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# A Numerical Methodology for Enforcing Maximum Principles and the Non-Negative Constraint for Transient Diffusion Equations

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**Abstract.** Transient diffusion equations arise in many branches of engineering and applied sciences (e.g., heat transfer and mass transfer), and are parabolic partial differential equations. It is well-known that these equations satisfy important mathematical properties like maximum principles and the non-negative constraint, which have implications in mathematical modeling. However, existing numerical formulations for these types of equations do not, in general, satisfy maximum principles and the non-negative constraint. In this paper, we present a methodology for enforcing maximum principles and the non-negative constraint for transient anisotropic diffusion equation. The proposed methodology is based on the method of horizontal lines in which the time is discretized first. This results in solving steady anisotropic diffusion equation with decay equation at every discrete time-level. We also present other plausible temporal discretizations, and illustrate their shortcomings in meeting maximum principles and the non-negative constraint. The proposed methodology can handle general computational grids with no additional restrictions on the time-step. We illustrate the performance and accuracy of the proposed methodology using representative numerical examples. We also perform a numerical convergence analysis of the proposed methodology. For comparison, we also present the results from the standard single-field semi-discrete formulation and the results from a popular software package, which all will violate maximum principles and the non-negative constraint.

**AMS subject classifications**: 65

**Key words**: Numerical heat and mass transfer, maximum principles, non-negative solutions, anisotropic diffusion, method of horizontal lines, convex quadratic programming, parabolic PDEs.

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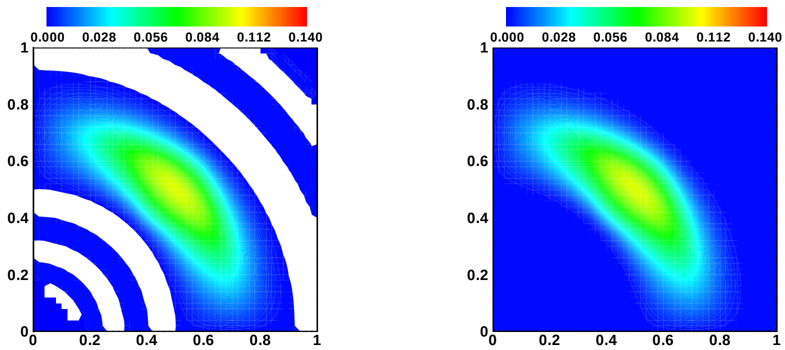


Figure 1: Diffusion in heterogeneous anisotropic medium: This figure shows the contours of the concentration under the Galerkin single-field formulation (left) and the proposed methodology (right) at time $=0.5$. The time-step is taken as $\Delta t = 0.5$, and XSeed = YSeed = 51. The regions that violated the non-negative constraint are indicated in white color.

## 1 Introduction and motivation

Certain quantities (e.g., concentration of a chemical species and absolute temperature) naturally attain non-negative values. A violation of the non-negative constraint for these quantities will imply violation of some basic tenets of physics. It is, therefore, imperative that such physical constraints are met by mathematical models and by their associated numerical formulations. In this paper, we shall focus on two popular transient mathematical models, in which physical restrictions like the non-negative constraint play a central role. The first model is based on Fick's assumption (commonly referred to as Fick's law) and the balance of mass. Fick's assumption is a simple constitutive model to describe the diffusion of a chemical species in which the flux is proportional to the negative gradient of the concentration. The second model is based on Fourier's assumption and the balance of energy, which describes heat conduction in a rigid conductor. Both these constitutive models combined with their corresponding balance laws give rise to transient diffusion equations, which are parabolic partial differential equations.

There has been tremendous progress in applied mathematics for these type of equations with respect to existence and uniqueness results, qualitative behavior of solutions, estimates, and other mathematical properties [21, 56]. In particular, it has been shown that transient diffusion equations satisfy the so-called maximum principles [56]. It will be shown in a subsequent section that the non-negative constraint can be shown as a consequence of maximum principles under certain assumptions. Analytical solutions to several problems have been documented in various monographs (e.g., see references [11, 54]). However, it should be noted that most of these solutions are for isotropic and homogeneous media, and for simple geometries. For problems involving anisotropic and heterogeneous media, and complex geometries; finding analytical solutions is not possible, and one has to resort to numerical solutions. Obtaining physically meaning-