

Fit for purpose models for metrology: a model selection methodology

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Abstract. We describe a model selection methodology for partial differential equation (PDE) based models and show the results of applying it to a test problem derived from a model of the laser flash thermal diffusivity measurement technique. A methodology for comparing and choosing simplified models is of benefit to the model development process in metrology. It is assumed that the computational aim is not only to solve the model to obtain the results that the metrologist requires, but to ensure that the model is no more complex than necessary to achieve this and that results can be obtained in a reasonable time using the available computing resources. The advantage of the proposed method is that it avoids the need to solve directly the underlying complex model. We present the results of comparisons of four models of the laser flash problem and identify the further work needed to extend the approach to a wider range of problems and to identify suitable measures for comparing residuals.

1. Introduction

This paper describes a model selection methodology for PDE based models, and shows the results of applying it to a simple test problem, derived from a model of the laser flash thermal diffusivity measurement technique. The majority of PDE models are not amenable to analytical solution, and must be solved using software implementations of numerical approximation techniques. For the purposes of this paper it is necessary to discuss briefly the following terms:

- model complexity: the more complex a model is, the more difficult it is to solve. Nonlinear models are more complex than linear models. Increasing the dimension of a model increases its complexity. Adding more unknown quantities to a model increases the model complexity.
- computational expense: the longer a model takes to solve using a given piece of software running on a given computer system, the more computationally expensive that model is. Increased model complexity leads to increased computational expense.
- computational aim: the computational aim of the model is a specification of the information, preferably including a required level of uncertainty, that the model needs to supply.
- fit for purpose: a fit for purpose model is a model that generates the required results to the necessary level of accuracy within a manageable amount of time, i.e., it achieves its computational aim at a reasonable computational expense.

One approach to model development that balances the need for a detailed description of the physical system and the need for low computational cost is to start from a simple model



and progressively add complexity until the model can be considered as validated and hence fit for purpose. Common assumptions used to simplify models include uniformity and constancy of material properties, linearity of boundary conditions and loads, neglect of thermal and electrical effects, and reduction of the dimensionality of the problem by assuming axisymmetry or planarity.

One difficulty with this approach to model development is identifying what change to the model will make the most difference to the results. This problem is particularly common when models have been simplified via assumption of constancy or linearity in their material properties, loads, and boundary conditions and it is not clear which assumption is most likely to be invalid.

Another problem is that it is difficult to know in advance that a given change to a model will have a significant effect on the results, so it is possible to waste a large amount of effort and time implementing and running a complex model, only to find that the new complexity has made no difference to the results. The development of multiphysics models from simpler models, transient models from steady-state models, and the extension of a two-dimensional model into a three-dimensional model are examples of labour-intensive model changes with no guarantee of improvement.

These challenges demonstrate that a methodology for comparing complex model changes that does not involve solution of complex models would be of benefit to the model development process.

2. Model selection

Model selection for PDE models is usually strongly application-driven and the choices made are often motivated by expert knowledge, so as a result there is little work in the literature on generic techniques for comparing different models.

Papers by authors such as Bär et al [3] and Guo and Billings [4] have investigated selecting a set of governing equations for dynamical systems from a parameterised family of nonlinear equations. Applications of this work include development of models of distributed parameter systems and of reaction-diffusion equations. The authors select the models by minimising the difference between model predictions and measured values. Other work [1] has evaluated best-fit values of a spatially varying diffusion coefficient at the nodes of a finite element (FE) mesh by matching model results to known values of the solution at the nodes.

The measured values used by these techniques typically need to be distributed throughout the spatio-temporal domain for a good fit to be possible. This requirement restricts the range of problems to which the approaches can be applied. Many measurement techniques take surface measurements or measurements of bulk behaviour, but cannot measure sub-surface values. Bamabach et al[2] proposed a methodology for choosing the best-fit model for a given experiment from a finite group of governing equations. The methodology does not require measurement results to be distributed throughout the domain, and so is more applicable to metrology problems.

The methodology proposed by Bamabach et al[2] employs optimisation to identify, for every possible pair of models in the group, a set of model input values and model results that create the biggest difference in the chosen results between the two models. It is then necessary to carry out an experiment for each set of input parameters and make measurements equivalent to the model results. The optimal model choice can then be obtained from the measured values and the model results. This approach is a good objective method for choosing amongst a group of models, but the optimisation process to identify the input values that cause most difference between the results of a pair of models will require repeated solution of each model, which will be computationally expensive. The methodology we propose avoids direct solution of complex models, making a significant saving in computational effort.

