Recent Advances in the Development of Computational Design Simulators for Deformation and Solidification Processes[1]

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Our current research efforts are devoted to the development of mathematically rigorous computational design techniques for materials processes. In this presentation, we will highlight some solution techniques for a number of complex mathematical problems of importance to the design of deformation processes for shape and microstructure control and of directional solidification processes that result in cast products of desired microstructures. Even though we are currently developing the two computational tools as independent design simulators, we anticipate that a unified simulator will eventually result that will enable us to control product quality and cost with proper simultaneous design of both processes.

In the first part of the presentation, a computational finite element framework will be introduced for the design of multi-stage deformation processes that lead to products of desired shape and material state with minimum material utilization rates and energy cost. The various design problems are posed as constraint optimization problems and the needed gradients are computed using innovative continuum parameter and shape sensitivity analyses for large deformations of hyperelastic-thermo-viscoplastic materials within an updated Lagrangian framework. The overall time-incremental linear sensitivity analysis can be used to efficiently compute the sensitivities of the temperature, deformation, stresses and material state with respect to any design variables. The sensitivity analysis is performed in an infinite-dimensional continuum framework that accounts for the non-differentiable nature of the frictional/contact conditions. Remeshing and data transfer techniques are being developed in the context of a design simulator where, in addition to transfer of direct fields, transfer of sensitivity fields is performed as well. The effectiveness of the developed design techniques will be demonstrated with several examples. We will finally mention a number of inves-

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tigations currently pursued to allow us to address the design of complex industrial multi-stage deformation processes.

In the second part of this presentation, we will discuss the computational design of solidification processes. Continuum adjoint and sensitivity problems are defined for solidification systems accounting for various transport mechanisms including heat and mass transfer, natural and solutal convection, thermo-capillary, electro-magnetic convection and other. In order to control the local to the freezing interface thermal and growth conditions, we have posed a number of design optimization problems that utilize the solution of these adjoint/sensitivity problems to compute the gradient of the underlying cost functionals. As an example, a method will be presented to calculate the thermal boundary conditions on the mold walls for directional solidification processes with thin mushy zones under the influence of buoyancy, thermocapillary and electromagnetic convection such that a desired stable solid-liquid interface growth is achieved throughout solidification.

The presentation will conclude with some thoughts on the directions to which this research is pointing mainly the real time control of materials processes using reduced order models of the various physical mechanisms, experimental sensing and data mining of continuum fields, sophisticated adaptive sensing and actuation, etc. Such information technologies based framework will allow us to robustly account for uncertainties in the physical and mathematical process/material modeling.