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The Importance of Properties in Modeling

A.F. Giamei

United Technologies Research Center
MS 129-22, Silver Lane
East Hartford, CT 06108

Abstract

Casting and welding of superalloys, stainless steel and titanium alloys are processes which can be improved through modeling of heat flow, fluid flow, residual stress development and microstructural evolution. These simulations require inputs of thermophysical data, some of which involves the partially or totally liquid state. In particular, these processes involve melting, flow in the liquid and solidification. Modeling of such processes can lead to an improved understanding of defects such as shrinkage, inclusions, cracks, incomplete filling (or penetration), macrosegregation, improper grain structure and deviations from dimensional specifications. Effective modeling can shorten process development time and improve quality.

An approach to these problems is to develop efficient models; validate through correlations with thermal, distortion and microstructural data; run parametric studies; extract knowledge based rules; and apply to adaptive closed loop control systems. With the appropriate pre- and post-processing, such analyses can be made "user friendly". This would include graphical user interfaces as well as realistic images and color maps. In such form, these models can be used for sensitivity analyses, which are useful in defining appropriate sensors and in the development of control strategies.

Such modeling can be done at several levels, e.g., the MARO level, modeling large scale phenomena such as heat and fluid flow or material deformation; the MICRO level, modeling the development of dendrites, grains or precipitates; or at the NANO level, modeling point defects, dislocations, stacking faults, etc. There are many computational issues associated with these simulations, e.g. computational efficiency and accuracy. In addition, there are many materials issues, not the least of which is the availability of accurate high temperature thermophysical data for complex alloys. This would include latent heat of fusion, temperature dependent heat capacity and thermal conductivity (for liquid and solid), viscosity, surface tension, thermal expansion, mechanical properties, etc. Preliminary data is frequently gathered from the literature; however, this is often not available for modern alloys. If additional data are required, measurements can be used; however, these are costly, time consuming and can be erroneous due to a lack of testing standards or impure materials.

Microstructural predictors can be extracted from thermal information, e.g. cooling rate

and thermal gradient; again, the prediction of microstructure is dependent on solidus and liquidus temperatures, mushy zone permeability, the solidification curve, volume changes, phase transformations, alloying effects (such as surface tension or viscosity), mold/metal reactions, metal/environment reactions, etc. Defect maps may be needed to predict the onset of shrinkage, hot cracking or "freckling". Constants may be needed for stress relaxation, dendrite coarsening, vaporization, etc. Visualization has been used as a tool to better comprehend complex data sets associated with the analysis of directional solidification (including crystal growth) and welding. Examples include not only isotherms, but also cooling rate, growth rate and thermal gradient. The latter two are not single valued scalars, but rather time and space dependent vector fields.

Efficient models have been developed for both casting and welding to predict heat flow and the relationship to dendrite and grain growth. These codes include many of the non-linear effects, e.g. radiation, which dominate these processes. The home-built FDM code(s) were designed to be useful not only to the scientist, but also to the process engineer. Special output can be requested to compare directly to experimental data. Visualization procedures were developed to visualize critical results, e.g. fusion zone width at the surface opposite that where the arc is applied ("penetration"). Both elaborate and simplified distortion analyses have been carried out. It is clear that extensive mechanical property data are critical in order to accurately predict residual stress patterns.

A scheme is currently being developed to integrate these modeling tools into a set of control algorithms; however, the success of this approach is critically dependent on the availability of accurate high temperature thermophysical data.

THE IMPORTANCE OF PROPERTIES IN MODELING

DEFECTS

CASTING	WELDING
SHRINKAGE INCLUSIONS CRACKING DIMENSION GRAIN NON-FILL MACRO SEGREGATION	CRACKING DISTORTION DROP-OUT POOR PENETRATION

APPROACH

Develop efficient models to enhance understanding and to correlate with IR, TC, Strain and Microstructural Data

Run parametric studies
Extract "rules"
Compare with "knowledge based" rules

Apply to control system

MODELING

- Preprocessing / analysis / post processing

- Color graphics with realism
- Animation

- Sensitivity analysis
- Model interrogation
- Artificial intelligence
- Comparision with experiment

