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We developed methodologies for the bifurcation detection and stability analysis of microscopic timesteppers (LB-based. lattice gas or Monte Carlo) based on the Recursive Projection Method (RPM). We demonstrated RPM-based "coarse" (macroscopic) bifurcation and stability computations for systems for which only microscopic evolution rules are available (LB. KMC, Brownian Dynamics -BD-). We were able to perform the coarse bifurcation analysis of KMC models of surface reactions, of LB models of multiphase -bubbly and of reaction diffusion problems, as well as of BD non- Newtonian rheological problems. New micro-Galerkin simulation methods based on Projective Integrators and Telescopic Projective Integrators were implemented. The "gaptooth" scheme and the "patch dynamics" schemes were developed and demonstrated. Methods for doing effective bifurcation analysis using timesteppers (thus sidestepping the necessity of deriving homogenized equations) were developed and demonstrated. Furthermore we implemented RPM around a state-of-the art massively parallel finite-element based code (codename: MPSalsa) at Sandia, as well as a state of the art chemical plant simulation code (gPROMS) which was used in problems of interest to UTRC (fuel cell reactor train modeling). We also developed and demonstrated methods for the computation of self-similar and "coarsely" self similar solutions, as well as methods for the coarse control of microscopic simulations.

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ENABLING DYNAMIC SIMULATORS: STABILITY, BIFURCATION and CONTROL COMPUTATIONS for DISTRIBUTED PARAMETER SYSTEMS

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3d Annual and Final Report

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Objectives

The objective of this project was to expand the capabilities of existing large scientific computational codes in order to enable advanced, computer-assisted analysis and design methods for complex, nonlinear, distributed (spatially varying) processes. The project, through the years, expanded to include techniques that would 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. Both the "large scale legacy code" side and the "unavailable macroscopic equation" side of the research objectives were successfully pursued, as testified to by the publications list at the end of the report.

Status of Effort

We developed methodologies for the bifurcation detection and stability analysis of *microscopic timesteppers* (LB-based, lattice gas or Monte Carlo) based on the Recursive Projection Method (RPM). We demonstrated RPM-based "coarse" (macroscopic) bifurcation and stability computations for systems for which only microscopic evolution rules are available (LB, KMC, Brownian Dynamics –BD-). We were able to perform the coarse bifurcation analysis of KMC models of surface reactions, of LB models of multiphase –bubbly—and of reaction diffusion problems, as well as of BD non-Newtonian rheological problems. New micro-Galerkin simulation methods based on Projective Integrators and Telescopic Projective Integrators were implemented. The "gaptooth" scheme and the "patch dynamics" schemes were developed and demonstrated. Methods for doing *effective* bifurcation analysis using timesteppers (thus sidestepping the necessity of deriving homogenized equations) were developed and demonstrated. Furthermore we implemented RPM around a state-of-the art massively parallel finite-element based code (codename: MPSalsa) at Sandia, as well as a state of the art chemical plant simulation code (gPROMS) which was used in problems of interest to UTRC (fuel cell reactor train modeling). We also developed and demonstrated methods for the computation of self-similar and "coarsely" self similar solutions, as well as methods for the coarse control of microscopic simulations.

Accomplishments

AC. 1 The "No-Equations" Framework for Multiscale Computations. We developed a general framework that can make a difference in the way multiscale computations are performed in science and engineering. This framework draws from

many ideas in numerical analysis, computational statistical mechanics and multiscale computational physics, but, to the extent that we can judge, has real generality in its formulation and novelty in its capabilities. More than anything else, ***it is a bridge between traditional numerical analysis and multiscale physics***: it enables the huge arsenal of techniques that have been developed in applied mathematics over the years to analyze continuum deterministic models (ODEs, PDEs, integrodifferential equations) to be brought to bear on microscopic models (molecular dynamics, Monte Carlo, kinetic models, models of microstructured media, stochastic PDEs etc.).

