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Dynamic time step and stability criteria comparison for the heat diffusion equation

Rabi H. Mohtar[a*], Larry J. Segerlind[b]

[a] *Department of Agricultural and Biological Engineering, Purdue University, West Lafayette, IN 47907*
[b] *Department of Agricultural and Biological Engineering, Michigan State University, East Lansing, MI 48824*

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Abstract — Dynamic time step estimates were determined for four single step numerical schemes in one dimension, and three finite element and three finite difference single step schemes in two dimensions. Unlike other stability-based time step criteria, the dynamic time step estimates are functions of grid size, material properties, and boundary conditions. For a certain problem, an initial coarse mesh is required to determine its lowest eigenvalue. The problem needs to be re-meshed and solved with the new mesh to satisfy a desired accuracy. Correlations between the dynamic time step and the stability criteria were conducted. A stability criteria equivalence was defined as the stability criteria that gives a time step estimate equivalent to the dynamic time step estimate. For the range of problems solved and for the central difference time stepping scheme, the stability criteria equivalence ranges from 0.5 to 2.7 for one-dimensional problems and 0.46 to 9.13 for two-dimensional problems, depending on the problem boundary conditions. The study shows that, unlike the dynamic time step estimate, the stability criteria used for selecting a time step is not adequate, since it does not change with the problem boundary conditions. © Elsevier, Paris.

dynamical time step / stability criterium / heat diffusion / numerical solution

Résumé — Comparaison du pas de temps dynamique et du critère de stabilité pour l'équation de diffusion de la chaleur. L'évaluation du pas de temps dynamique a été effectuée pour quatre schémas numériques en géométrie monodimensionnelle, ainsi que pour trois schémas à la fois d'éléments finis et de différences finies en géométrie bidimensionnelle. Contrairement aux critères de détermination du pas de temps basés sur la stabilité, l'évaluation du pas de temps dynamique est fonction de la dimension du maillage, des propriétés du matériau et des conditions aux frontières. Pour un problème donné, on doit d'abord utiliser un maillage grossier pour déterminer la valeur propre la plus faible. Pour des résultats précis, le domaine doit être ensuite remaillé et la solution reprise avec le nouveau maillage. On a réalisé une corrélation entre le pas de temps dynamique et le critère de stabilité. Un critère de stabilité équivalent a été défini comme étant le critère de stabilité donnant une estimation du pas de temps équivalente à celle du pas de temps dynamique. Pour la gamme de problèmes traités et pour une résolution en différences centrées, le critère de stabilité équivalent se situe entre 0,5 et 2,7 pour des problèmes à une dimension et entre 0,46 et 9,13 pour des problèmes à deux dimensions, dépendant des conditions aux frontières du problème. L'étude a montré que, contrairement à l'évaluation du pas de temps dynamique, le critère de stabilité n'est pas adéquat pour le choix du pas de temps, puisque celui-ci ne change pas avec les conditions limites du problème. © Elsevier, Paris.

pas de temps dynamique / critère de stabilité / diffusion de la chaleur / solution numérique

1. INTRODUCTION

The time-dependent heat conduction in solids is governed by the parabolic diffusion equation:

$$c\frac{\partial U}{\partial t} = k\,\nabla^2 U \qquad (1)$$

where c is the capacitance coefficient, k is the conductivity coefficient and U is the unknown temperature.

Applying finite element (FE) or finite difference (FD) numerical methods to (1), transforms the time and space-dependent partial differential equation (PDE) into a time-dependent system of ordinary differential equations (ODEs):

$$[C]\frac{\partial\{U\}}{\partial t} + [K]\{U\} - \{F\} = \{0\} \qquad (2)$$

* Correspondence and reprints.
mohtar@ecn.purdue.edu

where $[C]$ is the capacitance matrix coming from the transient term, $[K]$ is the stiffness matrix coming from the partial derivative with respect to spatial coordinants, and $\{F\}$ is the forcing function. Since there is no source term in the PDE, $\{F\}$ is zero before the boundary conditions are incorporated. The system of ordinary differential equations in (2) can be solved analytically using modal analysis or numerically using FE or FD methods. Despite the fact that many authors have presented and discussed solution procedures for the system of ODEs (2), there is still a lot of art and experience involved in selecting the proper scheme and the time step that is needed to reach an accurate solution. The numerical solution for the ODEs using single step schemes is defined as:

$$([C] + \theta\,\Delta t\,[K])\{U\}_{t+\mathrm{d}t} = ([C] - (1-\theta)\,\Delta t\,[K])\{U\}_t + \Delta t\,(\theta\,\{F\}_{t+\mathrm{d}t} + (1-\theta)\{F\}_t) \quad (3)$$

where $\theta = 0, 0.5, 0.67$, and 1 for Euler, central difference, Galerkin, and backward difference schemes, respectively. The central difference or the Crank-Nickolson scheme is second order accurate in time compared to the other schemes that are first order accurate in time.

