Efficient surrogate construction for response surfaces with steep gradients

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Phase field models are mathematical models used to describe the evolution of microstructures and phase boundaries in materials. In the context of fission gas predictions in nuclear fuel, for example, phase field models play an important role in capturing the intergranular gas phases. When constructing surrogate models of the phase field for uncertainty quantification purposes, specific challenges arise because the steep transitions in the phase field propagate into the parameter space. We investigate a new adaptive sampling scheme for dealing with such problems. In our method, the acquisition function, which plays a crucial role in guiding the selection of new data points to be sampled, is a combination of the surrogate mean and gradient. Furthermore, the massive phase field outputs (often $> 10^6$ grid points across space and time) pose challenges for classic surrogate construction methods such as Gaussian Processes. We discuss parallel partial emulation as a potential solution.