MSG: A Computer System for Automated Modeling of Heat Transfer

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Abstract

The task of modeling, i.e. of creating a set of equations that can be used to predict the behavior of a physical object, is a key step in engineering analysis. This paper describes a computer system, MSG, for generating mathematical models to analyze physical systems involving heat transfer behavior. MSG is motivated by the need for modeling in an automated design process. The models are sets of equations which may include algebraic equations, ordinary differential equations and partial differential equations. MSG uses the strong domain theory to guide model construction in three sequential tasks: identify regions of interests on an object, determine relevant heat transfer and energy storage processes, and transform these processes into equations. The decisions in these tasks are guided by estimates of variation in temperature and material property, and the relative strengths of heat transfer processes.

1 Introduction

The task of modeling, i.e. of creating a set of equations that can be used to predict the behavior of a physical object, is a key part of engineering analysis, which in turn is an essential part of doing design, diagnosis, etc. The form of a mathematical model may have a significant impact on both the cost and the results of its analysis. For example, the temperature of a thin plate under certain boundary conditions can be analyzed by a 1-dimensional model instead of a 3-dimensional model with minimum loss of accuracy and significant reduction in computational cost. While modeling is important in engineering design and analysis, it is still mostly viewed as an art, with little formalization of the process by which it is done, and taught mostly by experience and example.

This paper describes a computer system MSG (Model Selection and Generation). MSG generates mathematical models to assist engineers in their analysis of heat transfer in physical systems. The particular focus of this work is on the analysis tasks which arise in designing thermal manufacturing systems, such as those for casting and heat treatment. The input to MSG consists of a description of an object in terms of its geometry, its physical properties and its environments, and a description of a query in terms of its type (e.g. "temperature" or "heat flow"), its scope (e.g. "as a function of the x dimension and time") and its accuracy expressed as a set of *thresholds*. The output is a model, i.e. a set of mathematical equations, which may include algebraic, ordinary differential and partial differential equations in both linear and non-linear forms.

MSG uses the theory of the domain to construct models in three sequential tasks:

1. identify regions of interests, i.e. control regions, on an object,
2. determine relevant heat transfer and energy storage processes for these regions, and
3. transform this set of processes into equations.

The complexity and accuracy of a model is determined by decisions in choosing control regions and physical processes. To determine control regions and relevant processes, MSG uses a set of domain specific, very approximate methods to estimate the heat transfer behavior of an object in terms of its temperature variation and the relative strengths of its heat transfer processes.

Based on the information, MSG heuristically decides on a model for a query that the model is required to answer.

It should be noted that the focus of this paper is on mathematical formulation of physical problems. Once a model is produced its accuracy must still be validated by comparing its predictions with known results, because there are no known a priori methods for guaranteeing the accuracy of models in this domain. In this paper we will not look at the problems of validating the model's accuracy other than to note that if validation determines that a more (or less) accurate model is required, we can alter the *threshold requirements* that are input to MSG in order to increase (or decrease) the accuracy of the model it produces. We will also not look at the task of converting the equations MSG produces into a program that uses them to predict the behavior, nor will we look at the task of actually using such a program.

The method of selecting a model is based on the approach used by our domain experts, which has been shown to be adequate in their engineering practice in this domain. Furthermore, we believe analogous methods are used by engineers in other engineering disciplines.

The current implementation of MSG handles physical systems of single or multiple 3 dimensional objects. Objects handled include rectangular shapes and some extensions (e.g. L-shaped blocks).

The next section discusses the motivating context for our work on MSG, which is the problem of iterative design of thermal systems, and gives the specific requirements that arise in this context. Section 3 gives an overview of the heat transfer domain, and Section 4 will present the major tasks of MSG and give two examples showing how MSG carries out its tasks. Section 5 discusses several issues including the transfer of our ideas to other domains, and Section 6 discusses related work. Finally, we conclude with a summary.

2 The Design Context and the Modeling Requirements

2.1 Modeling in Iterative Design

The motivation of MSG is to support the design of thermal manufacturing systems. In particular, MSG is to support the analysis task in iterative design, as shown in Figure 1.

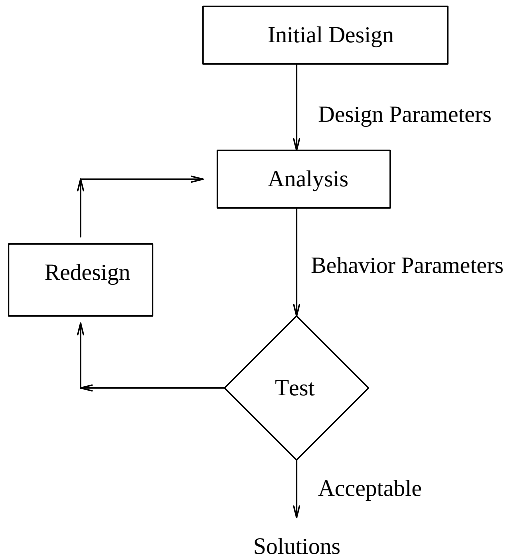

Figure 1: Iterative Design Process

In the domain of heat transfer, a system involves a complex, global interaction of heat transfer and energy storage processes on various parts of the system. Because of such global and complex interactions of processes, it is difficult to design one part of a system and evaluate the design of that part in isolation from the rest of the system. Instead, the design of a system has to be evaluated as a whole after the design of all its parts are completed. If the design does not meet the desired specifications, then it is modified and the whole evaluation is carried out again. This kind of design process is called "iterative design", where a design is successively modified and evaluated until it meets its required specifications.