Numerical integration in space and time of the time-dependent partial differential equation (1) produces a system of algebraic equations (3). A common problem during the numerical solution of these algebraic equations is to specify a time step that adequately and efficiently solves the problem. Several criteria are used to select the proper time step. Although the accuracy of the solution reaches its highest when the time step (Δt) approaches zero, an estimate of the time step that solves the problem within an error tolerance is useful but has not been found in a form for practical use. Smith [1] discusses the explicit Euler's scheme for solving the non-dimensional form of the PDE. He rearranged the difference equations, defined and named r as $\Delta t/(\Delta x)^2$, where Δt is the time step and Δx the grid space. During the discussion on stability, Smith stated that the explicit scheme is stable for 'r' values less than 0.5 and that the implicit Crank-Nickolson method has the advantage of being stable for all values of r. However, Smith recommends an 'r' value of one for an accurate solution for the Crank-Nickolson scheme. He discussed convergence and stability for some time stepping schemes and gave a time step expression that satisfies both criteria. No criterion was given for selecting time a step based on the accuracy of the solution. The r term defined by Smith does not include the material properties since the c_ρ/k term was defined as unity.

Allaire [2] defined stability in terms of the Courant number (C), which is similar to the 'r' value defined by Smith but it includes the material properties. To illustrate stable and non-stable schemes, Allaire defined an oscillatory stable scheme as having an oscillation that eventually dies out with the solution converging to the correct steady state values. Allaire showed the following criteria to be true for the single time step schemes:

$0 < C \leq 0.25$	no oscillation
$0.25 < C \leq 0.5$	oscillation but stable
$0.5 < C$	unstable (Euler's method only).

Allaire presented some examples to illustrate what he meant by his classifications. However, his solutions have no indication of instability for values of $C < 0.5$. Allaire discussed the weighted hybrid explicit implicit schemes defined in terms of a parameter theta, where, $0 \leqslant \theta \leqslant 1$. For $\theta = 0$, the scheme reduces to the explicit method and has the stability criterion of $C < 0.5$. He showed that the Crank-Nickolson and the fully implicit schemes are accurate for values of C up to 1.335.

Jaluria and Torrance [3] defined yet another stability parameter similar to Allaire's Courant number; they called it the Froude number, Fo. They suggested using values of $Fo < 0.5$ for the implicit scheme, although the lower the Fo values, the better the accuracy. However, they did not solve any examples using values of Fo lower than 0.5.

Rushton and Tomlinson [4] used the alternating direction approach as a numerical scheme to solve the discritized algebraic equations. They studied numerical stability for the solution scheme and found that the Courant number that generated accurate time step values changes with the problem boundary conditions. For a sudden change of pressure head on the boundary, the Courant number should be less than 1.0. For a draw down at a well, the Courant number should be less than 0.05. For a sudden change in discharge at a well, the Courant number should be less than 0.5. The authors suggested a trial and error procedure for selecting the optimal time step value.

Williams [5] and Fried [6] both studied the numerical solutions of the PDE and used the time step criterion that satisfied stability requirements. Williams used a term equivalent to the Courant number and stated that it should be less than 0.5. Fried used the stability criterion that the time step should be less or equal to 2 divided by the maximum eigenvalue of the system of ordinary equations. The analytical and numerical solution of the PDE requires a knowledge of eigenvalues for the eigenproblem: $([K] - \lambda[C])\{U\} = 0$, where $[K]$ is the stiffness matrix, $[C]$ is the capacitance matrix, and λ is the eigenvalue vector.

Patankar [7] presented a heat transfer computer program, CONDUCT. This program uses the backward difference scheme in time to solve the problem, but Patankar does not discuss selecting a time step.

The reason for the discrepancy of recommending different values of the same criterion represents one of the major limitations to the use of the stability criterion (such as the Courant number, Froude number or the r term as defined by Smith) for time step estimates. These criteria do not change with the boundary conditions of

the problem being solved. Each of the above authors has solved the heat equation for different boundary and initial conditions, and has recommended using a different value of the Courant and Froude numbers when solving a problem.

