PARALLEL LARGE-SCALE OPTIMIZATION FOR SOURCE INVERSION FOR CONVECTIVE-DIFFUSIVE TRANSPORT

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We consider the inverse problem of determining an arbitrary source in a time-dependent convective-diffusive transport equation, given a velocity field and pointwise measurements of the concentration. Applications that give rise to such problems include determination of groundwater or airborne pollutant sources from measurements of concentrations, and identification of sources of chemical or biological attacks. We formulate the inverse problem as a constrained least squares parameter estimation problem, in which the objective is to find a source function that minimizes an L_2 norm of the error between observations and predictions (continuous in time, pointwise in space), the constraint is the convection-diffusion initial-boundary value problem, and the inversion parameter is the spatio-temporal source function. To address ill-posedness of the problem, we employ Tikhonov or total variation regularization.

We present a variational formulation of the first order optimality system, which includes the initial-boundary value state problem, the final-boundary value adjoint problem, and the space-time boundary value source problem. We discretize in the space-time volume using Galerkin finite elements, and solve the three-field optimality system for the concentration field, adjoint concentration field, and source field. The solver is based on the Veltisto parallel PDE-constrained optimization library, which solves in the full space of unknowns, using an approximate reduction onto the space of inversion parameters, as well as an approximation of the reduced Hessian, as a preconditioner. Additional mechanisms for globalization and inexactness are incorporated. Veltisto is built from components of the PETSc library.

Examples are presented that study the influence of the density of the sensor array, the effectiveness of total variation regularization for discontinuous sources, the invertibility of the source as the transport becomes increasingly convection-dominated, the ability of the space-time inversion formulation to track moving sources, the convergence rate of the finite element approximation, and the scalability of the method to increasing problem size and number of processors.