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Autotuning E3SMv3

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- **Motivation**: Expedite and formalize E3SMv3 tuning.
  - Identify an optimal tuning parameter set for the atmosphere to assist expert model tuning.
  - Identify plausible alternative parameter sets.
  - Timeline: 6-12 months after code freeze in early 2023.
- **Setup:**
  1. Sample E3SM by running 100's of E3SM forward simulations with ~5 perturbed tuning parameters.
     - Prescribed present-day SST, ~5-10 yrs.
  2. Create a surrogate model.
     - Input: uncertain E3SM model parameters.
     - Output: climatologies of E3SM spatial fields on a 2-D grid.
  3. Optimize and calibrate parameters by sampling the surrogate model
     - Identify parameters that minimize the cost function between surrogate-predicted spatial fields and observational fields
  4. Confirm parameter selection by running surrogate-predicted optimal and alternative parameter sets in E3SM.

Expert manual tuning	Automated tuning
Time-consuming (6-12 months)	Less than 6-12 months
Deterministic: one set of "tuned" parameters per model release	Probabilistic: a distribution of parameters per model release OR observational target
Non-reproducible	Reproducible
Computationally expensive	Computationally expensive (upfront only)

E3SM Energy Exascale Earth System Model

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Prototype problem using E3SMv2

Prototype problem

- N=250 10-year E3SMv2 simulations, 5 uncertain atm. parameters
- Surrogate construction using PCA and polynomial chaos

Capabilities

- E3SMv2 parameter sampling (LHS) and ensemble generation using Dakota[1]
- Surrogate construction for E3SMv2 spatial fields using machine learning and reduced order modeling
- Deterministic and and Bayesian calibration for uncertain E3SMv2 parameters against an unlimited number of combined spatial fields
- Visualization as a function of atmosphere parameters

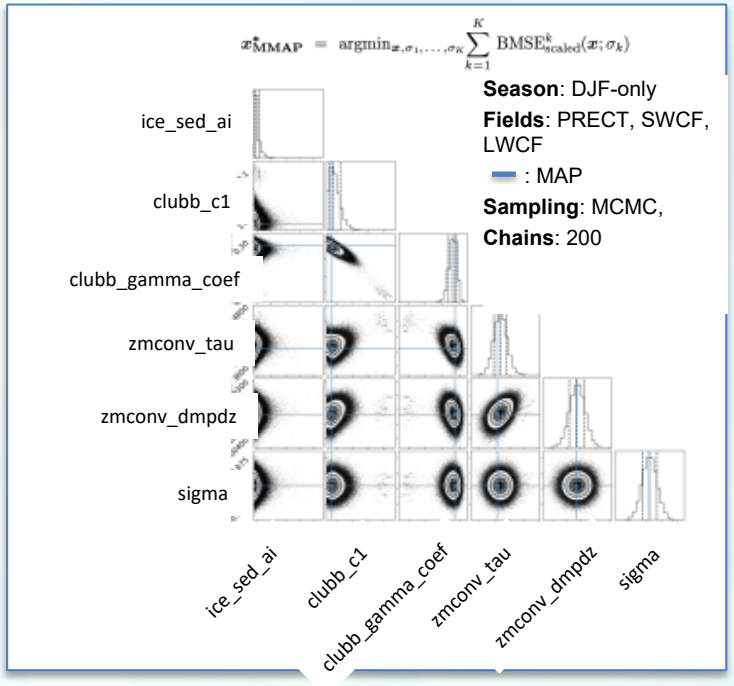

Figure: Corner plot of E3SMv2 parameter calibration against observations.

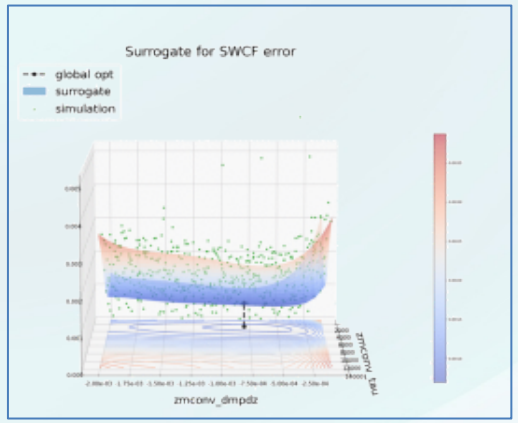

Figure: E3SMv2 SWCF error as a function of two E3SMv2 parameters as predicted by the surrogate (surface) and a ultra-low resolution configuration of E3SMv2 (green dots).

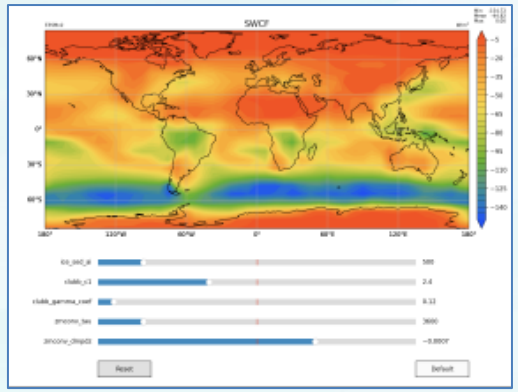

Figure: Screen shot from interactive visualization of fields as a function of E3SMv2 parameters.

Challenges

- Optimization
  - Surrogate errors are relatively large; multiple optimizations are needed to derive a parameter set with skill equal to the expertly tuned E3SMv2
  - Currently working to improve surrogate accuracy by experimenting with the surrogate construction loss function
- Calibration
  - Simple MSE-based objective function assumes fields and grid points are independent and model has no structural bias

More information

- B. Wagman, K. Chowdhary, A. Salinger. *E3SM Atmosphere surrogate construction and calibration using machine learning and reduced order modeling (talk).* SIAM UQ, April 2022
- Ensemble and surrogate software: https://github.com/E3SM-Project/Autotuning-NGD

1. Adams, B.M., Bohnhoff, W.J., Dalbey, K.R., Ebeida, M.S., Eddy, J.P., Eldred, M.S., Hooper, R.W., Hough, P.D., Hu, K.T., Jakeman, J.D., Khalil, M., Maupin, K.A., Monschke, J.A., Ridgway, E.M., Rushdi, A.A., Seidl, D.T., Stephens, J.A., Swiler, L.P., and Winokur, J.G., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.15 User's Manual," Sandia Technical Report SAND2020-12495, November 2021.