

Development of Exponential-Fitted Numerical Methods for Building Energy Simulation

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Abstract

Simulation of energy flows in buildings is computationally intensive. Consequently, improvements in computing power and algorithm efficiency can always be utilized. Commonly used implicit solvers require extensive matrix processing while standard explicit methods have limited stability and progress in very small time increments. In this work, a number of stable numerical methods are examined which are explicit in nature and therefore do not require the use of matrices. One such algorithm and two proposed developments of it are assessed using a building related test problem prepared for this purpose, and their performances are compared with that of an efficient implicit method. The proposed algorithms are found to be the best in their class with computational efficiencies approaching that of the implicit method. In addition, this class of method makes more efficient use of current computer resources and is particularly well suited to future (parallel) architectures.

Introduction

The practice of building services engineering involves the prediction of future thermal conditions and needs, and the design of buildings and plant to meet these requirements. More specifically, the engineer is required to determine peak heating and cooling loads, size thermal plant, analyse dynamic thermal performance, anticipate annual energy consumption and predict thermal comfort indices. The associated capital and running cost forecasts and the requirement to reduce the environmental consequences of energy conversion make this a non-trivial task. Nonetheless, it is important that designers and building owners have confidence in these predictions because of the great life spans of environmental systems and especially buildings. Assurance is particularly required when innovative buildings or systems are proposed or where margins are trimmed to reduce energy use. The dynamic and interconnected nature of the problem, as well as its scale and complexity, points to computer simulation as a solution method. The major mathematical techniques used for detailed dynamic simulation of energy flows in buildings are response function methods (and the related transfer function methods) and finite difference methods. A little known numerical method falling into the latter category is discussed here and some novel developments from it are proposed for this application.

Model Formulation and Discretization

A dynamic thermal model of a building consists of a set of partial differential equations and ordinary differential equations (ODE) for the dependent temperatures and heat fluxes, which generally cannot be solved analytically. For example, the diffusion of heat through a solid building element, such as a homogeneous wall layer, is most often treated as one dimensional and so the resulting temperature field can be described by the equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad [1]$$

The finite difference approach involves replacing the differential equations with consistent difference equations, which are tractable. Solutions are obtained at discrete points in space and time rather than as continuous functions. One way of implementing this approach would be to decompose Equation [1] into a set of ODEs by the method of lines (1), in which space is discretized but not time. A typical nodal equation would be

$$\frac{dT_i}{dt} = \frac{\alpha}{h^2} (T_{i-1} - 2T_i + T_{i+1}) \quad [2]$$

To these must be added ODEs for room air masses and other finite volumes of material assumed to have spatially uniform temperatures. Each volume is represented by a single nodal temperature which varies in time according to an equation of the form

$$mc \frac{dT_i}{dt} = \sum \phi(t, \mathbf{T}) \quad [3]$$

where the right hand side represents the sum of the thermal driving forces acting on that node. The ϕ are in general non-linear functions of \mathbf{T} . A complete building energy model can, therefore, be represented by the vector equation

$$\mathbf{T}' = \mathbf{f}(t, \mathbf{T}) \quad [4a]$$

or even more succinctly as

$$\mathbf{T}' = \mathbf{f}(\mathbf{T}) \quad [4b]$$

if t is included among the dependent variables. Equation [4b] is a first-order, autonomous system of non-linear ODEs of dimension $n + 1$ representing n nodes ($i = 1, 2, \dots, n$) and time ($i = 0$).

To complete the process of discretization, a numerical method for ODEs is applied to Equation [4b]. For instance, the commonly used theta method gives the difference equation

$$\mathbf{T}^{j+1} = \mathbf{T}^j + k \{ \theta \mathbf{f}(\mathbf{T}^{j+1}) + (1 - \theta) \mathbf{f}(\mathbf{T}^j) \} \quad [5]$$

Setting $\theta = 0$, $1/2$ and 1 gives Euler's rule (ER), the trapezoidal rule (TR) and the backward Euler method (BEM) respectively; the ODE equivalents of 'the explicit', the Crank-Nicolson and 'the implicit' schemes for partial differential equations. The equations generated by any explicit scheme are uncoupled and can be solved one at a time whereas those produced by an implicit scheme require simultaneous solution at each time step. The Crank-Nicolson scheme is, in fact, implicit in nature. The theta method is second-order for $\theta = 1/2$ but degrades to first-order for any other value of θ .