In iterative design, the analysis of a design is often the major bottleneck of the cycle because it may involve complex mathematical models that are time consuming to evaluate. One strategy to ease the bottleneck is to minimize the use of complex models by using models of varying accuracy and computational cost to suit the needs of iterative design process. For example, cheaper models can be used to get a preliminary design that is close to acceptable, and more accurate but expensive models can be used for evaluations of a final design. In particular, the use of approximate models is effective for the following activities:

- In order to start the design, we are interested in finding a good *initial design*, so that the iterative cycle can converge to a final design faster [Jamalabad *et al.*, 1990]. To obtain a good initial design, we may want to take a model that predicts behavior of a given structure, and *invert* it, so that given a specific behavior it tells us a structure that has that behavior. Such inversion is usually only possible for the simplest, and therefore most approximate models, but even so a structure derived from an approximate model is a good starting point for further design work.

- Similarly, approximate models can be used to analytically derive other information that is useful in various stages of design, such as sensitivities and tradeoffs among various physical parameters.

- In fact, at various stages of design, the designer is usually at least as interested in getting a broad understanding of what is feasible and of what the sensitivities and tradeoffs are, as in coming up with a specific design. If this information is not derivable analytically, it must come from a broad exploration of the design space, which means numerical evaluations of many designs. Doing so requires a behavior model that is relatively cheap to evaluate.

- At early stages of design, not enough may be known about an artifact to model it with high accuracy. Geometry and physical data are often lacking and inaccurate. No benefit is gained in using accurate models if the underlying data are incomplete.

Thus in the course of a single design we may need several models with differing tradeoffs between accuracy and computational cost.

2.2 Design Goals for MSG

The iterative-design context described above leads to three major considerations affecting the requirements for MSG.

1. MSG should generate models automatically, with minimum user assistance. MSG is embedded within the analysis task of the iterative design cycle. In order to allow the iterative design cycle to continue rapidly, it is

essential that the analysis task can proceed without interruptions. That implies that MSG must also be on its own with minimum human intervention. Therefore, MSG not only knows what knowledge is required for a model, but also how to put the pieces together into the complete model. This is in contrast to the objectives of interactive modeling systems, such as [Finn *et al.*, 1992] (see Section 6). Another motivation for producing as automated a system as possible is the hope that by doing so we will learn more about the basic nature of the modeling process, making it more of a science and less of an art.

2. MSG should be able to specify the applicability conditions of models that it generates. The applicability of a model is defined by a list of assumptions made by MSG in its model generation process. The list of assumptions serves several purposes. They may be used by an analysis system to determine if a model can be used for a problem at hand. Assumptions can also be used to support other parts of analysis, e.g. to do "sanity checking" of simulation results, and to guide the interpretation of numerical data. Assumptions provide justifications of a model, such that users can examine the assumptions to determine if MSG makes the appropriate modeling decisions for a problem at hand, and thereby feel more confidence about models that MSG generates. Finally, assumptions can be used as educating tools for novice engineers to acquire modeling expertise.

3. MSG should be able to generate models for a broad range of problems involving various queries and geometric configurations. Design often involves new materials and new geometry, which cannot be predicted a priori. That implies that MSG must embody enough physics of the domain such that when those situations arise, MSG can still create models for them.

While these requirements come from the use of MSG to produce models to be used in design, we believe that a system meeting these goals would also be useful for other purposes, e.g. diagnosis or training.

Having described the impact of the design context on MSG, we will now discuss the domain of heat transfer.

3 The domain: Heat Transfer

From the standpoint of modeling, one primary feature of the heat transfer domain is that it has a "strong theory". By that, we mean the basic heat transfer and energy storage processes are well understood and we have reasonable models for each process in isolation. In addition, we also know how these processes interact, i.e. their interaction is governed by the basic law of conservation of energy [Incropera and DeWitt, 1990] [Arpaci, 1966] [Jaluria and Torrance, 1986]. For a physical object and its environment, we can identify the processes that occur in that object, and, through the conservation law, we know how to combine those processes into a model representing the heat transfer behavior of that object. [1] In this section, we will briefly describe the basic heat transfer and energy storage processes and the conservation law. Then we will describe how this domain theory is used in MSG for model generation.

In the domain of heat transfer, there are basic types of heat transfer processes which include conduction, convection, and radiation. Each of them is governed by a domain specific law, giving conditions under which it should occur and how the magnitude of the heat flux is related to properties of the physical system such as temperature, heat conductivity and area. For example, conduction is modeled by the Fourier law, $Q_i = -kA\frac{dT}{dx_i}$, where k is the conductivity, A the surface area, $\frac{dT}{dx_i}$ is the temperature gradient along the direction x_i. and Q_i is the heat transfer by conduction in the x_i direction. Similarly, convection is modeled by Newton's law of cooling, radiation by the Stefan-Boltzmann law, etc.

While the domain specific laws govern the basic types of heat transfer processes, the conservation law of energy tells us how these heat transfer processes interact in an object, and all mathematical models are based on that conservation law. The law says that the net heat flux into a control region plus the net heat generation within the region is equal to the net change in internal energy within the region. Note that associated with the conservation law is the concept of a *control region.* A control region is a closed region we specify on an object, with respect to which we instantiate the conservation law. The control region focuses our attention on heat flows *across* its boundaries and generation and storage processes *within* its boundaries, and thus helps identify those processes in an object which are considered relevant in a model that we

[1] However, solving a model is a non-trivial task

are building. A typical model, then, is one or more equations describing the various heat transfer processes acting across the boundaries of a control region and internal energy change within that region.

Typical questions to be answered by a model include the temperature, the heat flux, or the internal energy change of a physical system. Among the common queries, temperature is the most important one since all other queries can be deduced from temperature. It is also important to know that temperature can be modeled either as a single value, i.e. average or lumped temperature, or as a set of values representing temperature distribution over space or time. For example, in a casting process it can be important to keep the temperature gradient in the casting below some value at every point in the casting, in order to prevent warping. This means that MSG has to construct not only models based on algebraic or ordinary differential equations, but also based on partial differential equations.

