Bayesian optimization and automatic differentiation techniques towards full nonlinear predictions of tokamak performance

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Predictions of fusion performance in upcoming burning-plasma machines such as SPARC and ITER require reliable models of turbulence and transport. However, the high computational cost associated with turbulence simulations has precluded the use of nonlinear gyrokinetic codes within transport solvers, except for a few benchmarking cases (e.g. [1, 2]). While nonlinear, gradient-driven, gryokinetic simulations are performed routinely for the analysis of tokamak experiments and validation studies, the self-consistent profile prediction often requires $10^2 - 10^3$ simulations to solve the inverse problem with standard gradient-based or Newton methods. For the first time, we present a framework based on Bayesian optimization (BO) and automatic differentiation (AD) techniques that can significantly reduce the number of simulations required to attain convergence when solving the transport equations. Gaussian process models with non-stationary kernels are used as surrogates to approximate quasilinear gyrofluid and nonlinear gyrokinetic transport fluxes with critical-gradient behavior and with multi-variate dependencies. The BO workflow ensures the efficient exploration of the parameter space to minimize the number of costly nonlinear simulations, and the use of AD enables the utilization of the exact Jacobian to solve the inverse transport problem with moving targets. Moving targets in the context of transport solvers refer to heating and fueling source profiles that depend on the predicted temperature and density profiles, as well as internal power flows (such as collisional energy exchange) and radiation. Prior to the implementation of this workflow with nonlinear gyrokinetic codes, tests are performed with the TGLF [3] quasilinear gyrofluid model and compared to standard inverse-problem solving methods. Progress on full-nonlinear profile predictions with the CGYRO [4] code will be presented.

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