LEVELS OF MODELING (LENGTH SCALES)

- MACRO (HF, FF, STR)
- MICRO (Grains, Dendrites, PPT)
- NANO (Dislocations, Point Defects)

MODELING PAYOFFS

- SHORTEN LEAD TIMES
- AVOID CAPACITY BOTTLENECKS
- IMPROVED QUALITY
- ACCELERATED COMPONENT DEMOS.
- INTELLIGENT PROCESSING

COMPUTER SCIENCE ISSUES

PHYSICAL MODELING
  Equations
  Assumptions
  IC, BC

COMPUTER PLATFORM
  Dimensionality
  Mesh Size
  Degree of Coupling

ALGORITHMS

ACCELERATION SCHEMES

VISUALIZATION TOOLS

MATERIALS ISSUES

- Reality
    - Assumptions
    - IC, BC
- Material Models
    - Solidification
    - Mechanical Behavior
- Parameters
    - $L, k, C_p, n, \alpha, \gamma, \varepsilon, , \eta, \upsilon$
- Parametric Studies and Assessment
- Validation

SOURCES OF THERMOPHYSICAL or MECHANICAL DATA:

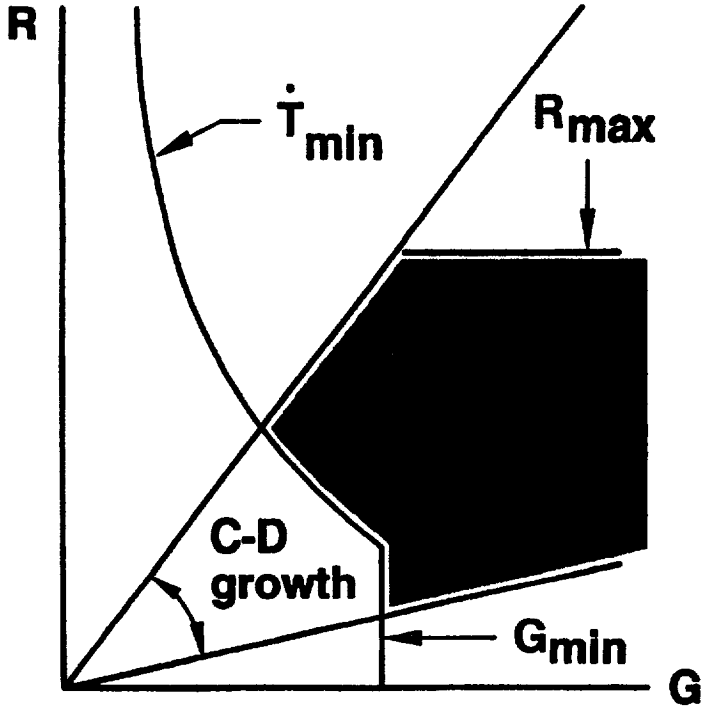
- Literature
- Experiment
- Thermodynamic Models
- Physical Models

CRITICAL LIQUID PROPERTIES

- THERMAL CONDUCTIVITY (vs. TEMP.)
- VISCOSITY & SURFACE TENSION "
- HEAT OF FUSION
- LIQUIDUS & SOLIDUS TEMP.
- SOLIDIFICATION CURVE
- MECHANICAL PROPERTIES OF "MUSH
- PERMEABILITY OF MUSH
- CHANGE IN VOLUME (L→S)
- MAJOR & MINOR ALLOYING EFFECTS
- ENVIRONMENTAL EFFECTS
- MOLD/METAL & GAS/METAL REACTIONS

