Interactive comment on “DATeS: A Highly-Extensible Data Assimilation Testing Suite” by Ahmed Attia and Adrian Sandu

K. Law (Referee)
lawkj@ornl.gov

Received and published: 18 May 2018

The authors and the first referee have done a very good job of summarising the contribution of this paper. I second the very relevant requests of the first referee, and I would like to additionally raise a few other points.

Perhaps the most important point to touch on here is the potential applicability of DATeS as a benchmarking tool. The most challenging aspect of developing community-wide benchmarks might be the abundance of tuning parameters required to get "optimal" performance. Please discuss this point, and initialise some default cases. For example, if you have Lorenz 63 with canonical parameters, observations every h time steps, and a given observational noise and prior, then the "best" you can do with EnKF is
using X set of tuning parameters. The best you can do with 4DVAR is with Y set of tuning parameters. And so on... Of course one has to define an error metric, and optimality of tuning parameters will presumably change, but something like RMSE and rank histogram of the innovation (or truth in the case of simulated data) is a good start. As the software is used this can then be updated by the community. When a new algorithm is proposed it can then be sized up against the community-endorsed benchmarks. This is of course asking a lot from both the software and the community, but it is good to aim high. Such benchmarking tool is needed and would be very useful.

Also, if you are aiming for the posterior distribution in a general non-Gaussian case, for example as a benchmark against which to evaluate other algorithms, or to compute higher moments, multiple modes, or tail probabilities, then the model and tuning parameters can again be recorded and the results can be challenged (for example, in case a mode has been missed) as new and improved methodology is introduced for general posterior inference and as computers getter bigger, stronger, and faster. This approach can in principle manifest reproducible, evolving, and community-endorsed gold-standard benchmarks, which can be used in addition to such metrics as RMSE and rank histograms in vetting existing and new algorithms in various scenarios.

Specific comments:

* p2, line 15: as a gateway for someone new to the field or interested in learning about the methodology without all the complexities, one could also mention some extremely simple software, for example the pedagogical applied mathematics reference on data assimilation Law etal 2015 provides a concise set of codes including examples of many of the modern data assimilation algorithms distilled to the level that they are single Matlab scripts of fewer than 50 lines which run in a fraction of a second.

http://tiny.cc/damat

* Sec 2: this presentation is not quite complete. It needs to be considerably cleaned up and made complete. For example, you do not state how the model enters the
picture: is it the case that there is a single state $x_k^a$, for analysis, and $x_{k+1}^b = \mathcal{M}_{k,k+1}(x_k^a)$? You do not define $^\text{rm true}$, and it vanishes in (3). Do you need it?

* p4, line 8: minimum variance estimator: even if the Gaussian background assumption holds, and you have an infinite ensemble, this is not the minimum variance estimator, which is the posterior mean. It is the minimum variance estimator among those which are linear in the observation. This does not include the posterior mean in case $\mathcal{H}_k$ is nonlinear. Same comment holds at the end of p4, relating to smoothing.

* p5, line 17: "not generally efficient" -> "not generally considered to be efficient". A lot of recent work has illustrated the potential applicability of particle filters for high-dimensional problems, although they have not yet been used operationally. In addition to the reference suggested by the other referee, see below references by Crisan, Jasra, van Handel, Poterjoy, Potthast, and van Leeuwen.

* p5, around line 20: it is important to point out here that MCMC is generally applicable only to static problems, i.e. a single posterior distribution for a single window of observations, with a known prior/background. Once you step forward to the next window, you will not in general have a closed form or even a good approximation for the new prior/background (and it will most likely not be Gaussian). One needs to therefore be careful when applying MCMC in a recursive/filtering context. I'm not familiar with the cited papers although I'm sure they deal with this in a sensible way. But it needs to be mentioned here. And, nonetheless MCMC methods are useful as a benchmarking tool for a single assimilation window with a known background – see Law and Stuart 2012.

* p7, line 6: "It is common in DA applications to assume a perfect forecast model, a case where the model is deterministic rather than stochastic." Perhaps you mean just "It is common in DA applications to assume the model is deterministic rather than stochastic."? Here inflation will of course be needed for ensemble methods in order
to have stability, and in any case the background covariance incorporates some sort of model error, so I don’t see this as a perfect model scenario.

* Related to the above point, localisation and inflation should be mentioned explicitly, due to their key roles in the field. Presumably they need to be incorporated within the analysis algorithm component.

*p8, line 14: state-size square matrices! Surely this is limited to very small problems, so some discussion of low-rank approximation of these matrices is important, and to be robust the code should not even try to construct these as full matrices if the state is high-dimensional.

* p14: define DEnKF


