A Framework for Virtually-Guided Certification of Die Cast Manufacturing Processes

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ABSTRACT

Die casting is an important process of metal manufacturing used in automotive, housing and other industries. The need of simulations to understand the physics and estimate the product quality in manufacturing is growing. It is convenient and financially viable to use computer simulations as replacements to real life experiments. There are uncertainties in the inputs like temperature, metal speed, thermal boundary conditions etc. which affect the product quality. In this paper, we present a computational framework developed to analyze the impact of these uncertainties in the simulations. The framework consists of fast numerical simulations, micro-structure characterization, experimental inputs, sensitivity analysis and uncertainty propagation from stochastically varying inputs to the quality of the cast product.

We are developing a 3D finite volume based Navier-Stokes solver running on an unstructured mesh of hexa-hedral elements. The unstructured hexa-hedral mesh helps to represent complex geometries with less number of control volumes while maintaining good accuracy. The flow solver includes computations of the fluid flow, natural convection, heat transfer and solidification. Multigrid methods are used to accelerate the convergence and the GPU is used to reduce the solution time. The temperature gradient, rate of cooling, velocities and other flow parameters are used to estimate the microstructure parameters such as primary and secondary dendrite arm spacings. These microstructure parameters govern the final quality of the cast product. Empirical models used in the simulation will be calibrated using experimental data, including effects of their uncertainty. The overall approach will be rigorously verified using published numerical results and validated using experimental results. Since there is a significant amount of uncertainty in process parameters and it is practically difficult to tightly control all parameters, uncertainty analysis is performed to quantify impact of variation of each process parameter on casting quality.

This overall framework will help in assessing importance of each process parameter, its effect on casting quality and amount of variation in input that can be allowed with a constraint of maintaining quality within given bounds.

INTRODUCTION

The manufacturing industry employs a variety of processes to produce a required finished product, out of which die casting is one important process. The advancement of high-speed computers and acquisition of real-time data has recently provided significant opportunities to understand and improve the processes by simulating the underlying physical phenomena using numerical techniques. There is now a vast amount of literature on efficient solution of the coupled mechanical, heat transfer and fluid flow phenomena in processes such as casting, welding, soldering and laser machining. Such models are highly
valuable in optimizing the processes and designing strategies to control the variances in part dimensions and residual thermal stresses. As the fidelity of the models grows, computer experiments can be used as proxies to real life experiments, leading to low cost design experimentation and quality improvement in small real times. Assurance of the simulations can therefore virtually certify the part before it is fabricated and tested. This is essentially the main impetus to our ongoing effort on “Virtually Guided Certification”.

Virtually guided certification implies performing enough computer experiments in which the role of physical experiments is replaced by simulations of the process phenomena. This therefore requires first constructing a mathematical model of the relevant physical process, defining the governing algebraic and differential equations, defining the various uncertainties and then developing a numerical algorithm to solve the comprehensive set of equations. Despite the high power of numerical algorithms and the availability of extensive property data, considerable uncertainties and errors exist in current day simulation techniques. In addition, gaps in the knowledge base also exist, especially in the interaction of material microstructure with physical property fluctuations. Spatial and temporal scale resolution is another important limitation of most simulations. The present effort, directed towards virtually guided certification, aims to reduce the uncertainty in the numerical simulation results through a) Verification and Validation; and b) Uncertainty Quantification.

MODELING APPROACH

Figure 1 shows the overall modeling approach. In the following sections, each of the blocks is described in detail.

DIE-CASTING EXPERIMENTS FOR CALIBRATION AND VALIDATION
Die-casting is a very complex process with interactions of numerous physical phenomena occurring at sub-grain length scales. Hence there is a necessity of empirical models to estimate the various micro-structure parameters and material properties. These empirical models have to be calibrated by using real life castings. After calibration, simulations can be run to estimate various output parameters. In order to have confidence in the developed approach, experimental data is used for validation. Actual castings are sectioned and micro-structure images are used to extract relevant microstructure parameter distributions from a micrograph by image processing techniques. Same parameters are estimated from simulations and compared with experimental data.
MICROSTRUCTURE MODELING
Microstructure parameters like dendrite arm spacing (DAS), grain size, shape, orientations etc. have a direct impact on the mechanical properties of castings. Hence it is important to estimate these parameters. Empirical models use the temperature and temperature gradients to estimate DAS. DAS is correlated to porosity and mechanical properties empirically.

