Hybrid System: Combing the Ising Model and an Ordinary Differential Equation

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Introduction

When trying to model molecular processes, one often comes against the problem of how to compensate between scales. On one hand, there is the fact that observable phenomena occur at the macroscopic scale, and so often times we average out the interactions to get a general equation for our appropriate scale. On the other hand, the microscopic interactions can and do perform interactions with each other. The result is that the deterministic macroscale approximation fails when interactions occur around the area of a phase transition or bifurcation point due to fluctuations.

Accounting for the occurrence of rare microscopic events, and their nonlinear contribution, is fundamentally important; but numerical constraints prevent a computational answer to any questions we may ask. The difference in scales is simply too large to allow our computers to calculate the results of all these interactions. Fortunately though, through the use of stochastic methods and statistical mechanics, such problems as the absorption of particles, can have their results approximated by treating the microscopic interactions as a continuous jump time Markov process and examining various closures. In order to understand one such approach, we looked at a paper by M.A. Katsoulakis, A.J. Majda, and A. Sopasakis [1] and attempted to reproduce the model set-up they described.

For the absorption of particles, we have particles existing along a surface which can move along the surface, can evaporate into a gas phase, or can condense back into a liquid state. The stochastic process of this phenomenon has a continuous time generator that is a functional on the current coverage densities of the particles and the coupled gas phase dynamics. The coverage densities microscopic interactions of the absorption of particles can be modeled using a spin flip stochastic Ising type model where the spin is used to represent the phase state (e.g., liquid or gas) of the molecule in that location.

The paper [1] also discusses two different closures can be obtained. First, by assuming that the stochastic system evolves with characteristic time faster than the deterministic gas phase system, we can use the stochastic averaging principle to obtain a system where phase transitions are absent from the system. Second by taking the asymptotic limit of long range interactions we obtain a spatially distributed deterministic closure, which is a mesoscopic model. In our work, we are not going into details of the closures of the hybrid model. The overall purpose of this paper is to explain the model set-up in detail and show some simulation results.

Mathematical formulation

We introduce the spin-flip stochastic Ising process $\{\sigma_t\}_{t \geq 0}$, modeling the absorption and release of particles on a one dimensional surface, coupled to an ordinary differential equation

$$\frac{dY}{dt} = f(Y, \sigma) \tag{1}$$

that serves as a caricature of an overlying gas-phase dynamics. In particular, here we consider only one example of possible ODE model: scalar equations with bistable behavior or saddle node bifurcations.

Ising Model

We consider a microscopic stochastic model defined on a periodic lattice of size N, which we denote as $\Lambda = \{1,2,..., N\}$. We have particles $\mathrm{P} = \{1,2,..., N\}$ that live on our lattice Λ. We assume a site at a lattice cannot be occupied by more than one particle (exclusion principle) and each site is occupied. In our implementation of the Ising Model, particle i is positioned at the lattice site i and it does not move.

Each particle $\rho \in \mathrm{P}$ has an order parameter $\sigma(\rho)$, called a spin, which is allowed to take values 0 or 1. On Figure 1, particles are represented by circles and spins are represented by their color: blue circle is 1, while red is 0. If the value of a particle's spin is 0, it is absorbed by the surface, while if it is one – it is released into the air.

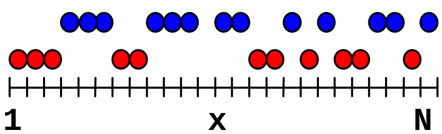

Figure 1: Configuration of an Ising Model at time t

A spin configuration σ is an element of the configuration space $\Sigma = \{0,1\}^{\Lambda}$ and we write $\sigma = \{\sigma(\rho) : \rho \in \mathrm{P}\}$. Physically, the mechanism of change of configuration (or co-called spin flip) may describe the release of a particle from a surface described by the lattice to the gas phase above and conversely the absorption of a particle from the gas phase to the surface.

