibrium Monte Carlo, on Molecular Dynamics as well as on legacy codes). We emphasized particularly the modifications that arise in the context of using coarse methods in a control context (a paper on coarse linear control of Brownian Dynamics, one on coarse linear control of lumped kinetic MC simulations, one on coarse linear control of LB distributed simulators). There is one publication on coarse, timestepper-based optimization, which is going to be submitted within a month or so; there is another paper on the "patch-dynamics" based control of distributed parameter systems that we expect to submit this calendar year. There were also several Proceedings papers which we simply did not mention (ACC, upcoming CDC etc.). In the second year we had successes in problems as diverse as evolutionary epidemiology (Cisternas et al.) and bacterial chemotaxis (Setayeshgar et al.), computational materials science (Haataja et al.) and equilibrium complex fluids (Kopelevich et al.). At the same time we proposed new links of the equation-free approach with control algorithms (Armaou et al., Siettos et al., collaboration with Christofides), the use of legacy codes (Siettos et al.); and worked on numerical analysis and new algorithms (Samaey et al., Kelley et al., Gear et al.). More recent accomplishments were made along three directions: The first was the equation-free approach to uncertainty quantification. The idea is simple: try to combine the best features of Monte Carlo sampling with the strength of the Polynomial (Wiener) chaos representation. Do short bursts of MC simulations, and use them to estimate, on the fly, the time- and parametric dependence of the appropriate obsevables – polynomial chaos projections of the result distributions. We already have, in addition to a first paper, another paper where the approach is used to develop algorithms for the study of homogenization problems. The second direction had to do with the coherent behavior of interacting entities (e.g. vehicles, swarms etc.). Here there are two options: are the interacting entities identical or different ? If they are similar, then "traditional" equation-free methods are used – we can observe the evolution of the statistics of brief microscopic simulations, and then use our equation-free approach for accelerated modeling or control purposes. But if the interacting entities have a distribution or properties, we can again take advantage of the computational chaos observables, and evolve not the statistics of the evolving distribution, but the projection of this distribution on polynomial chaos basis functions. There have been several papers along these lines including a recent *Phys. Rev. Lett.* The third direction has to do with novel data processing methods for determining the right observables from complex, high-dimensional data. Here, in collaboration with R. Coifman at Yale, we have developed methods for linking equation-free computation with *diffusion maps*: a computational approach based on harmonic analysis on graphs that allows for finding the "right coarse observables" from high dimensional simulation data; and the use of these results BOTH in accelerating simulations and in bootstrapping the data collection process. Finally, the methods we developed are already naturally applied to study the control of fluctuations in nanoscopic systems – a good example is provided by the parametric study of water filling-emptying transitions in carbon nanotubes, which also appeared in *Phys. Rev. Letters*. Overall, as the techniques mature and the application

list lengthens, the methods become more visible and start to be used by other people also – there was an article about this overall work program last month in SIAM News.

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Personnel Supported
Prof. Ioannis G. Kevrekidis, the PI, was partially supported during the summers of this period. Post-doctoral research associates partially supported were Dr. Costas Siettos, Dr. Jaime Cisternas, Dr. Ligang Chen and Dr. Sung-Joon Moon. Graduate students partiallyt supported included Mr. L. Qiao, Mr. J. Nehlsen and Ms. Joanne Chia; the latter two have graduated with PhD degrees, and the former is expected to graduate this academic year.

Interactions
Seminars by Prof. Kevrekidis: Several seminars at Universities (~30) and National Labs (~4), several invited/plenary talks (~30) and presentations at conferences (~50); Visits and discussions with UTRC personnel involved interactions with Drs. Dorobantu and Jacobson (complex system modeling techniques, model reduction in computational chemistry, also work on fuel cell dynamics modeling).

Transitions
A computational materials science company (CFDRC in Alabama) has used algorithms developed through this work with success in modeling fabrication of different types of CNT.

Honors/Awards
Crawford Prize of SIAM/Dynamical Systems (2003); Plenary lecture, SIAM Dynamical Systems meeting (2003); Plenary lecture, SIAM annual meeting, (2004); Plenary lecture, joint SIAM/SMB meeting (2006); NAS meeting (2005); also internationally (Bristol University, UK, the Weizmann Institute, Israel); Guggenheim Fellowship (precisely for the work on equation-free modeling of multiscale/complex systems performed under this grant, 2005). Moore Distinguished Fellowship at Caltech (2005). There was a full page article in SIAM News about this research program in 2005; also the PI was asked to join the Advisory Board of the Center for Cell Dynamics (at the Friday Harbor Lab, Univ. of Washington).

