# Physical Model Generation in Thermal Engineering Problems described by Partial Differential Equations

Donal P. Finn Hitachi Dublin Laboratory Trinity College University of Dublin Dublin 2, Ireland dfinn@hdl.ie

Abstract Model generation has emerged as a key task in engineering design and analysis. AI research in this area has focused on model based reasoning emphasising qualitative models in attempting to automate this process. In this paper, we propose that this work on the use of model based reasoning in model generation would benefit from the inclusion of case-based reasoning (CBR) techniques. We argue that the use of cases constrains the reasoning process as cases reflect known good routes in the solution space. Cases also have the advantage of facilitating the integration of heat transfer exemplars, approximations, formulae and correlations. In addition, much of human competence in this area is based on reusing solutions to previously solved problems and CBR emulates this. In the paper, we advance these arguments based on our experience with CoBRA, a CBR system for physical model generation for the domain of heat transfer described by partial differential equations.

### **1** INTRODUCTION

Model generation has been recognised to be one of the significant research challenges of the qualitative reasoning community [22, 23, 24] In recent years, research work has focused on different aspects of model generation including; modelling of engineering systems using compositional modelling [7,12], behavioural modelling of engineering phenomena using model abstraction switching [1], modelling across multiple ontologies using meta-modelling techniques [13], simplification of design analysis models using first principles reasoning [14], differential equation modelling using order of magnitude reasoning [25]. Although these projects have been motivated by different goals and adopt different artificial intelligence approaches, a number of general points can be made. Firstly, most work has interpreted model generation as a 'model switching' task between an initial complex model and some simpler but unspecified model. Consequently, this perspective has lead to the development of model generation systems that have been based on traversing a vast solution space of engineering knowledge using model-based reasoning techniques. Secondly, few of the research efforts appear to have been explicitly grounded on a cognitive understanding of how engineers in practise actually carry out modelling. This, we believe, has resulted in the overlooking of a large body of experiential engineering know-how and techniques. Thirdly, most of the research efforts have aspired towards automated modelling environments which aim to replicate the skills and expertise of engineers. This, we argue has resulted in the focusing on modelling tasks

Padraig Cunningham Dept. of Computer Science Trinity College University of Dublin Dublin 2, Ireland Padraig.Cunningham@cs.tcd.ie

that are often simplistic and therefore unrelated to modelling of real world engineering problems. Finally, it is noted that for some work, there appears to have been little effort in understanding the real needs of engineers from model generation tools and to apply these findings to the research efforts; this has resulted in the development of applications that are often of little practical use to the engineering profession. It is worth noting that these comments are not unique to this paper, in so far that they have been noted by other researchers commenting on the direction of research in the qualitative reasoning community [22,23,24].

In this work, we focus on the task of physical model generation associated with the analysis of engineering problems described by partial differential equations (PDEs). PDEs are nowadays analysed using numerical simulation techniques such as the finite element method. Prior to simulation engineers must create simplified spatial, phenomenological and temporal models of real world engineering problems to facilitate efficient computation. Thus, in this context, physical model generation can be regarded as one of the preliminary stages of numerical PDE analysis [9]. It has been acknowledged by both engineering [2, 8] and numerical analysis researchers [3, 18] that these preliminary modelling tasks form a crucial part of the overall simulation process and they call for increased research efforts in the development of knowledge based model generation tools. Although, there has been considerable work from the qualitative reasoning community in model generation, there has been little effort explicitly directed towards physical model generation in numerical simulation of PDEs.

In this paper, we present a novel approach to physical modelling in heat transfer analysis which aims to address many of the issues raised in the first paragraph including: What is the nature of modelling in PDE analysis? How do engineers carry out modelling and how does this influence our approach? What do engineers require from modelling systems? What type of tools assist engineers best with the model generation task? Our examination of these questions has led us to view model generation as an iterative design task that uses both experiential and model-based knowledge. Consequently we have developed a physical modelling system called CoBRA which exploits both model-based and case-based reasoning techniques within derivational analogy framework. We argue that this approach has a number of advantages over other work including; cognitive plausibility, computational tractability, ease of knowledge acquisition and a more pragmatic engineering approach to model generation. Finally, we believe that it addresses some of concerns raised by researchers from the qualitative reasoning community about the need to firstly, focus more clearly on significant engineering problems, and secondly, to tackle these problems in a manner that is beneficial to the engineering community [22].

