"Coarse" stability and bifurcation analysis using time-steppers: A reaction-diffusion example

Constantinos Theodoropoulos*, Yue-Hong Qian†, and Ioannis G. Kevrekidis**

*Department of Chemical Engineering, Princeton University, Princeton, NJ 08544; and †Department of Applied Physics, Columbia University, New York, NY 10027

Communicated by Andrew J. Majda, New York University, New York, NY, May 15, 2000 (received for review April 10, 2000)

Evolutionary, pattern forming partial differential equations (PDEs) are often derived as limiting descriptions of microscopic, kinetic theory-based models of molecular processes (e.g., reaction and diffusion). The PDE dynamic behavior can be probed through direct simulation (time integration) or, more systematically, through stability/bifurcation calculations; time-stepper-based approaches, like the Recursive Projection Method [Shroff, G. M. & Keller, H. B. (1993) SIAM J. Numer. Anal. 30, 1099–1120] provide an attractive framework for the latter. We demonstrate an adaptation of this approach that allows for a direct, effective ("coarse") bifurcation framework for the latter. We demonstrate an adaptation of this approach to illustrate how the so-called "time-stepper-based" bifurcation algorithms for PDE discretizations can be adapted to perform the "coarse" bifurcation analysis of models for which only microscopic evolution rules are available.

PDE steady states and their dependence on parameters can be obtained through Newton's method and its implementation in continuation/bifurcation algorithms. This implementation is easy and efficient if the right-hand sides of the PDEs can be explicitly obtained. If a transient integration scheme (a "time-stepper") is available, it can be used to locate stable steady states after (possibly long) integration. Shroff and Keller (1) introduced a scheme, named the Recursive Projection Method (RPM), which is built around an existing time-stepper. Steady states of the PDE are found as fixed points of the time-stepper. The scheme, by repeatedly calling the time-stepper for several (nearby) initial conditions and for short periods of time, effectively converts an available, possibly complicated (e.g., split step) time-stepper into a bifurcation code with minimal programming effort. Exploiting the dissipative nature of the PDE and the concomitant separation of time scales, RPM treats the time-stepper as a black-box and adaptively identifies a low dimensional subspace $P$, along which time-evolution is slowest (even slightly unstable). It performs Newton iterations with a (small) approximate Jacobian in this subspace and Picard iterations on its orthogonal complement $Q$. These small Jacobians are, in principle, easy to invert. The procedure is well-suited for the bifurcation analysis of large systems close to low-codimension bifurcations, because it sidesteps the problem of constructing and inverting large Jacobians (see also refs. 2 and 3).

PDE ("coarse") steady states correspond to stationary profiles, in space, of moments (e.g., concentrations) of populations in microscopic simulations. In other words, "coarse" steady states can be thought of as projections of the stationary states of microscopic simulations. The exact steady (not stationary, but actually steady) states of, say, an MD simulation (e.g., all molecules having zero velocity and zero acceleration) are not necessarily the same (in fact we do not expect them to be) as the averaged, coarse steady states of interest here, for which fluctuations at the molecular level persist.

Traditionally, the parameter-dependent behavior of a system is analyzed by first obtaining a "coarse" model (e.g., a mean-field PDE) and then performing bifurcation analysis of the PDE. Here we propose to adapt RPM-type methods in order to perform "coarse" bifurcation studies using microscopic evolution rules directly, i.e., to perform "coarse bifurcation calculations without first explicitly constructing a "coarse" model. The basic building block of the approach remains a call to a time-stepper. If a "coarse" model exists, this call involves (i) prescription of a "coarse" initial condition (concentration profile) and (ii) integration of the "coarse" model, the discretized PDE. The macroscopic time interval used (the time-stepper reporting horizon) is dictated by the dissipative nature of the PDE and corresponds to a natural separation between the "slow" and "fast" mode time scales (the gap between the corresponding linearization eigenvalues, see ref. 4). If the coarse model is not available, the evolution of a "coarse" initial condition (IC) can be obtained through (i) translating the coarse IC in one—or more—microscopic realizations consistent with it, (ii) evolving the realization(s) using microscopic rules for the same macroscopic time interval, and (iii) appropriately averaging the results over fine space and/or fine time and/or number of realizations to obtain the coarse time-$T$ map. Thus, coarse concentration profiles can be evolved through either coarse model (discretized PDE) time-steppers or microscopic time-steppers. This conceptual procedure is illustrated in Fig. 1. The structure of the RPM-based "coarse bifurcation" code remains unchanged, and a coarse bifurcation analysis is performed even in the absence of an explicitly derived and discretized mean-field PDE (or other evolutionary rule). A vital point, of course, is the translation of a coarse IC to one or more consistent microscopic ICs. While a multitude of consistent microscopic ICs exist, our illustration was chosen to be relatively insensitive to this major issue.