Stability

The stability of any numerical method, when applied to Equation [4b], is determined by the values of the products $k\lambda_i$, where the λ_i ($i = 1, 2, \dots, n$) are the eigenvalues of $\mathbf{J} = \partial\mathbf{f}/\partial\mathbf{T}$, the Jacobian matrix of \mathbf{f} . For Euler's rule, the products must lie within a unit circle in the complex plane centred at $(-1, 0)$. The trapezoidal rule is described as A-stable because its region of stability is defined by $\text{Re}(k\lambda) < 0$, that is, the whole of the left half-plane; though it is only marginally stable for large (negative) values of $\text{Re}(k\lambda)$. The backward Euler method is L-stable because it is A-stable and, additionally, its stability improves as $\text{Re}(k\lambda)$ approaches minus infinity. The size of the time increment k is limited if ER is applied to a building thermal model because, in this case, [5] is a *stiff* system of equations. An equation system is said to be stiff if

$$\text{Re}(\lambda_i) < 0 \quad [6]$$

and, in addition, the stiffness ratio σ satisfies

$$\sigma = \frac{\text{Max}_i |\text{Re}(\lambda_i)|}{\text{Min}_i |\text{Re}(\lambda_i)|} \gg 0 \quad [7]$$

The relatively large negative values of $\text{Re}(\lambda)$, implied by the definition of stiffness, necessitate small time steps k if ER or any other standard explicit method is to remain stable. L-stable methods, or at least A-stable methods, are considered appropriate for stiff systems because they are stable for all k . That is, TR and BEM are stable for any time step but, being implicit methods, they are computationally expensive requiring the storage, evaluation and factorization of large matrices.

When the physical entities or processes modelled by a set of equations have widely differing time constants [$1/|\text{Re}(\lambda_i)|$] stiffness ensues. Systems may be considered marginally stiff if σ is $O(10)$, while ratios of up to $O(10^6)$ are not unusual. A building thermal model is moderately stiff with stiffness ratios of $O(10^2)$ to $O(10^3)$ being typical. Stiffness is not uncommon in practical problems arising in such fields as chemical kinetics, nuclear physics, process control, electronics and mathematical biology.

Exponential-Fitted Methods

So stiff systems, including the building energy simulation problem, seem unavoidably costly to compute. Standard explicit solvers are compact and time stepping with them is cheap but many small time increments are required. Implicit solvers offer stability for any time increment at the cost of a lot of computation per step. What is needed is a method that can take long time steps cheaply. Exponential fitting seems to offer this Holy Grail of numerical simulation, that is, simultaneous L-stability and explicitness. Stiff systems are generally over-damped and exponential-fitted methods exploit this by fitting a suitably damped exponential rather than a polynomial to the next solution segment. Pratt (2) gives a comprehensive overview of this group of methods, suggests reasons for their relative obscurity and outlines some of the implementation difficulties associated with them. One of the few published algorithms for an explicit member of this family, RK2/EXP, is given by Ashour and Hanna (3). Their approach automatically partitions the equations into stiff and non-stiff groups at every step and subsequently integrates the first using a second-order exponential-fitted method:

$$z_i = \frac{f_i'(\mathbf{T}^j)}{f_i(\mathbf{T}^j)} \quad [8a]$$

$$T_i^{j+1} = T_i^j + f_i(\mathbf{T}^j) \left\{ \frac{\exp(kz_i) - 1}{z_i} \right\} \quad [8b]$$

and the second using a second-order Runge-Kutta method (RK2):

$$\hat{\mathbf{T}}^{j+1} = \mathbf{T}^j + k\mathbf{f}(\mathbf{T}^j) \quad [9a]$$

$$T_i^{j+1} = T_i^j + \frac{1}{2}k \{ f_i(\hat{\mathbf{T}}^{j+1}) + f_i(\mathbf{T}^j) \} \quad [9b]$$