The paper is laid out as follows: Section 2 discusses, firstly the issues associated with the physical modelling of heat transfer problems described by PDEs, and secondly our understanding of how engineers carry out physical model generation. Section 3 describes our approach and introduces CoBRA, a system for carrying out physical modelling in heat transfer analysis. Section 4 examines other related work and deals with some of the wider implications of our approach. Section 5 concludes the paper.

## 2 MODEL GENERATION

In this section we discuss the issues associated with the physical modelling of the heat transfer PDEs and outline our understanding and approach to model generation for this problem domain.

#### 2.1 Physical modelling in PDE analysis

Convection heat transfer problems can be defined as physical systems where heat transfer occurs between a solid body and a surrounding fluid medium, each at a different temperature. Numerical analysis of convection problems is usually carried out in a number of stages (see Figure 1) which have been identified as follows [3, 18]:



Figure 1 Physical Model Generation

• Behavioural Analysis This is the first task in most numerical engineering problems and it involves reasoning about the physical system with the objective of obtaining a behavioural understanding of the underlying phenomena. In this work, we assume that the engineer has already obtained a behavioural understanding of the physical system.

• **Physical Modelling** This phase involves applying idealisations and simplifications to spatial, phenomenological and temporal aspects of the physical

system with the objective of abstracting a mathematical model. This is the focus of the current work.

• Numerical Simulation This phase involves creating a numerical model and simulating using numerical techniques such as the finite element method.

• Visualisation This stage involves post processing and visualising of the numerical data produced by the simulation process.

Except for simple problems, it is neither feasible nor desirable to analyse all aspects of a physical system. This is because most real world problems contain complexities that render numerical simulation difficult and redundancies that are unnecessary to analyse. In practise, engineers simplify complexities thereby facilitating more efficient computation and ignore redundancies without loss to the integrity of the physical system. In physical model generation the major challenges to the engineer are: identifying the various complexities and redundancies in a physical system, applying appropriate modelling strategies to simplify or reduce these features and assessing the suitability of the resulting model. We consider physical modelling to consist of a number of subtasks including, spatial, phenomenological and temporal modelling.

Spatial modelling focuses on geometric features of the problem domain and involves applying modelling strategies such as: taking a two dimensional idealisation of a three dimensional physical system, finding geometric symmetries or carrying out feature modelling. Figure 2 illustrates feature modelling, and strategies can involve either replacing an existing complex feature with a simpler feature, removing the feature and substituting it with an equivalent boundary condition or removing the feature completely without any compensatory measures.



Figure 2 Feature modelling strategies

Phenomenological modelling deals with the construction of a PDE model that describes the thermal heat transfer process. Considering the full thermal PDE, it consists of three equations based on the physical laws of conservation of mass, momentum and energy. Each equation is in turn composed of terms, where each term describes a particular sub-phenomenon. In many heat transfer problems it is not necessary to model all these sub-phenomenon and therefore terms can be either simplified or even be ignored completely.

Temporal modelling involves choosing an appropriate transient or steady state model.

# 2.2 Our approach to physical modelling in PDE analysis

The central argument presented in this paper is that for physical modelling in finite element analysis the existing approach of using model-based reasoning should be augmented with case-based reasoning techniques. This argument is based on two assertions:

- This modelling task is based on a weak domain theory.
- When modelling engineers refer to exemplars and previously solved problems.

This first assertion requires some elaboration because, at first glance, heat transfer analysis is not normally considered to be a weak theory domain. This apparent contradiction exists because there is a strong theory for much of the interaction in heat transfer. The behavioural description that is the input to this modelling process is well understood as is the numerical simulation process (see Figure 1). However, the actual physical modelling process is not. The task of generating a physical model from a behavioural model is an abductive process and competence is based on experience rather than on any comprehensive theory that might be found in an engineering text. Instead, modelling skills and strategies are experiential in nature and are acquired by engineers through experience and practise. In conclusion, the models themselves are based on a strong domain theory but the process of producing and simplifying these models is not.

