Preface

Numerical simulations of dynamical problems in inhomogeneous solids are quite difficult for the case of moving discontinuities such as phase transition fronts or cracks. The origin of these difficulties is a constitutive deficiency in the thermomechanical description of the corresponding irreversible processes, which leads to an uncertainty in jump relations at moving discontinuities. Consequently, the construction of an appropriate numerical algorithm should be complemented by the development of the thermomechanical theory.

The aim of this book is to provide a framework for the description of moving discontinuities in solids and its implementation in a finite-volume numerical algorithm.

The macroscopic description of moving discontinuities in solids (such as phase-transition fronts or crack fronts) needs to go beyond the conventional local equilibrium approximation, since both phase-transition fronts and cracks propagate irreversibly accompanied by entropy production at their moving front.

The numerical simulation of thermomechanical processes supposes the application of a certain discretization method. Therefore, instead of infinitesimally small material "points", which are in local equilibrium, in numerical simulations we deal with finite-size computational cells, states of which are non-equilibrium ones in general. To keep the meaning of thermodynamic quantities well-defined, a projection of the non-equilibrium states onto an equilibrium subspace is used conventionally. This means that the non-equilibrium state of each computational cell is associated with an equilibrium state of the accompanying reversible process. The simplest projection is the averaging of corresponding fields over the computational cell. An averaging procedure over the control volume applied to appropriate conservation laws leads to a system of equations in terms of averaged quantities and corresponding fluxes at boundaries of cells. Such a procedure is a basis for Godunov-type finite-volume numerical schemes.

The main problem in the construction of a particular algorithm is the proper determination of numerical fluxes. However, even if we are able to determine the numerical fluxes in the bulk, their determination at moving fronts is highly questionable.

Throughout the book, all needed fluxes are determined by means of the local equilibrium jump relations. These local equilibrium jump relations are formulated in terms of excess quantities, which characterize the non-equilibrium states of computational cells. The continuity of excess quantities across the moving discontinuity is used for the closure of the model. This leads to the relation between the stress jump at the discontinuity and the corresponding driving force, which allows us to determine the velocity of a moving front. As a consequence, a thermodynamically consistent finite volume numerical algorithm is obtained, which can be applied to both wave and front propagation problems.

It is remarkable that similar considerations are applicable to another problem of moving discontinuity, namely, to crack dynamics. In the case of a moving crack, the local equilibrium jump relation at the crack front is complemented by another assumption regarding the excess quantities, which reflects the distinction between the problems of moving phase boundaries and cracks.

Examples of numerical simulations of phase-transition front propagation and straight brittle crack motion show the applicability of the developed non-equilibrium description to solve the problems of moving fronts.

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