A conservative $O(k^2)$ local truncation error (LTE) was used in RK2/EXP. A more accurate $O(k^3)$ estimate is desirable, and achievable because the numerical methods used are both second-order. Also, RK2/EXP produced spurious temperature spikes during some of the tests described below (Figures 1 and 2). Replacing RK2 with the second-order Taylor series method:

$$T_i^{j+1} = T_i^j + kf_i(\mathbf{T}^j) + \frac{1}{2}k^2 f_i'(\mathbf{T}^j) \quad [10]$$

was found to eliminate these spikes and improve the efficiency of the algorithm.

Two developments of RK2/EXP are therefore proposed here, both incorporating the Taylor series method in place of RK2. The first, designated PM1, includes LTEs established using Taylor series expansions in the usual way, with divided difference approximations in place of the higher derivatives. The second, PM2, employs yet another numerical solver, the second-order Adams-Bashforth method, to monitor the errors in both the stiff and the non-stiff methods.

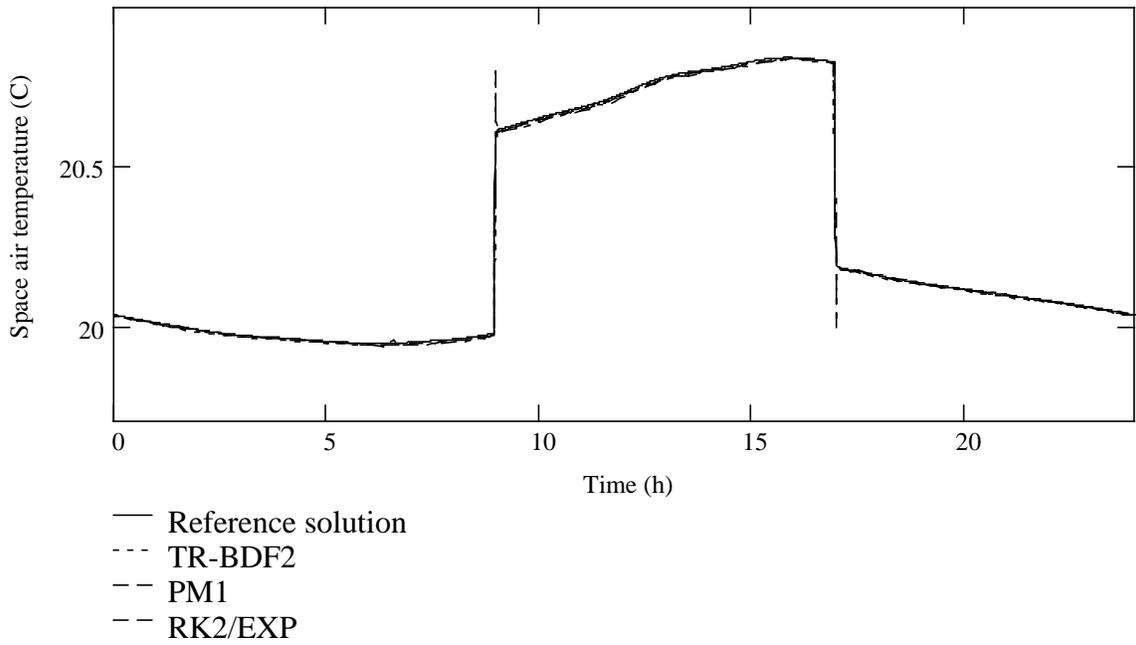


Figure 1 Air temperature predictions for test run 11, day 2. RK2/EXP performs poorly at step changes.