Abbreviations: PDE, partial differential equation; RPM, Recursive Projection Method; MC, Monte Carlo; MD, molecular dynamics; IC, initial condition; FD, finite difference; LB, Lattice–Boltzmann; FFH, FitzHugh–Nagumo.

†To whom reprint requests should be addressed.
For the reaction-diffusion system the evolution equations for colliding at a site). In the LB–BGK model we have implemented a lattice of fixed size, and of (non-reactive) collisions (particles of a single particle distribution function. Particle transport in LB equation (10), which describes the evolution in space and time implementation and solution. The LB models are based on a finite statistical noise inherent in lattice-gas models, but they are still macroscopic description of hydrodynamic systems; they lack the iii) RPM implementated around a “microscopic” time-stepper of the same FD spatial discretization, for con- ii) time-stepper employing an implicit Euler scheme for this dis- cretization. The time-stepper reporting horizon, T, should correspond to a time scale long enough for the fast modes (but not the slow stable ones) to decay; for our problem T ranged from 15 to 25. Let us clarify that this is not an economic alternative to direct bifurcation calculations for this problem; a single implicit integration step clearly costs as much as a direct steady time-stepper calculations. For a domain of length L = 20.0 with 200 discretization nodes, a Hopf bifurcation was found at \( \varepsilon \approx 0.015 \) and a saddle-node at \( \varepsilon \approx 0.944 \); the one-parameter diagram is shown in Fig. 2, where \( \langle u \rangle \), the spatial average of u, is plotted against \( \varepsilon \).

We then implemented an RPM-continuation code around a time-stepper employing an implicit Euler scheme for this discretization. The time-stepper reporting horizon, T, should correspond to a time scale long enough for the fast modes (but not the slow stable ones) to decay; for our problem T ranged from 15 to 25. Let us clarify that this is not an economic alternative to direct bifurcation calculations for this problem; a single implicit integration step clearly costs as much as a direct steady

\[
N_i^u(x + c_i t + 1) - N_i^u(x, t) = -\omega^u[N_i^u(x, t) - N_i^{ueff}(x, t)] + R_i^u(N_i^u, N_i^v) \tag{3}
\]

and correspondingly for v). Here, \( N_i^u(x, t) \) is the population density of activator (u) particles at position x on the lattice at time t, with velocity \( c_i \). In this one-dimensional system, particles can move only toward the two available adjacent sites (\( N_j^u \)) or (allowing for rest particles) stay in place (\( N_i^v \)). For unitary LB temporal and spatial increments, therefore, \( c_i = \{0, 1, -1\} \) and \( i = 1, 2, 3 \) respectively. \( N_i^{ueff} \) is the local equilibrium population, homogeneous in all velocity directions, and \( \omega^u \) is the BGK relaxation parameter; the first part of the right-hand side computes post-collision populations. \( R_i^u \) is the reaction term; we use the (strong) assumption (11) of local diffusive equilibrium for the reaction term. The left-hand side computes the particle streaming. In this case, there are 2 concentrations (u,v) at each lattice site and 3 discrete possible velocities per concentration (6 population densities overall). While concentrations can be uniquely computed as the 0th moments of the populations, e.g.,

\[
u(x, t) = \sum_{i=1}^3 N_i^u(x, t), \tag{4}
\]

the opposite is not true. If a “coarse” initial condition (concentrations, zeroth moments) is specified, any 3 random numbers (weights) \( w_i \) summing up to 1 would be a possible choice, i.e.,

\[
N_i^u(x, t) = w_i u(x, t). \tag{5}
\]

It so happens that in our LB–RPM the choice of initial weights is not critical; initial disturbances caused by such random choices decay much faster than the (macroscopic) time interval used in the time-stepper (as we will discuss below).

Results and Discussion

We first constructed the bifurcation diagram of a detailed FD discretization of the FHN model, to benchmark our RPM time-stepper calculations. For a domain of length L = 20.0 with 200 discretization nodes, a Hopf bifurcation was found at \( \varepsilon \approx 0.015 \) and a saddle-node at \( \varepsilon \approx 0.944 \); the one-parameter diagram is shown in Fig. 2, where \( \langle u \rangle \), the spatial average of u, is plotted against \( \varepsilon \).

