VALIDATION OF SOLUTION METHODS FOR BUILDING ENERGY SIMULATION

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ABSTRACT

The most commonly applied mathematical solution techniques for building energy simulation are response function methods and finite difference methods. The accepted validation methodology in this domain has as its main elements empirical validation, analytical verification and inter-model comparison. Of these, only analytical verification tests the solution method exclusively; but the test examples used are too confined to be representative of the building energy problem. A discriminating and comprehensive test method for the validation of solvers in this application is proposed here. It employs solutions of arbitrary accuracy for test problems of realistic scale and complexity in what are termed numerical experiments. The necessity for – and the effectiveness of – the proposed validation method is demonstrated by its application to a set of numerical solvers.

INTRODUCTION

A dynamic thermal model of a building and its associated heating/cooling plant is a set of differential equations describing energy flows between system components and from the environment. The equations originate in building physics, plant thermodynamics and control theory. Generally, they comprise conservation equations for energy and mass, equations of state for fluids and performance characteristics for plant. Simulation in this context corresponds to the solution of these equations going forward in time. The major mathematical techniques used to solve these equations are (time and frequency) response function methods and finite difference (numerical) methods.

The validation methodology used in this domain is well established. Most early developers of simulation software attempted to compare their program's predictions with measured data from a real building. A more general validation methodology began to emerge in the 1980s and papers by Judkoff et al (1983) and Bloomfield (1989) would be representative of this trend. This methodology, with some refinements and extensions, has become the accepted standard (ANSI/ASHRAE, 2001) and virtually all of the major validation exercises undertaken in recent years have used it (Gough and Rees, 2004; Witte et al, 2001; Strachan, 2000; Lomas et al, 1997; Jensen, 1995). The International Energy Agency (IEA) on whose work the ANSI/ASHRAE standard is based (Judkoff and Neymark, 1995) has recently described an ongoing research project (ECBCS News, 2003) aimed at further developing this same methodology. The main elements of the method are as follows:

(a) *Empirical validation* — in which calculated results from a program are compared to monitored data from a real building, test cell or laboratory experiment.

(b) *Analytical verification* — in which output from a program is compared with a known analytical solution.

(c) *Inter-model comparison* — in which the predictions of the target program are compared with those of other, better known, programs for the same (hypothetical) building. It is also used to make comparisons between a program and a previous version of itself – after a sub-model has been added or substituted for instance.

Empirical validation, though a necessary and appropriate application of the scientific method for whole model validation, is unsuitable for this project because it quantifies total (including measurement and modelling) error and not just the error due to the mathematical solution method which is sought here. Inter-model comparison does not involve an absolute standard and can, therefore, be rejected for this work. Analytical verification makes use of exact solutions to simple problems usually involving heat transfer within and at the surface of homogenous layers of material (Spitler et al, 2001; Bland, 1992; Carslaw and Jaeger, 1959). As such, they are of the type required to test solution methods in this application. However, being limited usually to linear problems with simple boundary conditions, they are too constrained to be representative of the problem in hand. Building energy flows are describe by a large set of coupled, non-linear differential equations driven by a great variety of boundary conditions; some of which are not even continuous. Nevertheless, rigorous and comprehensive testing of solution methods is imperative in that deficiencies in the solver have a global impact on performance whereas errors in any of the constituent models probably have a more limited effect.

NUMERICAL EXPERIMENTS

Proposed Validation Method

The test methodology proposed in the present study is the one almost universally used with newly developed numerical methods in the numerical/computational mathematics literature. There, *numerical experiments* are undertaken in which the proposed method is applied to a set of test problems possessing varying degrees of stiffness, non-linearity and other properties of interest (Cash, 2005 ; Mazzia and Iavernaro, 2003; Hairer and Wanner, 1996; Enright and Pryce, 1987; Enright and Hull, 1976; Enright et al, 1975). Exact solutions are known for some of the test problems and in the case of the others highly accurate reference solutions are generated by applying a convergent numerical method with a sufficiently small time step to the problem.