SUPERALLOY DENDRITE AND EUTECTIC STRUCTURES

PROCESS TARGET ZONE



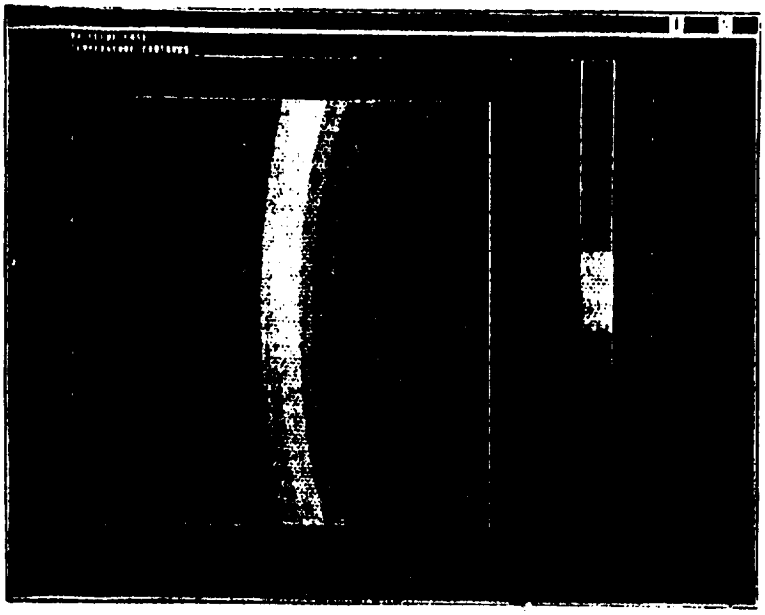
VISUALIZATION

VISA (FIELDVIEW), PATRAN and AVS

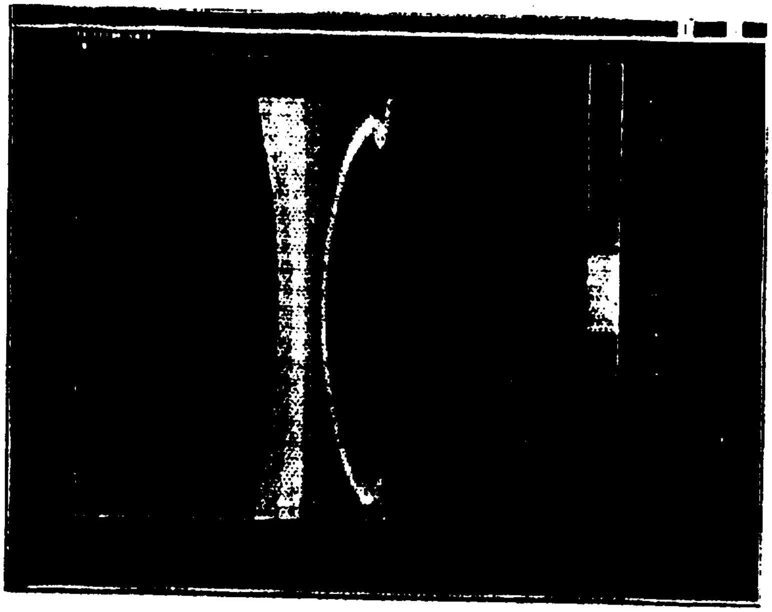
Run on Stellar GS-2000 & Dec-2100

Surface sections, Meshes
Isosurfaces, Contours
Translation, Rotation
User defined color maps
Animation

