dageo: Data Assimilation in Geosciences

- **Dieter Werthmüller**[1,2], 0000-0002-8575-2484
- **Gabriel Serrao Seabra**[1,3], 0009-0002-0558-8117
- **Femke C. Vossepoel**[1], 0000-0002-3391-6651

1: TU Delft, NL; 2: ETH Zurich, CH; 3: Petroleo Brasileiro S.A. (Petrobras), BR

This manuscript was submitted to the *Journal of Open-Source Software* (JOSS, joss.theoj.org) on 2025-03-06. It was rejected on a preliminary scope query on 2025-04-02, on the ground that the submission was deemed *«too small in terms of substantial scholarly effort to fit JOSS guidelines»*. See the pre-review issue on github.com/openjournals/joss-reviews/issues/7879.

We publish it here on EarthArXiv to make it nevertheless available to the community. We might consider re-submission to JOSS at a later stage, once more functionality is added to `dageo`.

`dageo` (at `v1.1.1` at the time of this pre-print):

- Repository: github.com/tuda-geo/dageo
- Zenodo: doi.org/10.5281/zenodo.14264408
- Documentation: tuda-geo.github.io/dageo

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Summary

Data Assimilation combines computer models with real-world measurements to improve estimates and forecasts of dynamical systems such as oceans, atmosphere, and subsurface reservoirs. The Python package `dageo` is a tool to apply data assimilation in geoscience applications. Currently, it encompasses the Ensemble Smoother with Multiple Data Assimilation (ESMDA) method and provides tools for reservoir engineering applications. The package includes localization to help with relatively small ensembles, Gaussian random field generation for generating heterogeneous parameter fields, and integration capabilities with external simulators.

An additional feature of `dageo` is a two-dimensional single-phase reservoir simulator that models pressure changes over time and well behavior for both injection and production scenarios. This simulator is particularly useful for educational purposes, providing a practical platform for students and researchers to learn and experiment with data assimilation concepts and techniques. The software features an online documentation, with examples that guide users through learning ESMDA concepts, testing new ideas, and applying methods to real-world problems.

ESMDA

Ensemble Smoother with Multiple Data Assimilation (ESMDA, Emerick and Reynolds (2013)) is the first data assimilation method implemented in `dageo`. However, `dageo` is general enough so that other data assimilation methods can and will be added easily at a later stage. While ESMDA is theoretically straightforward, practical implementation requires careful handling of matrix operations, ensemble management, and ensuring numerical stability. The algorithm works by iteratively updating an ensemble of model parameters to match observed data following

$$z_j^a = z_j^f + C_{\mathrm{ZD}}^f \left(C_{\mathrm{DD}}^f + \alpha C_{\mathrm{D}}\right)^{-1} \left(d_{\mathrm{uc},j} - d_j^f\right) \ , \qquad (1)$$

where z^a represents the updated (analysis) parameters, z^f the prior (forecast) parameters, and the C terms represent various covariance matrices for the data and the model parameters (subscripts D and Z, respectively). The ESMDA coefficient (or inflation factor) is denoted by α, the predicted data vector, which is obtained by applying the observation operator to the model output, is d^f and d_{uc} represents the perturbed observations (Burgers et al., 1998) for the j-th ensemble member, generated by adding random noise to the original observations for each iteration, as proposed in the original ESMDA method. Note that we assume to have an identity observation operator that translates the model state to the equivalent of the observations, so it is omitted in the equation (for more details in this regard see Evensen et al. (2022)). The equation is evaluated for i steps, where i is typically a low number between 4 to 10. The α can change in each step, as long as $\sum_i \alpha_i^{-1} = 1$. Common are either constant values or series of decreasing values. Note that while this explanation describes the parameter estimation problem, it could also be used to estimate the state estimation or both. The algorithm's implementation in `dageo` includes optimizations for efficient computation of the covariance matrix and allows to easily parallelize the forward model.

Key Features and Applications

Existing implementations often lack documentation and informative examples, creating barriers for unexperienced users of data assimilation methods. These challenges are addressed in `dageo` through several key innovations: it provides a robust, tested ESMDA implementation alongside a built-in, simple reservoir simulator, while offering and showcasing in the gallery, as a key feature, integration capabilities with external simulators. The gallery contains an example of this integration with the *open Delft Advanced Research Terra Simulator* `open-DARTS` (Voskov et al., 2024), a state-of-the-art, open-source reservoir simulation framework developed at TU Delft. It demonstrates how `dageo` can be used with industry-standard simulators while maintaining its user-friendly interface. The code itself is light, building upon NumPy arrays (Harris et al., 2020) and sparse matrices provided by SciPy (Virtanen et al., 2020), as only dependencies.

While other ESMDA implementations exist, e.g., `pyesmda` (Collet, 2022), `dageo` distinguishes itself through comprehensive documentation and examples, the integration of a simple but practical reservoir simulator, the implementation of advanced features like localization techniques for parameter updates, Gaussian random field generation for realistic permeability modeling, and a focus on ease of use, making it suitable for educational applications. This makes `dageo` a unique and valuable tool for both research and teaching. The software has been used in several research projects, including reservoir characterization studies at TU Delft, integration with the open-DARTS simulator for geothermal applications, and educational workshops on data assimilation techniques (e.g., Saifullin et al., 2024; Seabra et al., 2024). These applications highlight the software's versatility and its ability to address a wide range of challenges in reservoir engineering and geoscience.

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