Configuration σ changes as a function of time t, one spin flip at a time. Suppose a flip begins at t_n and completes at t_{n+1}. Then percentage of completion for that flip at time $t_n + \Delta t$ with $\Delta t \le t_{n+1} - t_n$ is $c(\rho,\sigma)\Delta t + O(\Delta t^2)$, where $c(\rho,\sigma)$ denotes the rate of the process.

In this model we implement spin flip Arrhenius dynamics. Therefore under this type of mechanism the configuration changes are driven based on the energy barrier a particle has to overcome in flipping from one state to another. The energy barrier makes it "easier" for a particle to get absorbed than released because the rate of absorption is greater. In other words, it will take less time for a flip from 1 to 0 to complete compared to the flip from 0 to 1. More specifically, we have the following relationship:

$$c(\rho,\sigma) = \begin{cases} c_r e^{-\beta(U_0 + U(\rho))} & \text{if } \sigma(\rho) = 0, \\ c_a & \text{if } \sigma(\rho) = 1. \end{cases} \tag{2}$$

In (2) $c_a = c_r = 1/\tau_I$, where c_a and c_r are absorption and release constants, while τ_I denotes the characteristic time of the process. We denote the inverse temperature by $\beta = 1/(kT)$, where $k = 1.38 \times 10^{-23} JK^{-1}$ is the Boltzmann constant. Here U_0 represents the energy associated with the surface binding of the particle ρ_i at location l_i.

The function $U(\rho)$ accounts for the potential associated with particle interactions on the lattice and the external potential $h(Y)$:

$$U(\rho, Y) = \sum_{\substack{z \neq \rho \\ z \in \Lambda}} \lambda J(\lambda \mid \rho - z \mid) \sigma(z) - h(Y) . \tag{3}$$

The parameter γ prescribes the range of microscopic interactions between particles. Here J is assumed to be even, $J(r) = J(-r)$ and can take a form

$$J(r) = \begin{cases} J_0 & \text{if } 0 \leq r \leq 1, \\ 0 & \text{otherwise,} \end{cases} \tag{4}$$

where J_0 is a parameter which, based on its sign, describes attractive or repulsive interactions. For attractive microscopic interactions J_0 is positive. We let $\gamma = 1/(2L+1)$, where L denotes the interaction radius. We assume that the external potential $h(Y)$ is linear, i.e. $h(Y) = cY + h_0$.

ODE: Scalar bifurcation

The form of the ODE (1) we choose for the numerical simulation is one of the most fundamental dynamical systems, a scalar (pitchfork) bifurcation:

$$\frac{dY}{dt} = a(\overline{\sigma})Y + \frac{\varphi}{\tau_c} Y^3 , \tag{5}$$

where we let

$$a(\overline{\sigma}) = \frac{1}{\tau_c}\left[z + (1 - \overline{\sigma})b\right] \tag{6}$$

and

$$\overline{\sigma} = \frac{1}{N} \sum_{i=1}^{N} \sigma(\rho_i) . \tag{7}$$

The constant τ_c represents the characteristic time of the ODE, while $\overline{\sigma}$ is the average spin value of the Ising model. Note that (5) has three nodes: $0, \pm\sqrt{-a(\overline{\sigma})\tau_c / \varphi}$ and the two main bifurcation states: super-critical, in the case of a stable node turning into one unstable and two stable nodes and sub-critical in the opposite situation.

Numerical simulations

The hybrid system is numerically solved by running the Monte Carlo simulation and ODE solver (4^{th} order adaptive Runge-Kutta-Fehlberg method) in parallel. We start from using a random initial configuration for the lattice and the gas state $Y(0) = 1$. This value is used in the Monte Carlo simulation through the external potential $h(Y)$. Each iteration of the Monte Carlo simulation produces a variable time step Δt and is immediately followed by applying the ODE solver. The solver iterates until the given time step Δt has been exhausted, producing a new value of the gas state that is going to be used in the following Monte Carlo step. This procedure repeats for a specified number of steps. More specifically, we applied the following algorithm for spin flip Arrhenius dynamics.

