Final Response to the Referee 1 (Report #2)

General Remarks

The following response is presented in a self–contained manner, *i.e.*, the response can be read without referring to the original review comments. Yet the original comment texts are also inserted with green. Please note that the Referee comments are quoted by »...« whenever they are quoted in the response text.

Response

We much thank to the present Referee, because the manuscript has been substantially augmented by adding the two further appendices in response.

After careful assessment, I have decided to recommend this manuscript for publication after a minor revision.

We are glad to learn that »After careful assessment«, the present Referee has »decided to recommend this manuscript for publication after a minor revision«.

Some of the points I previously raised have been addressed in the revised manuscript. A guide for applying the theory to more general forms of systems is now included in Sec. 5.3. The meaning of the output-constrained maximum-entropy principle is further elaborated. Additional details for clarification are provided throughout. All of which contributed to improving the manuscript's quality.

Also gladly the present Referee acknowledges that »Some of the points ... raised have been addressed in the revised manuscript«. Especially, »A guide for applying the theory to more general forms of systems is now included« as a standalone »Sec. 5.3«. Furthermore, »The meaning of the output-constrained maximum-entropy principle is further elaborated«, and »Additional details for clarification are provided throughout«. The Referee concludes that »All of which contributed to improving the manuscript's quality.«

What is still missing is a more thorough evaluation of the error in the derived model, as such information is crucial to understand the methodology's reliability. I agree, however, with the authors that deriving and evaluating the error systematically would be complex. To give readers a rough idea of when and how the derived model performs accurately, a more in-depth discussion of the error using simple examples would be valuable. For this purpose, I request the authors to expand the discussion related to Fig.2 (see also Comment (6) below). Additionally, I would suggest exploring other simple but qualitatively different cases, such as those involving fixed points (steady solutions):

- $d\phi/dt = -\phi$. Here, $\phi = 0$ is a globally stable fixed point.
- $d\phi/dt = \phi(1-\phi)$. Here, $\phi = 0$ is a stable fixed point, and $\phi = 1$ is an unstable fixed point.
- $d\phi/dt = \phi(1-\phi)(2-\phi)$. Here, $\phi = 0$, 2 are stable fixed points, and is $\phi = 1$ an unstable fixed point.

Yet, the Referee also points out that »a more thorough evaluation of the error in the derived model« is »still missing«. The Referee further emphasizes that »such information is crucial to understand the methodology's reliability«. At the same time, the Referee also agrees with us, as we responded previously, that »deriving and evaluating the error systematically would be complex«. As a compromise, this time, the Referee alternatively suggests »a more in-depth discussion of the error using simple examples« »To give readers a rough idea of when and how the derived model performs accurately«. As more specific proposals along this line, the Referee requests us more specifically two additional exercises:

1) »to expand the discussion related to Fig.2«: The Referee further elaborates on this exercise in the Major Comments 5) and 6) below. Thus, we also provide our response on this item below, only remarking for now that this exercise has been performed in revision, as explained below.

2) to explore »other simple but qualitatively different cases, such as those involving fixed points (steady solutions)«:

More specifically, the Referee suggests to consider the following simple dynamical systems:

(i) $d\phi/dt = -\phi$. »Here, $\phi = 0$ is a globally stable fixed point.«

(ii) $d\phi/dt = \phi(1-\phi)$. »Here, $\phi = 0$ is a stable fixed point, and $\phi = 1$ is an unstable fixed point.«

(iii) $d\phi/dt = -\phi(1-\phi)(\phi-2)$. »Here, $\phi = 0$, 2 are stable fixed points, and $\phi = 1$ is an unstable fixed point.«

These three dynamical systems have been thoroughly examined in revision in a newly–introduced Appendix C.

Some more comments are provided below.

The Referee further provides »Some more comments«:

Major Comments

1) [request] P.4 ll.118–119 "... f designates all ..."

It is not at all obvious to the readers that point here. I would explain can be space dependent. Please clarify this F is a functional of $\phi(x, y, z)$.

By following the suggestion, the following sentence has been inserted in revision (L119–120):

"The source, F, generally depends on the variable, ϕ, and also possibly on time t and space."

2) [comment] P.6 ll.139–140 "..., there is no closed analytical formula for reconstructing the original distribution from a given series of moments: ..."

For the authors' information, I found an interesting paper that is closely relevant to this problem. Chao Dang and Jun Xu, "Novel algorithm for reconstruction of a distribution by fitting its first-four statistical moments", Applied Mathematical Modelling, Volume 71, 2019, Pages 505-524, https://doi.org/10.1016/j.apm.2019.02.040.

We much appreciate the present Referee for pointing us out an existence of a very interesting paper by Dang and Xu (2019) on this subject: the essence of this paper is based on the fact that under an assumed PDF formulation (in our own terminology), it is indeed possible to define the PDF parameters from a given set of moments, *i.e.*, the operation of inverting the relations (3.4) to (3.3) in the manuscript, once a PDF form is pre–defined, as well known in the assumed–PDF community. Yet, the paper goes even further by asking a question of which PDF forms (or PDF models, in their own terminology) provides the best fit when several options of the PDF forms are considered.

Thus, this work is still short of resolving the issue in concern. Yet, we have decided to cite this paper in revision along with Daniels (1954) and Butler (2007), suggested in the previous round by the present Referee, so that extensive literature on the relations between the moments and the distribution can be suggested to the readers (L170).

3) [question] P.23 Eq.(5.10b):

I think we can solve the derived model in a slightly different way. Let us consider $\{\langle\sigma_l\rangle\}$, not $\{\sigma_l\}$, are the prognostic variables.