All useful methods, including those used to produce reference solutions in this work, have been shown to be convergent (Lambert, 1991; Isaacson and Keller, 1966) and consequently the reference solution approaches the exact solution as the time step is reduced. This is just as valid for large problems as it is for small ones. The test problems used in this project are of realistic scale and complexity. Test solutions generated using various mathematical techniques can then be compared with the reference solution and inferences drawn.

Clearly, the only significant error present in a numerical experiment is that associated with the solver under test. A wide variety of problems are typically used to test a new numerical method for general use. Here we seek the efficiency of solution methods in one specific application and consequently a test problem with the mathematical characteristics (Crowley, 2005) of the building energy problem was formulated and many variants of it were used in the evaluation process.

Test Problem

The hypothetical structure depicted in Figure 1 and specified below is used to test the performance of various numerical methods in this application.

Construction details and discretization

A typical office on an intermediate floor of a large office building is used for the work. It has one external wall facing due south and, other than the single glazed window, all enclosing masonary elements are made up of three homogenous layers. The dimensional data and thermophysical properties of these layers, together with other details which vary between versions of the test, are listed in Crowley (2005). Glass is represented by a single node because of its low Biot number and the small enclosed air mass is also characterised by just one node point. All other homogenous layers are represented by three nodes, one at the centre associated with half the mass and one at each surface representing a quarter of the mass in the case of a free surface or a quarter of each of two adjacent masses in the case of an interface. This is typical of building energy simulation software, as is the one dimensional representational of heat flow implied by it.

The total number of nodes required to represent the structure is apparently 44 but this can be reduced to 27 if the room is considered to be surrounded by identical rooms experiencing similar casual loads. In this case each floor/ceiling would clearly be irradiated identically (both spacially and temporally) by the sun and so the temperature distribution through each would be the same. For the same reason the temperature distribution through each side wall would be identical. If it is assumed that the internal design temperature is the same for all rooms and that solar flux never reaches the north wall, the temperature distribution through that wall would be symmetric about its centre-plane. Internal temperatures can, in fact, be expected to vary for the free running building because rooms facing north will not be directly irradiated but the assumption of uniformity is maintained to bring the computing burden within the constraints of the project. This or other minor modelling discrepancies should not invalidate the results provided all solvers are applied to the same problems and these problems are of an appropriate mathematical character. Figure 1 includes 27 distinct nodes numbered from inside the space to outside in all cases.

Thermal driving forces

The weather data used is taken from a test reference year (TRY) for Kew in England (CEC, 1985). A TRY is composed of hourly weather data for 12 typical months, forming a year. It is used in simulating the performance of buildings and HVAC systems so that annual energy consumption, indoor comfort conditions and other quantities of interest can be estimated. Two months of data were required for the present project because some of the test runs were 45 days in duration. May and June were used as these were the only consecutive months in the TRY that were taken from the same year (1963). Unrealistic discontinuities were thus avoided in progressing from one month to the next. The data columns used in this work contained dry bulb temperature (0.1ºC), global radiation (J/cm^2), diffuse sky radiation (J/cm^2), wind speed (0.1 m/s), month, day and hour. Where intermediate values are required the hourly meteorological data are interpolated using cubic splines.

The impact of short wave radiation on the test room requires knowledge of solar position and intensity. Solar altitude and azimuth angles are known functions of hour and month. Direct radiation from the TRY is assigned a direction using these and its influence on any building surface quantified. An anisotropic diffuse sky model (Perez et al, 1987) is used to distribute the given diffuse radiation data because it is known to be more intense around the solar disc and at the horizon. Direct and diffuse short wave radiation, together with a ground reflected fraction (0.2) of the global radiation, are then summed for each surface of the test room. Solar transmissivity and absorptivity of glass are calculated as functions of the angle of incidence; in this context, diffuse radiation is considered to have an incidence angle of 51º, representing the average approach angle for anisotropic sky conditions (Clarke, 1985; CEC, 1990). Self-shading by the building is considered. Solar radiation on internal surfaces is modelled as far as the first reflection.

