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DIGITIZING AMERICAN MANUFACTURING

DMDII FINAL PROJECT REPORT

VIRTUALLY-GUIDED CERTIFICATION OF DIE CAST MANUFACTURING PROCESSES

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EXECUTIVE SUMMARY

Modern manufacturing processes are very complex consisting of many steps and demanding high conformity to tolerances to maintain product quality and costs. Understanding and optimizing such processes are of critical importance for maintaining competitive advantage in the manufacturing industry. Recently, advances in computing hardware and software, and computational algorithms to simulate the manufacturing processes have helped in exploiting different materials, reducing product defects and meeting the tolerance goals. Such environments, if combined with experimental and computational methodologies to quantify uncertainties in process variables and input parameters can aid in developing virtual certification strategies such that bounds can be ascertained on the tight tolerances on mechanical, thermal and material integrity. The present work addressed this critical need.

The objective of this effort was to develop, implement and demonstrate methodologies that would estimate variations in product quality given stochastic variations in process inputs and process models, and help in product and process certification. A cyber environment called "OpenCast" was developed that can predict, identify and improve product quality by controlling off-design parameter variations as key inputs through uncertainty quantification of the key inputs. We demonstrated the technical approach by considering die casting manufacturing process. State-of-the art software like C++, MPI, GMSH, Paraview, OOF2 and Matlab were used to develop and drive the virtual certification methodology. The approach would also be seamlessly applicable to other manufacturing processes and software tools. The key takeaway of this project was the development of the virtual assessment and certification model that can be used by die casting engineers in designing the die and operational parameters for improving product quality. For the experimental geometries considered in this work, the OpenCast results agreed with experimental data within a few percent, typically less than 5%.

Our work addressed the goals mentioned by DMDII-15-07 as follows:

1. **Validation of Digital Manufacturing Tools**: Our work developed a comprehensive framework for assessing and improving the fidelity of digital manufacturing by integrating traditional simulation tools with Validation and Verification (V & V) and Uncertainty Quantification (UQ) tools to increase the fidelity of the predictions. On-design and off-design simulations were tested and where possible compared with laboratory and in-plant data.
2. **Demonstrate technologies that use advanced computing, modeling and simulations, and data analysis**: We integrated widely used various open source software for process modeling with tools for data analysis and techniques for uncertainty estimation and design optimization. Stochastic estimation techniques derived from recent research were combined with finite element and finite volume techniques to provide confidence levels in product quality and performance.
3. **Reduce cost of Certification through Virtual Experiments**: A microstructure and mechanical property prediction framework was developed which provided the properties and behavior of materials under various processing conditions by combining simulations with data analysis. The process parameter histories were linked to property variations and behavior of the materials. Our work shall reduce design-to-build time and associated costs.

We were successfully able to achieve the goal of this project which was to enhance as well as quantify the fidelity of computer-based predictive tools for a widely used process of die casting. The key innovation is the framework (OpenCast) by which a given product's performance can be predicted with bounds defined, thus leading to product certification.

I. PROJECT REVIEW

a. Project Scope and Objectives

The manufacturing industry employs a variety of manufacturing processes to produce a required finished product. These range from casting of raw materials in the form of billets and ingots to direct additive manufacturing through layer-by-layer deposition of the metal using laser or E-beam melting. Direct casting of machine parts is extensively employed in industry to produce near net shape products using liquid metals and die casters. Cast billets and steel ingots are converted into component form by a combination of machining processes such as milling, turning, drilling, etc. In all of these manufacturing processes, complex thermo-mechanical phenomena take place, which control the final quality of the finished product. In processes such as welding, the metal is melted first and then solidified to form the joined interface between two metal pieces. The integrity of such processes is a function of the residual stresses, and the infiltration of any impurities or gas bubbles from the outside. In order to produce components and material of high quality, it is necessary to understand the processes in detail and minimize events that lead to costly defects in the products.

