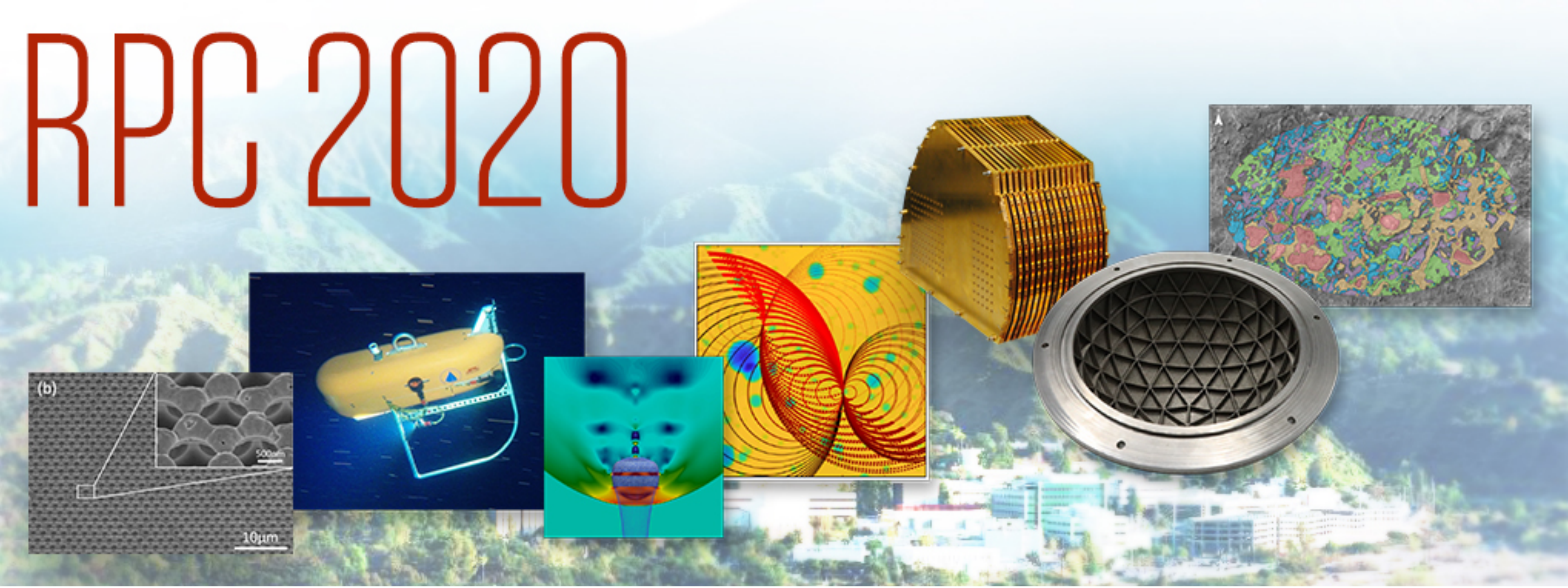


# Virtual Research Presentation Conference

## Advancing Uncertainty Quantification using new Nonlinear, non-Gaussian Mathematics

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**Program: SURP**

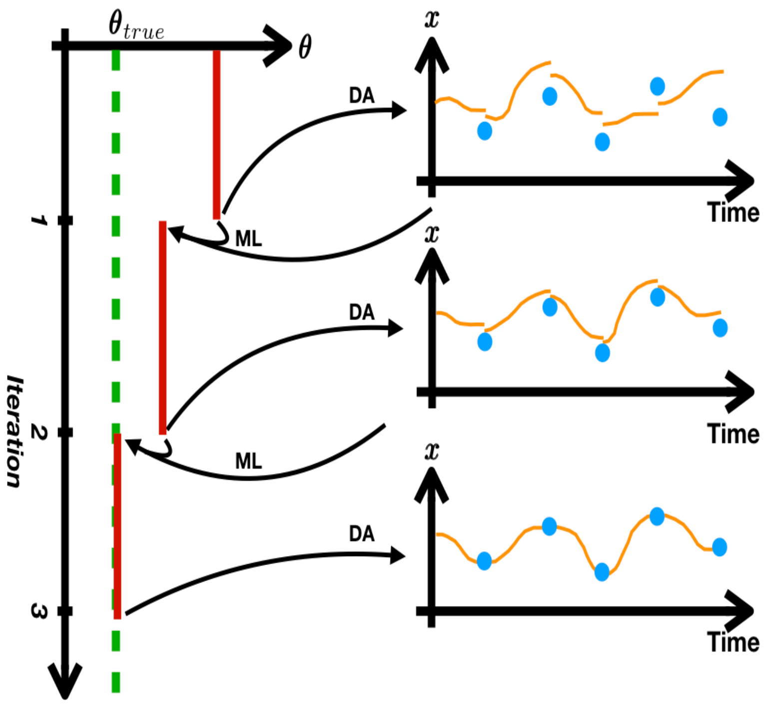
Assigned Presentation #RPC-130

**Jet Propulsion Laboratory**
California Institute of Technology

# Tutorial Introduction


### Abstract

This project brings new mathematics into practical data assimilation (DA) and uncertainty quantification (UQ) applications that commonly arise in Earth Science. We develop a joint atmospheric state and model parameter estimation framework that combines traditional data assimilation with machine learning. We apply the framework to idealized nonlinear models to quantify model sensitivity to changes in model construction and initial conditions. This research requires new mathematics, new computational methods, and an understanding of atmospheric physics. The methods developed for this particular research question are expected to be extensible to a wide range of remote sensing and numerical modeling topics.


Schematic for the proposed simultaneous state and parameter estimation algorithm. The left graph shows the iterations (vertically) of the machine learning (ML) algorithm as it optimizes the parameters θ. At each iteration, a data assimilation (DA) method is used to update the model outputs (orange lines) based on the observations (blue dots).

# Problem Description

**Context (Why this problem and why now)**

- In DA, typically the state of the system is updated, but the model construction is not. This means that the model error is not addressed. Estimation of the state is often straightforward, but the model error is often complex and nonlinear.
- It is necessary to develop new methodologies that are capable of informing both the state of the system and the model itself.

**SOA (Comparison or advancement over current state-of-the-art)**

- The state of the art in simultaneous state and parameter estimation is to simply re-use data assimilation methods, and append a list of model parameters to the model state vector.
- Our approach solves joint linear (state estimation) and nonlinear (model parameter estimation) using a combination of traditional data assimilation and machine learning methodologies. The techniques we are using have never before (to our knowledge) been applied to problems in Earth System Science.

**Relevance to NASA and JPL (Impact on current or future programs)**

- Quantification of uncertainty is a crucial part of the design of any new mission, and many UQ efforts founder on the rocks of nonlinearity and model error / state error interaction.
- The development of a new set of tools, generally applicable to a wide range of models and research questions, will enhance JPL’s ability to robustly determine in advance the information contained in a set of proposed measurements.
- A more robust treatment of uncertainty will lend additional credence to JPL’s mission proposals.