Our second assertion is less contentious; our experience with engineering modelling is that human experts refer extensively to heat transfer exemplars and previously modelled problems. Exemplars occur extensively in the form of fundamental scenarios that include heat transfer to plates, cylinders, fins, etc. Associated with these exemplars are a rich body of approximations and correlations which facilitate analysis and evaluation. Exemplars in the form of modelling episodes provide the basis for model generation as practised by engineers. These modelling episodes are used as building blocks for designing models for use in simulation. Engineers model by remembering these scenarios and then reason and modify them to fit the current context. These modifications usually involve 'first-principles' reasoning based around approximations and correlations associated with the exemplar. This anecdotal evidence is backed up by research in the related area of engineering design. While there has little work on the integration of CBR in engineering modelling there has been much work on using CBR in design. Arguments that human designers refer to past problem solving episodes are presented in [11, 20, 21].

Summarising then, we argue that the QR research on modelling would benefit from the integration of CBR techniques because that is the way engineers do it. In addition, we argue that the fact that modelling is based on a weak domain theory signals that a CBR approach will be fruitful.

# **3 PHYSICAL MODEL GENERATION IN COBRA**

In this section, we discuss the AI methodology adopted in this work, outline the conceptual architecture of our system and describe the CoBRA system for physical model generation.

#### 3.1 AI methodology

CBR is an AI methodology that serves the basic intuition that humans reuse solutions to previously solved problems during problem solving. The most obvious advantage of this approach is that competent systems can be developed based on shallow domain models, thus requiring little knowledge engineering. However, it is generally accepted that CBR systems for design require reasonably deep domain models and much work has been done in this area [4, 11, 15, 16]. CBR systems incorporating deep domain models still have advantages over systems based on first-principles reasoning. The case organisation helps focus the knowledge acquisition process and the cases encode known good routes through the solution space and thus constraining the solution search process [6].

One of the key issues in CBR is the manner in which the cases are adapted. The standard approach is to transform the solution of the old case to meet the specification for the new case. In some circumstances the interdependencies in the solution components are too complex for this to be practical. In this case generative adaptation (derivational analogy) can be used. This involves reworking the steps in the solution generation process in the context of the new problem specification. This is the strategy adopted in CoBRA.

#### 3.2 Conceptual architecture

An environment that facilitates interactive modelling between the user and the modelling system was considered to be the most suitable conceptual architecture for tackling physical model generation in heat transfer analysis. This decision was prompted by both design and pragmatic considerations. Design considerations arise from the knowledge that in finite element analysis the majority of users are expected to be

non-naive participants who will have a certain degree of understanding of physical modelling. Thus, this class of user is expected to be familiar with the various modelling tasks (outlined in Section 2.1) but will require expert advice in selecting modelling strategies and applying these strategies or actions in a particular problem context. For the task of physical modelling in finite element analysis, automated modelling or 'black box' approaches do not serve this user group well. Pragmatic considerations were prompted by the realisation of the significant implementational difficulties that were likely to be encountered if the entire modelling process was to be automated. Taking an automated approach would lead to additional formidable technical challenges (for example, feature recognition) which would have detracted from the core issue of examining whether case based reasoning techniques with derivational analogy can be applied to this domain.

Considering now how these ideas are incorporated with the CoBRA modelling system, we summarise our conceptual approach by the following points:

- Modelling is carried out in distinct stages which include phenomenological, spatial and temporal modelling.
- Within any modelling stage, modelling decisions are taken in a piecewise fashion by examining each modelling issue in turn. In this way a physical model is designed in a step by step manner.
- Case based reasoning with model-based generative adaptation forms the core AI approach.
- A case consists of a description of the modelling problem, a modelling solution and a derivational trace.
- Derivational traces consist of a model based reasoning trace by which a modelling solution was reached. They also act as a validation mechanism and explanation facility of the case solution.

Because the user is involved in the model creation process, physical modelling is considered to be a design task in itself. This perspective allows physical modelling to be viewed as an interpretation of the propose-critiquemodify design model as proposed by Chandrasekaran [27] for design. In this case, Chandrasekaran's approach is adapted for designing physical models, where, the user examines and *proposes* the sequence of modelling events, case based reasoning tools retrieve similar modelling scenarios with solutions, derivational analogy techniques adapt the solutions and also act as a *critiquing* mechanism in the context of the adapted solution and finally *modification* is carried out by the user applying the modelling action to the physical system.