MATERIAL PROPERTY AND BEHAVIOR PREDICTION
Two approaches are used to predict the material properties and behavior of the casting. First is to correlate the microstructure parameters to the mechanical property of the material (e.g. ‘Hall-Petch’ equation correlates yield strength to grain). Alternatively, a microstructure level finite element model can be used to accurately describe the local behavior of heterogeneous material such as a die-cast alloy including gradients of strains, stresses etc. This approach uses a simulated micrograph to synthesize individual constituents into a composite material and capture the material behavior of the alloy during metal deformation.

SOLIDIFICATION MODEL
Die casting consists of liquid metal flow, heat transfer, natural convection and solidification. An in-house finite volume based software is written to estimate the flow velocity and temperature. Unstructured mesh is used as it helps to have higher accuracy with less number of control volumes compared to a structured mesh. Initial liquid metal temperature, cooling rate etc. are inputs to the model.

Liquid metal is modelled as an incompressible fluid. Incompressible forms of Navier-Stokes equations are used with additional terms for solidification. A Darcy drag term \( \mu K \) is added in order to incorporate the effect of the mushy zone to the momentum equation. For example, the x-momentum equation is [8]:

\[
\rho \frac{\partial u}{\partial t} + \rho \nabla \cdot (\nabla u) = \mu \nabla^2 u - \frac{\partial p}{\partial x} - \frac{\mu}{K} u
\]

\( K \) is isotropic permeability of the dendritic array estimated using the Blaze-Kozeny model [8]:

\[
K = \frac{\lambda^2 (1 - f)^3}{180 f^2}
\]

Where, \( \lambda \) is the dendritic arm spacing and \( f \) is the solid fraction. Natural convection is modelled by Boussinesq approximation.

The solver is accelerated using a multigrid method. In multigrid method, varying grids of coarser levels are used to correct the solution at the finest level thus achieving accuracy corresponding to the finest level. It is known that by using the multigrid method [6] the rate of convergence is almost independent of the number of elements. The code is parallelized on a NVIDIA GPU using the CUDA language [7].

UNCERTAINTY QUANTIFICATION & SENSITIVITY ANALYSIS
During an actual die-casting process, there are several uncertainties causing statistical variations in the process conditions. Moreover, there are additional uncertainties due to the mathematical models used to represent the solidification phenomena as they take place due to temperature changes. These can eventually result in defective products. In addition, testing each and every product to determine its quality is not possible and counter-productive. Hence, in this effort, a computational approach is proposed which combines a statistical methodology of uncertainty quantification, validation and verification and microstructure evaluation with the fluid flow software.

In die casting, there are a large number of input parameters which affect the final product quality. Controlling all of them accurately is not economical. Hence sensitivity analysis is performed to estimate the impact of variation of each input parameter on the important output parameters. This quantifies a tolerance bound on each input parameter. So only a handful number of input process parameters need to be tightly controlled to maintain product quality.

RESULTS

DETERMINISTIC RESULTS
As a proof of concept, a sample geometry (Figure 2) is simulated. This section shows results generated by the in-house software for fixed values of process parameters.
The tub has outer dimensions of 4x4x4 cm³ and a cut out of 2x2x2 cm³. Initially, the cavity is filled with liquid aluminum at 1000K. All the bounding walls are held at 500K. Gravity is acting in –Y direction. This simulation takes just 3 minutes for 250,000 elements for 5000 time steps. In this problem, flow due to natural convection is also computed.