Note that the structure of the domain theory suggests a sequential approach to constructing models:

1. First we need to choose control regions of an object.
2. For each control region, we determine which heat transfer and energy storage processes are potentially active in it and across its boundaries, and choose which ones to include in the model and how to model them.
3. Finally, we instantiate the equations representing the conservation laws, using terms representing the processes. We now have a model in mathematical form on which we can perform mathematical simplifications.

The complexity and the accuracy of a model depend on how we model the heat storage and energy storage processes, which in turn are determined by the choices of control regions, the choices of processes, and the choices of how to model those processes. The next question is: how do we make these choices?

One way to make these choices is to use numerical simulations to evaluate the contributions of heat transfer and energy storage processes to the accuracy and complexity of a model (using empirical data or our most accurate model as a reference to determine accuracy), and then decide which ones should be included in the model. While this approach can find a model meeting specified accuracy and computational cost, it is expensive as many models have to be tried and tested, including some of high computational cost.

The approach taken in MSG follows from our informal observation of expert engineers. We find that expert engineers tend to use a set of domain specific rules to estimate the gross heat transfer behavior of an object, and then use that behavior to guide their choices of control regions and heat transfer and energy storage processes. These estimation methods, while not very accurate for detail predictions, often give sufficient information for making modeling decisions, and they are cheap to use. Many of the methods use "dimensionless" numbers and ratios. These were discovered by domain experts through dimensional analysis of governing equations and boundary conditions [Incropera and DeWitt, 1990] [Panton, 1984]. They give estimations of relative importance of the heat transfer and energy storage processes in an object based on the physical properties and the boundary conditions of the object. An example of these is the aspect ratio of an object which gives relative strengths of heat conduction along two directions in the object. Other examples include Biot number etc. The next section gives an account of what they are, and how MSG use them to make the choices.

4 MSG

In this section, we will give a detailed description of MSG. We first describe its input and output, followed by its architecture. Then we present two examples to show how MSG generates models, one model with ordinary differential equations and one with partial differential equations.

4.1 Input and Output

4.1.1 Input

MSG requires three kinds of input.

Geometry and properties: The first kind describes the geometry, the physical properties and the configuration of an object. The geometry specifies the type of object and its major dimensions, e.g. the dimension of x, y, z of a parallelepiped. The physical properties include conductivity, specific heat, density of the object. The configuration specifies how components of the object are joined together, e.g. two plates are joined by a common surface along a dimension.

Boundary and Initial conditions: The second kind gives the initial conditions and specifies the environment in terms of temperatures, heat fluxes, convection coefficients, etc.

Query: The third kind of input includes the type of a query, its spatial and temporal scope, and its accuracy requirements. The types of queries include heat flux, energy storage of an object, and temperature. The spatial and temporal scope specifies the spatial and temporal dimension along which variations are of interest. For example, the query of temperature distribution, $T(x, y, z, t)$ has the spatial scope in x, y, z direction and its temporal scope in time, t. That query indicates to MSG that temperature distribution along all spatial and time dimensions is required. A query of $T(x)$, on the other hand, asks how temperature varies in the x direction but does not ask how it varies with the y, z, or time dimensions. Finally, the accuracy requirement of a query is expressed in terms of a set of thresholds. They are spatial, temporal and linearity thresholds which govern the criteria under which choices on control regions and heat transfer processes are made.

4.1.2 Output

MSG produces two kinds of output.

Model: A model is a set of equations. At least one of them is a governing equation which describes the interaction of heat transfer processes on the control region. Other equations describe initial conditions and interaction of heat transfer processes at boundaries of the object, if necessary.

Assumptions: A list of assumptions MSG makes to produce the model. The assumptions specify conditions under which this model is valid.

4.2 System Architecture

MSG has three sequential tasks. They are:

1. **Choice of control regions:** The first task is to determine the types of the control regions. There are two essential types of control region: differential and finite. A differential control region is an infinitesimally

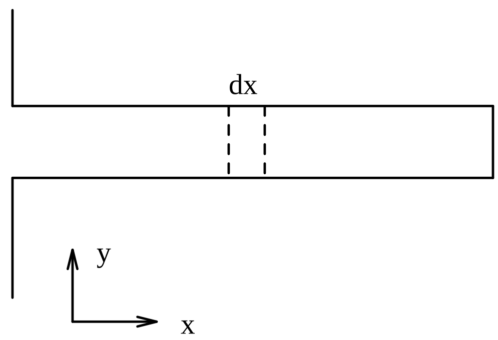

Figure 2: A control region for cooling fin

small region, for modeling interactions of heat transfer at each point in an object. A finite control region is a finite region for modeling overall interactions of heat transfer for that region. A control region can be finite on all dimensions of an object, or it can be finite in one dimension, and differential in other dimensions. An example of a finite control region for modeling a cooling fin is shown in Figure 2. The control region is differential in the x direction, but finite in other directions.

The choice of a control region is guided by the degree of temperature variation in spatial dimensions of objects. Temperature variation is defined as $\frac{\Delta_v T}{T_{ref}}$ where T is temperature, $\Delta_v T$ is the amount of temperature change as some dimension variable v varies over its range (e.g., v might be x, y, or z), and T_{ref} is some reference temperature in the range of v. The justification for choosing a differential control region is to capture temperature variation in a region. If temperature is sufficiently uniform, then a lumped model is as effective as a distributed model, with less computation cost.

MSG uses two different ways of estimating temperature variation in an object, depending on whether or not the object is a multi-component system. For a single component system, MSG uses Biot number [Incropera and DeWitt, 1990] to estimate temperature variation. It is a "dimensionless number", i.e. a ratio in which all physical dimensions such as length and time cancel out. The Biot number is derived from the balance of heat flux at the surface of an object. It is defined as

$$\frac{\Delta T_{solid}}{\Delta T_{boundary}} = \frac{hL}{k} \equiv \text{Biot Number}$$

where h, k, L are convection coefficient, conductivity, and thickness of an object along one spatial dimension. The formula for Biot number is derived from an estimate of the ratio of internal thermal resistance of a solid to the boundary layer thermal resistance, but it can be shown that this ratio is also roughly the ratio of temperature drop across thickness of the solid to temperature drop across the boundary. Thus, a small Biot number value implies a small temperature variation within the solid. If it is less than the specified threshold value, ϵ, a finite control region, i.e. a lumped model is chosen.