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 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 the proposed 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, was aimed to reduce the uncertainty in the numerical simulation models through three main approaches:

a) Verification and Validation; (Chapter 4 of the Appendix, A.1)

b) Uncertainty Quantification; (Chapter 6, 7 of the Appendix, A.1)

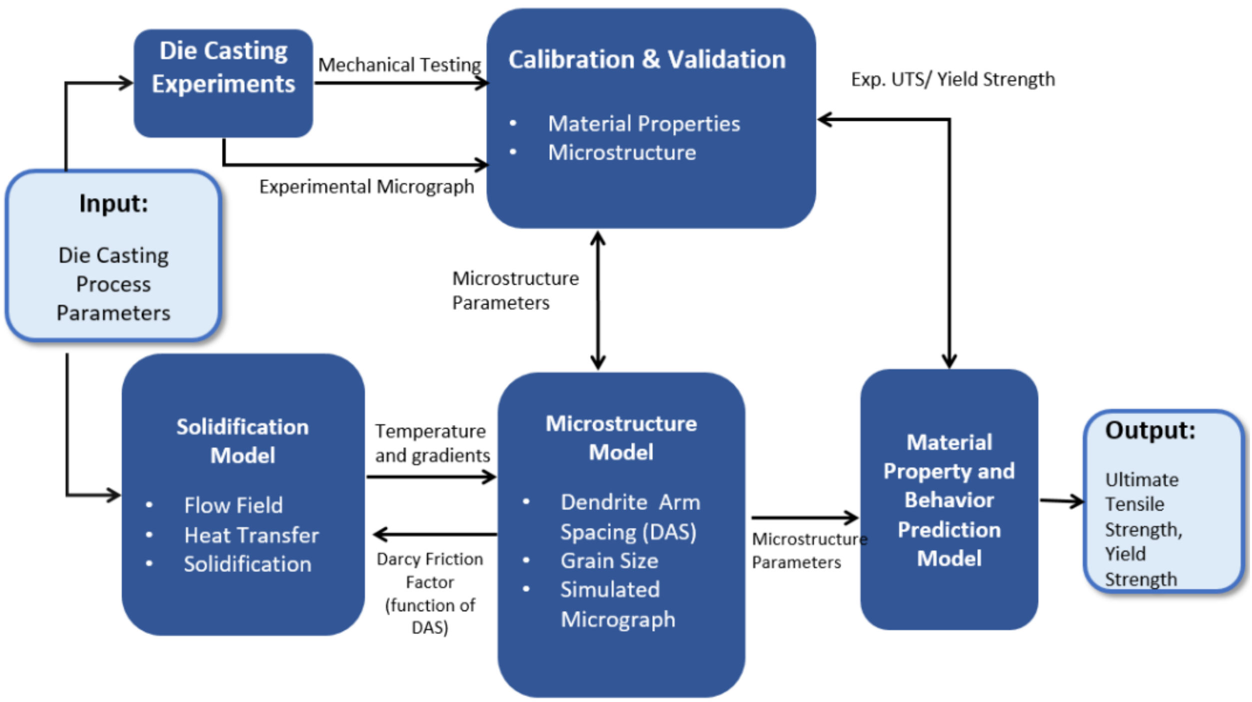
c) Virtual Experiments or Predictions. (Chapter 5 of the Appendix, A.1)

The main goals and objectives for the work were:

i) Develop an innovative methodology integrating data, computation, verification, uncertainty quantification, validation and prediction frameworks
ii) Provide a framework combining in-house/existing commercial software for solid, fluid, and thermal analysis with uncertainty quantification and microstructure modeling tools

Provide a virtual test bed to cast a given die cast geometry and predict its mechanical properties. The benefits of such simulations will be performance improvements through reductions in scrap castings, improvement in productivity, reduction in testing, and improved designs.

b. **Technical Approach and Planned Benefits**



The technical approach, summarized as shown in the figure above, is discussed in detail in the appendix (A.1) with a short overview here.

Individual components of virtual certification framework are shown in the above figure. The top and bottom links connect the input process parameters to outputs using experiments and numerical simulations, respectively. Real life die castings can be used to calibrate the empirical models for microstructure and material property parameters. Temperature gradients and cooling rates estimated using the numerical simulations are inputs to these models. The numerical software has been verified using published results for canonical problems and validated using available experimental results. Uncertainty quantification is a wrapper on the deterministic software in order to estimate the impact of stochastic variation in the process parameters on the final product quality. Below, we briefly describe, each module of the framework.