Publications

(includes publications acknowledging the support of the previous contract, that appeared after its final report).

1. ``Coarse" Integration/Bifurcation Analysis via Microscopic Simulators: micro-Galerkin methods, C. W. Gear, I.G.K and C. Theodoropoulos,; Comp. Chem. Engng. 26 pp.941-963 (2002)
2. "Coarse" stability and bifurcation analysis using stochastic simulators: Kinetic Monte Carlo Examples, A. Makeev, D. Maroudas and IGK, J. Chem. Phys. 116 10083-10091 (2002)
3. Some twists and turns in the path of improving surface activity, A. G. Papathanasiou, J. Wolff, IGK, H.H. Rotermund and G. Ertl, Chem. Phys. Lett. 358(5-6) pp.407-412 (2002)
4. Coarse bifurcation analysis of kinetic Monte Carlo simulations: a lattice gas model with lateral interactions, A. G. Makeev, D. Maroudas, A. Z. Panagiotopoulos and I.G.K., J. Chem. Phys. 117(18) pp.8229-8240 (2002)
5. CO oxidation on thin Pt. Crystals: Temperature slaving and the derivation of lumped models, J. Cisternas, P. Holmes, I.G.K. and X. Li, J. Chem. Phys. 188(4) pp.1-17 (2003)
6. Nonlinear model reduction for dynamic analysis of cell population models, Y. Zhang, M. A. Henson and IGK, Chem. Eng. Sci., 58 pp.429-445 (2003)
7. ``Focusing Revisited: a Renormalization/Bifurcation approach", C. Siettos, I.G.K. and P. G. Kevrekidis, Nonlinearity, 16 pp. 497-506 (2003)
8. Adaptive detection of bifurcations: an experimental feasibility study, R. Rico-Martinez, K. Krischer, G. Flaetgen, J. S. Anderson and IGK, Physica D, 176 (1-2), pp.1-18 (2003)
9. Gentle dragging of reaction waves", J. Wolff, A. G. Papathanasiou, H. H. Rotermund, G. Ertl, X. Li and I. G. Kevrekidis, Phys. Rev. Lett., 90(1) 018302 (2003)
10. Buckling in response to applied heat sources, J. Cisternas, P. Holmes and IGK, Physica D, 177(1-4), pp.71-100 (2003)
11. Projective Methods for Stiff Differential Equations: problems with gaps in their eigenvalue spectrum. C. W. Gear and IGK, SIAM J. Sci. Comp.24(4) pp.1091-1106 (2003).
12. Telescopic Projective Integrators for Stiff Differential Equations, C. W. Gear and I. G. Kevrekidis, J. Comp. Phys., 187(1) pp.95-109 (2003)
13. ``Coarse Brownian dynamics for nematic liquid crystals: Bifurcation, projective integration and control via stochastic simulation" C. Siettos, M. D. Graham and I. G. Kevrekidis, J. Chem. Phys.118(22) pp.10149-10157 (2003)
14. ``Wave Initiation through Spatiotemporally Controllable Perturbations", J. Wolff, A. G. Papathanasiou, H. H. Rotermund, G. Ertl, M. A. Katsoulakis, X. Li and I.G.K., Phys. Rev. Lett.,90(14) 148301(4) (2003).
15. ``Local manipulation of catalytic surface reactivity", J. Wolff, A. G. Papathanasiou, H. H. Rotermund, G. Ertl, X. Li and I. G. K., J. Catal., 216 pp.246-256 (2003)

