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#### Yannis G. Kevrekidis

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Princeton, July 22, 2013

TO: Prof. Marsha Lester, Editor, *J. Chem. Phys.*

RE: submission of a manuscript to the Journal

Dear Professor Lester

Attached please find a manuscript entitled

*Nonlinear Intrinsic Variables and State Reconstruction in Multiscale Simulations*

co-authored by Ms. C. Dsilva, Dr. R. Talmon, Dr. N. Rabin, Dr. R. R. Coifman and myself, that we would like to ask you to consider for publication in the Journal. I will be the corresponding author

Possible reviewers might be (a) Professor Shekhar Garde, Department of Chemical and Biological Engineering, RPI; (b) Professor Dimitrios Maroudas, Department of Chemical Engineering, University of Massachusetts-Amherst; (c) Dr. Radek Erban of Applied Mathematics, Oxford University; (d) Professor Andy Ferguson, Materials Science and Engineering, University of Illinois and (e) Prof. Prodromos Daoutidis, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis.

We will *not* be able to pay the open access fee.

The main contribution of the manuscript is the exploitation of a novel “twist” in nonlinear data mining that allows one to merge simulation data from different sets of partial observations and/or at different levels of granularity for atomistic multiscale simulations; the approach has the potential to allow the merging of computational and observational data, and the reconstruction (under appropriate conditions/data) of unmeasured variables.

We hope that you and the referees will find our contribution worthy of publication to *J. Chem. Phys*. If there is something else I can add, please do not hesitate to contact me (yannis@princeton.edu)

Sincerely



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