For a multi-component system, MSG calculates the lumped thermal resistance of each component in the system and the environment. Then it calculates the ratio of the lumped thermal resistance of each component to the total lumped thermal resistance of the system and the environments. If the ratio of that component is less than the specified spatial threshold, that component is lumped.

2. **Determining relevant physical processes:** After a control region is selected, the system can deduce the heat transfer and energy storage processes acting on the surface of and within that control region. The decision is to choose which of these processes to incorporate into the model, and the choice is based on the following rules.

   Reduction of Transient to Steady State: Reduction of a transient model to a steady state model is done by removing the process of internal energy change from the model. This is guided by the relative amount of temperature variation over time, defined as $\Delta_t T/\Delta_{max} T$, where $\Delta_t T$ is the difference in temperature at the start and end of the time interval we are modeling, calculated by using an algebraic lumped model of heat flow, and $\Delta_{max} T$ is the maximum temperature difference between initial and environment temperature. If $\Delta_t T/\Delta_{max} T \leq \epsilon$, then T is assumed to be constant with respect to time t. Therefore, $\partial T/\partial t = 0$, and the equations we eventually produce will have no term for heat storage, resulting in a steady state equation. Suppose that in some problem if we did not remove the energy storage process, the equation we eventually produced would be:

$$k\frac{\partial^2 T}{\partial x^2} = \rho C\frac{\partial T}{\partial t}$$

Then if we do remove the energy storage process the resulting equation will be:

$$k\frac{d^2 T}{dx^2} = 0$$

Spatial Dimension Reduction: Reduction from a 3D to a 2D or 1D model is done by removing conduction processes within solids along certain spatial dimensions. It is based on inferring that heat conduction in some dimension, say x, is much smaller than in other dimensions. If so, we can drop the process of heat conduction in x from our model, and hence from the resulting heat equation. If the only term in the equation mentioning x is the one arising from conduction in x, then if this term is dropped the number of spatial dimensions in the equation is reduced. Suppose that in some problem if we did not drop conduction in x the equation we eventually produced would be:

$$k\frac{\partial^2 T}{\partial x^2} + k\frac{\partial^2 T}{\partial y^2} + k\frac{\partial^2 T}{\partial z^2} = 0$$

Then if we do drop conduction in x the resulting equation will be:

$$k\frac{\partial^2 T}{\partial y^2} + k\frac{\partial^2 T}{\partial z^2} = 0$$

MSG estimates the ratio of heat conduction in one dimension to heat conduction in the other dimensions using a kind of order-of-magnitude reasoning; the resulting rule of thumb is based on the aspect ratio of the object, i.e. the ratios of its lengths in x, y, and z.

Non-linear to Linear Equations: Using the Fourier law in its full form to model conduction results in a *non-linear* PDE. If we can assume that physical properties such as thermal conductivity, specific heat, and density are independent of location, we can use a simplified form of the Fourier law which results in a *linear* PDE which is much easier to solve. Without this simplification conduction, e.g., in the y direction will be instantiated by the term

$$\frac{d}{dy}(k(y)\frac{dT}{\partial y})$$

whereas with the simplification, it becomes

$$k\frac{d^2T}{dy^2}$$

This simplification is based on estimating conductivity variation with respect to temperature. The conductivity variation is defined by $\Delta_T k/k_{average}$, where $\Delta_T k$ is difference of conductivity at maximum and minimum temperatures and $k_{average}$ is the average of these conductivities. If $\Delta_T k/k_{average} \leq \epsilon$, then the conductivity is assumed to be independent of temperature, and therefore also independent of x, y, and z (assuming a homogeneous material), which justifies using the simpler model of conduction.

3. **Transformation and Simplification:** After the decisions on physical processes and material properties have been made, their mathematical representations are fetched and put together in form of equations. To ensure the mathematical model is properly formed, MSG will generate relevant initial and boundary equations for the model according to the following rules:

   Initial condition: If an internal energy storage process is present, MSG generates an equation which represents the initial temperature distribution of an object.

   Boundary condition: If a differential control region is present in some dimension, and there are conduction processes in that dimension, then MSG generates equations which represent all boundary heat interactions in that dimension.

   Continuity condition: If differential control regions are present in two adjacent components of an object, MSG generates a equation representing the condition that the temperatures of of the joining surfaces of two components be the same.

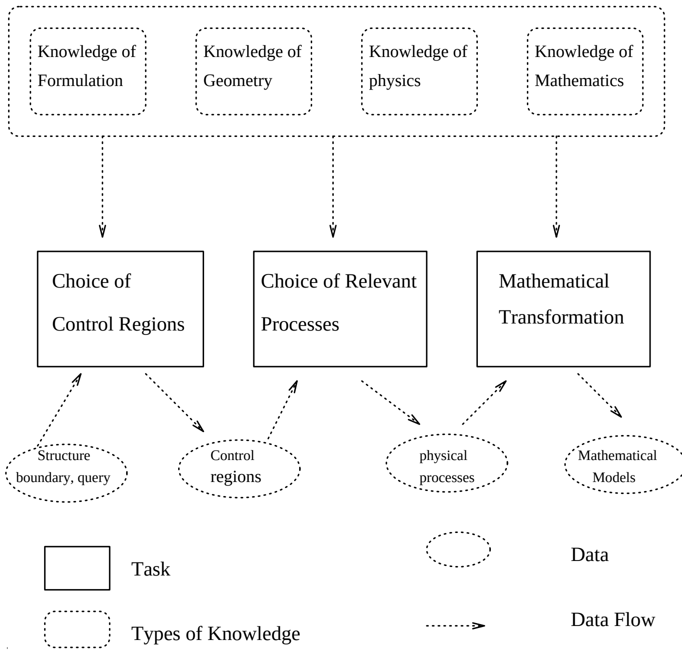

Figure 3: Tasks in Model Generation

A few basic mathematical simplifications are also carried out on these mathematical representations, such as cancelling common symbols on both sides of an equation.

