Review of ‘Application of ensemble transform data assimilation methods for parameter estimation in nonlinear problems’, by Sangeetika Ruchi, Svetlana Bubinkina and Jana de Wiljes.

Generall comments

This manuscript describes an overview and comparison of a number of data-assimilation methods for parameter estimation in nonlinear problems. It describes the tempered ensemble transform particle filter as an alternative to Ensemble Kalman Inversion. To reduce computational costs, the authors introduce an entropy-inspired regularisation factor to underlying transport problem. The application of a Sinkhornfixpoint iteration reduces the computational costs considerably. This is a new addition to existing particle filters. The manuscript further discusses two different hybrid approaches that apply a Kalman-inversion proposal step in the particle filter. The menchmark of these methods against a Markov-Chain Monte Carlo approach as well as the assessment of their computational costs is a valuable and significant result. The description of the computational complexity help to quantify the efficiency of the methods. An example of Darcy flow through a synthetic reservoir (aquifer) illustrates the quality of the parameter estimate and the general performance of the methods.

This is an interesting manuscript that deserves publication. The comparison of the different methods, and the clear explanation of the underlying mathematics will help data-assimilation practitioners to make a balanced choice between several data-assimilation methods. By presenting original solutions, the manuscript inspires those who develop data-assimilation methods to further refinement of methods or innovative approaches. The language is clear and concise, but not all symbols used are explained, and some terms could be clarified further. The paper puts the obtained results into context, but could relate the results more to the field of the proposed application and include relevant references of that field. The text reads well and the figures are of good quality.

I hesitate between ‘accepted with minor revision’ and ‘accepted with major revision’. The manuscript would be publishable with only minor text adaptations, but I feel it could have a much larger impact if the authors would change the manuscript more substantially. There are two main items that I would encourage the authors to address. In addition to this, I have a list of minor issues, mostly textual.

Specific comments

<u>Terminology and description of example</u>: As this paper could be of particular use to practitioners in the reservoir-engineering domain, I would encourage the authors to make the text more accessible to those. This could be done by changing or clarifying the use of certain terms and adding key references to explain the methods. For example, in reservoir engineering, the term Ensemble Kalman Filter is more commonly used than the term Ensemble Kalman Inversion; adding a number of key publications on this method and derived methods would help to set the scene and provide the reader with further background information. Also, those using data assimilation in practical applications will be

interested in the actual values of the properties, and less likely to work on dimensionless problems. Relating the symbols to physical quantities would make this manuscript more accessible and relevant to them.

Presentation of the methodologies: The mathematical rigour and expertise of the authors would allow them to not only compare the performance of the methods in an empirical sense, but also place them in the overall framework of data-assimilation methods for parameter estimation. The manner in which the hybrid EKI-TETPF method is presented, is presented as a particle filter with several 'fixes' (namely a) tempering, b) a Sinkhorn approximation, and c) an EKI proposal). Can the authors think of a way to present the methods from a holistic viewpoint, making clear that these 'fixes' are essential ingredients of the methods in order to perform a consistent and also effective parameter estimation? The abstract reads "Gaussian approximations [….] often produce astonishingly accurate estimations despite the inherently wrong underlying assumptions": Can you discuss more explitly how the assumption of Gaussianity affects the outcome, perhaps by illustrating how non-Gaussian the distributions really are, or how the different methods deal with non-Gaussianity and/or non-linearity?

Technical corrections (language, minor items)

- Please pay attention to the use of hyphens in compound modifiers. For example, the title could read 'Application of ensemble-transform data-assimilation methods for parameter estimation in nonlinear problems'. Other places where this would help: 'high-dimensional problems', 'entropy-inspired', 'highly-correlated samples', 'an easy-to-sample form', etc.
- The term 'ensemble Kalman inversion' is used to a method that is known by many as 'ensemble Kalman filtering'. I suggest to clarify that EKI is used as equivalent to the ensemble Kalman filter. Page 2, line 38 and/or in the paragraph startig on p.8, line 201: suggest to add one of the key references for ensemble Kalman inversion or ensemble Kalman filtering, so readers can find out more about the method.
- Page 1, line 3: abstract: 'inherently wrong': the Gaussian assumptions are not always wrong, so suggest to reformulate: 'depsite the simplifying assumptions' or something along these lines. Alternatively, demonstrate in the manuscript that these assumptions are actually wrong.
- Page 2, line 55: "the number of required intermediate steps and the efficiency of ETPF still depends on it". What does "it" refer to?
- Page 5, line 118: Crank-Nicholson pcn-MCMC: explain what pcn means here.
- Page 5 line 130: the scalar theta -> the scalar theta in Equation 5
- Page 6, line 152: where the minimum is compute -> where the minimum is computed
- Page 7 line 181 One the other hand -> on the other hand
- Page 8, line 204: estimation of posterior -> estimation of the posterior
- Page 8, line 205-215: make sure to list and clarify all symbols used.
- Page 9, line 232: make clear how to choose beta
- Page 9, line 239: EKI as an more elaborate -> as a more elaborate

- Page 9, line 240: Computational complexity: the estimates of computationa complexity of the various methods is very useful. I suggest to include a table that illustrates the computational complexity of all methods/variations and include a few sentences on this in the 'Conclusions' part.
- Page 9, line 244: the example is dimensionless. Suggest to relate this to an example in which you list a number of typical values. You can then also mention that channels such as shown in Fig 1 can be found in fluvial rock formations that form aquifers or reservoirs.
- Page 9, line 247: please make clear what physical variable (rate, pressure) the source term represents
- Page 9 line 267: on an NxN grid: a potential user would like to know what is the scale, and spatial dimension. Suggest to give the value of N earlier than you do now (on page 10, line 273).
- Page 10, line 255: the choice of P for parameterisation is not very practical, as you are also using this letter for pressure
- Page 11, line 285: please make clear what property is being observed
- Page 12, line 310: we plot box plot -> we plot a box plot; using Sinkhorn approximation -> using a Sinkhorn approximation
- Page 12, line 313: TESPF outperforms: has a lower RMSE? Is smoother? How do you define a good performance?
- Page 12 line 320: estimate well mot -> estimate well not
- Page 13, figure 2: it is good to see the box plots for permeability, I would have liked to also see this for rate (observed state variable)
- Page 14 figure 4: please label the x axis (it is described in the caption but would be good to see in the figure, too).
- Page 14, line 332: these are very interesting results. I would value a discussion on how to find the best beta value in a realistic application of the hybrid method. In a synthetic case, this value can be determined, but how would you deal with this when assimilating real data? This discussion could be added in 'conclusions' (page 17)
- Page 14 line 344: we plot box plot -> we plot a box plot (or 'the box plot shows…')
- Page 15, line 363: the application that you show, would be referred to as a 'reservoir engineering' application, or a 'hydrological' application, not as a 'geophysical application'. (In oil- and gas industry, reservoir engineering is about flow in porous media, while geophysics is about the use of seismic and other geophysical data and propagation of sound waves. In hydrology, permeability is usually replaced by hydraulic conductivity, so by using permeability your example would be more familiar to those working in reservoir engineering.)