The first module is the calculation of temperature distribution in the die cast part as a function of space and time. Solidification phenomena of die casting involves interplay between heat transfer and flow due to natural convection. Temperature distribution and flow patterns during solidification of pure metals or binary alloys are needed for estimating the microstructure. Hence the Navier-Stokes equations and energy equations are solved using finite volume technique. Efficient multigrid based techniques provided rapid convergence so as to test may different input conditions.

For die casting, the microstructure parameters like grain size and dendritic arm spacing are important as they affect the final product quality. After the temperature distribution is calculated, models are needed to estimate the grain size distribution as a function of the local rate of cooling. Phase field modeling is a popular method used to study the evolution of the microstructure during solidification. The phase field method simulates the growth of each dendrite and thus, it is computationally expensive at the length scale of die cast products. In this research, an empirical relation is used to estimate secondary dendritic arm spacing. There are various models suggested for grain size estimation during solidification. Here, the isothermal crystal growth model is used. The temperature gradients and cooling rates are used to estimate the micro-structure parameters like grain size and mechanical properties like yield strength. This is the second module developed in this effort.

A third module developed in this study is for uncertainty quantification. Use of deterministic simulations alone to analyze the engineering systems is incomplete due to the lack of precisely defined input data. Thus, there has been a growing interest in coupling uncertainty propagation techniques with the deterministic numerical simulations to estimate the effects of stochastic variations in the input process parameters on the outputs. The polynomial chaos expansion is a popular method used to estimate the relation between input and output parameters. Stochastic Galerkin projection and collocation are two strategies to estimate the coefficients of the polynomial chaos expansion. Stochastic Galerkin method is an intrusive method since it requires solution of a new set of equations and thus, modification of the underlying deterministic code which becomes a significant additional effort. Hence, recently non-intrusive stochastic collocation methods have been developed which need multiple evaluations of the deterministic simulation at predefined collocation points obtained by sampling from the probability distribution function of the input parameters. Values of outputs estimated at these samples are then used to estimate the coefficients of the polynomial chaos expansion.

The present effort aims to reduce the uncertainty in the numerical simulation results through verification, validation and uncertainty quantification. Verification, calibration, and validation is done by published numerical and experimental results. Uncertainty quantification is used to assess the impact of stochasticity in the input parameters on the output parameters.

Thus, a framework with calibration, verification, validation and uncertainty quantification coupled to numerical simulation is developed in this effort.

The technical approach was accomplished with a collaborative team comprising the University of Illinois at Urbana-Champaign (UIUC), North American Die Casting Association (NADCA) and its member companies which include Chicago White Metal Casting, Mercury Castings, RCM Industries, Twin City Die Castings Company and Visi-Trak Worldwide. The UIUC team developed the OpenCast software and technical methodologies that were incorporated into OpenCast, and the experimental structures and Data were provided by NADCA and its member companies.

III. KPI'S & METRICS

This project established new tools for verification, validation and uncertainty quantification in the area of die casting. The key metrics that have been achieved in verification, validation and uncertainty quantification are summarized below.

Verification: At the start of our project, there were no tools to establish rigorous verification of die casting software. To establish verification, we have identified and developed approaches such as analytical theories and code-to-code comparison. We have established verification of OpenCast by considering a number of real-life die castings. Verification is performed using numerical results of the three dimensional natural convection problem (details in Appendix A.1 Chapter 4.1).

Validation: Similar to verification, at the start of our project, there were no tools to establish rigorous validation of die casting software. To establish validation, we have performed experiments of real-life die castings. We have established validation of OpenCast by considering a number of real-life die castings. Validation with uncertainty quantification is performed using the temperature time history from the solidification of a block. This study validates the fluid flow due to natural convection, heat transfer and solidification aspects of OpenCast (details in Appendix A.1 Chapter 4.2).