Global Update Scheme

1. Calculate transitional rate $c(\rho, \sigma)$ for each site on the lattice.
2. Calculate totals: $R_a = \sum_{\forall \sigma(\rho)=1} c(\rho, \sigma)$, $R_d = \sum_{\forall \sigma(\rho)=0} c(\rho, \sigma)$, and $R = R_a + R_d$.
3. Generate the random spin using Bernoulli distribution

$$p\left(\sigma(y), \frac{R_d}{R}\right) = \begin{cases} \frac{R_d}{R} & \text{if } \sigma(y) = 1, \\ \frac{R_a}{R} & \text{if } \sigma(y) = 0, \\ 0 & \text{otherwise.} \end{cases}$$

4. Randomly pick a particle ρ_i with a spin opposite to $\sigma(y)$ and flip it.
5. Update time to $t = t + \Delta t$, where $\Delta t = 1/R$.
6. Repeat from step 1 until equilibration or dynamics of interest have been captured.

As mentioned earlier, both the ODE system and the Ising Model have their own time scales, τ_c and τ_I respectively. We define $\tau = \tau_c / \tau_I$ and explore the following three cases:

- $\tau << 1$
  ODE equilibrates faster compared to the spin dynamics;
- $\tau \approx 1$
  ODE equilibrates at similar times with the spin dynamics;
- $\tau >> 1$
  ODE equilibrates slower compared to the spin dynamics.

Without the loss of generality, we fix $\tau_I = 1$ and vary τ_c to see the effects. By doing so, we can see how the phase portrait of our dynamical system is going to change when the parameter $\bar{\sigma}$ goes through its bifurcation value.

The Table 1 below summarizes the parameters used in the simulation of the hybrid model.

Name	Value
N	1000
β	1
τ_I	1
U_0	0
L	20
λ	1/41
J_0	0.01
c	-1
h_0	1
$Y(0)$	1
φ	-0.025
b	4
z	-1

Table 1: Parameters for the hybrid model

In our simulations, we explored the effects of different time scales on the overall behavior of the model.

Simulation Results and Observations

We implemented the global update scheme described earlier in MATLAB 7 and ran it for different values of parameters to see the effects of the change of scale. Figure 2 shows a typical behavior of the system for each of the three cases for the ratio of the scales. We show two pictures for each of the values of parameters to highlight that even though the simulation results of two independent runs can never be identical, the overall patterns do look alike. On Figure 2.1 we can see that if the characteristic time of the ODE is smaller than one for the Ising Model, the hybrid model is going to be severely impacted by the effects of noise produced by the Ising Model. The Figure 2.2 shows the case, where the characteristic time of the ODE is about the same as one of the Ising Model. In this case, we can observe that even though the noise does affect the overall behavior, the shape of the curve looks consistent. The last case shows a scenario where the characteristic time of the ODE is larger than one for the Ising Model, so the ODE equilibrates much slower compared to the Ising Model. In this case, we can see that there are fewer sudden "jumps" in the solution compared to what we see in the previous two cases.