#### 3.3 Case Descriptions in CoBRA

In CoBRA, a target case consists of a frame based representation of the physical system. Frames are created on the basis of geometric information obtained through an AutoCAD interface. In a target frame, representation is organised according to the different modelling stages, spatial, phenomenological and temporal. This representation is built up component by component by the user, in this case (see Figure 3), a base fin (longitudinal rectangular fin), a secondary appendage (longitudinal rectangular fin) and the additional minor features associated with the appendages (cavities, features, etc.). In spatial modelling, this involves choosing from the user interface, the appropriate qualitative descriptors to define each feature. Feature indices are based on qualitative engineering terms that are used by engineers to describe and distinguish fundamental modelling scenarios. In addition to the feature indices, problem parameters such as geometric data are included in the target cases. However this information is not used as indices, but is included for use in the derivational traces.



Figure 3 A case in the CoBRA system

A base case consists of a representation of the real world physical system, the solution in the form of a simplified model, and a reasoning trace of the justifications for the transformations in going from the real world problem to the simplified model. Cases are constructed at the level of fundamental modelling scenarios and this determines directly the type of indices used as well as the contents of the derivational traces. Figure 3 illustrates a typical convection heat transfer problem that can be tackled by the modelling system. The physical system is a finned heat exchanger that dissipates heat to the surrounding ambient air, such exchangers are often used as heat sinks in electronic devices. The heat exchanger consists of a base appendage with an associated secondary appendage. Each appendage has additional minor features. The task being addressed by CoBRA in this example is to produce a simplified model of the physical system. The frame definition on the right of Figure 3 illustrates the problem description, the problem solution and the derivational trace that provided this solution. Indices are based on qualitative engineering terms that are sufficient to distinguish the fundamental modelling scenarios. A target case contains only the problem description; this is the specification of the physical system. Modelling progresses by firstly examining the role of the minor features, and then the importance of the secondary and complex appendage.

Case retrieval is implemented in a two stage process, matching (or base filtering) and mapping. Matching is carried out using an activation network which is made up of activation units which correspond to the indices of the base cases. A feature vector is created for each target case which contains the relevant indices of the problem. The feature vector is the basis by which the activation units are initialised and on completion, each case in the case base contains a value of how many indices it shares with the target case. The mapping stage is concerned with establishing the correspondences between the base cases and the target cases. Mapping based on establishing the full set of matching features between the target and base cases is the criteria used for retrieving cases.

# 3.4 Generative Adaptation using Model based Reasoning

Derivational traces are exploited in this domain, because, although the target and base cases may map qualitatively, small differences between physical parameters such as spatial or medium data can lead to significantly different solutions. Such differences cannot be expected to be captured in the initial qualitative classification of the problem, furthermore, to index all episodes based on both descriptive and parametric indices would result in an intractably large case base. In CoBRA, a derivational trace links the start and goal state of a case and describes the basis of the modelling solution. Each reasoning trace has two main components; a decision part and a resulting action part (after [5]). The decision part contains:

- Alternative modelling strategies considered and rejected
- Assumptions and justifications for the decisions taken.
- Heat transfer approximations and correlations to allow evaluation of a particular modelling strategy.
- Heat transfer domain knowledge describing dependencies of later decisions on earlier ones.

The action part holds the steps taken as a result of the reasoning trace of the decision part. A typical action is, "Remove the feature which faces into the flow". A sample reasoning trace is shown in Figure 4. Each node in the reasoning trace represents a decision point in the model simplification process. In this example, the solution in the base case was derived in two ordered stages. The first stage examines the influence of the feature on the flow field and consists of Goals 1 and 2. This involves determining whether the feature is actually fully contained within a turbulent boundary layer, and if so, whether the influence of the feature on the flow field is deemed negligible. Goal 3 examines the contribution of the feature to overall heat transfer. In the base case, the heat transfer contribution of the feature was of the order of 4% of total heat transfer well within the 5% constraint, so therefore the fin was removed. In the target case, this contribution was of the order of 3.5% thereby permitting the feature to be removed.



Figure 4 A model-based derivational trace

Derivational traces are based on fundamental modelling scenarios and are created at this level of complexity. Thus the contents of the derivational trace are determined by the context of each scenario in question and this can vary from exemplar to exemplar. Because the derivational traces are created at according to each fundamental modelling scenario, the issue of trade-off between the sufficiency of the indices and the complexity of the derivational traces is essentially predetermined by the engineering nature and content of the exemplars.

Currently, the derivational traces are constructed and organised on a case by case basis, in other words, a generalised approach based on a common vocabulary and structure has not been used. Because of the varying nature and complexity of the derivational traces, it is likely that such a generalised approach would be organised at a planning rather than at a modelling level. This is an issue that will be investigated in future work.