AC.1.1 A framework for the stability/bifurcation analysis of microscopic / stochastic timesteppers. We have used our "lift-evolve microscopically-restrict" approach, integrating it with the Recursive Projection Method to perform the stability/bifurcation analysis of both lumped and distributed systems. In the lumped case, since the number of degrees of freedom for the coarse contraction mappings is small, it is not necessary to "do RPM". *Variance reduction* has emerged as a very important component in the identification/estimation of the coarse description derivatives that underpin the bifurcation capabilities. In chronological order the results can be found in (a) Theodoropoulos, Qian and Kevrekidis, *PNAS* (2000). This is the first paper, illustrating coarse bifurcation computations on a one-dimensional kinetic model (a Lattice-Boltzmann model of the FHN PDE (b) Theodoropoulos, Sankaranarayanan, Sundaresan and Kevrekidis, Conference Proceedings (2001) and *Phys. Rev. Lett*, submitted (2002) A truly two-dimensional, multiphase flow simulation for what is an open problem (instabilities of arrays of rising gas bubbles in liquids). It is worth noting that testing the results/predictions with traditional, continuum, front-tracking Navier Stokes methods led to a collaboration with Prof. G. Tryggvasson of WPI, and a joint paper with him from the comparison work will be forthcoming. (c) Makeev, Maroudas and Kevrekidis, *J. Chem. Phys.* **116** (23) 10083-10091 (2002). This is the first paper we have on stochastic timesteppers. The problems studied are lumped surface science models, studied through Gillespie Monte Carlo simulations; the bifurcation analysis of the "expected value" equations as well as their multiparameter continuation is accomplished. The Discussion Section of this paper contains a long and (we hope) informative account of shortcomings of the approach as well as **(and we believe this is one of its strong points)** ways to test on-line the validity of the models and the necessity to "augment" the dimensionality of the description as conditions/parameters change. (d) Gear, Kevrekidis and Theodoropoulos, *Comp. Chem. Eng.* In press (2002). This is a "manifesto" of our distributed system bifurcation approach (and also of our coarse integration approach.. (e) Makeev, Maroudas, Panagiotopoulos and Kevrekidis, *J. Chem. Phys.* in press, 2002). This is also lumped, but now "real" lattice kinetic Monte Carlo as opposed to the Gillespie approach – this paper clarifies many issues of "maturation of higher moments" and has some impressive results in regimes where the traditional closures (Mean Field, Quasi-Chemical) fail. (d) Siettos, Graham and Kevrekidis (almost completed, 2002) Also lumped, this problem is the first to produce a bifurcation diagram for a stochastic PDE (which arises in the closure of the rheological behavior of nematic liquid crystals in shear). The paper also contains a test of various levels of closure. It constitutes only the beginning of a collaboration with Prof. Michael Graham, a Non-Newtonian fluid mechanics researcher at the U. of Wisconsin as well as with Prof. Robert Armstrong, chairman of Chemical Engineering at MIT, also working in this area. AC.1.2 A

framework for the "long-time" integration of microscopic/stochastic timesteppers. Here we have been extremely fortunate: we initiated a collaboration with Professor C. William Gear, *the* world expert in numerical integration, who retired from being the Director of the NEC Research Institute and took an interest in our work. With him we have developed the "numerical analysis of legacy integrators" (which does bear relations to explicit Runge-Kutta methods for stiff problems) in a sequence of papers: (a) Gear and Kevrekidis, *SIAM J. Num. Analysis*, in press (b) Gear, Theodoropoulos and Kevrekidis, *Comp. Chem. Eng.* in press, 2002. (c) Gear and Kevrekidis, *J. Comp. Phys.* submitted, 2001. This paper introduces *telescopic* projective integrators as well as (d) Setayeshgar, Gear, Othmer and Kevrekidis (in preparation, 2002). These papers discuss the coarse integration of distributions for stochastic problems, especially the issues of lifting and special functions for the restriction. The application in the second paper is bacterial chemotaxis (an internal variable model developed by Prof. Othmer).

AC.1.3 A framework for the "large-space" integration of microscopic/stochastic timesteppers The idea is to use simulators of a process over *small spatial domains* coupled together through boundary conditions (assuming that the overall process is described by a smooth field) to be able to evolve the full coarse field over the "entire space". This work initially resulted in what we call **"the gaptooth scheme"**. We already have some numerical analysis for these hybrid schemes, determining the boundary conditions that provide the communication between the "small boxes" is a very important task, where again identification and traditional numerical analysis play a very important role. (a) I. Kevrekidis, C. W. Gear, J. M. Hyman, P. Kevrekidis, O. Runborg and C. Theodoropoulos, in preparation, (2002). This paper is our first attempt to present our entire framework. It will be submitted within a couple of weeks.