Internal long wave radiation calculations take into account multiple diffuse reflections directly between each pair of surfaces and reflections between the pair involving any third surface (Clarke, 1985). View factors are calculated using an area weighting method since the space approximates a cube. Net external long wave radiation exchange is estimated using a mean black body equivalent temperature of the surroundings (sky, ground and adjacent buildings) which requires calculation of the mean sky temperature as a function of time. The expression of Berdahl and Martin (1984) is used here and it reduces to the clear sky formula of Swinbank (1963) when the cloud cover factor is zero. Ground temperature and that of adjacent buildings are estimated as in Clarke (1985).

The formulae of Alamdari and Hammond (1983) are used to calculate the natural convection coefficients for internal surfaces. To calculate the forced convection coefficient at an external surface the local wind direction and speed are first estimated using the algorithm in ESP-r and described in CEC (1990). This is substituted into Allen's (1987) expression for the surface coefficient.

Infiltration due to wind pressure and air density difference, acting on the perimeter crack around the window, is included as a set of algebraic equations which are solved at every time step. A casual heat gain to the internal air mass is switched on in the morning and off again in the afternoon. A proportionally controlled convective air-conditioning terminal unit can be activated for any desired period. Its capacity is 20% in excess of the cooling load and the proportional band of the controller is variable. The 27 differential equations representing the test room (plus one for time to make the set autonomous) are too lengthy to reproduce here and can be found in Crowley (2005).

Evaluation of Numerical Methods

In order to show the necessity for – and the effectiveness of – the proposed validation method, a collection of recently developed implicit numerical methods, together with some more traditional ones, were ranked using it. Ten variants of the test problem specified above were used for the assessment. Descriptions of slow thermal response (heavyweight) buildings and fast response (lightweight) buildings due to CIBSE (1999) were used to produce extreme versions of the problem and the other eight lie between these limiting cases.

In the domain of building energy simulation, the most commonly used implicit numerical methods include the trapezoidal rule (TR) [the Crank-Nicolson method], the backward Euler method (BEM) and the second-order backward differentiation formula (BDF2). Some newer methods that are *prima facie* suitable for this application (Crowley, 2005) include Kvaerno3 (Kvaerno, 2004), TRX2 (Hosea and Shampine, 1996), Carroll (Carroll, 1989), TR-BDF2 (Bank et al, 1985) and Alex2 (Alexander, 1977). Adaptive step size versions of all of these numerical methods were programmed and applied to the test problem with an error tolerance of 0.1 K to produce test solutions.

During a typical test run, two independent solutions were generated using library differential equation solvers and a reference solution was formed by averaging them. Both of these methods, the method of Rosenbrock and the fourth order Runge–Kutta method (Press et al, 1992), include adaptive step size control and the tolerance variable was set to 10^{-6} K in each case. The agreement between these two solutions was excellent – see Table 1 which presents accuracy statistics for a typical medium weight variant of the test problem (test 3). The reference solution was subtracted from each of the test solutions in turn at every node and every hour over a four day period following the pre-conditioning period. Switch on/off events for the terminal unit and for the casual gain were arranged to occur just before some of these assessment points. Mean absolute difference (Table 1) gives an overall measure of accuracy but it was felt that maximum absolute difference should be used lest a small number of unacceptable errors be concealed by the averaging process. These might be anticipated at times of rapid change in the solution. Mean difference detects any bias towards over- or under-estimation of the solution and the cross-correlation coefficient gives a measure of the phase relationship between the reference solution and each of the other solutions.

The performance of a numerical method should be judged not just by the accuracy achieved but also by the computational effort expended because one can usually be traded for the other by changing the requested error tolerance. The measure of computational efficiency used here is $\mathrm{CE} = 1 \Big/ \left(\left| \hat{d} \right| \cdot ET \right)$, where $\left| \hat{d} \right|$ is the maximum absolute temperature difference between the reference solution and the test solution (Table 1) and *ET* is the execution time for the test run. Each of the test programs was equipped to keep a tally of the most expensive steps in the solution process. They are LU decomposition (factorisation), forward/back substitution, matrix evaluation and derivative function evaluation. Table 2 lists these measures of computational effort and gives their frequencies for a typical test run (test 3). LU decomposition of the system matrix was found to be the dominant computational task in terms of execution time, even when the frequencies of the various linear algebra operations were factored in (Crowley, 2005). Consequently, *ET* can be taken to be approximately proportional to the number of LUs – especially as the problem gets larger because of the scaling properties of the four operations. Average computational efficiencies for the above mentioned numerical methods are presented in Figure 2. Each is scaled to the CE for TR because this method is probably the most widely applied to stiff systems of differential equations in this domain and many others. The more traditional methods (BEM, TR and BDF2) were found to be far from optimal for building energy simulation. Alex2, a very stable and robust member of the Runge-Kutta family, was shown to be more efficient than TR by a factor of 4.27.