16. ``Coupling Fields and Underlying Space Curvature: an Augmented Lagrangian Approach", P. G. Kevrekidis, F. L. Williams, A. R. Bishop, I.G.K. and B. A. Malomed, Phys. Rev. E, 67 047602(4) (2003)
17. The gaptooth method in particle simulations, C. W. Gear, J. Li and I.G.K., Physics Letters A, 316 pp.190-195 (2003). Can be obtained as physics/0303010 at arXiv.org
18. An exploding Glass ?, P. G. Kevrekidis, S. Kumar and I.G.K., Phys. Lett. A, 318 pp.364-372 (2003); Can be obtained as cond-mat/0302102 at arXiv.org
19. Equation-free coarse-grained multiscale computation: enabling microscopic simulators to perform system-level tasks", with C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg and K. Theodoropoulos, Comm. Math. Sciences, 1(4) pp.715-762 (2003); original version can be obtained as physics/0209043 at arXiv.org.
20. Enabling Dynamic Process Simulators to Perform Alternative Tasks: A Time-Stepper Based Toolkit for Computer-Aided Analysis, C. I. Siettos, C. C. Pantelides and I.G.K. Ind. Eng. Chem. Research,42(26) pp.6795-6801 (2003); Can be obtained as math.OC/0302040 at arXiv.org
21. Optimal Sensor Location and Reduced Order Observer Design for Distributed Process Systems", A. A. Alonso, I.G.K., J. R. Banga and C. E. Frouzakis, Comp. Chem. Eng. 28(1,2) pp.27-35 (2004)
22. Time-steppers and coarse control of microscopic distributed processes, A. Armaou, C. I. Siettos and I. G. Kevrekidis, Int. J. Robust and Nonlinear Control, 14} pp.89-111 (2004).
23. Computing in the Past with Forward Integration, C. W. Gear and I. G. K., Physics Letters A., 321 pp.335-343 (2004) Can be obtained as nlin.CD/0302055 at arXiv.org
24. Application of wavelet-based reduction techniques to nonlinear reaction-transport problems, J. Krishnan, O. Runborg and I. G. Kevrekidis, Comp. Chem. Engineering, 28 pp.557-574 (2004)
25. Coarse Bifurcation Diagrams via Microscopic Simulators: a State-Feedback Control-Based Approach", C. I. Siettos, D. Maroudas and I. G. Kevrekidis, Int. J. Bif. Chaos, 14(1) pp.207-220 (2004)
26. Apparent hysteresis in a driven system with self-organized drag", M. Haataja, D. Srolovitz and I.G.K., Phys. Rev. Lett. 92(16) 160603 (2004); can be found as cond-mat/0310460 at arXiv.org.
27. Coarse Projective kMC Integration: Forward/Reverse Initial and Boundary Value Problems", R. Rico-Martinez, C. W. Gear and I.G.Kevrekidis, J. Comp. Phys., 196(2) pp.474-489 (2004); can be found as nlin.CG/0307016 at arXiv.org.
28. Equation-Free multiscale computations for a lattice-gas model: coarse-grained bifurcation analysis of the NO+CO reaction on Pt(100)", A. G. Makeev and I.G.K., Chem. Eng. Sci., 59(8-9) pp.1733-1743 (2004).
29. Coarse Bifurcation Studies of Bubble Flow Lattice Boltzmann Simulations, C. Theodoropoulos, K. Sankaranarayanan, S. Sundaresan and I.G.K., Chem.Eng.Sci., 59 pp.2357-2362 (2004), can be obtained as nlin.PS/0111040 at arXiv.or\

