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A Robust and Efficient Adaptive Multigrid Solver for the Optimal Control of Phase Field Formulations of Geometric Evolution Laws

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Abstract. We propose and investigate a novel solution strategy to efficiently and accurately compute approximate solutions to semilinear optimal control problems, focusing on the optimal control of phase field formulations of geometric evolution laws. The optimal control of geometric evolution laws arises in a number of applications in fields including material science, image processing, tumour growth and cell motility. Despite this, many open problems remain in the analysis and approximation of such problems. In the current work we focus on a phase field formulation of the optimal control problem, hence exploiting the well developed mathematical theory for the optimal control of semilinear parabolic partial differential equations. Approximation of the resulting optimal control problem is computationally challenging, requiring massive amounts of computational time and memory storage. The main focus of this work is to propose, derive, implement and test an efficient solution method for such problems. The solver for the discretised partial differential equations is based upon a geometric multigrid method incorporating advanced techniques to deal with the nonlinearities in the problem and utilising adaptive mesh refinement. An in-house two-grid solution strategy for the forward and adjoint problems, that significantly reduces memory requirements and CPU time, is proposed and investigated computationally. Furthermore, parallelisation as well as an adaptive-step gradient update for the control are employed to further improve efficiency. Along with a detailed description of our proposed solution method together with its implementation we present a number of computational results that demonstrate and evaluate our algorithms with respect to accuracy and efficiency. A highlight of the present work is simulation results on the optimal control of phase field formulations of geometric evolution laws in 3-D which would be computationally infeasible without the solution strategies proposed in the present work.

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1 Introduction

The optimal control of geometric evolution equations or more generally free boundary problems arises in a number of applications. In image processing the tracking of deformable objects may be formulated as the optimal control of a suitably chosen evolution law [1]. A number of applications arise from problems in material science such as the control of nanostructure through electric fields [2, 3]. An important and topical application area is the image driven modelling of biological processes, such as tumour growth [4] or cell migration [5], in which parameters (or functions) in a model are estimated from experimental imaging data. In a recent study we proposed an optimal control approach to whole cell tracking [6], i.e., the reconstruction of whole cell morphologies in time from a set of static images, in which the cell tracking problem was formulated as the optimal control of a geometric evolution equation [6]. In general the approximation of such optimal control problems is computationally intensive both in terms of central processing unit (CPU) time and memory. Hence, the development of robust and efficient solvers for such problems with a view to reducing CPU time (or simply wall-clock time) and memory requirements is a worthwhile research direction.

In the current work we consider the optimal control of geometric evolution laws of forced mean curvature flow type. We denote by $\Gamma(t)$, a closed oriented smoothly evolving $d-1$ dimensional hypersurface in $\mathbb{R}^d$, $d=2,3$ with outward pointing unit normal $\boldsymbol{\nu}$. The motion of $\Gamma(t)$ satisfies a volume constrained mean curvature flow with forcing, i.e., given an initial surface $\Gamma(0)$, the velocity $\boldsymbol{V}$ of Γ is given by

$$\boldsymbol{V}(\boldsymbol{x},t)=(-\sigma H(\boldsymbol{x},t)+\eta(\boldsymbol{x},t)+\lambda_V(t))\boldsymbol{\nu}(\boldsymbol{x},t), \quad \boldsymbol{x}\in\Gamma(t), \ t\in(0,T], \tag{1.1}$$

where $\sigma>0$ represents the surface tension, H denotes the mean curvature (which we take to be the sum of the principal curvatures) of Γ, η is a space time distributed forcing and λ_V is a spatially uniform Lagrange multiplier enforcing volume constraint. We assume we are given an initial interface Γ^0 and a target interface Γ_{obs} both of which are smooth closed oriented $d-1$ dimensional hypersurfaces.

The optimal control problem, which is the focus of the current work, consists of finding a space time distributed forcing η in (1.1) such that with $\Gamma(0)=\Gamma^0$, the interface position at time T corresponding to the solution of (1.1), $\Gamma(T)$, is "close" to the observed data Γ_{obs}. We have deliberately refrained from stating precisely what is meant by $\Gamma(T)$ being close to Γ_{obs} as in the sharp interface setting it is not obvious what constitutes a good choice of metric to measure the difference between two surfaces. In particular standard measures such as the Haussdorff distance are typically non-smooth and this complicates the approximation of the optimal control problem. Moreover, the theory of optimal control of geometric evolution laws is in its infancy, in fact only recently has progress been