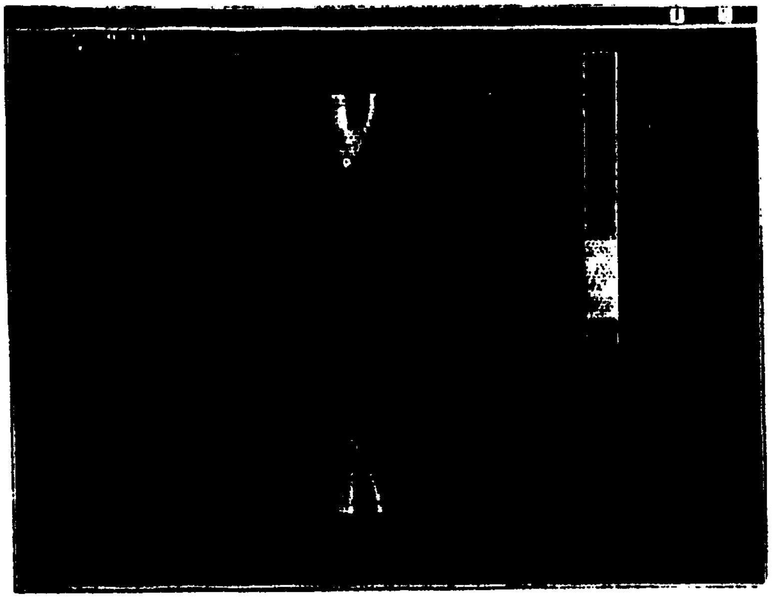
BASELINE CASE: TEMPERATURE CONTOURS



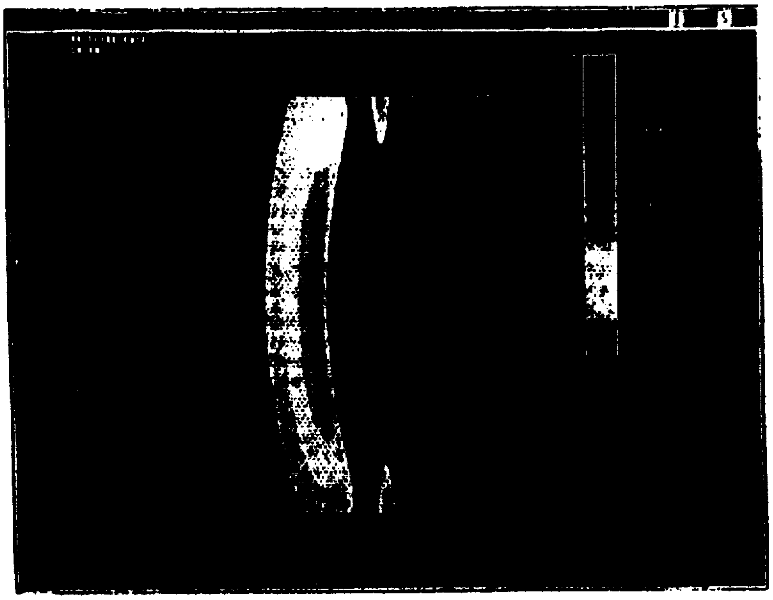
BASELINE CASE: G_n



BASELINE CASE: R_n



BASELINE CASE: G_n/R_n



WELD MODELS

Finite Difference Method (FDM)

Home built, Fast, User-Friendly, Temp Only
1 min to 1hr runtimes

Finite Element Method (FEM)