30. Equation-free: the computer-assisted analysis of complex, multiscale systems, I. G. Kevrekidis, C. William Gear and G. Hummer, A.I.Ch.E Journal, 50(7) pp.1346-1354 (2004)
31. Optimal sensor placement for state reconstruction of distributed process systems", A. A. Alonso, C. E. Frouzakis and I. G. Kevrekidis, A.I.Ch.E. Journal 50(7) pp.1438-1452 (2004)
32. The stirred tank reactor polymer electrolyte membrane fuel cell, Jay B. Benziger, E. Chia, E. Karnas, J. Moxley, C. Teuscher and I. G. Kevrekidis, AIChE Journal 50 pp.1889-1900 (2004); can be obtained as physics/0310037 at arXiv.org pp.451-455 (2004)
33. From Molecular Dynamics to coarse self-similar solutions: a simple example using equation-free computation", L. Chen, P. G. Debenedetti, C. W. Gear and I. G. Kevrekidis, JNNFM 120 pp.215-223 (2004)
34. Steady State Multiplicity in a Polymer Electrolyte Membrane Fuel Cell", E.-S. Chia, J. B. Benziger and I. G. Kevrekidis, AIChE J. 50(9) pp.2320-2324 (2004).
35. Equation-free modeling of evolving diseases: coarse-grained computations with individual-based models, J. Cisternas, C. W. Gear, S. Levin and I.G.K., to Proc. Roy. Soc. London, 460 (2050) pp.27621-2779 (2004);nlin.AO/0310011
36. Asymptotic States of a Smoluchowski Equation, P. Constantin, I.G.K. and E. S. Titi, Arch. Rat. Mech. Anal. 174 pp.365-384 (2004)
37. Coarse-Grained Computations for a Micellar System, D. I. Kopelevich,A. Z. Panagiotopoulos and I. G. Kevrekidis, J. chem. Phys. 122 044907 (2005); can be found as cond-mat/0407219 at arXiv.org
38. Coarse-Grained kinetic computations of rare events: application to micelle formation, D. I. Kopelevich, A. Z. Panagiotopoulos and I. G. Kevrekidis, J. chem. Phys.122 044908 (2005); can be found as cond-mat/0407220 at arXiv.org
39. Effective equations for discrete systems: A time stepper based approach, J. Moeller, O. Runborg, P. G. Kevrekidis, K. Lust and I.G.Kevrekidis, Int. J. Bifurcations and Chaos 15(3) pp.975-996 (2005); can be found as physics/0307153 at arXiv.org.
40. An equation-free, multiscale computational approach to uncertainty quantification for dynamical systems, D. Xiu, R. Ghanem and I. G. Kevrekidis, IEEE Computing in Science and Engineering, 7(3) pp.16-23 (2005)
41. Equation-free, gaptooth-based controller design for distributed complex - multiscale processes, A. Armaou, I. G. Kevrekidis and C. Theodoropoulos, Comp. Chem. Engineering 29 pp.731-740 (2005)
42. The dynamic response of PEM fuel cells to changes in load, J. Benziger, E. Chia, J. F. Moxley and I. G. Kevrekidis, Chem. Eng. Sci., 60(6) pp.1743-1759 (2005)
43. Coarse Master Equation from Bayesian Analysis of Replica Molecular Dynamic Simulations, S. Sriraman, I. G. Kevrekidis and G. Hummer, J. Phys. Chem., 109(14) pp.6479-6484 (2005)
44. The gap-tooth scheme for Homogenization Problems, G. Samaey, D. Roose and I. G. Kevrekidis, SIAM MMS 4(1) pp.278-306 (2005); also physics/0312004

45. Application of Coarse Integration to Bacterial Chemotaxis S. Setayeshgar, C. W. Gear, H. G. Othmer and I. G. K., SIAM MMS, 4(1) pp.307-327 (2005); also physics/0308040 at arXiv.org
46. Parrinello-Rahman Dynamics for Vortex Lattices, R. Carretero-Gonzalez, P. G. Kevrekidis, I.G.Kevrekidis, D. Maroudas, D. J. Frantzeskakis, Phys. Lett. A., 341(4) pp.128-134 (2005)
47. Equation-free/Galerkin-free POD-assisted computation of incompressible flows, S. Sirisup, D. Xiu, G. E. Karniadakis and I. G. Kevrekidis, J. Comp. Phys., 207(2) pp.568-587 (2005)
48. Constraint-defined Manifolds: a Legacy-Code Approach to Low-Dimensional Computations", C. W. Gear and I. G. Kevrekidis, J. Sci. Comp.25, pp.17-28 (2005)
49. Projecting on a Slow Manifold: Singularly Perturbed Systems and Legacy Codes, C. W. Gear, T. J. Kaper, I. G. Kevrekidis and A. Zagaris, SIADS, 4, pp.711-732(2005) Physics/0405074 at arXiv.org
50. Equation-free, multiscale computation for unsteady random diffusion, D. Xiu and I. G. Kevrekidis, SIAM MMS 4, pp.915-935 (2005)
51. The power performance curve for engineering analysis of fuel cells, J. B. Benziger, B. Satterfield, W. H. J. Hogarth, J. P. Nehlsen and I. G. Kevrekidis, J. Power Sources, 155, pp.272-285 (2006)
52. Optical Imaging and Control of Genetically Designated Neurons in Functional Circuits", G. Miesenboeck and I. G. Kevrekidis, Ann. Rev. Neurosci. 28, pp.533-563 (2005).
53. Equation-free optimal switching policies for bistable reacting systems using coarse time-steppers, A. Armaou and I. G. Kevrekidis, Int.J. R.N.C., 15, pp.713-726 (2005) (math.OC/0410467 at arXiv.org).
54. Coarse-grained numerical bifurcation analysis of Lattice Boltzmann Models, P. van Leemput, K. W. A. Lust and I. G. Kevrekidis, Physica D.210, pp.58-76 (2005)
55. Equation-free, coarse grained computational optimization using time-steppers, A. Bindal, M. G. Ierapetritou, S. Balakrishnan, A. Armaou, A. G. Makeev and I. G. Kevrekidis, Chemical Engineering Science, 61, pp.779-793 (2006)
56. Diffusion Maps, Spectral Clustering and the Reaction Coordinates of Dynamical Systems, B. Nadler, S. Lafon, R. C. Coifman and I. G. Kevrekidis, Appl. Comp.Harm. Anal., 21, pp.113-127 (2006), math/0503445 at arXiv.org
57. Patch dynamics with buffers for homogenization problems, G. Samaey, I. G. Kevrekidis and D. Roose, J. Comp. Phys., 213, pp.264-287 (2006)
58. An equation-free computational approach for extracting population-level behavior from individual-based models of biological dispersal, R. Erban, I. G. Kevrekidis and H. G. Othmer, Physica D 215, pp.1-24 (2006)
59. An equation-free approach to nonlinear control: Feedback linearization with pole-placement", C. I. Siettos, I. G. Kevrekidis and N. Kazantzis, International Journal of Bifurcations and Chaos, 16, pp.2029-2041 (2006); nlin.CG/0412006 at arXiv.org