DISCUSSION AND RESULT ANALYSIS

A building energy model is a set of coupled equations, representing energy flows between system components and from the environment. It is constructed using mathematical models of the various heat/mass transfer processes present. Then a mathematical solution process is selected or developed.

Validation of mathematical models is a classic application of the scientific method. Model predictions are compared with field measurements and the model is revised as necessary. It is considered good practice to have just one active processes in such a validation experiment lest error cancellation occur. This is not always possible. The mathematical solver, however, can be tested in isolation by use of numerical experiments.

Application of the proposed validation method revealed that some commonly used numerical methods were far from optimal for this application and a number of very efficient, potential replacement methods were identified. The great range of efficiencies found for the set of numerical methods assessed demonstrates the benefits of being able to choose between them.

It would be of interest to test time and frequency response function methods in this way. They do not produce exact solutions, as is sometimes stated, because the number of time divisions or frequencies used has to be finite.

CONCLUSION

A discriminating and comprehensive test method for the validation of mathematical solvers in the context of building energy simulation has been proposed. The necessity for it and its effectiveness in this application have been demonstrated. It is recommended for inclusion in standards dealing with the validation of building energy analysis software.

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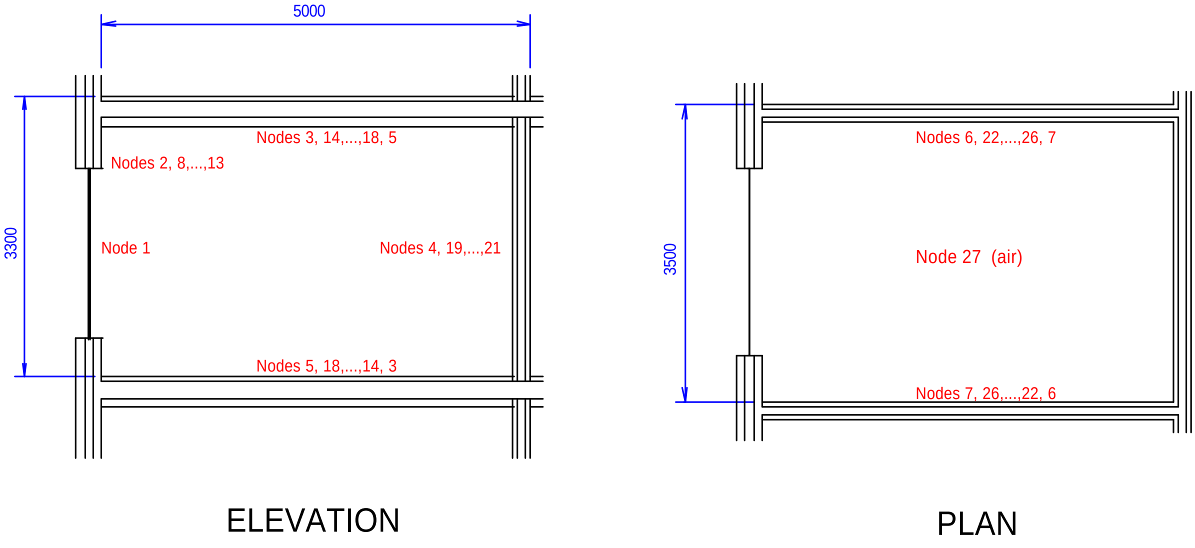

Figure 1. Test room for detailed test problem.