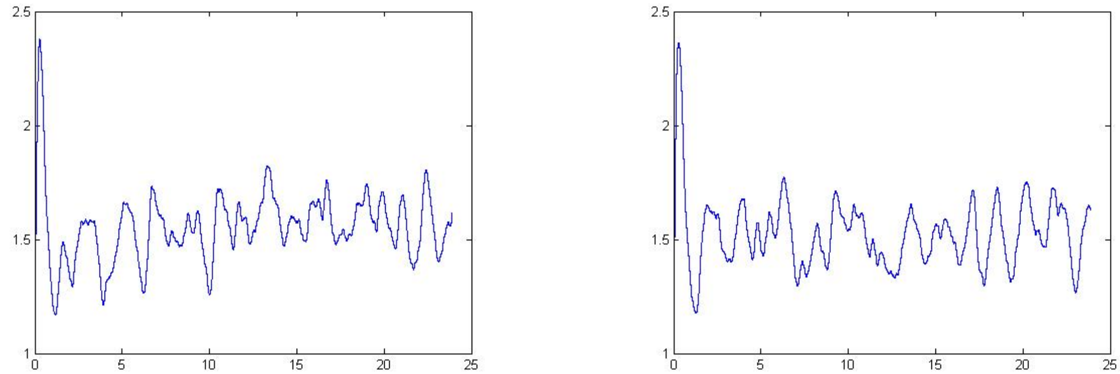

Figure 2.1 $\tau_c = 0.1$, $\tau << 1$

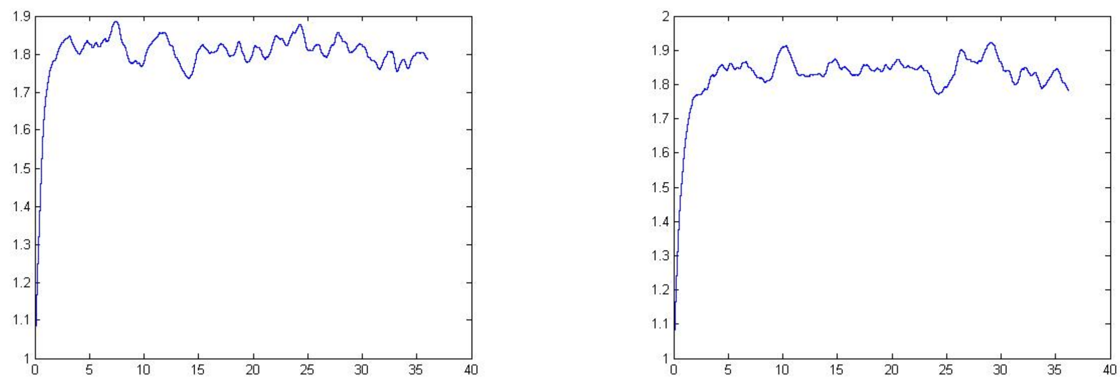

Figure 2.2 $\tau_c = 1$, $\tau \approx 1$

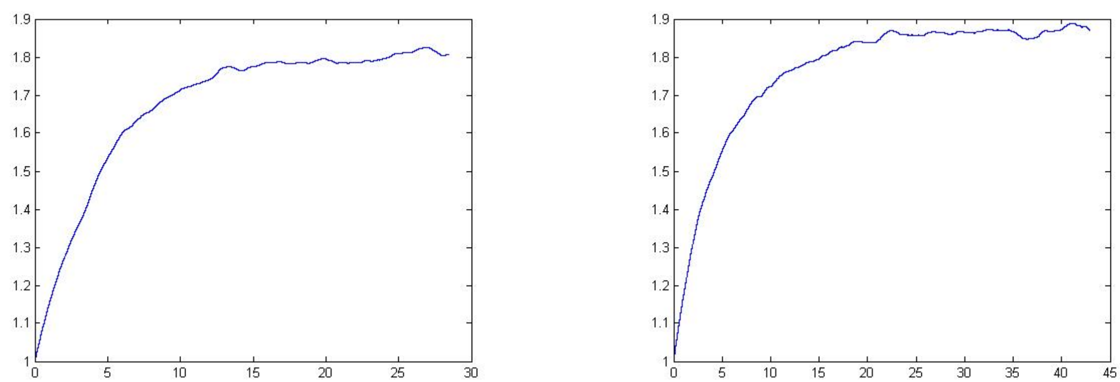

Figure 2.3 $\tau_c = 5$, $\tau >> 1$

Our numerical simulations of the hybrid system confirmed that the value of the ratio of characteristic time scales of stochastic and deterministic parts of the hybrid system makes a noticeable impact on the solution. The behavior of the overall system is highly susceptible to changes in such ratio.

Reference

[1] M.A. Katsoulakis, A.J. Majda, A. Sopasakis, *Multiscale couplings in prototype hybrid deterministic/stochastic systems: Part I, Deterministic closures.* Comm. Math. Sci. Vol. 2, No. 2, pp. 255-294, 2004.