Uncertainty Quantification: Similar to verification and validation, the baseline for identification of important uncertainties and incorporating them into die casting software was minimal. As part of this project, we have established rigorous uncertainty quantification by performing systematic experiments and sensitivity analysis. A number of key uncertainties were identified in the boundary temperatures, initial temperature and alloy composition. The results of propagation of these uncertainties on the outputs like grain size, SDAS and yield strength are discussed in the chapter 7 of appendix A.1.

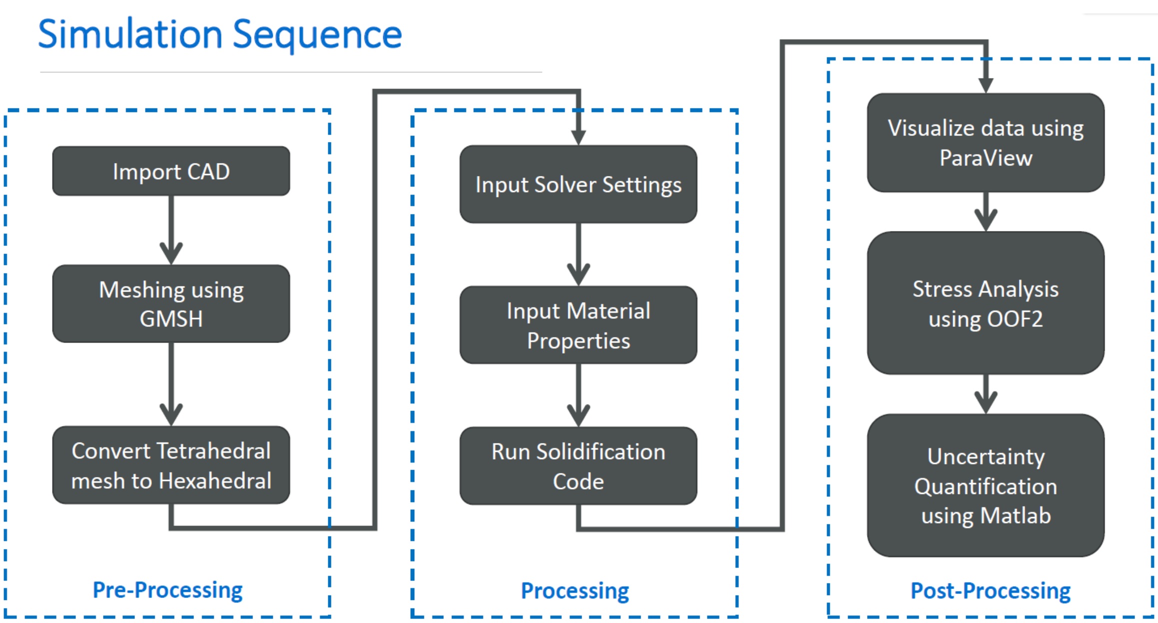
IV. TECHNOLOGY OUTCOMES

a. Product Features

We developed a numerical software OpenCast that models fluid flow, heat transfer and solidification. The software uses the finite volume method on an unstructured mesh that has been demonstrated on multiple practical casting geometries. It is coupled with surrogate modeling techniques like polynomial chaos expansion and neural networks. Parameter and boundary condition uncertainty quantification and sensitivity analysis have also been integrated. Design optimization using pattern search and genetic algorithm together with machine learning methods are also included in the software. The developed software environment also includes a python based GUI which is capable of

- Pre-processing of user-defined geometry
- Providing input material properties
- Running the solidification code on multiple processors
- Visualization of output generated
- Representative microstructure generation and stress analysis
- Generation of response surfaces for a 2D UQ analysis

A detailed manual on installing dependencies and capabilities of the GUI is included as Appendix A.6. Details of the input variables and their format are also given in Appendix A.6. A diagram of the simulation sequence is given below. It includes calls to various modules through a GUI, as follows. First, a input geometry corresponding to the cast is provided as a CAD file. This geometry is supplied in Solid works format. It is then meshed, through a GUI command, using open source software GMSH. The GMSH generates a combination of tetrahedral and hexahedral elements. However, the convergence of fluid flow solution on tetrahedral elements is slower than on hexahedral elements, hence the tetrahedral elements are converted to hexahedral elements. The GUI then provides commands to prescribe solver settings, and material properties. Given these, the next action is to run the solidification (fluid flow and heat transfer) code and predict the time evolution of the temperature field. This spatio-temporal evolution can be visualized using the open source software ParaView. The GUI provides a command to launch the Paraview software. The temperature distribution can then be used to also conduct a stress analysis using the software OOF2 (also open source). The final step is the uncertainty and optimization study, which requires multiple runs of the software through a wrapper. This UQ analysis is done through Matlab. Matlab scripting is the only non open source software required to conduct the UQ analysis.



