UQ study of parameter sensitivity in POP

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OMWG

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Outlines

• Introduction – LLNL UQ pipeline
• Climate Model Uncertainty Quantification @ LLNL
  ➢ UQ studies across CESM components
• UQ sensitivity study of POP:
  ➢ Methodology – learning from POP failures
  ➢ Examples and applications
• Conclusions
• Future work
Climate Model Uncertainty Quantification @ LLNL

- Perturbed parameter ensembles of the Community Earth System Model (CESM)
- Constrain parameter PDFs with satellite observations
- Calculate PDF of climate sensitivity
- Climate change UQ using coupled models and LLNL's UQ Pipeline

Example of a sensitivity map calculated using the Morris method on CAM3 in a high dimensional parameter space.

Example of a response surface generated using polynomial chaos expansions on CAM3 ensembles. (rendering by Kwei-Yu Chu)
UQ simulations across *Community Earth System Model* (CESM) components

- CESM is one of the most widely used “high end” climate models in the United States
- 3-D models for the ocean, atmosphere and sea ice

Our UQ ensembles
- >5,700 simulations
- >92,000 climate model years
- 54 parameters sampled
- >450 TB of monthly-avg data
# UQ Simulations Across CESM Components

<table>
<thead>
<tr>
<th>CESM Components</th>
<th>Purpose</th>
<th># of Params</th>
<th># of Sims</th>
<th>Sim-years</th>
<th>Archive</th>
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</thead>
<tbody>
<tr>
<td>CAM</td>
<td>Parameter sensitivity, calibration of CAM</td>
<td>21-29</td>
<td>over 3,300</td>
<td>over 40,000</td>
<td>~50TB</td>
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<tr>
<td>CAM+CICE+SOM</td>
<td>Parameter sensitivity, calibration of CICE</td>
<td>7</td>
<td>70</td>
<td>2,800</td>
<td>~5TB</td>
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<tr>
<td>CAM+CICE+SOM</td>
<td>Climate sensitivity UQ</td>
<td>12-36</td>
<td>~600</td>
<td>~19,000</td>
<td>~35TB</td>
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<tr>
<td>POP+CICE+data Atm</td>
<td>Parameter sensitivity of POP</td>
<td>18-22</td>
<td>~540</td>
<td>~6,200</td>
<td>~105TB</td>
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<tr>
<td>CAM+CICE+POP</td>
<td>UQ on fully-coupled system</td>
<td>up to 53</td>
<td>on-going</td>
<td>on-going</td>
<td>on-going</td>
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</tbody>
</table>

Computing resources for UQ ensembles provided through Livermore Computing
POP Set up

- Coupled CICE 4.0 + POP 2.0 runs with data Atm
- gx1v6, 60 vertical levels, 1h time step
- Normal year Large and Yeager climatology forcing
- 540 runs, 20-yr integration
- Anisotropic viscosity horizontal mixing (Smith and McWilliams, 2003),
- G&M isopycnal tracer horizontal mixing (Gent and McWilliams, 1990),
- KPP vertical mixing (Large et al., 1994),
- Sub-mesoscale and mixed layer eddies (Fox-Kemper et al., 2008)
- Abyssal tidal mixing (Jayne, 2009)
- Diffusion type of convective adjustment
# POP parameters used in the UQ study

<table>
<thead>
<tr>
<th>#</th>
<th>Parameter Name</th>
<th>Range</th>
<th>Description</th>
<th>Namelist File</th>
<th>Namelist</th>
<th>Src*</th>
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<td></td>
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<td>Low</td>
<td>Default</td>
<td>High</td>
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<td>hmix_gm</td>
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<td>0.13</td>
<td>0.50</td>
<td>pop2_in</td>
<td>vmix_kpp</td>
</tr>
</tbody>
</table>

* Source => D: Danabasoglu, G; J: Jochum, M; T: Tokmakian, R
^ Values correlated; varied with identical values.
Ocean Heat Transport – Ensembles and Observations

Northward Heat Transport (Global) [1993-2003]

Observations from Fasullo & Trenberth, 2008
Analysis of Failed POP Runs

- About 10% of our simulations failed
  - 540 simulations
  - 494 succeeded
  - 46 failed
- Lack of convergence
- What parameter combinations caused the failures?
- Can we predict (assign probabilities) future failures?

\[ P(\text{fail}) = 1 - P(\text{success}) \]

Used SVMs to Train Probabilistic POP Classifiers
- 18 features
- 1 = fail, 0 = success
- cross validation
- bootstrapping to assess performance
Failure Probability

- Binary classification problem
  \( C_f = \text{simulation failure} \)
  \( C_s = \text{simulation success} \)