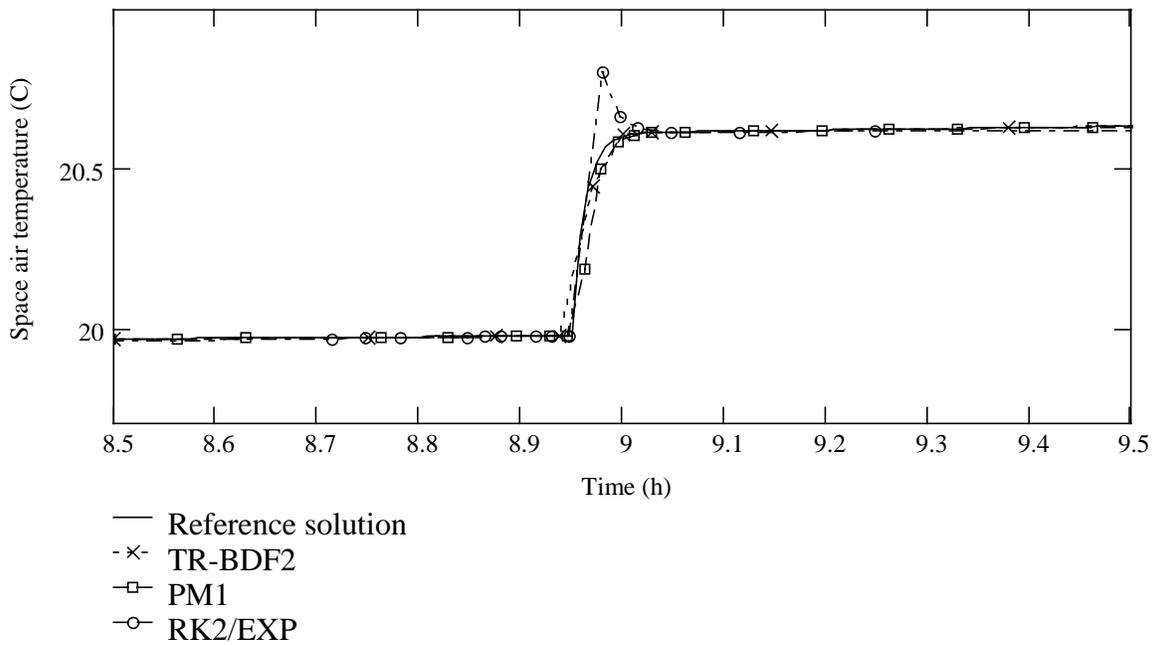


Figure 2 Air temperature predictions for test run 11, day 2, 8.30 am to 9.30 am. Here, a short time interval around the first step change is examined to highlight the performance of RK2/EXP.

Evaluation Of Numerical Methods

The three exponential-fitted algorithms RK2/EXP, PM1 and PM2 were tested and, for comparison, TR-BDF2 was also included in the assessment. The latter is a composite of TR and the second-order backward differentiation formula (4) and was previously found to be the most efficient of the implicit numerical methods in this application (5). Its LTE was estimated in the manner described for PM1 above.

Test Problem

Analytical tests (6), based on physically simple heat transfer problems with known solutions, are decisive but very limited in scope. They are essentially tests of the conduction model. Convection and radiation are linearized so that an exact solution can be obtained. Empirical validation using measured data from a real structure is inappropriate here because it is difficult to separate the error due to the numerical method, which is sought, from errors in other parts of the model and in the input data. A mathematical test was used in which the methods were applied to an equation set with the characteristics of the building energy problem (5). The test equations were generated by considering the heat flows at a cubic space enclosed by five identical plane slabs and one vertical glass sheet. Typical internal and external heat loads were applied and a proportionally controlled terminal unit was included. This is a demanding problem, which includes step changes and discontinuous derivatives in the thermal driving terms. It consists of 17 differential equations, which are, in general, non-linear, and stiffness ratios ranging from $O(10)$ to $O(10^4)$ were generated during the testing process.

Computational Procedures

Adaptive step size versions of the four algorithms were programmed in which the time increment was varied until the LTE was within a specified tolerance which was set to 0.1 K per step for this work. Two different interpolation methods were included in each program. They were linear interpolation (LI) and computation of intermediate values (CIV) using the numerical method under test.

