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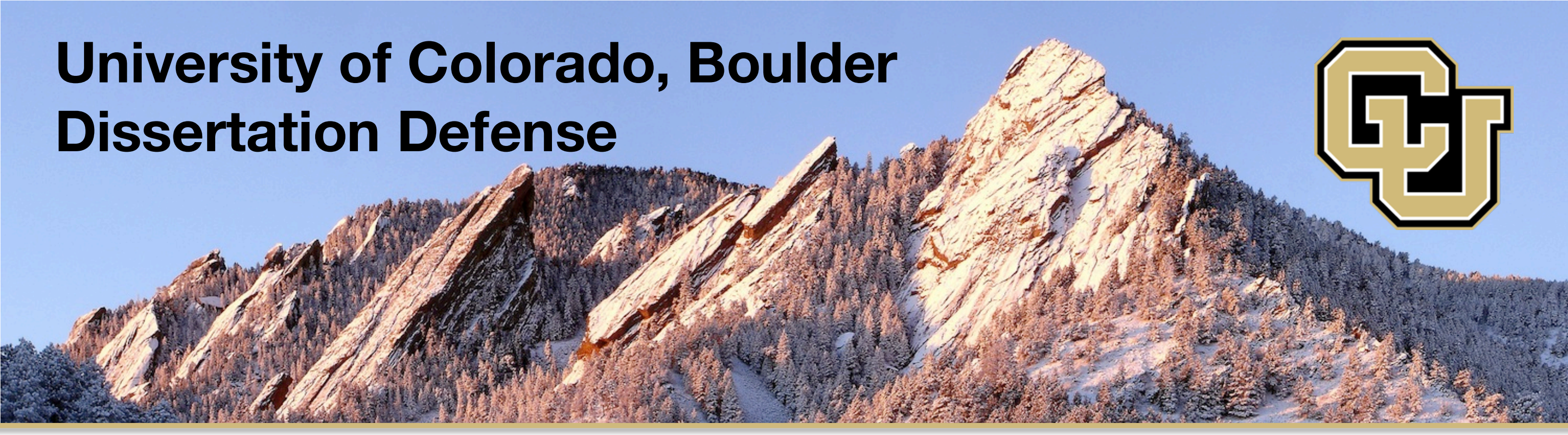

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Approximate Bayesian Computation for Parameter Estimation in Complex Thermal Fluid Systems

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A major challenge in computational fluid dynamics (CFD) simulations of real-world flows is the accurate assignment of boundary, initial, and geometric conditions, as well as fluid and material properties. Despite advances in experimental techniques, however, acquiring the information necessary to simultaneously set each of these conditions and properties remains a considerable challenge. As a potential solution to this difficulty, recent advances in data-driven parameter estimation techniques have provided flexible and increasingly sophisticated methods for improving the fidelity of simulation configurations using experimental data. This dissertation applies, for the first time, a technique called approximate Bayesian computation (ABC) to complex thermal-fluid flows in order to determine numerical simulation parameters from experimental or other reference data.

In this dissertation, the ABC approach is demonstrated for several engineering test cases to demonstrate its efficacy at determining unknown parameters in a wide variety of settings. As a simple initial case, the logistics equation is used to demonstrate the technique. This is followed by the case of a two-dimensional turbulent buoyant jet with variable inlet velocity. The jet is modeled using a large eddy simulation (LES), and reference data is obtained from ensembles of both LES (serving as a benchmark for the technique) and direct numerical simulation (DNS) cases. The reference parameters are correctly identified based on either velocity or temperature measurements at various heights. Using a similar setup, but now with a lightly forced helium plume, the puffing frequency of the jet is identified and used to match experimental observations to predict inlet composition.

Moving on to industrial engineering applications, a three-dimensional turbulent buoyant jet with unknown temperature conditions is simulated using a Reynolds-averaged Navier Stokes (RANS) simulation. In this application, reference observations come from the same RANS case with known parameters. The ABC procedure correctly identifies the inlet temperature boundary conditions. In the next case, a rotating cylinder above a high-temperature turbulent buoyant jet is investigated. Here the reference observations come from a two-dimensional RANS simulation. In particular, the initial reference case has known jet inflow and cylinder rotational velocities, and the ABC approach is shown to correctly identify the reference values of these parameters using sparse temperature statistics within the domain. In an additional test using the two-dimensional rotating cylinder case, the reference case has known species concentrations at the jet inflow and we show that ABC can correctly identify the reference concentrations using sparse species and temperature measurements within the domain.

The ultimate application of ABC in this dissertation uses the technique to determine three- dimensional LES parameters based on comparisons with experimental observations. The experimental temperature data are obtained above an industrially-relevant catalytic burner using laser absorption spectroscopy. This final application identifies parameters that are not able to be measured experimentally, including inlet velocity and heat addition due to continued combustion within the flow field.

These successes indicate that ABC can be extended to additional real-world engineering systems, even when only sparse observational data is available. Using ABC and reference data, one can accurately drive the selection of boundary conditions, as well as model parameters, in numerical simulations. Furthermore, ABC can provide insights into quantities that are not easily measured experimentally.