b. System Requirements *

Recommended operating system and CPU configuration:

- Linux based operating system: OpenCast is tested on Ubuntu 16.04.3 LTS and 18.04.1 LTS. But it may work on other linux operating systems.
- RAM: At least 8GB
- Processor Frequency: At least 1500 MHz

c. System Architecture *

Discussed in the appendix A.6 in details

d. Features & Attributes *

Discussed in the appendix A.6 in details

e. Modes of Operation *

Discussed in the appendix A.6 in details

f. Software Development Documentation/Design Document *

Discussed in the appendix A.1 in details

a. Background Intellectual Property

None

Installing Dependencies

- OS
  - Ubuntu
- GUI Interface
  - pyQT4
- C++
  - Mpi
  - Make
  - Hypre
  - parallel
- Mesh generation and viewing
  - GMSH
- Output visualization
  - Paraview
- Microstructure and Stress Analysis
  - OOF2
- UQ
  - MATLAB with UQLab
  - GQN sparse grid for different dimensions and accuracy levels

g. **Users & Use Cases**

Opencast can be used by any engineer that works in die casting and manufacturing. The engineer uses Opencast to simulate the die casting process so that the engineer can do tradeoff analyses to determine the manufacturing time and determine best casting manufacturing process to produce a quality part and decrease the number of prototype iterations. The software will ultimately decrease manufacturing time and cost.

II. ACCESSING THE TECHNOLOGY

As computational scientists, we wanted to develop virtually-guided certification tools to significantly minimize manufacturing costs and improve product quality. The integrated software environment for virtual die casting, along with appropriate user interface tools have been developed and are provided to DMDII. Any organization that has access to this tool through DMDII should be able use it for die casting and other manufacturing applications that will be supported by the tool. Manufacturing engineers should be able to use the software environment to design products with reduced uncertainty, improved strength, longer life-time, reduced waste, etc. The software will be supplied both to DMDII and NADCA for distribution as open source software. However, there is no maintenance provided at this time. We are currently not looking into commercial avenues for the software. However, other third party vendors may develop marketable software in conjunction with UIUC, NADCA and DMDII. Currently UIUC is not claiming any IP to the developed flow software.

VI. INDUSTRY IMPACT & POTENTIAL

a. **Impact to the specific market the project was addressing and size of that market**

The software can be used by all die casting manufacturing engineers to optimize the process conditions, and estimate the uncertainties in product quality because of parameter uncertainties. The market for die casting is large but consists of small and big industries. Current costs of similar but less-sophisticated costs are large and discourage them from using the strength and advantages of mathematical modeling. An open source software can encourage more industry engineers to adopt this technology. The market for diecasting products is estimated to be in the billions of dollars, and market for existing commercial software for casting is a few hundred million dollars.

b. How could this technology be used in other industries

The framework can be applied to other manufacturing processes like additive manufacturing, welding, sand casting etc. with modifications to OpenCast.

c. Next step based on other use potential

The software has been delivered to NADCA for beta-testing. We will also provide a copy of the software to DMDII for distribution, if desired. Currently no plans exist for commercialization and product maintenance by UIUC.

