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A hybrid machine learning and reservoir simulation approach to modeling gas hydrate systems using open-source software

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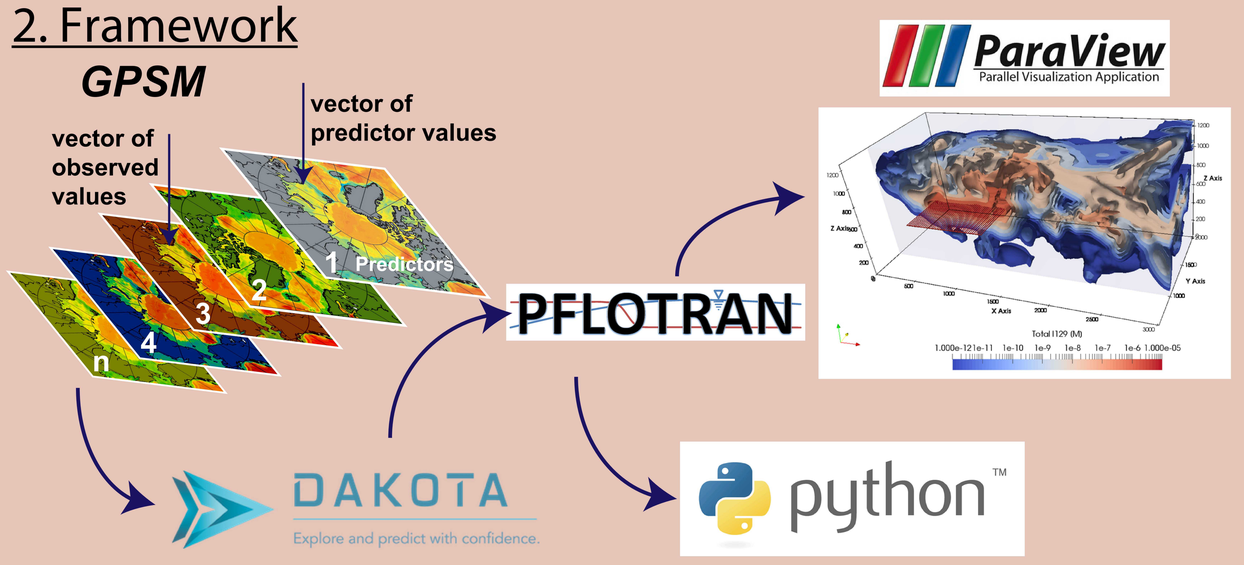
1. Outline

We introduce a framework (**Section 2**) for integrated probabilistic gas hydrate systems modeling, which includes:
- ***parameter distribution prediction*** (e.g. using maching learning with the Global Predictive Seabed Model [GPSM])
- ***parameter sampling*** (using Dakota)
- ***mechanistic simulation*** (using the massively parallel subsurface flow and reactive transport simulator PFLOTRAN)
- ***statistical analysis*** (using Python packages)
- ***3D visualization*** (with ParaView).

For this project (see Frederick et al. poster for more details), we are ultimately interested in predicting occurrence of shallow free gas accumulations in the Arctic. Coarse mapping of gas hydrate and free gas can yield insight into which locations to sub-sample for more rigorous uncertainty quantification.

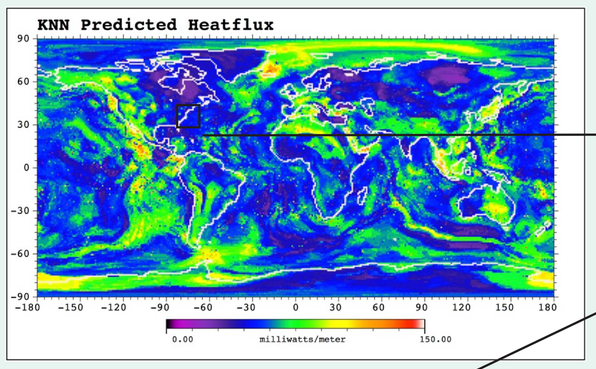
Applying the framework (**Section 3**), we use machine-learned maps (**3A**) of quantities that provide the expected values and distributions of boundary and initial conditions for a series of 1D simulations (**3B**). For a given example, we look at the sensitivity of the base of the gas hydrate stability zone to various inputs (**3C**). This procedure can be followed everywhere on the globe (**3D**). The 1D models run here are non-isothermal, multiphase, and consider in-situ microbial methane generation, sedimentation, and methane diffusion/advection.