The objective of this study is to compare a dynamic time step estimate that changes with problem boundary conditions with a commonly used stability criterion to estimate the time step.

2. METHODOLOGY

2.1. Dynamic time step estimate equations

Dynamic functional estimates for the time step to be used in the numerical solution of field problems using the single time step schemes were developed based on a 5% error tolerance by Mohtar [8] and Mohtar and Segerlind [9, 10, 11]. The time estimate equations were developed for the unit step change problem through a numerical experimental procedure by varying the grid size and finding the time step that accurately integrated the problem within the error tolerance. These time steps were fitted by a power function and a regression equation determined the unknown coefficients. The equations estimate the time step using the number of nodes and the lowest eigenvalue of the system of ordinary differential equations. The numerical experimentation was repeated for the four schemes: forward difference, central difference, Galerkin, and backward difference in time, and for the finite element and the finite difference methods in space. A coarse grid was generated over the solution domain to determine the lowest eigenvalue of the system of ordinary differential equations. This parameter was also used to estimate the time to steady state and time domain sampling points used to evaluate the error relative to the analytical solution. A finer grid was generated for the numerical solution to ensure accuracy. The time step estimate equations were successfully tested and were used to solve problems other than those used in their development.

The time step estimate equations for the four single time stepping numerical schemes in one dimension are:

Euler	$\Delta t\,\lambda_1\,N^{1.6} = 0.27$	(4)
Central difference	$\Delta t\,\lambda_1\,N^{1.2} = 1.13$	(5)
Galerkin	$\Delta t\,\lambda_1\,N^{3.8} = 70$	(6)
Backward difference	$\Delta t\,\lambda_1\,N^{3.9} = 30.6$	(7)

where Δt is the time step, N is the number of nodes in the grid and should be greater than seven for all schemes to reduce spatial discritization error, λ_1 is the lowest eigenvalue of the system of ordinary differential equations.

The time step estimates for the three finite element, and the three finite difference single time stepping schemes are:

Galerkin forward difference

$$\Delta t\,\lambda_1\,N^{1.05} = 1.8 \text{ for } N \geq 25 \tag{8}$$

Galerkin central difference

$$\Delta t\,\lambda_1\,N^{0.6} = 1.6 \text{ for } N \geq 25 \tag{9}$$

Galerkin backward difference

$$\Delta t\,\lambda_1\,N^{0.1} = 0.05 \text{ for } N \geq 25 \tag{10}$$

Forward finite difference

$$\Delta t\,\lambda_1\,N^{1.05} = 1.2 \text{ for } N \geq 9 \tag{11}$$

Central finite difference

$$\Delta t\,\lambda_1\,N^{0.6} = 1.6 \text{ for } N \geq 9 \tag{12}$$

Backward finite difference

$$\Delta t\,\lambda_1\,N^{0.1} = 0.05 \text{ for } N \geq 9 \tag{13}$$

The first three equations (8–10) use the finite element method for space discritization, while the last three (11–13) use the finite difference for space discritization. In one-dimension the finite element and the finite difference generate similar equations and only one set is presented. The Galerkin scheme, representing a θ value of 0.67 is not reported for two dimensions.

2.2. Stability criteria

The stability criteria is a common criteria used in the selection of time step in transient field problems, particularly heat transfer, and is defined as:

$$\frac{k\,\Delta t}{\rho\,c\,\Delta x^2} < C \tag{14}$$

where k, c, and ρ are material dependent parameters in the PDE and are often taken as unity for simplicity, and C is a constant, Fried [6].

The stability criterion is a function of grid size Δx, time step Δt, and material property $k/\rho c$. It does not change with the boundary conditions. Therefore, the time step criterion developed using the stability criteria does not change if the boundary conditions of the problem changed, even though the boundary conditions have an impact on the dynamics of the problem. The speed at which the problem moves to steady state is a function of the lowest eigenvalue (λ_1) that is a function of the boundary conditions [12].