3. Proposed methodology

The methodology has been developed to compare and assess changes to a model that solves a PDE model using a numerical approximation technique. Throughout the following it is assumed that the same discretisation has been used for all models. At its current stage of development the methodology only addresses steady-state models, so the numerical approximation technique will result in a matrix of equations of the form

$$A(\mathbf{u})\mathbf{u} = \mathbf{b}, \quad (1)$$

where $\mathbf{u} = (u_1, u_2, \dots, u_N)^\top$ is a vector of unknown solution parameters, \mathbf{b} is a known vector that implements the loading and boundary conditions and is independent of \mathbf{u} , and $A(\mathbf{u})$ is a matrix that will be dependent on \mathbf{u} if the model is nonlinear. It is assumed that all matrices that define models are non-singular, so all models are solvable, and that a given model has a unique solution. It is further assumed that all of the entries in the matrix A , the functions $a_{ij}(\mathbf{u})$, are infinitely differentiable functions of the u_k . The majority of physical models lead to functions such that the $a_{ij}(\mathbf{u})$ are either polynomials or can be expanded as polynomials within the range of solution values likely to occur within a given model, so this assumption is unlikely to restrict the validity of the proposed methodology.

Suppose that the solution \mathbf{u}^0 to a simple model $A^0(\mathbf{u}^0)\mathbf{u}^0 = \mathbf{b}^0$ is known, and that we wish to assess how different from \mathbf{u}^0 the solution to a more complex model $A^1(\mathbf{u}^1)\mathbf{u}^1 = \mathbf{b}^1$ is. Then the i th component of the vector of residuals \mathbf{r} obtained from putting the known solution \mathbf{u}^0 into the new model is given by

$$r_i = [A^1(\mathbf{u}^0)\mathbf{u}^0 - \mathbf{b}^1]_i = [A^1(\mathbf{u}^0)\mathbf{u}^0 - A^1(\mathbf{u}^1)\mathbf{u}^1]_i \quad (2)$$

$$= \sum_{j=1}^N a_{ij}^1(\mathbf{u}^0)u_j^0 - \sum_{j=1}^N a_{ij}^1(\mathbf{u}^1)u_j^1. \quad (3)$$

The assumption of the uniqueness of the solution to each model means that these residuals can only be uniformly zero if \mathbf{u}^0 and \mathbf{u}^1 are identical. We can expand the value of $a_{ij}^1(\mathbf{u})$ as a Taylor series about \mathbf{u}^0 :

$$a_{ij}^1(\mathbf{u}^1) = a_{ij}^1(\mathbf{u}^0) + \sum_{k=1}^N (u_k^1 - u_k^0) \left\{ \frac{\partial a_{ij}^1}{\partial u_k} \right\}_{\mathbf{u}^0} + \sum_{l=1}^N \frac{(u_l^1 - u_l^0)}{2} \frac{\partial^2 a_{ij}^1}{\partial u_k \partial u_l} \Big|_{\mathbf{u}^0} + O((u_m^0 - u_m^1)^3) \quad (4)$$

so that, abbreviating terms above the linear, the i th component of the residual vector becomes

$$r_i = \sum_{j=1}^N \left(a_{ij}^1(\mathbf{u}^0)u_j^0 - a_{ij}^1(\mathbf{u}^0)u_j^1 - u_j^1 \sum_{k=1}^N (u_k^1 - u_k^0) \left\{ \frac{\partial a_{ij}^1}{\partial u_k} \right\}_{\mathbf{u}^0} + O((u_m^0 - u_m^1)^2) \right) \quad (5)$$

$$= \sum_{j=1}^N \left[a_{ij}^1(\mathbf{u}^0) + \sum_{k=1}^N u_k^1 \left\{ \frac{\partial a_{ij}^1}{\partial u_k} \right\}_{\mathbf{u}^0} + O((u_m^0 - u_m^1)) \right] (u_j^0 - u_j^1), \quad (6)$$

which is a weighted sum of the components of $\mathbf{u}^0 - \mathbf{u}^1$. The ℓ^2 norm and the ℓ^∞ norm can be used to compare residuals from different models.

Many numerical approximation methods produce matrices and vectors such that the residuals are strongly dependent on the local mesh size. This dependence makes comparison of values within the same vector misleading unless the residuals are weighted by mesh size in some way. All results in this paper have been normalised by multiplying by V_i/V where V_i is the integral of the i th basis function over the domain, and V is the total volume of the domain of the model.

Note that individual residuals are not a direct measure of the difference between the results in a given region. For instance, for models created using finite element analysis, all pairs of models that differ only in boundary conditions have zero residuals for points that do not lie on the boundary.