The work was carried out on a personal computer using a general purpose mathematical software package (7). During a typical test run two independent solutions were generated using built-in 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 (7, 8), include adaptive step-size control and the tolerance variable was set to 10^{-6} in each case. The agreement between these two solutions was excellent. The test solutions were statistically compared with the reference solution over a four day period following the pre-conditioning period. A total of 30 test runs were analysed which included test spaces with slabs of various thicknesses, and thermal diffusivities virtually spanning the range encountered in building materials. Discontinuities in the heat gains were moved in time, and in all cases tests were carried out first with the free running test space and then repeated with the terminal unit active.

The performance of a numerical algorithm 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. The measure of computational efficiency (CE) used here was $CE = 10^5 / (\varepsilon N)$ where ε is the maximum absolute temperature difference between the reference solution and the test solution and N is an estimate of the number of machine operations per node/equation for the test run, taking a floating point addition as one

operation. CE can be thought of as the accuracy attained per unit computing time. The results obtained for the test runs outlined above are given in Table 1. The CE for the most efficient method, TR-BDF2 + CIV, was divided into the CEs of each of the other methods in turn. The geometric mean values of these ratios, calculated for the full set of test runs in each case, are presented in Table 2. Figures 3 and 4 allow visual comparison of the solutions for a representative test run.

TABLE 1
Computational Efficiency for the Test Problem

Test run	Test space construction	Slab thickness d [m]	Characteristic conduction time d^2/α [s]	Average stiffness ratio	Terminal unit status	Time delay prior to assessment [s]	Displacement of casual heat gain [s]	CE for the following numerical methods							
								TR-BDF2		RK2/EXP		PM1		PM2	
								CIV	LI	CIV	LI	CIV	LI	CIV	LI
1	Concrete	0.100	1.02×10^4	309	On	180	0	17.07	3.50	4.95	6.93	3.63	7.47	14.52	18.63
2	Concrete	0.100	1.02×10^4	49	Off	180	0	0.96	4.04	0.99	0.46	1.09	0.79	0.88	1.01