In summary, the system architecture is shown in Figure 3. It incorporates three major kinds of approximation:

- choice of control regions based on temperature variation,
- choice of heat transfer and energy storage processes based on the relative strengths of these processes, and
- choice of linear or non-linear models based on material property variation.

4.3 Examples

We will use two examples to illustrate how MSG carry out the tasks described in the previous section. The first example involves heat transfer analysis of a composite made of two plates of different materials. The second one involves quenching of a metal cube. The queries in both examples are temperature in x, y, z spatial dimensions and in time. The first example results in a model of two coupled partial differential equations, which describe one dimensional transient heat transfer for both plates. The second example results in an ordinary differential equation model which describes the overall heat transfer for the cube.

In the description of the examples, the following units are used: kg for kilogram, m for meter, s for second, K for degrees kelvin, J for joule, and W for watt ($1J/s = 1W$). The following symbols are used in the mathematical equations of the examples: A_i for surface area i, ρ_i for density of component i, C_i for specific heat of component i, k_i for conductivity of component i, V_i for volume of component i, T_i for temperature of component or surface i, and h_i for convection coefficient for surface i.

4.3.1 First Example: 1-dimensional transient model

The first example will show how differential control regions instantiated on the two plates of a composite object result in a partial differential equation model for one dimensional transient heat transfer.

The example involves heat transfer analysis of a composite made of plates of two different materials: plate A of brick and plate B of gypsum, as shown in Figure 4. Both plates A and B have the same width and height dimensions, 0.3 m on all sides, and the same thickness, 0.02 m. Plate A has conductivity of 0.72 $W/m.K$, specific-heat of 835 $J/kg.K$, and density 1920 kg/m^3. Plate B has conductivity of 0.22 $W/m.K$, specific-heat of 1085 $J/kg.K$, and density 1680 kg/m^3. Their initial temperature is 273.15 K. They are exposed to an environment of temperature 473.15 K with convection heat coefficient of 50 $W/m^2.K$. The query involves the temperature of both plates with respect to all three spatial dimensions and time, i.e. $T(x, y, z, t)$. The thresholds for spatial and temporal variation and for non-linearity are all 0.1.

1. **Choice of control regions:** MSG first computes the effective thermal resistance of two plates along the direction of connections, in this case, along the x-direction. They are 0.091 $K.m^2/W$, and 0.028 $K.m^2/W$. The effective thermal resistance of the environment at each side of the plate is 0.02 $K.m^2/W$. Therefore, the total thermal resistance is 0.159 $K.m^2/W$.

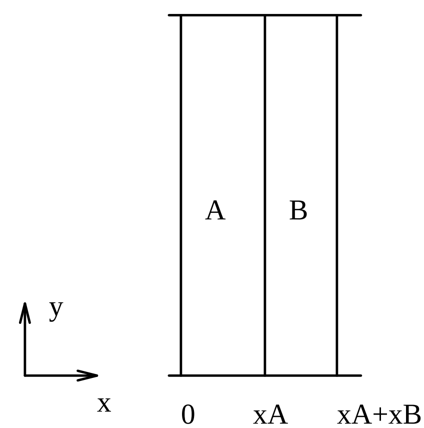

Figure 4: Example of two plates

Then MSG takes the ratio of the thermal resistance of each plate with respect to the total thermal resistance, and checks if they fall below the spatial threshold of 0.1. Neither of them fall below the spatial threshold, so neither can be lumped.

Since the query $T(x, y, z, t)$ has a spatial dependency requirement in x, y, z, and since the thermal resistance analysis does not justify lumping either plate, MSG will instantiate differential control regions, CV_A, CV_B within the plates.

2. **Determining relevant physical processes:** For the control region CV_A, MSG instantiates a set of conduction processes $\{\dot{E}, Q_x, ...Q_{z+dz}\}$, where $\dot{E}$ is energy storage, and $Q_x, ..Q_{z+dz}$ are conduction heat flux on the surfaces of the differential control region.

   After the instantiation, MSG uses aspect ratio of the plate to estimate the order of magnitude values of conduction processes within the plate. In this example, MSG finds that conduction heat fluxes along the x dimension dominates the conduction processes along other dimensions. Therefore, the conduction processes $Q_y, Q_{y+dy}, Q_z, Q_{z+dz}$ are removed from the set, with the elements of processes in the final set reduced to $\{\dot{E}, Q_x, Q_{x+dx}\}$

   Similar choices are made with respect to the control region CV_B.

3. **Transformation and Simplification:** For CV_A, MSG maps $\{\dot{E}, Q_x, Q_{x+dx}\}$

Governing Equation:

$$k_A \frac{\partial^2 T_A}{\partial x^2} = \rho_A C_A \frac{\partial T_A}{\partial t}$$

$$k_B \frac{\partial^2 T_B}{\partial x^2} = \rho_B C_B \frac{\partial T_B}{\partial t}$$

Initial conditions:
$T_A(x, 0) = 273.15$
$T_B(x, 0) = 273.15$
Boundary conditions:
$x = 0 : h_{e1}(T_{e1} - T_A) = -k_A \frac{dT_A}{dx}$
$x = xA : k_B \frac{dT_B}{dx} = k_A \frac{dT_A}{dx}$
$x = xA : T_A = T_B$
$x = xA + xB : h_{e2}(T_{e2} - T_B) = k_B \frac{dT_B}{dx}$

Figure 5: 1-D Transient Model

into a mathematical equation $Q_x - Q_{x+dx} = \dot{E}$. Similarly, MSG maps another governing equation for CV_B.