4. Test problem

A simple steady-state test problem was developed to demonstrate the proposed methodology. The problem was designed such that increases in complexity could be introduced in its boundary conditions and material properties, and potentially an increase in dimension could be introduced. The problem was a two-dimensional steady-state thermal simulation of a cylinder with thermal conductivity $\lambda(T)$, of radius R and thickness H , being heated by a specified flux Q on one flat face, and losing heat via a heat transfer coefficient $h(T)$ to an atmosphere at fixed temperature T_a from its other faces. The problem was created by considering a steady-state version of a model of the laser flash thermal diffusivity experiment, a problem studied before [5].

The full specification of the problem is:

$$\frac{\partial}{\partial r} \left(\lambda(T) \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(\lambda(T) \frac{\partial T}{\partial z} \right) = 0, \quad 0 \leq r \leq R, 0 \leq z \leq H, \quad (7)$$

$$\lambda(T) \frac{\partial T}{\partial z} = -Q(r), \quad 0 \leq r \leq R, z = 0, \quad (8)$$

$$\lambda(T) \frac{\partial T}{\partial z} = h(T)(T_a - T), \quad 0 \leq r \leq R, z = H, \quad (9)$$

$$\lambda(T) \frac{\partial T}{\partial r} = h(T)(T_a - T), \quad 0 \leq z \leq H, r = R. \quad (10)$$

The residuals of the discretised form of the equation have units of watts (W).

The initial model fixed λ to be constant, with $\lambda = 55.5$ W/(m K), and fixed Q and h to be constants related to the ambient temperature T_a , the emissivity ϵ (set to 0.8), and the Stefan-Boltzmann constant σ via $Q = 12\epsilon\sigma T_a^3(628 - T_a)$ W/m² and $h = 4\epsilon\sigma T_a^3$ W/(m² K). The definition of h was derived from a linearisation of the nonlinear boundary conditions for radiative heat loss. The expression for heat flux was developed by using a one-dimensional model that took surface area into account to estimate a heat flux that would give a temperature of 628 K on $z = H$. Two different ambient temperatures were used: $T_a = 528$ K and $T_a = 618$ K.

Two different changes to the initial model were identified, each of which would lead to additional complexity if the model were solved directly. The first change introduced radiation boundary conditions on $r = R$ and on $z = H$ so that $h(T) = \epsilon\sigma(T_a^3 + T_a^2T + T_aT^2 + T^3)$. The second change used temperature-dependence of the thermal conductivity, specified as $\lambda(T) = 55 + 0.1(T - \bar{T})^2$, where \bar{T} is the average temperature of the simple model for a given ambient temperature. For the model with $T_a = 528$ K, $\bar{T} = 630.55$ K, and for the model with $T_a = 618$ K, $\bar{T} = 628.41$ K.

The simple models were solved as a finite element problem using a uniform mesh of 16 linear quadrilateral elements in each direction. The results of the simple model with $T_a = 528$ K are shown in figure 1. The models with added complexity were also solved using the same finite element mesh so that differences in results could be calculated directly.

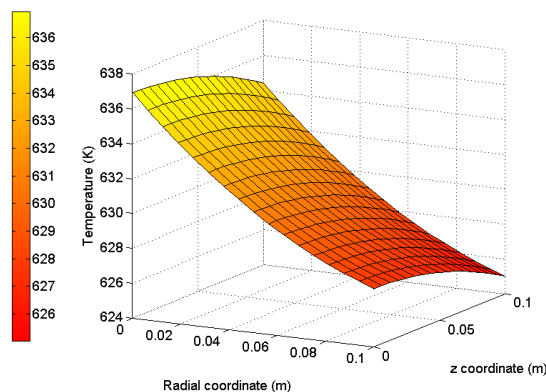


Figure 1. Temperature results for $T_a = 528$ K. The temperature results for $T_a = 618$ K show a similar spatial distribution, but vary between 627.6 K and 629.4 K.

5. Test problem results

The values of the residuals associated with the basis function associated with each node are plotted in figures 2 to 4. Note that these figures plot the results in different orientations so that the interesting features can be seen more clearly: the axes show the orientation of each plot.

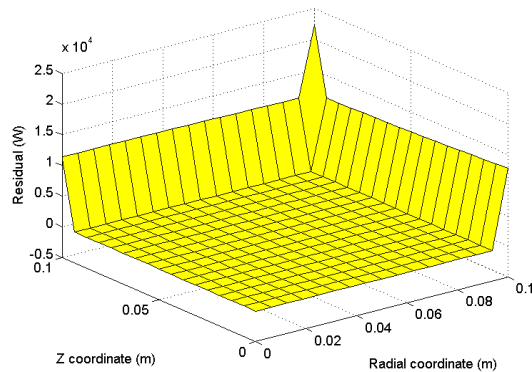


Figure 2. Residuals from the radiation boundary condition model for $T_a = 528$ K. The residuals for $T_a = 618$ K have a similar spatial distribution, but are an order of magnitude smaller.