# 4.0 COMPARISON WITH RELATED WORK

In this section we briefly review related work and in this context, compare our approach to model generation.

Addanki [1] describes an automated modelling approach using a methodology called the "graph of models". The basic idea is that system behaviour can be represented by a series of interlinked models which exist at different levels of abstraction. Modelling progresses by automatic selection and changing of analysis models on the basis of assumption satisfaction and model accuracy.

Iwasaki [12] describes a system called Device Modelling Environment that formulates a behavioural model of a device, simulates its behaviour and interprets the results. An input description of the device topological structure is given and a compositional modelling approach formulates the appropriate mathematical model.

Yip [25] describes a system for simplifying the Navier Stokes fluid equations using order of magnitude reasoning within a qualitative reasoning framework. The conceptual approach adopted is rather similar to the way an engineering academic would engage in deriving simplified models. PDE models produced by the system are mathematically complete, but may in some cases have no physical meaning. This modelling task in similar to the phenomenological modelling stage described in Section 2.1

Ling [14] discusses a system for generating sets of PDEs for designing thermal systems described by either algebraic equations, ordinary differential equations and PDEs. Order of magnitude and dimensional analysis techniques are used to heuristically derive a mathematical model. Currently they have implemented their approach for conduction heat transfer problems.

Shephard et al. [17] discuss the various modelling decisions that must be considered when specifying a mathematical model for numerical analysis. They describe an approach based on a rule based expert system for the domain of stress analysis in aircraft structures. Attention is focused on the use of different idealised behavioural models at different levels of abstraction.

Falkenhainer and Forbus [7] describe an approach based on compositional modelling. By using explicit modelling assumptions, domain knowledge can be to be decomposed into semi-independent fragments, each describing various components of the physical system.

In our work, we deal with physical model generation associated with engineering problems described by PDEs; to date only the work of Yip [25] and Ling [14] have dealt with this class of problem. Our approach however has some significant differences.

Firstly, rather than deriving models from first principles, we use cases which are based on tried and tested episodes. One advantage is that, in practise for finite element analysis, engineers do not normally derive physical models from first principles (as described by Yip [25]). Instead, our observations have been, that they choose between known good models and then 'tweak' these models to satisfy the problem at hand [9]. Cases with model-based generative adaptation support this approach to modelling more readily. Another advantage is that, cases encode known good routes through weak domain solution spaces thereby avoiding extensive backtracking often associated with model-based approaches [6].

Secondly, we argue that by using case based reasoning techniques, we can capture a body of experiential engineering skills and know-how, that is otherwise difficult to represent by model-based techniques. Our studies of modelling have indicated that engineers make extensive recourse to this type of knowledge when carrying out physical modelling in numerical analysis [9].

Thirdly, from a knowledge engineering perspective, the use of derivational traces means that the knowledge acquisition process is carried out in the context of episodes. This we found provided no special difficulties for our domain expert, which is in contrast to experiences for elicitation of generalised knowledge associated with model based approaches [26].

Fourthly, we argue that this approach meets more closely the needs of engineering practitioners in a number of ways. For instance, compared to the work of Iwasaki [12] which aims to develop a complete modelling and simulation environment, we believe that the emergence of modelling tools that can be integrated between existing CAD and numerical packages will serve engineering needs most usefully [2,3,8,18]. In addition, we believe that such tools should aim to empower engineering analysts, and therefore, it is likely that interactive modelling support systems as advocated in this paper will achieve this aim more readily [9].

### 5.0 CONCLUSIONS

In this paper we presented an approach to physical model generation that adopts both case based and model based reasoning. This approach has been based on the assertion that physical modelling generation is a poorly understood process and is often carried out using a combination of episodic and first principles reasoning. This argument is backed up by our belief, not only that physical modelling is based on a weak domain theory but also that engineers make extensive use of previous modelling episodes and experiential knowledge when modelling. Furthermore we argue that for physical modelling in PDE analysis, interactive modelling tools that operate between CAD and numerical analysis systems are likely to be most useful for engineers in physical modelling tasks. Currently the case base consists of about twenty cases and future work will focus on expanding the number of cases so as to increase the coverage of the system. In addition we intend to examine the issue of creating a common vocabulary and structure for more efficient and transparent implementation and representation of the derivational traces.

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