Since the query involves temperature, and both the control regions involve internal energy storage and conduction heat fluxes along the x dimension, MSG will instantiate equations for initial conditions of plates A and B and equations for boundary conditions along the x dimension. Note that because of the joining of plate A and B only one equation is instantiated for the boundary heat flux between the plates. Furthermore, an equation for temperature continuity is instantiated for the interface of the plates. The final model is shown in Figure 5.

4.3.2 Second Example: lumped model

The second example will show how a totally finite control region i.e. finite in all spatial dimension x, y, z, will result in an ordinary differential equation model, as opposed to a partial differential equation model.

The example involves forging of a hot metal cube A of dimension 0.03 meter on all sides. It is made of steel with conductivity of 20.0 $W/m.K$, specific-heat of 477.0 $J/kg.K$, and density of 7900.0 kg/m^3. Its initial temperature are 373.15 K, and it is quenched by immersing in water of temperature 273.15 K with convection heat coefficient of $50W/m^2.K$.

The query involves the temperature of the cube with respect to all spatial dimension and time, i.e. $T(x, y, z, t)$. The thresholds for spatial, temporal, and non-linearity are 0.1.

1. **Choice of control regions:** MSG computes the Biot number of the cube for all its spatial dimensions, x, y, z. In this case, it is 0.075 and is the same for all spatial dimensions. Since it is less than the spatial threshold of 0.1, MSG chooses finite control region, covering the entire cube.

2. **Determining relevant physical processes:** MSG instantiates heat flux on the control region. Since the control region covers the whole solid, the heat fluxes on the control region are just the convection heat fluxes on the surface of the cube. Since there are no conduction heat fluxes across the control region boundaries, MSG does not need to consider pruning any conduction processes.

3. **Transformation and Simplification:** Since the query involves temperature, the equations have to be in terms of temperature rather than simply heat storage and flux. So, MSG expands the definition of internal energy and the definitions of convection heat fluxes for the control region. The control region involves an instance of internal energy, so MSG generates an equation for initial condition. The resulting model is shown in Figure 6

4.4 Implementation Status and Testing

The system described in this paper has been implemented in Common Lisp and CLOS. It is also interfaced with a symbolic mathematical system, Maple, for mathematical manipulations of equations. The three main tasks are implemented as procedures, as are the approximation rules. Entities such as control

The Initial condition: $T_A(0) = 373.15$
The Governing Equation:
$h_{e1}A_{e1}(T_{e1} - T_A) + h_{e2}A_{e2}(T_{e2} - T_A) + h_{e3}A_{e3}(T_{e3} - T_A)$
$+h_{e4}A_{e4}(T_{e4} - T_A) + h_{e5}A_{e5}(T_{e5} - T_A) + h_{e6}A_{e6}(T_{e6} - T_A)$
$= \rho_A C_A V_A \frac{dT_A}{dt}$

Figure 6: ODE Transient Model

volumes and heat transfer and energy storage processes are represented as objects.

The system has been tested for both single-component and multi-component objects. It has generated 12 examples, with 2 algebraic models, 2 ODE models and 8 PDE models (of which one involves 2 coupled PDEs, and another one is non-linear). The examples cover cooling fins, extrusion processes, and heat treatment of flat plates. The types of heat flow include conduction and internal heat generation within solids and radiation and convection at surfaces of solids. The CPU time for these examples for MSG running on a Sparcstation 1 ranges from 1 second for an algebraic model to 4 seconds for a model of two coupled PDEs.

5 Discussion

Having described the architecture, we now turn to a discussion of several issues: a general characterization of the kinds of approximation MSG uses, a discussion of the kinds of knowledge MSG uses, some comments on why MSG uses the computational approach it does, and some comments on the limitations of MSG and directions for future research.

5.1 Kinds of approximation

Approximations used in MSG fall into two types: those based on variation of temperature and material properties, and those based on relative strengths of heat transfer processes.

Variation of a property f is defined as $\frac{\Delta_v f}{f_{ref}}$, where $\Delta_v f$ is the amount of changes in f as v varies over its range (i.e. $|\min f(v) - \max f(v)|$). If this is much smaller than some reference value for f, we can ignore the variation, and treat $f(v)$ as if it were independent of v, and equal to $f(v_0)$ where v_0 is some fixed value in the range of v. Examples of this type of approximation are:

- lumping of control regions using Biot number where temperature is assumed constant in certain spatial directions,
- transient to steady state approximation where temperature is assumed to be constant over time, and
- nonlinear to linear approximation where material properties are assumed to be independent of temperature, i.e. independent of space and time too.

The other type of approximation is by comparing the relative strengths of a set of processes that have an additive effect, e.g. the heat flows into some control region. Suppose we have such a set of processes $\{a, b\}$, where A and B are their strengths (amount of energy flowing per unit time). If $A \ll B$ then we can ignore process a. An example of this type of approximation is in pruning conduction processes in spatial dimensions.

In practice, we often do not compute A and B directly. Rather, we use a dimensionless number or ratio to estimate, e.g., $\frac{A}{B}$. If the dimensionless number or ratio is below the relevant threshold (given as input to MSG), we assume $A \ll B$.

5.2 Kinds of Knowledge Needed

Modeling involves diverse kinds of knowledge. At least four kinds of knowledge are used, explicitly or implicitly, in MSG.

1. MSG relies on strong domain theory, in particular a strong theory of heat flow. The domain has a set of well-defined heat transfer and energy storage processes with specific laws governing the behavior of each type of processes. Furthermore, there is a well-defined relation governing how these processes interact, i.e. the conservation law. These processes and the governing law form the basis of all models in the domain. Finally, there are cheap methods that MSG can use to estimate the degree of variation of temperature and the relative strengths of heat flows.