1. From $\{\langle\sigma_l\rangle(t)\}$, we can estimate the PDF $p(\phi, t)$ by using the maximum entropy principle.
2. Using the estimated $p(\phi, t)$, we can calculate the $\{\langle F_{\sigma_l}\rangle(t)\}$.
3. Using Eq.(5.10b), we can numerically calculate $\{\langle\sigma_l\rangle(t + \Delta t)\}$.

By repeating this procedure, we can numerically calculate the time evolution of weights $\{\langle\sigma_l\rangle(t)\}$. Isn't this easier than solving Eq. (5.8a)?

Here, the present Referee argues that at every time step, once the values of $\{\langle\sigma_l\rangle(t)\}$ are updated, we can evaluate the updated distribution form simply by by invoking the maximum entropy principle without performing a time integral of the parameters. The proposal, indeed, sounds appealing with a first glance.

However, the Referee is unfortunately missing some key issues behind.

First, the maximum entropy principle can merely define a general distribution form, as given by Eq. (3,15) in the manuscript, once the constraints, $\{\langle\sigma_l\rangle(t)\}$, are specified. However, as explicitly pointed out immediately following this formula, the maximum entropy principle itself does not provide specific values for the distribution parameters, $\{\lambda_l(t)\}$. Those are still to be determined by inverting the relations (3.4) into (3.3). This inversion is precisely the main difficulty with the standard assumed–PDF approaches, because the relations (3.4) are often highly nonlinear, and their inversions into the form (3.3) are hardly trivial, as already suggested in the introduction, and also more specifically discussed in Sec. 3.2.1. The proposed prognostic formulation circumvents the difficulty of this inversion problem.

To make this point clearer, in revision, the following short remark is added towards the end of Sec. 5.1 (L654–656):

"Realize that the key step introduced in the formulation here is to prognose the PDF parameters, $\{\langle\lambda_l\rangle(t)\}$, by Eq. (5.8a). In this manner, we circumvent the principal difficulty of the current assumed–PDF approaches of inverting the relations (3.4) into the form (3.3)."

4) [comment] Sec.5.3 "Generalization to the PDE system (2.1)":

I appreciate that the authors added this section; we can now see that the generalization of the proposed theory is indeed straightforward. From the derivation provided in this section, I also feel that we may not need to bring the Liouville equation.

The present Referee appreciates »that the authors added this section«. The Referee further remarks that »I also feel that we may not need to bring the Liouville equation.« Yes, it is indeed true that Eq. (5.11d) can be derived without invoking the Liouville equation. However, we still believe it important to invoke the Liouville equation explicitly so that we can also explicitly demonstrate that we are indeed solving the Liouville equation under this approach, albeit with an extremely truncated form. Furthermore, without directly invoking the Liouville equation, it would be rather difficult to identify the middle expression in Eq. (5.11d), that explicitly links the temporal tendency of $\langle \sigma_l \rangle$ to that of the PDF parameters, λ_l.

5) [comment] P.28, ll.787–790 "... the solution breaks down beyond this point ...":

I think this behavior is reasonable. Please note that the solution of $d\phi/dt = \phi^2$, $\phi(0) \neq 0$ blows up in finite time if $n > 1$.

No, this behavior is not reasonable. Curves for the exact solutions have been added in green in revision to Fig. 2, and a full discussion of this system has also been presented in the Appendix B in revision. As the Referee correctly points out, the system with »$d\phi/dt = \phi^2$, $\phi(0) \neq 0$ blows up in finite time if $n > 1$«. However, as explicitly discussed in the newly–added Appendix B, this merely translates into a strong tendency of the distribution to stretch towards the larger values with time, and the distribution itself continues to evolve without singularity.

6) [question, request] Fig.2:

Is Fig.2b correct? If I understand Eq. (5.17e) correctly, $\lambda_1(t)$ does not depend on n when $m = 1$.

For each $m = 0, 1, 2, 3$, please plot the true $\lambda_1(t) = 1/\langle \phi \rangle(t)$ and discuss which choice of n is the most accurate.

We much appreciate a question concerning this figure, because there was a totally stupid error in the code, in which the definitions of the parameters, m and n, are swapped round everywhere, that also led to additional errors. The figure has been thoroughly modified in revision: the four panels now show the cases for $m = 0$, 2, 3, and 4, because the case with $m = 1$ is trivial, as the reviewer correctly pointed out. As already remarked in response to 5), the exact PDF solutions for those systems have been evaluated in revision in the Appendix B, and furthermore, the values of λ_1 diagnosed from $\langle \phi^n \rangle$ obtained by using the exact evolution of the distributions are also added as green curves in Fig. 2.

Minor Comments

7) [request] P.5 ll.139–140 (L140–141 in revisoin) "Furthermore, in the present study, the source term, F, is assumed to be deterministic":

This is not correct. Brownian motion is considered in Sec. 4.4. Please rephrase.

By following the suggestion of the Referee, the phrase "but except for the case of the Brownian motion considered in Sec. 4.4" has been added in revision.

Typo

8) P.8 l.219 "... be be . . . "

9) P.11 l.314 "... to constraint . . . " → "... to constrain . . . "

10) P.21 l.582 "... with by . . . "

11) P.22 l.622 "... "$\ldots \partial^2\phi/\partial\phi^2$" → "$\ldots \partial^2 p/\partial\phi^2$"

12) P.26 l.730 "... questioned form"

Various typos have been corrected as pointed out by the Referee. We much appreciate the careful proof reading given. Furthermore, for finalizing our manuscript thorough proof reading has also been applied to remove further typos and grammatical errors.