AC.2 "On the fly" homogenization/effective medium computations When we make computations of dynamics in complicated media (e.g. heterogeneous catalysts, porous media) the traditional approach is to obtain *effective equations* – equations for the averaged, effective behavior of a uniform medium, with properties computed from the properties and geometry (distribution of properties) of detailed realizations of the actual complicated medium. After this is done, the effective equations are analyzed through traditional PDE techniques. We already have done the first demonstration of such a coarse bifurcation study: (a) Runborg, Theodoropoulos and Kevrekidis, *Nonlinearity*, (2002). This contains the analysis of an instability involving reactive front propagation on heterogeneous composite catalysts. It sets the stage for many studies of composite media, both reactive and unreactive. (b) Moeller, Runborg, Lust, P. Kevrekidis and I. Kevrekidis (in preparation). This contains the analysis of an effective continuum description of a *spatially discrete* medium. Such problems are vital to studies of coupled neuronal or cellular tissue, where again we can computationally study averaged, continuum tissue behavior directly from neuronal/cellular models. The first such study of a chain of thalamus neurons is contained in this paper.

AC.3 The computation (and "no equations" computation) of self-similar solutions This has been one of the most fortunate new developments of our research program. In studying the rising bubbles in our multiphase flow application above, we needed to adapt RPM to traveling solutions (finding a way to dynamically travel along with the solution of a problem with translational invariance, so that the solution eventually appears steady). The visit of Clancy Rowley (then a grad student at Caltech, now a professor in MAE in

Princeton) gave us the missing link: a "template based" pinning condition. It was a relatively small step to realize that the approach of Rowley and Marsden, which was useful for traveling problems, was also useful for another class of problems with a continuous symmetry group: self-similarity. In collaboration with Professor Don Aronson and Dr. S. Betelu from the U. of Minnesota we were able to realize this development: a general procedure for the computation and stability/bifurcation analysis of self-similar (exploding or collapsing) solutions. We have already been able to revisit and obtain new insights for the classic focusing problems in dispersive equations (the nonlinear Schroedinger, see below). The fact that we can do these computations not only when we have the equations (as we have done so far) but also, through our coarse timestepper procedure (with lifting and restriction) when the equations are not available, will, we believe, have important consequences in fields as diverse as computational materials science, interfacial fluid mechanics, cell biology, mathematics and cosmology, and we will continue pursuing it vigorously.

AC.4 A framework for the stability/bifurcation analysis of large scale legacy codes The original motivation for our multiscale work comes, as we said above, from the "numerical analysis of legacy codes" – enabling complicated legacy simulation codes (timesteppers) to perform tasks (like finding steady states) in ways they were not intended to. While our work opens, we believe, new directions in computational multiscale phenomena, we have also pursued, in collaboration with UTRC, the "original" motivation: enabling commercial design codes to do additional tasks like bifurcation, "long integration" and optimization. In particular, we have worked with Process Systems Enetrprises (the developers of gPROMS, a state-of-the art industrial simulator) to do the stability analysis of components of the UTRC/IFC fuel cell power train. We are very proud of this development, and we are continuing our collaboration with UTRC along these lines. We have also done something we believe is really important. In collaboration with Prof. Pantelides of PSE we have managed to perform fixed-point calculations of Pressure Swing Absorption (a large scale periodically forced problem) literally hundreds of times faster than traditional simulation. PSA is a $10 billion industry, and the slowness of simulation is absolutely the bottleneck in design and performance optimization.

AC.5 Realization of an "addressable medium": a testbed for real-time "infinite" sensing / actuation. For many years we have been pursuing this elusive goal: an experimental system that is distributed in space, has rich open-loop dynamics (spatiotemporal pattern formation), over which we have "infinite" (extremely resolved) sensing capability and comparably resolved actuation authority. This past year, the dream became a reality. In our October 5 *Science* article we showed how, through the combination of spatially resolved optical techniques, a pair of computer controlled galvanometer mirrors and a laser beam, we were able to create, annihilate, guide, and in general control reaction fronts (the basic building blocks of spatiotemporal patterns) on a catalytic surface in real time. The article (along with the web-accessible videos of its movies) opens, we believe, many possibilities in the study of problems with "infinite sensing and actuation". In particular, we have used this capability to implement (through feedback laws) new types of spatiotemporal dynamics. More importantly, we have used this ability in order to come up with spatiotemporal policies that would optimize overall reaction rates. Both of these developments (papers a and b below) suggest the need for a

lot of real time image processing and distributed optimal control, and we are eager to pursue these new –for us- paths in the coming years.

AC.6 Realization of adaptive bifurcation detection. Here we have been after the following challenge: can we come up with a diskette that will allow an experimentalist to get his system to find and converge on its bifurcation points "by itself" ? That is, can we construct a program which, when executed on a computer connected with an experiment through real-time I/O, will give us a closed loop system that will identify and converge on what, for the open loop experiment, was a bifurcation point (a point of marginal stability) ? The procedure involves state measurements, low-dimensional model identification, and use of what would be the open loop bifurcation parameter as the control variable. We had demonstrated this computationally in the past. We now were able to show it experimentally. This work has certain common features with the optimum-seeking controllers of Krstic (this can be thought of as a "bifurcation-seeking" controller).