2. MSG's entire architecture is based on a particular modeling strategy, using control regions to instantiate a conservation law, and approximate models to provide information about strengths of heat flow processes and variation in quantities such as temperature. While the particular conservation law and other details are part of the domain theory, this modeling strategy is at least somewhat domain-independent.

3. MSG uses some simple geometric reasoning, e.g. to figure out the surface area of the interface between components of objects.

4. MSG uses mathematical knowledge to do some symbolic simplifications and to provide the right kinds of boundary and initial conditions to ensure that a model is properly formed.

5.3 The Computational Approach

MSG's computational approach has three features worth commenting on

- It is procedural, rather than being based on search or non-procedural rules, or on Case-Based Reasoning.
- It is compositional, that is it builds models from pieces, rather than selecting a model from a library of complete models.
- It uses approximate numerical models, rather than either Qualitative Physics or highly accurate numerical models, to decide which physical processes are significant.

We will explain how these features are affected by the task and the theory of the domain.

It is natural to implement MSG using an procedural approach because of the ordering and constraints imposed by the domain theory on the modeling decisions. For example, a set of heat transfer and energy storage processes can only be identified after a control region is chosen, and pruning of these processes can only be carried out after the set of processes is identified. Similarly, proper initial and boundary conditions can be provided only after decisions on heat transfer and energy storage processes have been made. Because of this dependency, an ordering is established for groups of modeling decisions which is reflected in the three sequential tasks in MSG. Furthermore, choices made in earlier tasks constrain the choices in the later tasks. For example, if a totally lumped control region is chosen in the first task, pruning of heat transfer process in the second task is not necessary because a lumped model can be efficiently solved even with many heat transfer processes. Similarly, additional equations need not be generated to provide boundary conditions for a totally lumped control region. The result is an efficient architecture, which structures the set of modeling decisions and which avoids making unnecessary decisions.

This strong domain theory also explains why Case-Based Reasoning (CBR) is not needed. Since we can make the decisions in an procedural manner there is no need to pay the overhead of retrieving specific cases and adapting them to the new problem. It should be noted, however, that MSG's approach does not lend itself to handling problems for which there is no strong theory.

The compositional nature of MSG's approach is motivated by our desire to provide systematic coverage of models for a wide range of problems and queries. In this domain, the number of models can be combinatoric. A simple calculation can illustrate the combinatoric nature of the problem. Let us assume that we are modeling total heat storage in a single cube using algebraic equations. Let us assume each face of the object has one of six possible combinations of boundary conditions, namely, insulation (no heat flux), constant heat flux, radiation, convection, combined constant heat flux and convection, and combined radiation and convection.[2] Even counting rotations and reflections of a situation (e.g. interchanging the x and y axis) as a single problem, there are 1771 different problems each of which results in different equations, i.e. a different model. That number has not even included the numbers of possible partial and ordinary differential equations models, and models for other types of queries. A library of all possible models would be time consuming and error prone to produce, at least without the kind of automated modeling system described in this paper.

Finally, MSG uses approximate numerical techniques to to decide which heat transfer and energy storage processes are significant. On the one hand, "pure" qualitative techniques which focus on the signs of values are not adequate, since we need to compare the relative magnitudes of values. On the other hand, using numerical simulators to obtain values for differential equa-

[2]Each of these conditions is possible, depending on the environment of the object. Constant temperature is excluded because it is often difficult to achieve physically in a practical situation.

tions can be very expensive. To get around this, MSG calculates rough estimates of these values through simple algebraic models and the use of domain specific dimensional numbers.

5.4 Limitations and Future Research

In this subsection we will first discuss the limitations of MSG. Then we will address two possible directions for future research

5.4.1 Limitations

MSG current implementation can handle rectangular shaped objects and some extensions (e.g. L-shaped blocks). It can handle single or multiple components, stacked next to each other or in concentric shells. To handle spherical and cylindrical components it will be necessary to extend the geometrical reasoning ability of MSG to handle these geometries, and it will also be desirable to incorporate domain physics expressed in the spherical and cylindrical coordinate systems. We expect that these additions will not be too hard to do. However, handling arbitrary shapes or free-form objects will raise more difficult issues both because geometric reasoning becomes much harder and because issues of shape approximation arise.

5.4.2 Model validation and refinement

MSG relies on variations and order of magnitude values to make a heuristic guess at the specific set of approximations that will achieve the desired overall accuracy of the resulting model. As far as we can tell, this is all human engineers can do also. Thus, if for some reason it is necessary to *ensure* that the model is within some specific accuracy its results must be compared with those of other, more accurate, models to determine whether the new model is accurate enough. If it is not accurate enough, or if it is more accurate than needed and more expensive to run than desired, we must go back, modify the threshold values, and produce a new model. A few groups are looking at this process of iterative model refinement, e.g. [Addanki *et al.*, 1991, Weld, 1990], but much more work is needed, especially for the kind of distributed (non-lumped) models that are important in heat transfer and other fields.

5.4.3 Transfer to other domains

Another important question for future research is the degree to which the methods used in MSG will transfer to other domains. The key things that make MSG work in this domain include the existence of a strong domain theory and a conservation law that ties the individual processes together. These features are present in other domains as well, such as fluid mechanics [Panton, 1984], where the conservation laws are the conservation of mass and momentum, and the basic physical processes are stress, pressure, force, and momentum etc. Furthermore, their model formulation is based on a control region formulation, like that used in the heat transfer domain. Our current hypothesis is that the three sequential tasks in the architecture of MSG may be transferable to other domains such as fluid mechanics. The approach of pruning physical processes using approximate models may also be transferable. However, the types of approximations and the methods of estimating variations and order of magnitude values of physical processes will be domain specific.

One possible problem with some domains is that they involve more than one conservation law. Some mechanics problems may be formulated using either the law of conservation of energy or the law of conservation of momentum. A method may have to be found for choosing which conservation laws are used in which ways to build a given model.

