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# Preconditioning for a Phase-Field Model with Application to Morphology Evolution in Organic Semiconductors

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**Abstract.** The Cahn–Hilliard equations are a versatile model for describing the evolution of complex morphologies. In this paper we present a computational pipeline for the numerical solution of a ternary phase-field model for describing the nanomorphology of donor–acceptor semiconductor blends used in organic photovoltaic devices. The model consists of two coupled fourth-order partial differential equations that are discretized using a finite element approach. In order to solve the resulting large-scale linear systems efficiently, we propose a preconditioning strategy that is based on efficient approximations of the Schur-complement of a saddle point system. We show that this approach performs robustly with respect to variations in the discretization parameters. Finally, we outline that the computed morphologies can be used for the computation of charge generation, recombination, and transport in organic solar cells.

**AMS subject classifications**: 65F08
**Key words**: Preconditioning, phase–field models, organic solar cells, Cahn–Hilliard, finite element analysis.

## 1 Introduction

We consider a model for solvent-based fabrication of organic solar cells. A thin-film of a dilute blend containing electron-acceptor, electron-donor and solvent is deposited on

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a substrate. As the solvent evaporates, the initially homogeneous mixture undergoes phase separation into electron-acceptor rich and electron-donor rich areas. In order to simulate the evolution of the morphology we use a phase-field model based on the Cahn–Hilliard equation [14], which is a fourth order partial differential equation (PDE). The equations are derived from the minimization of the Ginzburg–Landau energy function via a gradient flow. The original Cahn–Hilliard equation models the evolution of two phases while in our case we require a system of three components and follow the model introduced in [32]. Our aim in this paper is to focus on equipping the phase-field system with a suitable discretization and a general preconditioning strategy as this is important for enabling three-dimensional simulations required for realistic solar cell morphologies. As these will be of large scale and the system will be ill-conditioned, the convergence of any iterative solver will be slow unless we introduce a suitable preconditioning strategy. Our preconditioning approach for the ternary Cahn–Hilliard system is based on applying block-preconditioners [9–11,34] and these rely on the coupling of well studied components such as algebraic multigrid methods. Finally, in a proof-of-concept study we demonstrate how these morphologies can be incorporated into 2D electrical device simulations of organic solar cells. We demonstrate that our generated morphologies can significantly affect both the current voltage curves and the charge density within the active layer.

## 2 Phase–field model

The mathematical description of the morphology evolution can be done by a phase field model [28, Chapter 10], that consists of a domain $\Omega \subset \mathbb{R}^3$ and three scalar fields

$$\phi_p, \phi_{\mathrm{NFA}}, \phi_s \colon \Omega \times [0,T] \to [0,1] \subset \mathbb{R} \tag{2.1}$$

representing the volume fractions of polymer, non-fullerene acceptor (NFA) and solvent, respectively, at a given point in the domain at a given time in the interval $[0,T]$. In this work, we focus on the numerical treatment of the model and leave the scaling of physical dimensions to future work. The conservation relation

$$\phi_p + \phi_{\mathrm{NFA}} + \phi_s = 1 \tag{2.2}$$

applies for all $x \in \Omega$ and every $t \in [0,T]$. The Ginzburg–Landau energy functional forms the basis for the Cahn–Hilliard equation and is given by

$$F(\phi_p,\phi_{\mathrm{NFA}},\phi_s) = \int_\Omega \left[ f(\phi_p,\phi_{\mathrm{NFA}},\phi_s) + \frac{\epsilon_p}{2}\left|\nabla\phi_p\right|^2 + \frac{\epsilon_{\mathrm{NFA}}}{2}\left|\nabla\phi_{\mathrm{NFA}}\right|^2 \right] \mathrm{d}x + F_s(\phi_p,\phi_{\mathrm{NFA}},x), \tag{2.3}$$