3	Insulation	0.100	9.35×10^3	57	On	180	0	6.10	2.12	2.00	2.26	3.46	3.30	3.65	3.76
4	Insulation	0.100	9.35×10^3	49	Off	180	0	2.62	1.39	0.44	2.24	0.19	0.36	0.21	0.37
5	Wood	0.100	9.09×10^4	700	On	180	0	7.17	0.71	4.30	6.32	27.23	12.21	6.53	17.23
6	Wood	0.100	9.09×10^4	122	Off	180	0	1.36	1.66	0.89	2.17	0.57	4.87	0.90	0.84
7	Aluminium	0.100	1.23×10^2	1769	On	180	0	15.03	3.03	0.08	0.11	0.05	0.05	0.04	0.04
8	Aluminium	0.100	1.23×10^2	1881	Off	180	0	0.92	2.08	0.06	0.08	0.04	0.04	0.04	0.04
9	Concrete	0.050	2.55×10^3	146	On	180	0	12.38	3.77	2.06	2.19	8.74	6.52	3.37	2.86
10	Concrete	0.050	2.55×10^3	43	Off	180	0	0.98	1.67	0.73	1.78	0.45	0.70	0.47	0.52
11	Concrete	0.200	4.08×10^4	690	On	180	0	9.63	3.07	6.75	5.99	6.29	2.34	9.54	9.10
12	Concrete	0.200	4.08×10^4	120	Off	180	0	1.43	4.87	1.07	0.49	1.12	3.03	0.92	0.46
13	Concrete	0.100	1.02×10^4	309	On	180	-3600	9.10	2.22	6.10	5.58	7.09	2.74	11.33	7.19
14	Concrete	0.100	1.02×10^4	49	Off	180	-3600	3.30	2.04	1.05	1.03	0.41	0.79	0.52	0.45
15	Concrete	0.100	1.02×10^4	310	On	180	+3600	12.53	3.79	5.12	5.77	3.65	7.70	16.62	21.24
16	Concrete	0.100	1.02×10^4	49	Off	180	+3600	0.99	5.67	5.81	1.86	0.58	0.94	0.56	0.97
17	Concrete	0.100	1.02×10^4	309	On	120	0	3.79	3.54	1.45	9.04	1.36	14.48	13.80	13.85
18	Concrete	0.100	1.02×10^4	49	Off	120	0	1.91	4.12	0.74	0.80	0.40	0.37	0.41	0.80
19	Concrete	0.100	1.02×10^4	309	On	240	0	13.95	3.52	8.88	7.46	10.87	21.32	21.13	20.81
20	Concrete	0.100	1.02×10^4	49	Off	240	0	1.35	3.97	0.57	1.21	0.66	2.25	0.51	1.22
21	Concrete	0.100	1.02×10^4	309	On	300	0	10.89	3.43	5.57	9.08	40.68	21.32	18.26	21.44
22	Concrete	0.100	1.02×10^4	49	Off	300	0	1.47	3.91	1.39	0.72	1.36	1.14	0.74	1.56
23	Concrete	0.100	1.02×10^4	309	On	360	0	18.38	3.47	5.64	6.62	42.14	20.67	17.81	19.77
24	Concrete	0.100	1.02×10^4	49	Off	360	0	2.32	3.85	1.61	1.79	0.65	0.88	0.76	1.72
25	Concrete	0.100	1.02×10^4	309	On	420	0	18.22	3.65	5.28	7.56	39.96	40.31	18.41	19.49
26	Concrete	0.100	1.02×10^4	49	Off	420	0	2.43	3.81	2.13	2.41	1.38	1.46	2.11	2.32
27	Concrete	0.100	1.02×10^4	309	On	480	0	14.90	3.64	4.86	4.87	27.93	28.27	13.32	7.23
28	Concrete	0.100	1.02×10^4	49	Off	480	0	3.42	3.77	2.50	2.64	1.18	1.76	1.16	2.54
29	Wood	0.500	2.27×10^6	9311	On	180	0	15.70	2.57	6.21	6.86	25.13	22.69	18.18	9.32
30	Wood	0.500	2.27×10^6	1745	Off	180	0	1.03	1.94	1.01	0.45	0.41	2.96	0.89	0.97
31	Aluminium	0.010	1.23	17530	On	180	0	11.84	2.93	*	*	*	*	*	*
32	Aluminium	0.010	1.23	19580	Off	180	0	1.33	3.82	*	*	*	*	*	*