Figure 2 shows the residuals obtained by putting the solution to the simple model into a model with radiation boundary condition with $T_a = 528$ K. The residuals are zero away from the boundary because the boundary condition change has not altered the equations linking nodes away from the boundary. The residuals are almost uniform where they are non-zero. There is a sharp spike in value at the corner $r = 0.1, z = 0.1$. This spike probably occurs because that corner is affected by the change in boundary condition in two directions. The spike suggests that a different residual scaling strategy is required for nodes affected by boundary conditions.

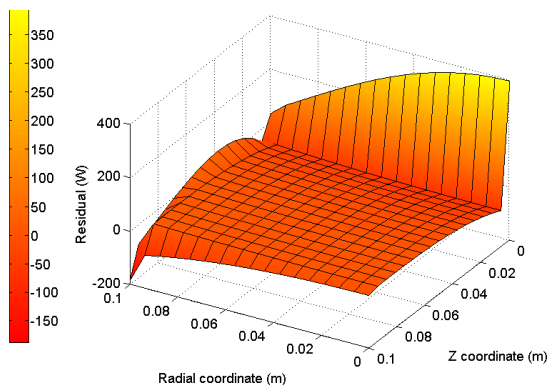


Figure 3. Residuals from the temperature dependent thermal conductivity model for $T_a = 528$ K.

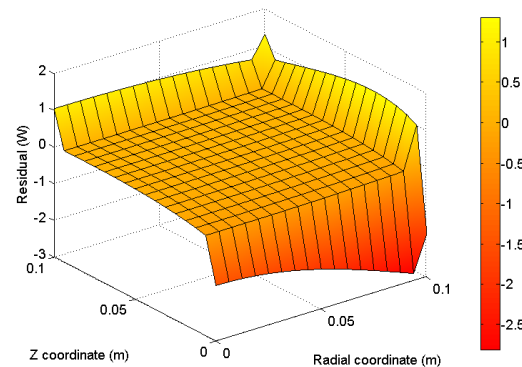


Figure 4. Residuals from the temperature dependent thermal conductivity model for $T_a = 618$ K.

Figures 3 and 4 show the residuals obtained by putting the solution to the simple model into a model with temperature-dependent thermal conductivity. Both plots show that the largest residuals are close to the face $z = 0$. A comparison of the temperature differences from the finite element solutions show that this is the region of largest temperature difference. Figure 5 shows the temperature difference for $T_a = 528$ K as an example.

Table 1 shows the root mean square (RMS) and maximum absolute values of residuals and of difference in nodal temperature ΔT for all four models with added complexity. The numbers

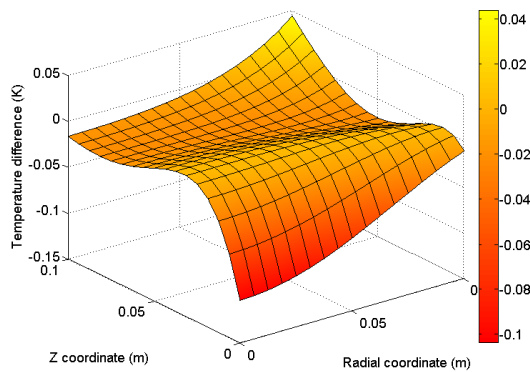


Figure 5. Temperature difference between the results of the simple model and the model with temperature-dependent thermal conductivity and $T_a = 528$ K.

in each row of the table decrease from left to right, showing that the ordering of the models from “most changed” to “least changed” given by the residuals is the same as that given by the temperature results.

Table 1. Maximum absolute values and root mean square averages of changes in temperature caused by a model change, and of the residuals obtained by putting the solution of the original model into the changed model.

	$T_a = 528$ K Radiation b.c.	$T_a = 618$ K Radiation b.c.	$T_a = 528$ K $\lambda(T)$	$T_a = 618$ K $\lambda(T)$
Max. abs. residual	5650	649	97.3	0.704
RMS residual	1020	118	17.9	0.150
Max. abs. ΔT	20.1	0.236	0.104	0.0116
RMS ΔT	20.1	0.234	0.0244	0.00525

6. Conclusions

A methodology has been proposed for choosing between different changes to a model. The proposed methodology does not require solution of the changed model, enabling model changes to be assessed before solution. The methodology has been demonstrated on a test problem, and has been shown to rank possible model changes in an order consistent with the changes in model results.

More work is needed to identify a correct scaling to remove area and volume effects, to investigate the most suitable measure for comparison of residuals, and to demonstrate the methodology on a more complicated problem.

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