Commercial (MARC), Temp and Stress
3hr to 40 hr runtimes

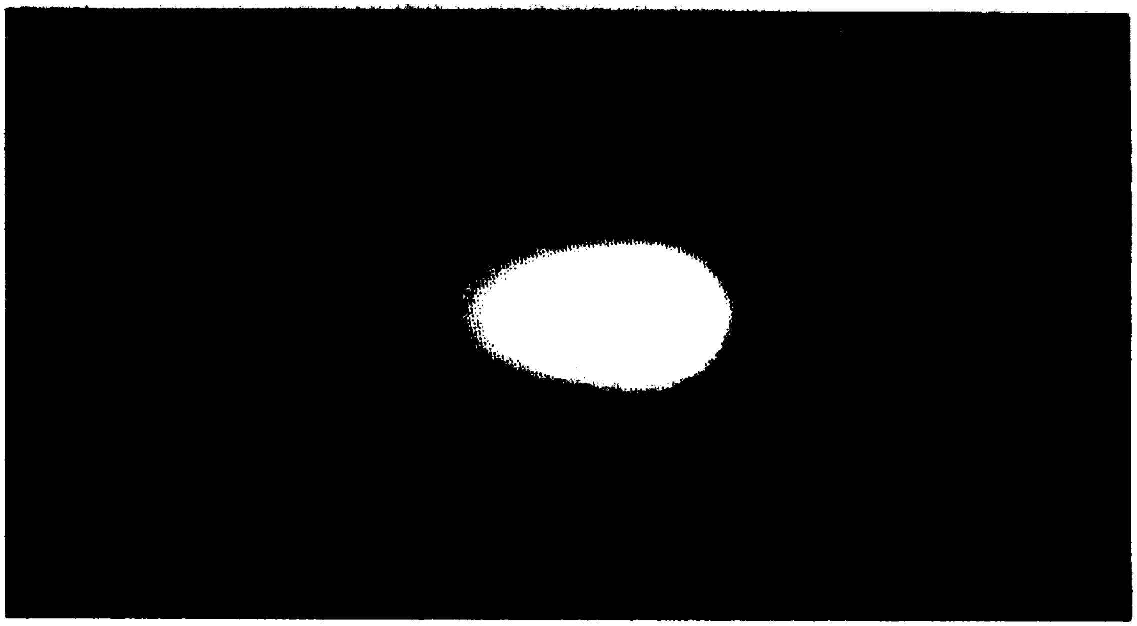
FDM Code

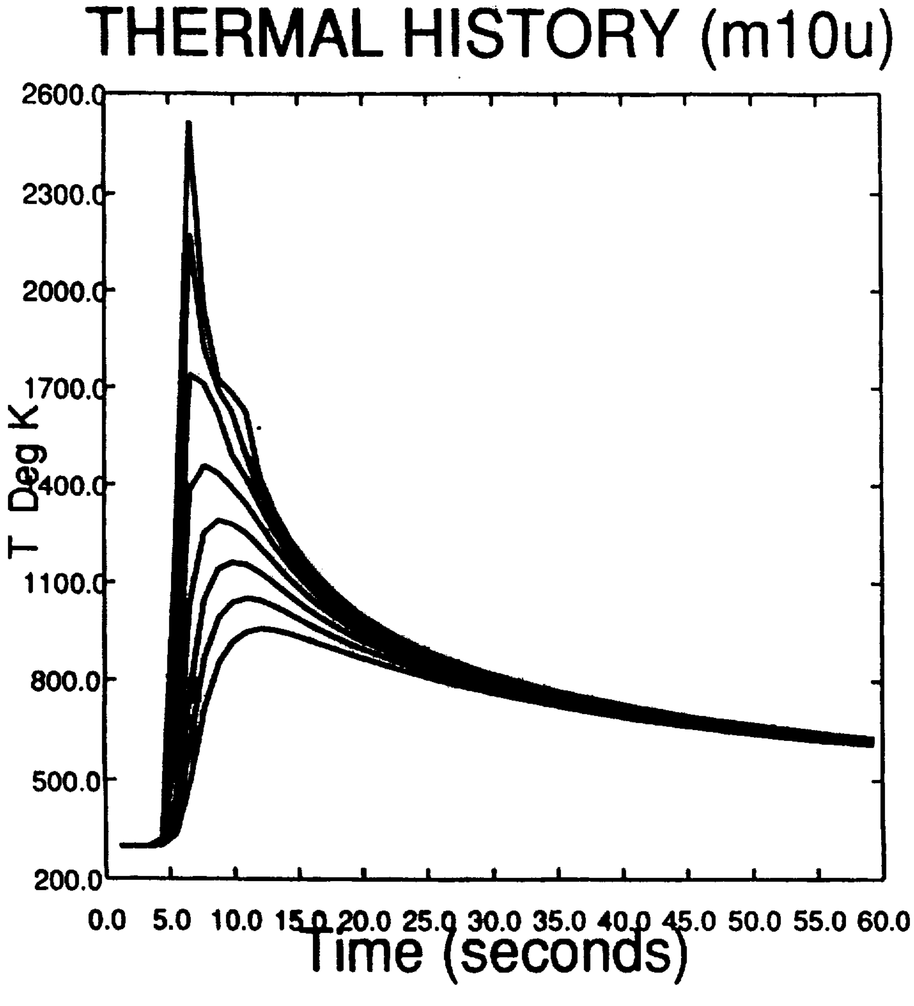
Includes Heat of Fusion, Temp dependent Sp. Heat &
Thermal Cond., Cond./Conv. & Radiation to Atm.
"Top Hat" or Gaussian Heat Input & Evaporation
Output for volume dependent data at a given time
and/or time dependent data on a given surface

Checkout and estimator provided for input data

Code broken down by function; Makefile provided

Derivative quantities (thermal gradient, cooling rate)
and microstructural predictors added