*Unacceptably small time increments.

TABLE 2
Mean Computational Efficiencies Relative to TR-BDF2 + CIV

Method of interpolation	Relative CE for the following numerical methods			
	TR-BDF2	RK2/EXP	PM1	PM2
CIV	1.00	0.43	0.48	0.50
LI	0.69	0.49	0.64	0.58

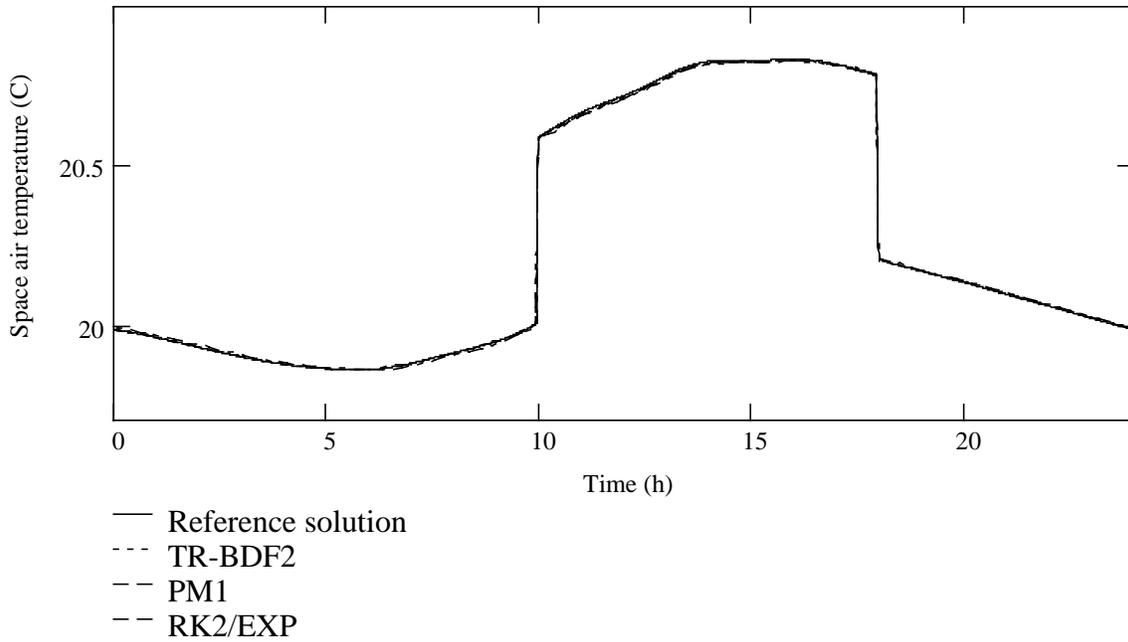


Figure 3 Comparison between reference solution and test solutions for a representative run (test run 15, day 2).

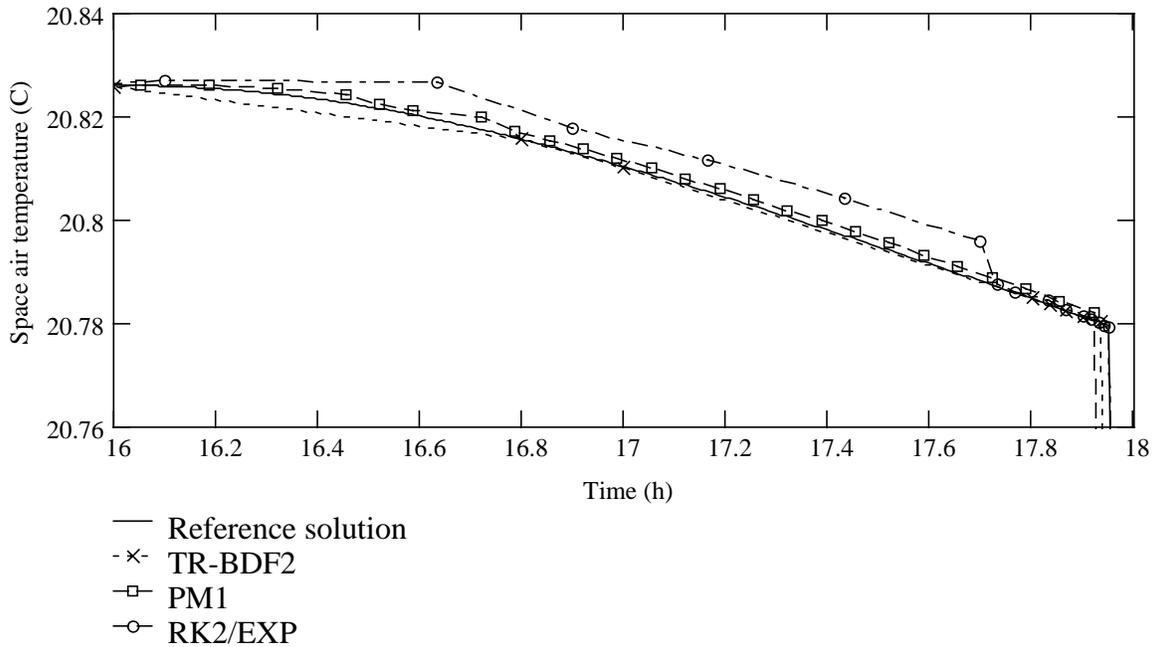


Figure 4 Comparison between reference solution and test solutions for a representative run (test run 15, day 2, 4.00 pm to 6.00 pm). A small part of the test run has been magnified to allow closer inspection of the solutions.