VII. TECH TRANSITION PLAN & COMMERCIALIZATION

We are collaborating with industry partners to obtain real-life die-cast process data for validation. The integrated software environment will be shared with industry partners. A manufacturing organization can use our software, provide feedback and share useful experimental data to extend the fidelity of the predictive models. DMDII members interested in other manufacturing applications can contact us for collaboration opportunities. A detailed software training session was organized for DMDII members and industry partners.

a. Identify Future Plans

We are currently not looking into commercial avenues for our software. However, we are open to the idea.

b. Identified Barriers to Adoption

Currently existing commercial software do not have all the features developed in this work. This software combines uncertainty quantification and sensitivity analysis with numerical modeling of solidification during die casting using polynomial chaos expansion method and machine learning techniques. The linear solver is a blend of algebraic multigrid with Krylov subspace solvers for speedy convergence. However, existing commercial software provide professional level maintenance and support that are helpful to the user. We currently do not have any staff to maintain and provide instructions on use of software. This is one major barrier to product adoption. We are willing and interested in partnering with any third party vendors interested in commercializing the software.

c. Additional Information to Consider

For calibration and validation, experimental data would be useful. Since it was difficult to measure temperature and velocities during solidification in die casting, we used temperature measurements from a published work for validation. However, in future, the models can be improved if any actual die casting data is available.

VIII. WORKFORCE DEVELOPMENT

The North American Die Casting Association consists of approximately 400 small, medium and large die casting companies and manufacturers of die casting equipment. It is the main industrial body representing die casting in North America. The participation of NADCA in this work attests to the value this research brings to the community. Computer simulations are rated highly by the die casting industry for their utility to process design, but many member companies in NADCA do not have necessary knowhow and training to use existing simulation software. NADCA offers a large number of educational courses and training workshops for the member companies. Current courses cover all aspects of die casting, ranging from introduction to die casting to computer simulations. Courses on die cast problem solving, formation of defects and strategies for their reduction, thermal design and cost estimation are taught as one-day or two-day short courses and/or as workshops. Problem solving is emphasized than basic mathematical and/or physical aspects. These courses are well attended by members of the consortium. Capitalizing on the resources and contacts available through NADCA, this team will transfer results of proposed research to member industries through various channels available at the University and at NADCA.

First, the university team in collaboration with NADCA organized a workshop that presented the results of this research to member companies (Appendices A.2-A.5). This workshop was scheduled and managed in much the same way as other courses taught by NADCA. In addition, the webinar was recorded and will be electronically transmitted as per the demand from member companies. These activities are expected to contribute towards work force development and increased productivity. The webinar is uploaded at
https://www.diecasting.org/wcm/Technology/OpenCast/wcm/Technology/OpenCast.aspx?hkey=a510d2f1-5c6b-489e-b40d-82e16aa745b9

IX. CONCLUSIONS/RECOMMENDATIONS

This project led to the development of OpenCast – an open source multiphysics code that can simulate real-life die castings. The key features are:

1) OpenCast has been rigorously verified with existing analytical and simulation results
2) OpenCast has been rigorously validated with experimental data for real-life die castings
3) Uncertainties that play an important role have been identified and they have been incorporated into OpenCast

The present effort generated an open source software for die and material casting that currently does not exist. The DMDII investment is valuable to the industry who wish to conduct thermal/mechanical analyses. Further, we also have provided UQ wrapper on the main software. The key recommendation is to continue the validation of the software with more experimental data measured across the globe, and by the industries themselves. This should be an ongoing effort in future years.

X. LESSONS LEARNED

Solidification software with fluid flow and natural convection was verified and validated. Uncertainty quantification was also been integrated into the software framework. However, we had limited experimental data for die cast products. If we had more data, we could have performed more extensive validation, thereby expanding the prediction capability of the tool. It is also necessary to instrument the die with thermocouples to measure the temperature distribution, which has to be supplied to the Opencast software environment. Also, an integrated thermal analysis of the die must be performed along with the solidification analysis to input the boundary conditions. The main lesson learned is the lack of experimental data on actual die casting geometries. However, currently many die casting companies are using commercial software for “what if” kind of analysis. Open cast can be used in the same vein.

XII. APPENDICES

See appendices for more details on the theory, validation, results, and the user interface.

- A.1 OpenCast Theory Manual
- A.2 Gov Eqns Numerics UQ (NADCA Webinar)
- A.3 Deterministic Solidification Results (NADCA Webinar)
- A.4 Experimental Testing (NADCA Webinar)
- A.5 Uncertainty Quantification and Optimization (NADCA Webinar)
- A.6 OpenCast GUI Manual