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## Princeton University

#### Yannis G. Kevrekidis

Pomeroy and Betty Perry Smith Professor of Engineering

Professor of Chemical and Biological Engineering &

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Princeton, November 1, 2013

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

RE: small corrections on manuscript proofs

Dear Professor Lester

Thank you and the production staff for the careful effort in preparing our work for publication. Attached please find our annotated proofs (the annotations are in the form of yellow “sticky notes” on the .pdf) of the 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.

We have made every effort to address the comments and questions from the production staff. We hope that our edits will make our manuscript suitable for publication. If there is something else I can add, please do not hesitate to contact me (yannis@princeton.edu)

Sincerely



Yannis G. Kevrekidis

Professor, Chemical and Biological Engineering &

Program in Applied and Computational Mathematics

Associated Faculty, Mathematics

**RESPONSES TO PROOF COMMENTS**

*1. Is the title of your article accurate and spelled correctly?*

Yes

*2. Are the author names in the proper order and spelled correctly?*

Yes

*3. Please check afﬁliations including spelling, completeness, and correct linking to authors.*

Everything is correct

*4. Did you remember to include acknowledgment of funding, if required, and is it accurate?*

Line 674 should read

“…US Department of Energy Computational Science Graduate Fellowship…”

*Q1: Please provide zip code for afﬁliations 1, 2, and 4.*

Affiliation 1: zip code 08544

Affiliation 2: zip code 06520

Affiliation 4: zip code 08544

*Q2: Please check deﬁnition of ODE.*

This is correct.

*Q3: Please check the insertion of labels (a)–(d) in the caption of Fig. 3.*

This is correct

*Q4: Please verify the changes made in the volume in Refs. 1 and 2.*

This is correct

*Q5: Please provide volume and page no. in Ref. 8.*

Volume 9, pages 3515-3526

*Q6: Please provide a digital object identiﬁer (doi) for Ref(s) 8. For additional information on doi’s please select this link: http://www.doi.org/. If a doi is not available, no other information is needed from you.*

The doi is 10.1021/ct400137q

*Q7: Please verify the publisher’s name in Ref. 13, as we have inserted the required information*

This is correct

*Q8: Please check the presentation of Ref. 19 for correctness.*

The citation should read

M. Hein, J. Y. Audibert, in *Proceedings of the 22nd International Conference of Machine Learning* (ACM, 2005), p. 289.

*Q9: Please verify the volume number in Refs. 42 and 46, as we have inserted the required information*

These are correct

In addition, we would make the following edits:

1. On line 122, we would like to change “…manifestation in an observable domain of a…” to “manifestation, in an observable domain, of a…”
2. We would like to change Equation 1 from “\mathbf{Y}(t) = f(\mathbf{x}(t)),” to “\mathbf{Y}(t) = \mathbf{f}(\mathbf{x}(t)),”
3. On line 124, we would like to change “where $f:\mathbb{R}^d \rightarrow \mathcal{M}$ is an unknown…” to “where $\mathbf{f}:\mathbb{R}^d \rightarrow \mathcal{M}$ is an unknown…”
4. On lines 130-131, we would like to change “…and $\dot{w}\_i(t)$ are independent white noises.” to “…and $w\_i(t)$ are independent Brownian motions.”
5. On line 236, we would like to change “The diagonal entries of $D$ serve as estimates…” to “The diagonal entries of $\mathbf{D}$ serve as estimates…”
6. On line 281, we would like to change “…and $\dot{\mathbf{w}}(t) \in \mathbb{R}^d$ is a vector consisting of independent white noises.” to “…and $\mathbf{w}(t) \in \mathbb{R}^d$ is a vector consisting of independent Brownian motions.”
7. On line 283, we would like to add a comma after ∞.
8. On line 314, we would like to change “…but $D$ appears with coefficient -1 rather than $-1/2$.” to “…but $\mathbf{D}$ appears with coefficient -1 rather than $-1/2$.”
9. In Equation 12, “l” in “scale l” should be italicized.
10. On line 385, we would like to change “…a new data point $\Psi(\tilde{i})$ is find the…” to “…a new data point $\Psi(\tilde{i})$ is to find the…”
11. In the caption of Figure 2, we would like to change “the LP approximation is shown in black…” to “the LP approximation in black…”
12. On line 482, we would like to change “Gillespie SSA example” to “chemical reaction network example”
13. On line 540, we would like to remove the word “direct”