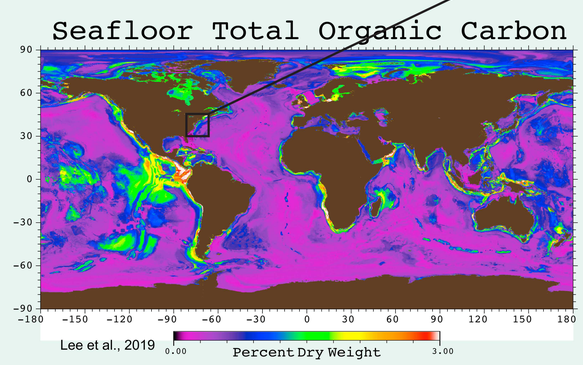
2. Framework



3. Applying the Framework

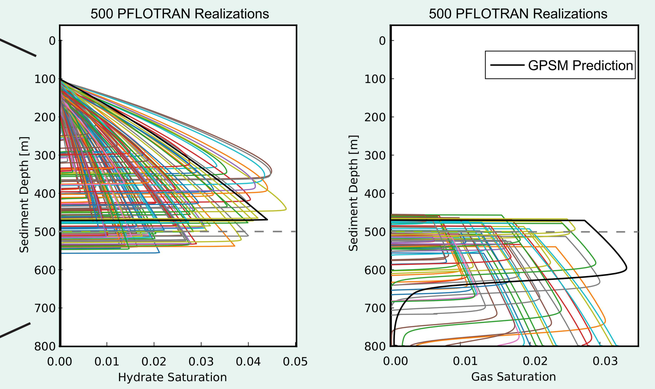
A) **GPSM**



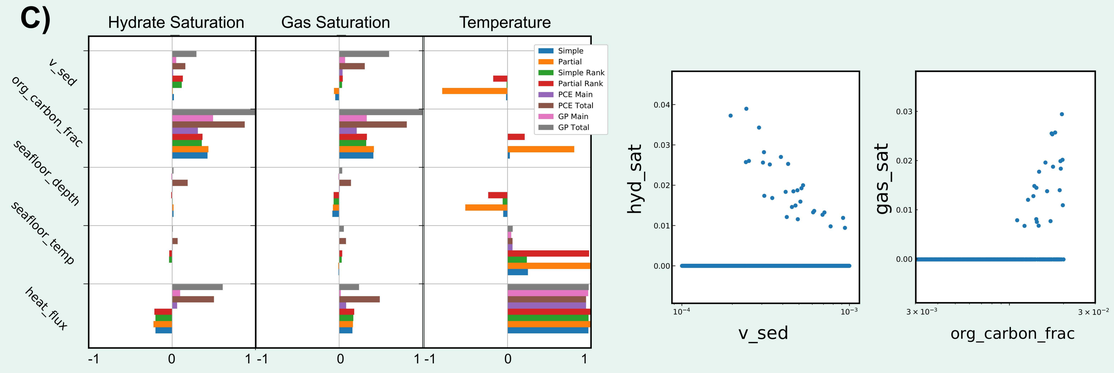


B) DAKOTA Explore and predict with confidence. PFLOTRAN

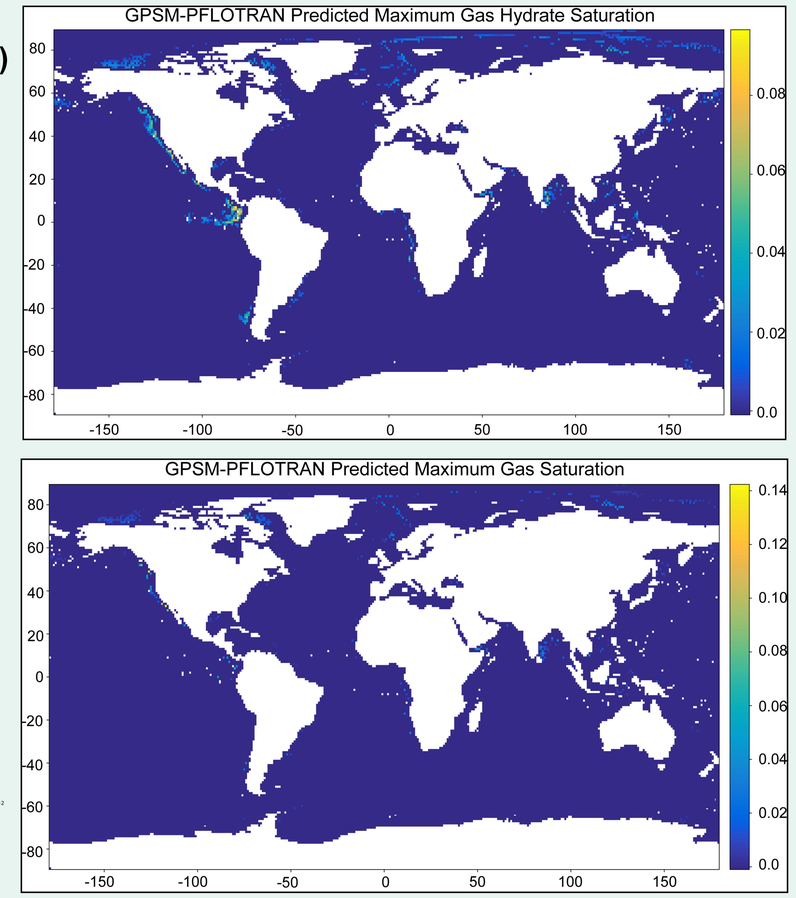
Parameter	Distribution	Min	Max	Current (GPSM)
Seafloor Depth (m)	Uniform	2760	2800	2780
Seafloor Temperature (C)	Uniform	3	5	4
Heat Flux (W/m^2)	Uniform	0.03	0.08	0.06
Sedimentation Rate (m/yr)	Log-uniform	$1x10^{-4}$	$1x10^{-3}$	$2x10^{-4}$
Seafloor Organic Carbon Fraction	Log-Uniform	$1x10^{-3}$	$2x10^{-2}$	$1x10^{-2}$



C)



D)



4. Discussion

We introduce and demonstrate a framework for gas hydrate systems modeling that incorporates geospatial machine learning and mechanistic reservoir simulation to generate probabilistic maps of shallow gas and gas hydrate accumulations in marine environments. Early results indicate that siginificant amounts of gas and gas hydrate could form in Arctic regions due to in-situ microbial generation of methane, but that for most regions of the globe this mechanism is insufficient by itself to generate significant amounts of hydrate or gas.

5. References & Acknowledgements

Lee, T. R., Wood, W. T., & Phrampus, B. J. (2019). A machine learning (kNN) approach to predicting global seafloor total organic carbon. Global Biogeochemical Cycles, 33(1), 37-46.

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