Discussion

PM1 proved to be the most efficient explicit exponential-fitted algorithm and LI the most effective means of interpolation for this group. The CE for PM1 was 31% greater than that of RK2/EXP for the chosen test example (Table 2). PM2 was 18% better than RK2/EXP. For comparison, standard low-order explicit methods have relative CEs in the range 0.18 to 0.34. Even though all of the exponential-fitted methods are L-stable, none of the algorithms including them could complete test runs 31 or 32 (Table 1) in reasonable time. However, these same tests can also be problematic for some currently used methods such as TR and the Hopscotch method. Persistent, unrealistic temperature oscillations result if long time steps are used (9, 10, 11). Tests 31 and 32 are, admittedly, stiffer than would normally be encountered in building energy simulation. The exponential-fitted algorithms, in fact, performed as though they had extended rather than infinite stability regions, which may be adequate for this moderately stiff problem.

The efficiency of the best implicit method was approached but not matched mainly because evaluation of the derivative function f is expensive in this application. However, because matrices are not used, a much larger fraction of the problem can be held in fast memory thus greatly increasing the processing rate. Also, being explicit in nature, these methods do not require simultaneous solution of equations and are therefore ideally suited to parallel processing. Computers with this capability are increasingly available and computation rates can be increased by a factor approaching the number of processors present. Neither advantage has been quantified in this evaluation.

Increased computational efficiency can always be applied to advantage. It allows faster simulations at the same error tolerance or, by tightening the tolerance, greater accuracy for the same computing time. Alternatively, it could facilitate a finer sub-division of the building; for example: (i) local two- or three-dimensional modelling of thermal bridges and building junctions; (ii) further sub-division of planar surfaces such as floors; or (iii) more nodes per homogeneous material layer. Or the additional computational power might be utilized to remove some modelling simplifications such as the linearization of convection and radiation terms. One further use for it might be to include more of the building's surroundings in the model so as to portray more accurately any local distortions of the recorded weather data.

Conclusions

An explicit exponential-fitted numerical algorithm and two proposed developments of it have been evaluated for the simulation of energy flows in buildings and plant, and their performances compared with an efficient implicit method. The proposed algorithms were found to be the best in their class with computational efficiencies approaching that of the implicit method for a representative set of test problems. None of the exponential-fitted algorithms performed well for the stiffest of the tests; however, these particular tests are more demanding than would normally be met in building energy simulation.

Perhaps of most interest is the potential of these methods. They are compact enough to run mostly in core memory and, being explicit, they are far more suited to parallel processing than implicit methods. The enhanced computing power can be used to reduce simulation times, improve the accuracy of solutions, increase the scale of problem tackled or allow more detailed modelling.

Nomenclature

c	Specific heat of material represented by a node [J/(kg·K)]
$f_i(\cdot)$	Derivative function
$f_i'(\cdot)$	Time derivative of f_i
$\mathbf{f}(\cdot)$	Vector of derivative functions
h	Space increment [m]
i	Space step level or node number
j	Time step level
\mathbf{J}	Jacobian matrix of \mathbf{f}
k	Time increment [s]
m	Mass of material represented by a node [kg]
n	Total number of equations
N	Number of machine operations per node/equation for a test run
t	Time [s]
T	Nodal temperature [K]
\mathbf{T}	Vector of dependent variables
\mathbf{T}'	Time derivative of \mathbf{T}
x	Space co-ordinate [m]
z	Exponent

Greek Symbols

α	Thermal diffusivity [m ² /s]
ε	Maximum absolute temperature difference between reference solution and test solution [K]
θ	Weighting factor
λ_i	Eigenvalue of \mathbf{J}
σ	Stiffness ratio
ϕ	Nodal heat gain [W]

Acronyms

BEM	Backward Euler method
CE	Computational efficiency
CIV	Computed intermediate values
ER	Euler's rule
LI	Linear interpolation
LTE	Local truncation error
$O(\cdot)$	Order of magnitude
ODE	Ordinary differential equation
PM1	Proposed method one
PM2	Proposed method two
$\text{Re}(\cdot)$	Real part of a complex number
RK2	Runge-Kutta method

RK2/EXP Ashour and Hanna's algorithm
TR Trapezoidal rule
TR-BDF2 Trapezoidal rule – backward differentiation formula composite method

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