Personnel Supported

Prof. Ioannis G. Kevrekidis, the PI, was partially supported in the summer of 2001. Post-doctoral research associates supported were Dr. Costas Siettos and Dr. A. Armaou. Several students were also partially supported through this grant: Ms. Joanna Chia (a second year student), Mr. J. Nehlsen (also 2nd year) and in part Ms. Xiujiang Li (4th year).

Interactions

Seminars by Prof. Kevrekidis: 10 seminars in Universities, 9 presentations at the AIChE annual meeting, Invited Talks (IPAM at UCLA, LANL, AFOSR D&C 50th meeting, Oxford University, U of Warwick, FHI der MPG (Berlin)).

There were repeated visits and discussions with UTRC personnel; mainly this involved Dr. S. Ghosh (fuel cells modeling, continuation and bifurcation algorithms, issues of dynamics and model reduction), and Banaszuk (discussions on possibilities of "coarse modeling" of mixing).

Transitions

(1) This year, in collaboration with staff from Process Systems Enterprises and Dr. C. Siettos, we were able to significantly accelerate an industrial process simulator (gPROMS) to analyze Pressure Swing Adsorption processes The contact is: Professor Costas Pantelides **(2)** We also used our approach and gPROMS to analyze the stability of reactor trains in hydrogen fuel cells for UTRC/IFC (Drs. Siettos and Theodoropoulos) The contact is: Dr. Shubhro Ghosh.

Honors/Awards **(a)** Plenary Lecture, Fields Institute, Dec. 2001; **(b)** Dynamics Days Europe, July 2002; **(c)** Inaugural Othmer Symposium, Polytechnic U; **(d)** Control activity group meeting, Leuven. **(e)** O. A. Hougen visiting professorship, U. of Wisconsin, 2002.

Publications

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3. C. W. Gear, I. G. Kevrekidis and C. Theodoropoulos, "Coarse Integration/Bifurcation Analysis via Microscopic Simulators: micro-Galerkin methods" *Comp. Chem. Eng.* In press, (2002)
4. C. W. Gear and I. G. Kevrekidis, "Projective Methods for Stiff Differential Equations: problems with gaps in their spectrum", *SINUM in press* (submitted 2001)
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6. I. G. Kevrekidis, J. M. Hyman, C. W. Gear, P. G. Kevrekidis, O. Runborg and C. Theodoropoulos, "Equation-Free Multiscale Computation: Enabling Microscopic Simulators to Perform Macroscale Tasks", in preparation.
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8. D. G. Aronson, S. I. Betelu and I. G. Kevrekidis, "Going with the Flow: a Lagrangian approach to self-similar dynamics and its consequences, *PNAS in review* (submitted 2001)
9. C. I Siettos, I. G Kevrekidis and P. G. Kevrekidis, "Focusing Revisited: a renormalization-bifurcation Approach", *Nonlinearity* submitted.
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12. X. Li, I. G. Kevrekidis, M. Pollmann, A. G. Papathanasiou and H. H. Rotermund, "Front initiation on micro designed composite catalysts", *Chaos* **12**(1) 190-203 (2002).
13. R. Rico-Martinez, K. Krisher, G. Flätgen, J. S. Anderson and I. G. Kevrekidis, "Adaptive Detection of Instabilities: an Experimental Feasibility Study", *Physica D* in review, submitted 2001
14. S. Setayeshgar, C. W. Gear, I. G. Kevrekidis and H. Othmer, "Application of Coarse Integration to Monte Carlo Simulation of Bacterial Chemotaxis", in preparation for *PNAS*
15. C. W. Rowley, I. G. Kevrekidis, J. E. Marsden and K. Lust "Reduction and reconstruction for self-similar dynamical systems" *Nonlinearity* submitted (2002)
16. C.I. Siettos, A. Armaou, A. G. Makeev and I. G. Kevrekidis "Microscopic/ Stochastic Timesteppers and "Coarse" Control: a Kinetic Monte Carlo example", *AIChE J.* submitted (2002).
17. A. G. Makeev, D. Maroudas, A. Z. Panagiotopoulos and I. G. Kevrekidis "Coarse bifurcation analysis of KMC simulations: A lattice gas model with lateral interactions", *J. Chem. Phys.* in press (2002).