2.3. Time step estimates comparison

The dynamic time step estimates of equations (4)–(13) were compared with the stability criteria time step estimate of equation (14). Since the dynamic time step estimate changes with the boundary conditions, the comparison has to be based on a fixed value of λ_1. Using a Cartesian coordinate with the number of nodes on the x-axis, and the time step on the y-axis, the stability criteria (equation (14)) plots as a series of power curves similar in shape to the dynamic time step equations. For a certain boundary condition, a regression fit was performed for each scheme to find the optimal stability criteria that minimizes the difference between the two time step estimates, using equation (14) and equations (4)–(13). The resulting optimal stability criterion was defined as the stability criteria equivalence. A sample of the regression for $\lambda_1 = 9.8$ is shown in *figure 1* for the Galerkin scheme of equation (6). Similar results were produced for the other schemes and various λ_1 values. The Fo/N^2 in the figure refers to the time step estimate based on the stability criteria.

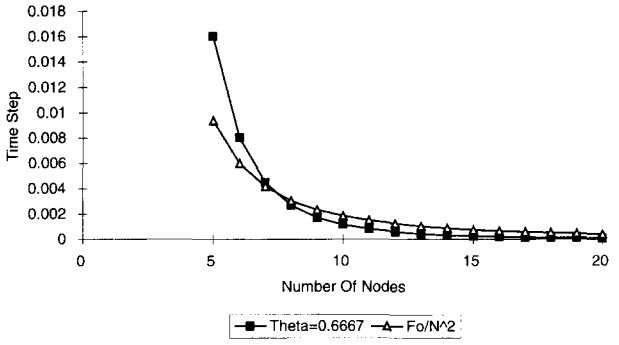

Figure 1. Comparison between estimated time step and stability criteria for the Galerkin scheme.

3. RESULTS

3.1. One-dimensional problems

The stability criteria equivalence for the four one-dimensional schemes (equations (4)–(7) at three values of λ_1 are shown in *figure 2*. The distribution in this figure for each curve is symmetric about the central difference. Although there is an infinite series of such curves, the figure shows important features and characteristics of the comparison between the two time step estimate approaches. The figure shows that the central difference scheme ($\theta = 0.5$) is superior to the other schemes. This is because when using the central difference time stepping scheme, larger time steps are permissible for the same accuracy. The difference

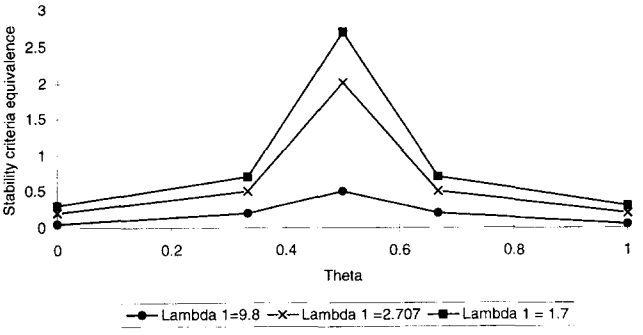

Figure 2. Stability criteria equivalence and its variation with λ_1.

between the central difference scheme and the other schemes is significant. The other important feature is that the stability criteria equivalence is not a fixed parameter and is not sufficient to describe the dynamic behavior of the time-dependent solution of the parabolic equation. In addition, the difference between stability criteria equivalence for each λ_1 value is significant, especially for the central difference scheme. *Figure 2* also shows that the stability criteria equivalence for the backward difference and Euler forward difference schemes was the same. This suggests that the two schemes have comparable accuracy. This result is not a surprise from the theoretical point of view since both schemes stand at equal distance but opposite sides of the center of the approximation domain in the Mean Value Theorem. The values also confirm an earlier observation that the Euler and backward difference schemes run with parallel accuracy and that there is no real advantage in using the backward difference scheme from an accuracy point of view. The backward difference is inaccurate in the region where the Euler scheme is unstable [8]. The values in this figure are within the range of recommended values of stability criteria given in the literature. They also explain why different studies recommend different values of stability criteria.

3.2. Two-dimensional problems

The dynamic time step estimates for the six schemes (equations (8)–(13)), were correlated against the stability criteria of equation (14). Similar to the one-dimensional problems, the stability criteria equivalence was determined by solving for the stability criteria that minimizes the sum of absolute differences between the two time steps estimates. *Figure 3* shows the regression fit between the Galerkin central difference scheme (GCD) (equations (9) and (14)), in order to find the stability criteria equivalence. The comparison in this figure is for certain boundary conditions. The time step estimate of equations (8)–(13) are dynamic and change with problem boundary conditions as well as grid size and material properties. On the other hand, the time