THERMAL HISTORY (m10u)
T Deg K
2600.0
2300.0
2000.0
1700.0
1400.0
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800.0
500.0
200.0
0.0
5.0
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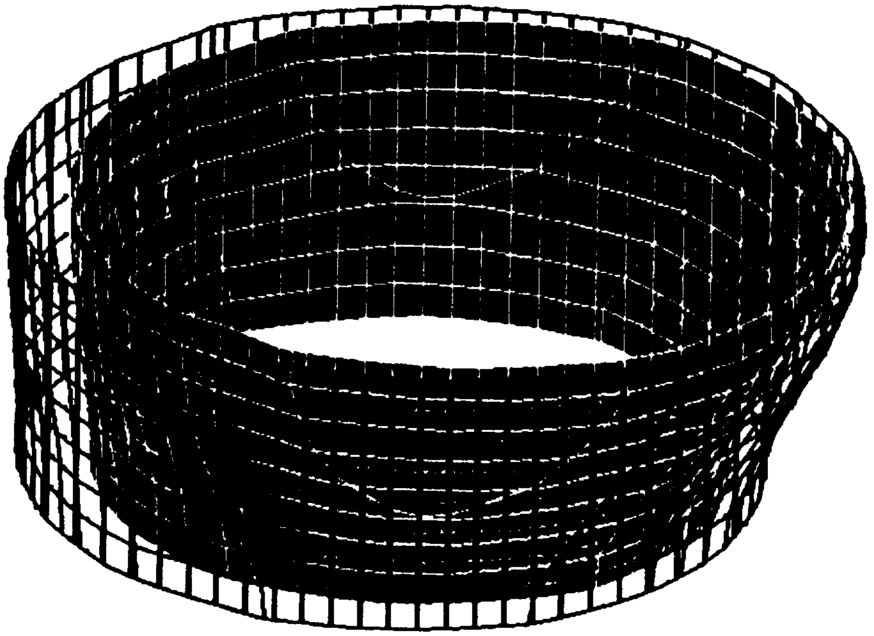
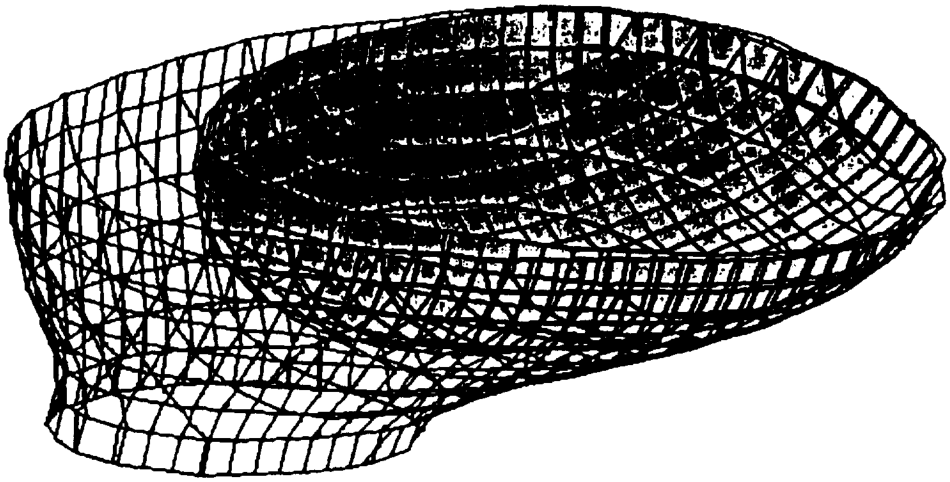
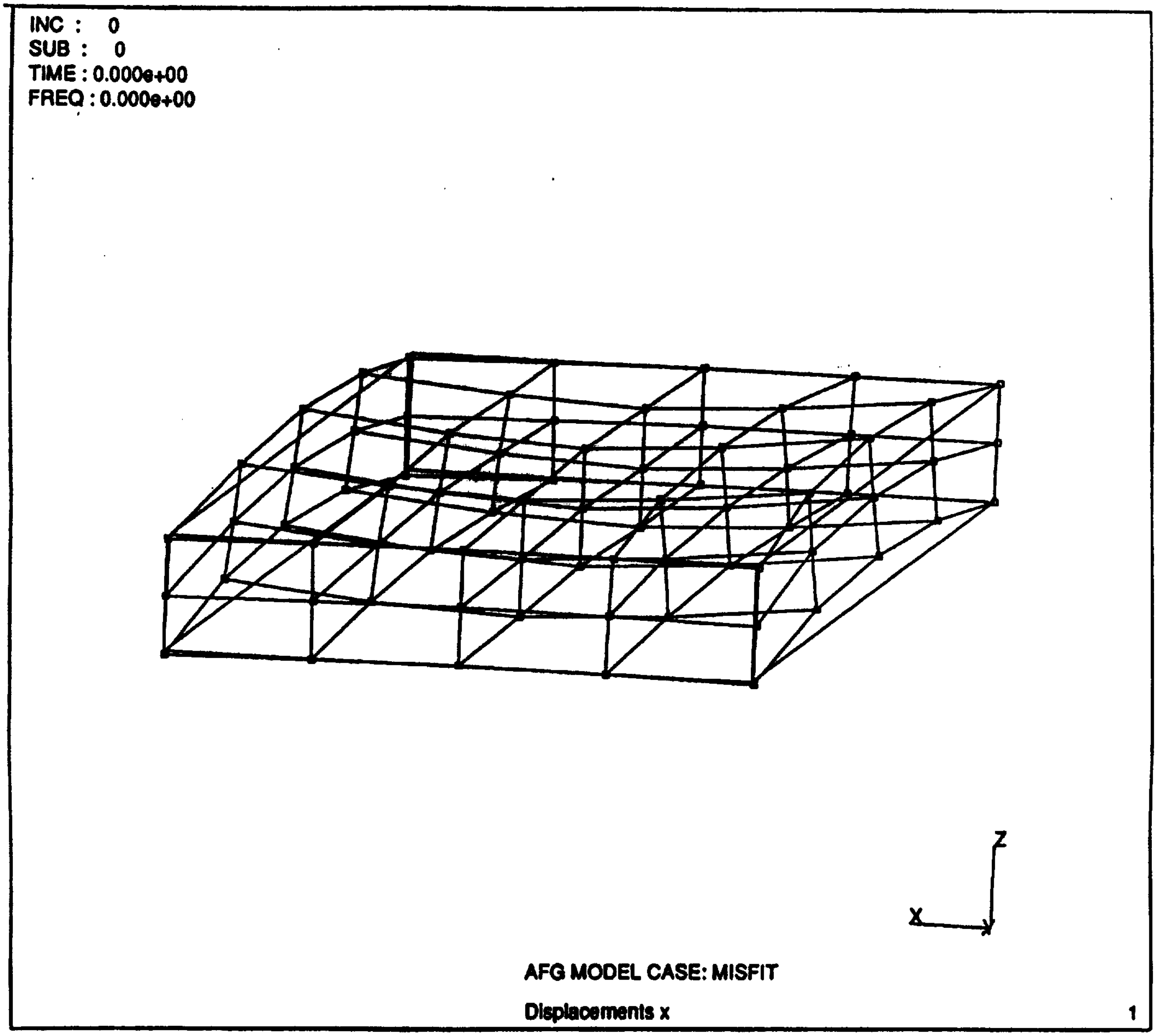
50.0
55.0
60.0
Time (seconds)