Table 1
Accuracy statistics for test run number three

NUMERICAL METHOD	TEMPERATURE DIFFERENCE BETWEEN REFERENCE SOLUTION AND OTHER SOLUTIONS (K)			CROSS-CORRELATION AT ZERO TIME DELAY (AIR POINT NODE ONLY)
	MEAN DIFFERENCE d	MEAN ABSOLUTE DIFFERENCE $\lvert d \rvert$	MAXIMUM ABSOLUTE DIFFERENCE $\lvert \hat{d} \rvert$	
Rosenbrock	3.12×10^{-6}	4.64×10^{-6}	2.04×10^{-4}	1.0000
Runge-Kutta	-3.12×10^{-6}	4.64×10^{-6}	2.04×10^{-4}	1.0000
Alex2	0.00059	0.0010	0.051	1.0000
BDF2	0.00244	0.0045	0.097	1.0000
BEM	-0.00740	0.0228	0.295	1.0000
Carroll	0.00022	0.0030	0.155	0.9998
Kvaerno3	0.00352	0.0055	0.145	0.9998
TR	0.00061	0.0044	0.242	0.9995
TR-BDF2	0.00097	0.0038	0.170	0.9998
TRX2	0.00219	0.0040	0.122	0.9999

Table 2
Measures of computational effort for test run number three

NUMERICAL METHOD	LU DECOMPOSITIONS	FORWARD/BACK SUBSTITUTION PAIRS	MATRIX EVALUATIONS	DERIVATIVE FUNCTION EVALUATIONS
Alex2	395	2788	298	2788
BDF2	414	1054	388	1028
BEM	330	1202	280	1152
Carroll	205	1124	194	1124
Kvaerno3	208	1576	208	1838
TR	268	850	243	1248
TR-BDF2	197	1398	185	1228
TRX2	187	1255	183	1008

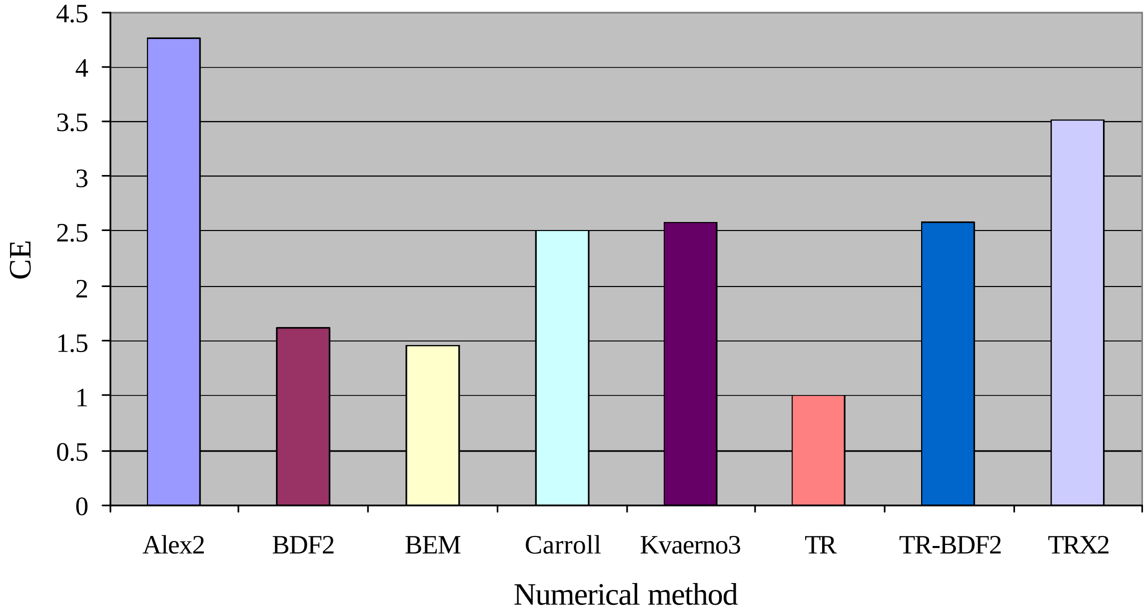

Figure 2. Computational efficiencies (CE) of selected numerical methods (re TR).