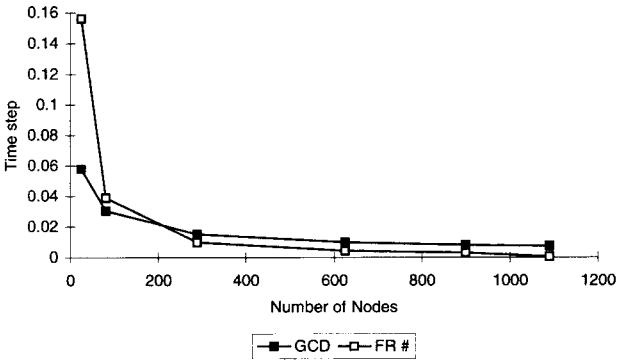

Figure 3. Finding a stability criteria equivalence through best fitting the GCD time step estimate equation and the FR time step estimate for a fixed boundary condition and material properties, i.e. fixed λ_1.

step estimate using the stability criteria of equation (14) is static and changes only with material properties and mesh size. This suggests that for every λ_1, there exist different stability criteria equivalence.

This study was conducted where λ_1 was allowed to vary and the regression procedure above was repeated. Results of the study are shown in *figures 4* and *5*. These figures represent different views of the same data and suggest that the finite element and finite difference methods have very similar stability criteria equivalence, and hence, similar accuracy. They also suggest that the central difference schemes have the largest stability criteria equivalence and are more accurate than the other schemes. The backward difference and forward difference schemes produce similar stability criteria equivalence suggesting similar accuracy. The backward difference and forward difference schemes are clustered together and can almost be combined into single stability criteria equivalence number that is independent of the problem type. The central difference scheme is more sensitive to the problem type and could only be represented by an equation through regressing stability criteria equivalent and λ_1. The variation in stability criteria equivalence for the central difference scheme is

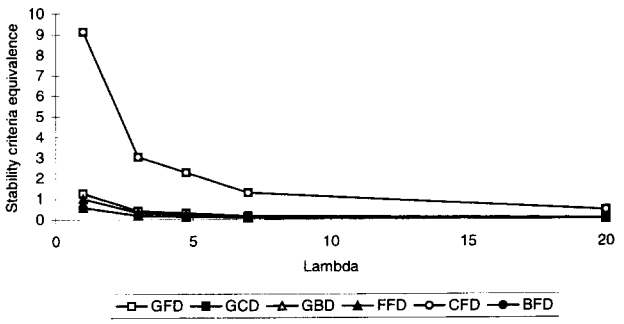

Figure 4. The stability criteria equivalence and its variations with λ_1 for the six schemes.

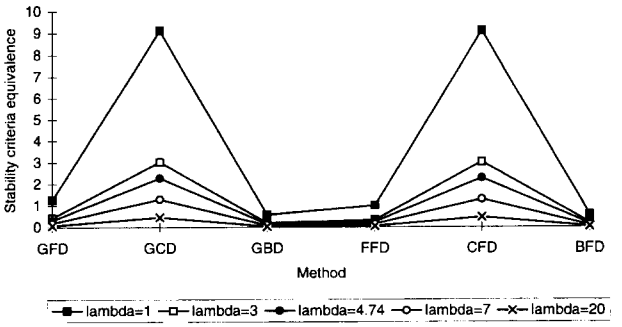

Figure 5. The stability criteria equivalence variations for the different schemes and different values of λ_1.

too large to be captured in a single number, as in the case of backward and foreword difference schemes.

4. SUMMARY AND CONCLUSIONS

The dynamic time step estimates were correlated with the stability criteria. A major observation was made during this correlation process that the stability criterion is problem independent. It only changes with the mesh size and material property. However, the dynamic time step estimate changes for each problem boundary condition, as well as mesh size and material properties. These later characteristics were captured by the smallest eigenvalue (λ_1). Therefore, any particular correlation between the stability criteria and the time step estimates changes with the problem being solved. Regression fit of the two time step estimates for various problems were presented.

Compared to the other schemes, the central difference scheme showed large sensitivity in the stability criteria equivalence corresponding to different problems and was proven to be more accurate.

This analysis also revealed that a non-oscillation criterion, such as the Froude number, is very conservative. It was originally designed for the conditionally stable explicit schemes [1]. It has been widely used to estimate the time step for all other schemes, including the unconditionally stable schemes. Furthermore, it could be computationally very inefficient for an accurate scheme such as central difference. The stability criteria could be used for the forward or backward difference schemes where it would still be slightly conservative. There is experimental evidence that Euler's scheme is always accurate when its stability requirements are satisfied [8]. On the other hand, the backward difference schemes are not accurate for a time step above those of the Euler's stability criteria.

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