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ROBUST BIFURCATION DETECTION FOR KINETIC MONTECARLO SIMULATIONS

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Traditionally, transport and reaction processes are modeled by constitutive equations like mass and energy balances. However, often one has only available microscopic, molecular- level dynamic models capable of describing the physics of the phenomena taken place at different levels of coarse graining. In spite of the proven capacities of these microscopic simulators, they exhibit limitations.

The bifurcation detection for any type of molecular simulation cannot be addressed with traditional, model- based, computational methods. Recently, the introduction of model-free calculations (see e.g [1]) allows one to devise strategies to tackle these problems. Some of the mathematical and computational tools that are available for the bifurcation analysis of macroscopic models could also be used to achieve the non-linear characterization of microscopic simulations, if a macroscopic equivalent can be constructed. Such macroscopic equivalent can, indeed, be formulated by considering a coarse time-stepper formulation [1].

We use the strategy for bifurcation detection proposed by Rico-Martínez et al. [2]. The procedure consists of four modules: i) the trajectories of the system (e.g. coarse time stepper) are used to obtain a low order model that describes the behavior of the system; ii) the identified model is used to estimate the location of the bifurcation point; iii) define the conditions that describe the specific type of bifurcation sought; iv) use the estimated critical parameter value to device a parameter variation policy that will direct and keep the system close to the desired bifurcation point.

The low order model proposed is based on an Artificial Neural Networks (ANN) approximation corrected with a Kalman Filter type estimator [3]. This robust identification technique is demonstrated to represent a better option for the identification of the non-linearities of microscopic simulations, giving robustnees to the technique yo make it capable of characterizing Monte Carlo simulations.

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[1] A. G. Makeev, D. Maroudas, A. Z. Panagiotopoulos, and I. G. Kevrekidis, *J. Chem. Phys., 117, 8229 @ S 8240, (2002). Kevrekidis, Int. J. of Bif. and Chaos, 14, 207-220, (2004).*

[2] R. Rico-Martínez, K. Krischer, G. Fltgen, J. S. Anderson and I. G. Kevrekidis, Physica D, 176, 1-18, (2003).

[3] C. González-Figueredo and R. Rico- Martínez, Int. J. Chem. Reac. Eng, 3, A63 (2005).