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Large-scale stabilized FE computational analysis of nonlinear steady-state transport/reaction systems ☆

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Abstract

The solution of the governing steady transport equations for momentum, heat and mass transfer in fluids undergoing non-equilibrium chemical reactions can be extremely challenging. The difficulties arise from both the complexity of the nonlinear solution behavior as well as the nonlinear, coupled, non-symmetric nature of the system of algebraic equations that results from spatial discretization of the PDEs. In this paper, we briefly review progress on developing a stabilized finite element (FE) capability for numerical solution of these challenging problems. The discussion considers the stabilized FE formulation for the low Mach number Navier–Stokes equations with heat and mass transport with non-equilibrium chemical reactions, and the solution methods necessary for detailed analysis of these complex systems. The solution algorithms include robust nonlinear and linear solution schemes, parameter continuation methods, and linear stability analysis techniques. Our discussion considers computational efficiency, scalability, and some implementation issues of the solution methods. Computational results are presented for a CFD benchmark problem as well as for a number of large-scale, 2D and 3D, engineering transport/reaction applications.

Keywords: Stabilized finite elements; Transport-reaction; Parallel; Newton-Krylov; Domain decomposition; Multilevel; Steady-state; Continuation; Bifurcation; Stability analysis

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1. Introduction

Physical problems in a number of scientific and engineering fields can be described by a system of coupled nonlinear PDEs. One of the main interests in these fields is the problem of determining steady and/or time dependent states evolving with changes of characteristic parameters. These parameters arise in various ways. The parameters can be coefficients of the PDEs, characteristic values from the boundary conditions, or characteristic dimensions from the domain of the solution. Our discussion focuses on applications involving steady-state solution of transport/reaction systems. However, the methods, algorithms, and parallel implementations presented have broad applicability to many scientific fields.

The numerical challenge for transport/reaction system simulation is the solution of the partial differential equations (PDEs) describing momentum, heat, and multicomponent mass transfer with chemical reaction source terms. These governing PDEs are outlined in residual form in Table 1, and are valid for low Mach number flows operating at a thermodynamic system pressure of $\widetilde{P}$. In these equations the transport properties are the mixture density, ρ, mixture viscosity, μ, mixture specific heat, $\widehat{C}_P$, the mixture thermal conductivity, λ, the kth species mass diffusivity, D_k, and thermal diffusivity, D_k^{T}. The source terms are defined by the molecular weight, W_k, the specific enthalpy, $\hat{h}_k$, and the molar production per unit volume, $\dot{\omega}_k$ for the kth species. This system of PDEs is non-self adjoint, strongly coupled, highly nonlinear, and characterized by physical phenomena that span a large range of length and time scales. The high degree of coupling and nonlinearity in this system is generated from the convection terms, the chemical reaction source terms, and the strong dependence of the transport properties and chemical kinetics on the thermodynamic state, $(T, \widetilde{P}, Y_k)$.

Our discretization of the governing transport/reaction equations employs stabilized finite element (FE) methods. This formulation is based on the developments of Hughes et al. (see e.g., [34,5,33,31,38,30,36,35,66]) in a seminal set of papers that developed this very successful and powerful discretization methodology. The stabilized formulation circumvents the Ladyzhenskaya–Babuska–Brezzi condition (see e.g., [4,24]) for compatible discretization for mixed finite element formulations of the saddle point problem arising from discretization of the incompressible Navier–Stokes equations. The stabilized FE formulation allows for equal order interpolation of the incompressible Navier–Stokes equations and eliminates spurious pressure modes. Our formulation implements a simplified form of a consistently stabilized FE method [1]. In the current context of transport/reaction systems, the use of equal order interpolation simplifies the data structures of a parallel unstructured FE code and the linear algebra interface for iterative solution methods.

Additionally, a stabilized FE strategy is also used to control instability in the Galerkin FE formulation for highly convected flows. The methodology that we employ is based on a variation of the stabilized FE

Table 1
Residual form of governing transport/reaction PDEs and simplified constitutive equations

Momentum	$\mathbf{R}_m = \rho(\mathbf{u}\cdot\nabla\mathbf{u}) - \nabla\cdot\mathbf{T} - \rho\mathbf{g}$
Total mass	$R_P = \nabla\cdot(\rho\mathbf{u})$
Thermal energy	$R_T = \rho\widehat{C}_p[\mathbf{u}\cdot\nabla T] + \nabla\cdot\mathbf{q} + \sum_{k=1}^{N_s}\hat{h}_k W_k\dot{\omega}_k$
Mass fraction for species k	$R_{Y_k} = \rho[\mathbf{u}\cdot\nabla Y_k] + \nabla\cdot\mathbf{j}_k - W_k\dot{\omega}_k,\ k = 1,2,\ldots,N_s-1$
	$R_{Y_{N_s}} = \sum_{k=1}^{N_s} Y_k - 1$
Newtonian stress tensor	$\mathbf{T} = -P\mathbf{I} + \boldsymbol{\Psi} = -P\mathbf{I} - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I} + \mu[\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}]$
Heat flux vector	$\mathbf{q} = -\lambda\nabla T + \sum_{k=1}^{N_s}\hat{h}_k\mathbf{j}_k$
Mass species flux vector	$\mathbf{j}_k = \rho D_k\nabla Y_k - D_k^{\mathrm{T}}\frac{\nabla T}{T}$

The primitive variables are the velocity vector $\mathbf{u}$, the temperature T, the hydrodynamic pressure P, and the N_s species mass fractions Y_k. The physical and transport properties are a function of the local T and Y_k and a global system pressure $\widetilde{P}$.