We then implemented an RPM-continuation code around a time-stepper employing an implicit Euler scheme for this discretization. The time-stepper reporting horizon, T, should correspond to a time scale long enough for the fast modes (but not the slow stable ones) to decay; for our problem T ranged from 15 to 25. Let us clarify that this is not an economic alternative to direct bifurcation calculations for this problem; a single implicit integration step clearly costs as much as a direct steady
As mentioned above, a systematic way of converting nearby coarse (macroscopic) initial conditions to consistent ICs of the microscopic integrator is a vital issue for coarse stability calculations. We had to translate 400 numbers (two concentrations at 200 points each) to 2,400 numbers (three densities each for two quantities at 400 lattice points, respectively). All of our initialization tests were performed for $\epsilon = 0.8$, starting from a “coarse” steady state profile on the stable branch, obtained by 200-node FD simulations at a nearby parameter value ($\epsilon = 0.5$). We used three equal weights in Eq. 4 as well as random weights summing up to 1. We performed both “fine” and “coarse” initializations. For “fine” initializations, starting from the (interpolated) steady state coarse concentration profile, three equal weights ($w_1 = 1/3$) were first used as in Eq. 5 to initialize each population at each lattice site. Triads of random weights ($w_i$) with sum 1, different for each site, were also employed. For coarse initializations, starting from the same coarse steady state profile, locally averaged values of $u$ and $v$ ($\bar{u}$ and $\bar{v}$) every 10 consecutive FD nodes were calculated. These averages were used to initialize (in a “step” fashion) the corresponding lattice site populations through both equal and random weights. Even in the more severe “coarse” case with random weights, the discrepancy between (the projections on the zeroth moments of) different trajectories, caused by the different initializations, were practically eliminated after times much shorter than the RPM-time-stepper reporting horizon (after $t \approx 0.1$ as compared to $T = 15 - 25$).

The LB time-stepper was then coupled to RPM, taking enough microscopic collision/streaming steps to match the macroscopic reporting horizon. The LB–RPM “microscopic” system was able to accurately reproduce the “coarse” PDE bifurcation diagram in the neighborhood of the Hopf bifurcation (Fig. 3a). Both stable and unstable branches converged on, were essentially the same as the steady states computed through the “coarse” code (the FD PDE discretization). This also holds in the neighborhood of the saddle-node bifurcation; in this case the discrepancy between the stationary states of the LB–RPM and the steady states of the PDE was slightly more pronounced.

A natural byproduct of RPM-type methods applied to a discretized PDE time-stepper is the leading eigenspectrum of the PDE Jacobian, reconstructed from the eigenvalues and eigenvectors of the small Jacobian in the slow subspace. The eigenvalues $\mu_i$ of this small “coarse Jacobian” at a fixed point of the time-stepper are related to the eigenvalues $\lambda_i$ of the “full” coarse Jacobian of the system: $\mu_i = \exp(\lambda_i T)$. An attractive feature of the LB–RPM technique is that it correspondingly approximates the leading “coarse” eigenspectrum of the system in question, from the approximated small “coarse” Jacobian. In these simulations the dimension of this small Jacobian ranged from 0 to 3. RPM also accurately predicted the value of $\epsilon$ where eigenvalues cross the imaginary axis (here $\approx 0.015$). Finally, the leading eigenvectors of the system linearization were also successfully reconstructed. They are depicted in Fig. 5 a and b for $\epsilon = 0.01$. In all cases the eigenvectors compare well with the
ones from the FD code despite the fact that they were reconstructed from a small (three-dimensional) LB simulation-based subspace.

Conclusions

What was illustrated here for LB-based time-steppers can, in principle, also be accomplished for other microscopic (MC, MD) or hybrid simulators [e.g., CONNEFESSIT, Brownian configuration fields (12–14), and DSMC (15)]; the action of the (coarse) Jacobian on the presumably low-dimensional subspace of slow (or slightly unstable) coarse system modes can be approximated through a (microscopic) time-stepper and used in (macroscopic, “coarse”) bifurcation calculations. The use of repeated, relatively short-term calls to the microscopic/hybrid time-stepper sidesteps the necessity of deriving (and closing) a macroscopic (coarse) equation for the system moments. What the approach extracts from the microscopic time-stepper is precisely the minimal information required to perform the computational bifurcation analysis of a coarse PDE (or other types of coarse deterministic evolution rules). Vital issues for the success of the scheme are (i) the translation of coarse initial conditions to “good” consistent microscopic realizations, and (ii) averaging (if necessary) the evolution result of these microscopic ICs over fine space and/or fine time and/or realizations to obtain the corresponding coarse short term integration result (an accurate coarse time-T map). We believe that the approach holds promise for the systematic stability and parametric analysis of the coarse dynamic behavior of a large class of systems described through microscopic evolution rules. In a similar spirit (averaging “detailed” time-stepper results over realizations of heterogeneous media rather than microscopic time-stepper results over microscopic initial conditions) it may also play a role in the stability/parametric analysis of the coarse dynamic behavior of phenomena in complex media for which effective equations are difficult to obtain [e.g., reaction and diffusion on composite catalysts (16)].

This work was partially supported by the Air Force Office for Scientific Research, Sandia National Labs and UTRC.