- Failure probability from Bayes’ rule
  \[ P(C_f|x) = \frac{1}{1 + \exp(-\lambda(x))} \]
  where \( x = \text{model parameter values} \) and \( \lambda = \log(\text{likelihood-odds ratio}) \).
Descriptive Analysis

Scatter plots of 540 simulation outcomes versus pairs of normalized values of four parameters. Simulation failures strongly correlate with parameter values, but also overlap with many successful simulations. Advanced statistical methods are used to separate the overlaps.
SVM Classification

Support Vector Machines (SVMs) are used to assign a simulation to $C_f$ or $C_s$ for input vector $\mathbf{x}$.
- effective for high dimensions
- nonlinear classification (see left)

Use \texttt{LIBSVM} package ($C$-SVC, radial basis kernels, probability estimates)

Committee of SVM classifiers through bootstrap aggregation ("\textit{bagging}").

$$
\mu_c = \frac{1}{N_b} \sum_{i=1}^{N_b} \mathcal{P}_i(C_f|\mathbf{x})
$$

$$
\sigma^2_c = \frac{1}{N_b} \sum_{i=1}^{N_b} \left[ \mathcal{P}_i(C_f|\mathbf{x}) - \mu_c \right]^2
$$
Classifier Performance

- Studies 1 & 2 ⇒ train SVM classifiers
  Study 3 ⇒ independent validation

- Study 3 simulation outcomes predicted using three decision criteria
  \( D \equiv \text{variable} \geq \text{threshold} \).
  \[
  D_{\text{avg}} \equiv \mu_c \geq 0.5 \\
  D_{\text{sum}} \equiv \mu_c + \sigma_c \geq 0.5 \\
  D_{\text{snr}} \equiv \mu_c / \sigma_c \geq 3.53
  \]

- Results summarized in “confusion matrix” on the right.

- SVM classifiers successfully predict simulation failures (accuracy 96.7% and 97.8%).

<table>
<thead>
<tr>
<th>Actual</th>
<th>True Positives</th>
<th>False Positives</th>
</tr>
</thead>
<tbody>
<tr>
<td>Failure</td>
<td>( D_{\text{avg}} = 9 )</td>
<td>( D_{\text{avg}} = 1 )</td>
</tr>
<tr>
<td>Success</td>
<td>( D_{\text{sum}} = 11 )</td>
<td>( D_{\text{sum}} = 3 )</td>
</tr>
<tr>
<td></td>
<td>( D_{\text{snr}} = 12 )</td>
<td>( D_{\text{snr}} = 2 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Predicted</th>
<th>False Negatives</th>
<th>True Negatives</th>
</tr>
</thead>
<tbody>
<tr>
<td>Success</td>
<td>( D_{\text{avg}} = 5 )</td>
<td>( D_{\text{avg}} = 165 )</td>
</tr>
<tr>
<td>Failure</td>
<td>( D_{\text{sum}} = 3 )</td>
<td>( D_{\text{sum}} = 163 )</td>
</tr>
<tr>
<td></td>
<td>( D_{\text{snr}} = 2 )</td>
<td>( D_{\text{snr}} = 164 )</td>
</tr>
</tbody>
</table>

14 actual failures | 166 actual successes
Sensitivity Analysis of the Simulation Failures

Network Diagram of Sobol Indices

Total variance is decomposed:
\[ v_t = \sum v_i + \sum v_{ij} + \sum v_{ijk} + \ldots \], where
- \( v_i \) = variations from parameter \( i \)
- \( v_{ij} \) = co-variations from parameters \( i \) and \( j \)

Variance contributions on a network graph.
- node diameter \( \propto \frac{V_i}{V_{tot}} \) (main effects)
- edge width \( \propto \frac{V_{ij}}{V_{tot}} \) (interactions)

(higher orders can also be displayed on the same graph)

Sensitivity analysis methods in the UQ Pipeline were applied to the POP.

Sensitivity measures are used to identify important model parameters.

We ranked the importance of 18 uncertain parameters across 34 climate model outputs of interest.

++ = important to many outputs  + = important to at least one output
POP MOC

Global

Atlantic

MAXMOC_GLO_YR10

MAXMOC_ATL_YR10
Drake Passage Transports
Conclusions

UQ technology potential:

- To use the probability classifiers in future planning of ensembles by prediction the model failure or success given a certain input parameters combination;
- To reduce the uncertainty of the input parameters;
- To study the model solution sensitivity to input parameters variations and their combinations across the different modules of the model component or the fully coupled climate system.
Future work

Data Archive @ LLNL
Contact: Don Lucas, lucas26@llnl.gov
    Curt Covey, covey1@llnl.gov
Future Plans: Data available at LLNL ESG Portal
THANK YOU!

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