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UNCONDITIONALLY ENERGY STABLE AND FIRST-ORDER ACCURATE NUMERICAL SCHEMES FOR THE HEAT EQUATION WITH UNCERTAIN TEMPERATURE-DEPENDENT CONDUCTIVITY

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Abstract. In this paper, we present first-order accurate numerical methods for solution of the heat equation with uncertain temperature-dependent thermal conductivity. Each algorithm yields a shared coefficient matrix for the ensemble set improving computational efficiency. Both mixed and Robin-type boundary conditions are treated. In contrast with alternative, related methodologies, stability and convergence are unconditional. In particular, we prove unconditional, energy stability and optimal-order error estimates. A battery of numerical tests are presented to illustrate both the theory and application of these algorithms.

Key words. Time-stepping, finite element method, heat equation, temperature-dependent thermal conductivity, uncertainty quantification.

1. Introduction

Demand for superior predictions of scientific and engineering problems is ever increasing. Improvement of available computational resources and both development and application of numerical methodologies work synergistically to meet the aforementioned demand. In particular, numerical schemes are devised to improve model accuracy (e.g., via inclusion of additional physics), replicate additional properties of the continuous problem (e.g., long-time stability), incorporate uncertainty quantification via statistical techniques, etc. The focus of this manuscript is on improving the efficiency of ensemble simulations, which facilitate uncertainty quantification, applied to heat conduction dynamics with increased model physics.

The crisis of predictability in numerical weather prediction, led to the discovery of chaos and the use of ensemble simulations to produce predictive results with uncertainty quantified. Some key figures include, Charney [5], Philips [41], Thompson [45], Lorenz [34, 35, 36]; see, e.g., [27, 32] and references therein for a historical perspective. Ensemble calculations typically involve J solves of a set of equations with slightly perturbed initial data. Calculations are performed as either J sequential, fine mesh runs or J parallel, coarse mesh runs of a given code. The ensemble average tends to perform better as a prediction than any of the individual realizations; see, e.g., Chapter 6 Section 5 of [27] or [2, 13, 28]. Evidently, increased computational resources are needed over a single realization run. Moreover, since both increased ensemble size J and mesh density h yield superior results, there is an inherent competition for available computational resources.

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The last six years have seen increased focus in improving efficiency of ensemble calculations [21, 22, 23, 24, 40, 43, 14, 15, 16, 17, 10, 8, 12, 9, 33, 6, 26, 38, 39, 42] and references therein. The driver for much of this work is owed to a breakthrough work by Jiang and Layton [21], as applied to non-isothermal fluid flow. Therein, they recognized that a consistent modification of the convective term, utilizing the ensemble mean and fluctuation of the viscosity together with lagging of the fluctuation term, would yield a shared coefficient matrix independent of the ensemble member j. The result was a reduction in both storage requirements and solution turnover time.

Recent years have seen increased focus towards problems with uncertain parameters and considerations of alternative physics. Of particular interest here, first- and second-order ensemble algorithms for iso-thermal fluid flow with constant viscosity were developed in [14, 15]. Further, first-order methods were presented for the heat equation with constant thermal conductivity under mixed boundary conditions in [42] and both space and time dependent thermal conductivity under Dirichlet boundary conditions in [38]. Moreover, first and second-order methods were developed for spatially dependent thermal conductivities in [9]. Notably, stochastics were incorporated in [38, 39] via the Monte Carlo method and in [33] for the convection-diffusion equation via stochastic collocation.

In each of the above works, both stability and convergence were conditionally dependent on the ratio between the fluctuating and mean values of the relevant parameter. In contrast, the ensemble methods presented herein are unconditionally, nonlinearly, energy stable and first-order accurate, with $\Delta t = \mathcal{O}(h)$. Moreover, we consider the heat equation with uncertain temperature-dependent thermal conductivity due to uncertain initial conditions. Physically, this is more realistic as most materials' thermal conductivity exhibit non-trivial temperature-dependence. Mathematically, the resulting equation becomes nonlinear, in the diffusive term, presenting new challenges over the analogous linear problem.

Let $\Omega \subset \mathbb{R}^d$ be an open, bounded, Lipschitz domain. Given initial temperature $T^0(x) = T(x,0)$, thermal conductivity κ and heat source f, find $T(x,t) : \Omega \times (0,t^*] \to R$ satisfying

$$\frac{\partial T}{\partial t} - \nabla \cdot (\kappa \nabla T) = f \ in \ \Omega. \tag{1}$$

We consider two boundary configurations: mixed and Robin. Throughout, κ is the thermal conductivity of the solid medium which depends on the temperature profile; that is, $\kappa \equiv \kappa(T)$. For the mixed boundary condition, the boundary $\partial\Omega$ is partitioned such that $\partial\Omega = \overline{\Gamma_D} \bigcup \overline{\Gamma_N}$ with $\Gamma_D \bigcap \Gamma_N = 0$ (Γ_D for Dirichlet condition and Γ_N for Neumann condition). Let n denote the outward normal, then

$$T = 0 \ on \ \Gamma_D, \ \nabla T \cdot n = 0 \ on \ \Gamma_N. \tag{2}$$

Moreover, the Robin condition is prescribed via

$$\alpha T + \kappa \nabla T \cdot n = \beta \ on \ \partial\Omega, \tag{3}$$

where $\alpha \in [0,1]$ is the emissivity, and β a prescribed function on the boundary.

The paper is organized as follows. In Section 2, we introduce mathematical preliminaries required in the analysis, including semi-discrete numerical schemes and