60. Equation-free dynamic renormalization in a glassy compaction model, L. Chen, I. G. Kevrekidis and P. G. Kevrekidis, Phys. Rev. E 74, 016702, cond-mat/0412773 at arXiv.org
61. An equation-free approach to coupled oscillator dynamics: the Kuramoto model example, S.-J. Moon and I. G. Kevrekidis, Int. J. Bifurcations and Chaos, 16, pp.2043-2052 (2006)
62. Coarse nonlinear dynamics of filling-emptying transitions: water in carbon nanotubes, S. Sriraman, I. G. Kevrekidis and G. Hummer, Phys. Rev. Lett., 95, 130603 (2005)
63. Equation-free dynamic renormalization: self-similarity in multidimensional particle system dynamics, Y. Zou, I. G. Kevrekidis and R. Ghanem, PRE, 72, 046702 (2005) math.DS/0505358 at arXiv.org).
64. Equation-free Dynamic Renormalization of a KPZ-type Equation, D. A. Kessler, I. G. Kevrekidis and L. Chen, Phys. Rev. E. 73, 036703 (2006) cond-mat/0505758 at arXiv.org

Also:

65. Nonlinear Dynamics Analysis Through Molecular Dynamics Simulations I. G. Kevrekidis, J. Li and S. Yip, in Multiscale Modeling and Simulation, S. Attinger and P. Koumoutsakos eds., Lecture Notes in Computational Science and Engineering, 39, Springer Verlag, pp.69-80 (2004)
66. Exploration of Coarse Free Energy Surfaces templated on continuum numerical methods, D. Passerone and I. G. Kevrekidis in Multiscale Modeling and Simulation} S. Attinger and P. Koumoutsakos eds., Lecture Notes in Computational Science and Engineering, 39, Springer Verlag, pp.81-92 (2004)
67. Damping Factors for the gap-tooth scheme, G. Samaey, I. G. Kevrekidis and D. Roose, in Multiscale Modeling and Simulation, S. Attinger and P. Koumoutsakos eds., Lecture Notes in Computational Science and Engineering, 39, Springer Verlag, pp.93-102 (2004)
68. Equation-free, coarse grained feedback linearization, C.I. Siettos, I. G. Kevrekidis and N. Kazantzis, Proceedings of the 2005 ACC, September 2004.
69. Higher order accuracy in the gap-tooth scheme for large-scale solutions using microscopic simulators. A. J. Roberts and I. G. Kevrekidis, Proceedings of CTAC 2004; can be found as math.DS/0410310 at arXiv.org
70. Diffusion maps, spectral clustering and eigenfunctions of Fokker-Planck Operators, B. Nadler, S. lafon, R. R. Coifman and I. G. Kevrekidis, Proceedings of the 2005 Neural Information and Processing Systems conference, Tuebingen, Germany, 2005.
71. Equation-Free Modeling for Complex Systems", I. G. Kevrekidis, C. W. Gear and G. Hummer, in Handbook of Materials Modeling, Vol.1 S. Yip, editor, Kluwer (2004).
72. Equation-Free Modeling for Complex Systems", I. G. Kevrekidis (with C. W. Gear and G. Hummer)in Reports from the 2004 NAE Symposium on Frontiers in Engineering, pp.69-77, The National Academies Press, Washington D.C.