ARTICLE IN PRESS

Computers and Mathematics with Applications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

A hierarchical computational model for moving thermal loads and phase changes with applications to selective laser melting

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ARTICLE INFO

Article history:
Received 9 August 2017
Received in revised form 2 November 2017
Accepted 12 November 2017
Available online xxxx

Keywords:
Additive manufacturing
hp-FEM
Transient thermal problems
Dynamically changing meshes

ABSTRACT

Computational heat transfer analysis often involves moving fluxes which induce traveling fronts of phase change coupled to one or more field variables. Examples are the transient simulation of melting, welding or of additive manufacturing processes, where material changes its state and the controlling fields are temperature and structural deformation. One of the challenges for a numerical computation of these processes is their multi-scale nature with a highly localized zone of phase transition which may travel over a large domain of a body. Here, a transient local adaptation of the approximation, with not only a refinement at the phase front, but also a de-refinement in regions, where the front has passed is of advantage because the de-refinement can assure a bounded number of degrees of freedom which is independent from the traveling length of the front.

We present a computational model of this process which involves three novelties: (a) a very low number of degrees of freedom which yet yields a comparatively high accuracy. The number of degrees of freedom is, additionally, kept practically constant throughout the duration of the simulation. This is achieved by means of the multi-level *hp*-finite element method. Its exponential convergence is verified for the first time against a semi-analytic, three-dimensional transient linear thermal benchmark with a traveling source term which models a laser beam. (b) A hierarchical treatment of the state variables. To this end, the state of the material is managed on a separate, octree-like grid. This material grid may refine or coarsen independently of the discretization used for the temperature field. This methodology is verified against an analytic benchmark of a melting bar computed in three dimensions in which phase changes of the material occur on a rapidly advancing front. (c) The combination of these technologies to demonstrate its potential for the computational modeling of selective laser melting processes. To this end, the computational methodology is extended by the finite cell method which allows for accurate simulations in an embedded domain setting. This opens the new modeling possibility that neither a scan vector nor a layer of material needs to conform to the discretization of the finite element mesh but can form only a fraction within the discretization of the field- and state variables.

1. Introduction

The computational analysis of powder bed fusion processes such as e.g. selective laser melting (SLM) is challenging due to many reasons. The most prominent include:

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https://doi.org/10.1016/j.camwa.2017.11.014
0898-1221/

1. highly localized and moving strong temperature gradients
2. non-linearities due to temperature dependent coefficients and phase changes of the material
3. growing and possibly geometrically complex computational domains
4. large range of scales in both space and time
5. coupled multi-physics.

This article presents a methodology for the prediction of the temperature evolution in a powder bed fusion process taking into account the first three issues. While we incorporate the non-linearities due to temperature dependent coefficients and phase changes of the material using the rather standard latent heat model first presented in [1], special focus lies on the discretization of the highly localized and moving strong temperature gradients and on the representation of growing computational domains.

The evolution of temperature fields in space is a diffusion dominated process which can be well resolved by the finite element method. Many commercial packages are available on the market and provide a wealth of physical models, but their discretizational technology is mostly limited to linear, at most quadratic finite elements. Therefore, the resolution of local gradients is limited to *h*- refinements, i.e. refining the mesh size towards singularities.

Strong gradients, however, can most efficiently be resolved by *hp*-finite elements which vary the size of the element h locally as well as the polynomial degree of the trial/test space p [2,3]. While *hp*-fem leads to efficient discretizations where error estimators are used to drive an adaptive scheme, it also provides excellent accuracy in cases where the solution characteristic is known a priori. This is the case for the simulation of powder bed fusion processes because the area of refinement is well defined by the location of the laser spot where sudden, high temperatures cause phase changes in the material.

Moreover, most simulations of powder bed fusion processes use static discretization schemes, i.e. the mesh is refined towards the entire laser path and kept fixed at all time-steps. As a consequence, the necessary number of degrees of freedom is directly proportional to the length of the laser path. However, high gradients are local to the laser spot itself and not distributed along all of its path. Therefore, the number of degrees of freedom should be independent of the length of the laser path and at best constant over time. To this end, transient refinement and de-refinements of the discretization throughout the runtime of the simulation is necessary to keep the refinement local to the current position of the laser. Only recently, discretizations have appeared that utilize these kind of transient meshes for computational SLM analysis, see e.g. [4–6] and references therein. To the authors' knowledge, all of these contributions exploit *h*-refinements for low order polynomials, only.

Another important aspect is the treatment of the state variables. While the evolution of temperature is a diffusive process, the evolution of the material state is not. Solidified material does not diffuse into regions containing powder. Additionally, material interfaces may not coincide with the boundaries of the finite elements. For example, material may need to be added in form of powder in a way which does not necessarily conform to the finite element discretization. In the paper at hand, we propose to provide this flexibility by discretizing the material coefficients *independently* of the underlying discretization of the field variables.

The article is structured as follows: We start by introducing the governing equations in Section 2.1 and present its discretized weak from in Section 2.2. We then give a quick introduction into the recently introduced multi-level *hp*-finite element method [7], which provides *hp*-discretizations on transient meshes. To evaluate its accuracy, we first present results for a transient but linear, three-dimensional benchmark resembling a SLM process in Section 2.4.1 before proceeding to evaluate the scheme against a transient non-linear benchmark involving phase changes and latent heat in Section 2.4.2.

We then proceed to combine the multi-level *hp*-method with the finite cell method in Section 3.1 which was initially designed to avoid boundary conforming mesh generation for complex domains. We use this concept to treat state and field variables on different discretizations. Section 3.2 then presents an example computing the evolving interface of a structure. Herein, two independent and transiently changing discretizations are used for state and field variables. Their separate treatment combined with the multi-level *hp* method allows for a relatively low number of degrees of freedom which stay almost constant throughout the simulation process.

2. Thermal analysis with phase changes

This section sets out to describe a new discretizational scheme for thermal analysis with phase changes. To clear the view, we neglect effects of radiation and mass transfer even though they have physical relevance in practical examples.

2.1. Governing equations

In this spirit, let us consider a domain, $\Omega \subset \mathbb{R}^n$ with boundary $\partial\Omega$, where n is the number of space dimensions. The governing nonlinear transient heat conduction equation with phase-change, written in terms of volumetric enthalpy $H = H(T)$ and temperature $T = T(\mathbf{x})$ fields, has been investigated by many researchers. In the sequel, we closely follow the presentation given in [8] which reads:

$$\frac{\partial H}{\partial t} - \nabla \cdot (k \nabla T) = Q \quad \text{in} \quad \Omega, \tag{1}$$

Please cite this article in press as: S. Kollmannsberger, et al., A hierarchical computational model for moving thermal loads and phase changes with applications to selective laser melting, Computers and Mathematics with Applications (2017), https://doi.org/10.1016/j.camwa.2017.11.014.