Furthermore, while the approach of MSG may *work* in another domain, it still may not be the *best* approach for that domain - e.g. in some domains there may be only a few models that are ever used, and the difficulty may be in the numerical solution methods, which are beyond the scope of MSG. In such domains a library-based approach would make more sense.

Thus, while the MSG's methods look promising for other domains, further research is needed to verify their usefulness.

6 Related Work

Related work in model formulation and selection includes work by Addanki *et al* [Addanki *et al.*, 1991], Weld [Weld, 1992], Viswanath *et al* [Viswanath and Jaluria, 1991], Falkenhainer [Falkenhainer, 1992], Falkenhainer and Forbus [Falkenhainer and Forbus, 1991], Finn *et al* [Finn *et al.*, 1992], and Gelsey [Gelsey, 1989].

Both Addanki *et al* [Addanki *et al.*, 1991] and Weld [Weld, 1990] [Weld, 1992] present methods for choosing among alternative models, but neither focuses on automatically generating the alternative models to choose from. The approach of Addanki *et al* involves traversing a graph whose nodes are the alternative models and whose arcs indicate how changing from one model to the next will effect the values computed. Weld uses a kind of Qualitative Reasoning to determine whether an approximate model will give answers that are an lower (or upper) bound on those computed by a more accurate model. In both cases model equations are explicitly input to the system, and they both mention the need for model generation and abstraction[Addanki *et al.*, 1991], [Weld and Addanki, 1990]. Our work discussed in this paper is a step in that direction.

Viswanath *et al* [Viswanath and Jaluria, 1991] describes a program which designs ingot casting systems using a small library of analysis models. Each model is a complete model of a casting system, in the form of an executable program. The system uses expert rules to choose which model to use. Since the models are not constructed compositionally but must be provided as complete programs, only a small number of models are available, covering a fairly narrow set of problems.

Falkenhainer [Falkenhainer, 1992] essentially presents a method of *building* such a library of complete models, along with rules about when to use each one. He starts with the equations for a full model and with constraints on the possible values of the parameters. The models are produced using two syntactic approximation operators:

$A + B \Rightarrow A$ if it is possible that $|B| \ll |A|$

$\partial x/\partial y \Rightarrow 0$ if it is possible that $\partial x/\partial y \approx 0$

The full equations are checked syntactically for every place that these operators might apply, consistent with the given ranges of parameter values ($B \ll A$ is taken to mean $B \leq 10 * A$), and every subset of these applications that involves consistent assumptions leads to a different model. Each model is then solved for a range of parameter values, the results are compared to the results of the full model, and a "credibility domain" is derived for each model which characterizes the range of parameter values over which the model's error is within some given tolerance (e.g., 5%).

This approach is promising when the cost of numerical evaluation can be amortized over much use of the resulting models, and when the cost of evaluating the models is not too high, i.e. models are not too complex, and the number of likely-useful models is not too high. However, in our domain there are a combinatorially large number of possible models (see Section 5.3), and the cost of evaluating the more complex models can be very high. Furthermore, the kinds of syntactic operators in this approach do not cover all approximations in our work, e.g. the choice of a totally finite control regions which leads to an ordinary differential equation or an algebraic model.

Rather than using a pre-computed library of complete models, the approach taken by Falkenhainer and Forbus [Falkenhainer and Forbus, 1991] is to have a library of "model fragments" and to compose these into a complete model only after we have been told what query the model is to answer. An initial set of necessary model fragments is derived from the terms mentioned in the query, and a "domain theory" is used to infer additional fragments which must be included to make a consistent model. This process gives a number of alternative models, and simple heuristics are used to choose the one that is lowest in cost. This is very promising work, especially in its compositional approach and in its use of the query to guide the modeling process. However, it does not handle distributed physical quantities (e.g. the way temperature varies with position inside a given solid) and as a result it does not produce *partial* differential equations. Furthermore, this work is focused on modeling of large heterogeneous systems with relatively loosely coupled parts, such as a shipboard steam-powered propulsion plant. The main goal is to model only as much of this complex system as is needed to answer a query. Our focus is on smaller, more homogeneous, more tightly coupled systems such as modeling the heat transfer through an oven window made of several layers of differing materials.

Finn *et al* [Finn *et al.*, 1992] describes an intelligent modeling assistant for analysis in the domain of heat transfer, the same domain as ours. The system is an *interactive* system which uses features of a new modeling problem to extract possibly-relevant cases from a library of previous modeling decisions. It provides the user with some advice on the applicability of these previous modeling methods to the new case, but leaves the final decision up to the user. Since it is an interactive system, it does not meet the needs of our design context. On the other hand, since it does involve a human user it appears more amenable than a totally automatic system would be to handling issues that are currently not well formalized such as approximating complex geometry.

It should be noted that as of [Finn *et al.*, 1992] this system was only in early stages of implementation; furthermore, the methods by which it will provide advice to the user are not described in any detail.

Also related to our work is that by Gelsey[Gelsey, 1989], which deals with the problem of inferring the behavior of such mechanical devices as simple clocks, starting with a CAD/CAM-like model of their structure. For this task, the set of physical processes is known (they are just the contact forces between parts of the device), and the primary problem is to instantiate these forces, along with motion constraints imposed by the kinematics of the joints between the parts. A further difficulty arises because the set of parts in contact changes over time, so that in addition to building a model, there is the problem of controlling the simulation so that when the contacts change, this can be detected, the simulator stopped, and the model can be revised.

7 Summary

Modeling is a key step in analysis, which in turn is an essential part in design and other engineering activities. This paper describes a computer system, MSG, for generating mathematical models for analyzing heat transfer behavior. The models include algebraic, ordinary and partial differential equations. MSG uses the strong theory of this domain to guide model construction in three sequential tasks: identify regions of interests on an object, determine relevant heat transfer and energy storage processes, and transform those processes into equations. The decisions in these tasks are guided by a set of domain specific methods which estimate the variation of temperature and material properties and the relative strengths of heat transfer processes.

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