Temperature and Solid Fraction

Figure 3 shows temperature contours at a cross-section in the YZ plane. Red color is above 950K and blue indicates below 550K. As expected, the metal adjacent to the boundaries cools down first, whereas the core cools last. Figure 4 shows corresponding solid fraction. Red indicates the completely solidified region and blue indicates complete liquid region. Again, the core solidifies last. Similarly, figures 5 and 6 show temperature and solid fraction plots respectively along the XZ plane.
Microstructure and Mechanical Properties

Empirical relations from literature are used to estimate the microstructure and mechanical properties. Secondary Dendritic Arm Spacing (SDAS) is computed by [1]:

$$SDAS = \lambda_2 = 44.6 \left( \frac{\partial T}{\partial t} \right)^{-0.359}.$$  

Figure 7 shows SDAS estimated along the planes YZ and XZ at three different cross-sections. Red color indicates SDAS of 11 µm and blue indicates SDAS of size 1 µm. It can be seen that SDAS is higher in the core region which solidifies at the end. The 0.2% proof strength is estimated by [2]:

$$\text{Proof Strength} = 59 \cdot \text{SDAS}^{-0.5} + 120.3 \text{ MPa}.$$  

Figure 8 shows contours of proof strength. Higher SDAS values indicate lower proof strength. Hence the core region is weaker (140 MPa) compared to the boundaries (200 MPa). Shrinkage and gas porosity are important defects which affect the cast quality. There are models in the literature which estimate the porosity. For instance, model by Khalajzadeh, Vahid, et al.
[9] is the latest one which estimates both gas and shrinkage porosity in one dimensional casting. Such a model will be added to the software for defect prediction.

Figure 7: SDAS
Figure 8- 0.2% Proof Strength (MPa)

UNCERTAINTY QUANTIFICATION

Stochastic variations in material properties and the process boundary conditions are the main sources of uncertainty in casting properties. In this example, the latent heat (material property) and wall temperature (boundary condition) are chosen as uncertain inputs. The deterministic problem mentioned in the previous section is studied for each stochastic variation. It is assumed that the relative uncertainty in both is 1%. It is assumed that both the input parameters follow a normal distribution. Four output parameters are chosen: solidification time, max, min and average of SDAS.

Polynomial chaos expansion is used to estimate the change in the output parameters due to the variation in the input parameters. Stochastic collocation is used to estimate the coefficients of the polynomial chaos expansion of each output. The roots of the Hermite polynomials are used as nodes for collocation whereas, Hermite polynomials are used as basis for the polynomial chaos expansion. Hermite polynomial and its roots are an optimal choice because the input parameters are assumed to follow a normal distribution and Hermite polynomials are orthogonal with respect to a normal distribution [3]. Since this is a two-dimensional stochastic problem, a sparse grid algorithm is used. The sparse grid nodes are taken from the website by Heiss and Winschel [4] based on the research paper by Heiss and Winschel [5]. It is assumed that the inputs are independent.

Figure 9 plots the response surfaces for each of the four output parameters as a function of the two input parameters. In each figure, x axis is latent heat and y axis is wall temperature. Response surfaces can be used to come up with optimal regions of
input parameters. For example, to increase productivity, it is good to have lower solidification time. From figure 9, lower values of latent heat and wall temperatures help increase productivity. Sensitivity can also be qualitatively estimated from the response surface contours. For example, the contour lines of solidification time are steep which means that the solidification time is more sensitive to latent heat than the wall temperature. On the other hand, the contour lines of maximum of Min(SDAS) are horizontal which implies that this parameter is independent of latent heat. The contours of Max(SDAS) are non-linear. This implies that the sensitivity is a function of the input parameters. At lower values of input parameters (lower left corner), Max(SDAS) is equally sensitive to both inputs whereas, at higher values (upper right corner), it is more sensitive to latent heat.

CONCLUSIONS

This paper presents a general framework for verification, validation and uncertainty quantification in numerical simulations of the die-casting process. A finite volume method based software with multigrid acceleration on GPU is developed to simulate the fluid flow, heat transfer, natural convection and solidification. The software predicts metal flow velocities, temperature and solid fraction as a function of space and time. Microstructure parameter like dendrite arm spacing and a mechanical property such as proof strength are estimated using empirical relations. These empirical relations are calibrated using experimental data. Uncertainty quantification and sensitivity analysis are done using the stochastic collocation method. This methodology can be used as a wrapper on any deterministic numerical method. Overall this framework improves the computational method by estimating the impact of stochastic variations in the input parameters on the final product quality. It gives information about which input parameters should be tightly controlled to get a desired product quality, thereby reducing rejection rate.

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