mv9E MUSHY ZONE (VEL. 1mm/s)

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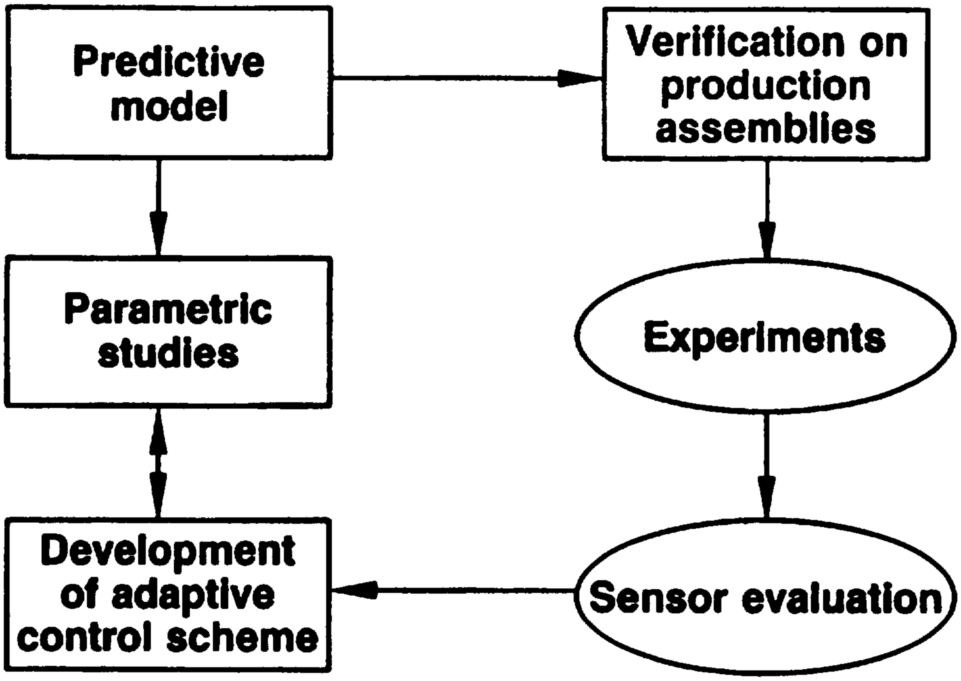
Z
X
AFG MODEL CASE: MISFIT
Displacements x
1

ADAPTIVE CONTROL DURING WELDING WILL REQUIRE IDENTIFICATION OF OF KEY PROCESS VARIABLES



Predictive model

Verification on production assemblies

Parametric studies

Experiments

Development of adaptive control scheme

Sensor evaluation

GIGO

Thermophysical Property Issues: Now and for the Future

by

J.W. Zindel
Research Laboratory
Ford Motor Company
Dearborn, MI

Abstract

Ford Casting Operations is using a finite difference model to simulate mold filling and solidification. The goal of the modeling is to reduce product cycle time, improve both prototype and production casting quality, and reduce tooling costs. This effort is complicated by the fact that numerous materials (gray iron, nodular iron, and aluminum) and mold materials (green sand, precision sand, semi-permanent mold and permanent mold) are currently used in production. The model requires various parameters such as heat transfer coefficients, conductivities, heat capacities and viscosities by specified as a function of temperature. The cost and time associated with generating this data for all the alloys and mold materials being used impedes the modeling process. In the future, as more sophisticated simulations become available, the required accuracy and resolution of the data will most certainly increase. Efforts aimed at making this type of data available in a timely, cost effective manner would be of great benefit to all.

Casting Operations
Ford Motor Company

Processes	Materials
Green Sand	Grey Iron
Precision Sand	Nodular Iron
Permanent Mold	Al 319
Evaporative	Al 356
Shell	Al F16
	Al 332

Why Model Casting Processes?

- **Reduce Cycle Time**
- **Improve Quality**
- **Reduce Costs**
  Eliminate Tooling Revisions
  Robust Design Reduces Scrap
- **Improve Yield**

Software Feature Considerations

- Accuracy
- 3-D
- Fill Cycle
- Ease of Implementation
  Geometry
  Material Properties
  Mesh Generation
- Speed of Execution

Required Data

- Conductivity
- Heat Capacity
- Density
- Viscosity
- Interface Heat Transfer Coefficient

- The Question:
- At what point does a marginal improvement in precision and accuracy of the data not result in an observable improvement in the prediction with current models?
- The Answer:
- Sensitivity analyses must be performed with existing software in order to determine the level of accuracy and precision required to make useful predictons. Validation experiments need to be conducted in concert with the sensitivity analyses.

Future Goals

- Mechanical Property Prediction
- Strategic Planning
  New process cycle times
  Capital requirements
- Residual Stress Prediction

Solidification Simulation Users and Support Group

R. Mrdjenovich	Champion
K. Blackmore	Systems
J. Dudley	Small parts
S. Huang	Small parts
J. Lapeus	Blocks
S. Zimdars	Heads
M. Martin	Manufacturing CAE
V. Nara	
D. Dewhirst	Research
J. Zindel	
R. Mueller	Technical Administration