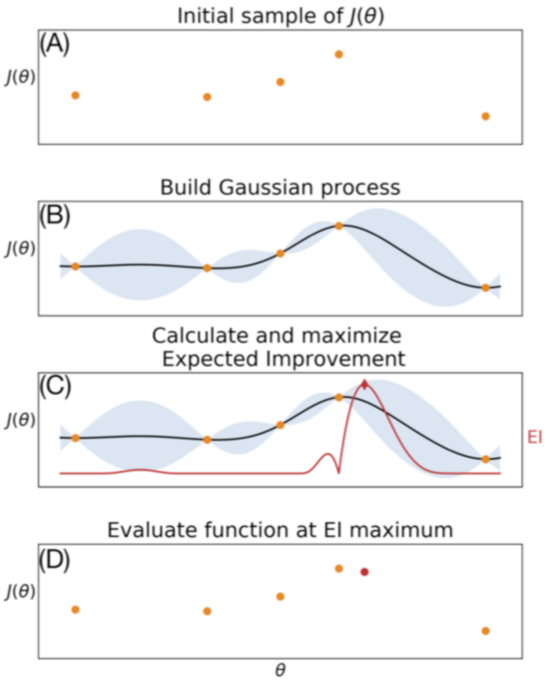
# Methodology

**Formulation, theory or experiment description**

- Utilize ensemble Kalman filter methods for (linear) state estimation
- Implement Global Bayesian Optimization for (nonlinear) model parameter estimation. GBO uses statistical emulators to approximate the model-observation mismatch and find optimal parameter values
- Test the combined EnKF – GBO methodology in two well-known nonlinear models (Lorenz, 1963; 1996)

**Innovation, advancement**

- While EnKF has been used extensively for state estimation, it often fails for nonliear model parameters
- GBO has been used in optimizing advertising schemes online, but has not yet been applied to Earth System Science




Schematic depicting a single GBO. (A): begin with a set of realizations of the objective function J(θ) (orange dots). (B): Fit a Gaussian process to these points; shown are the GP mean (black) and 2-sigma (blue). (C): Calculate Expected Improvement (EI; red line), and propose a new parameter sample θ∗ (red dot). (D): Evaluate the objective function at the proposed sample, and add the point (θ∗,J(θ∗)) to the set of objective function realizations.

# Results

### Accomplishments versus goals

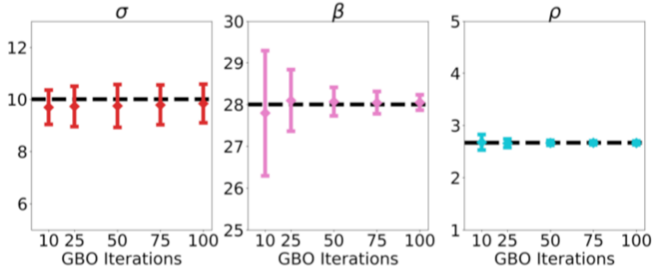
- We have met all of the first year goals for this collaborative project. The GBO algorithm was successfully applied to both numerical models, and the results were presented at the 2019 American Geophysical Union Fall Meeting, and have been written up for submission to peer review.
- We will not be able to meet our year 2 and 3 goals, as the student and moved on to bigger and better things.

### Significance

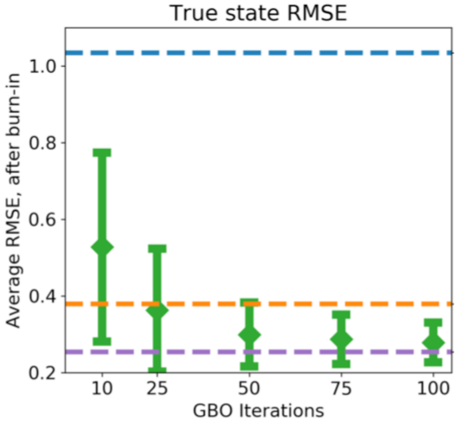
- The GBO algorithm functioned far better than traditional parameter estimation methods
- The combination of linear + nonlinear algorithms has great potential for application to a suite of problems with jointly linear and nonlinear characteristics.

### Next steps

- Submission of a manuscript describing the results for peer review
- Seeking continued funding to support continuation of this work and application to atmospheric models




Parameter estimates from GBO, as a function of GBO iteration for each of 3 parameters in the Lorenz ‘63 model.




RMS error between the EnKF estimates and the true state of the system as a function of number of GBO iterations. Best guess from a priori (blue), augmented state (orange), GBO results (green), and perfect model (purple).

# Publications and References

Lunderman, S., M. Morzfeld, and D. J. Posselt, Simultaneous parameter and state estimation by derivative-free optimization of ensemble Kalman filter residuals. Poster presented at the 2019 American Geophysical Union Fall Meeting, San Francisco, CA, 9-13 December 2019.

Lunderman, S., M. Morzfeld, and D. J. Posselt, 2020: Global Bayesian Optimization in Data Assimilation. J. Discrete and Continuous Dynamical Systems, In Preparation.