Solutions of Linear and Nonlinear ODEs in Time Resulting from Decoupling of Space and Time in IVPs

By

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Abstract

This thesis presents considerations for determining a meritorious time integration strategy for a system of linear and nonlinear ordinary differential equations (ODEs) in time resulting from decoupling space and time in initial value problems (IVPs) using GM/WF for the spatial discretization. It is shown that Wilson's θ and Newmark's methods are meritorious over the others. It is further established that Newmark's method is meritorious over Wilson's θ method for integrating ODEs in time resulting from non-structural applications such as the mathematical models in Eulerian description for fluid mechanics. Newmark's linear method is considered for integrating linear and nonlinear first order and second order ODEs in time resulting from decoupling space and time for IVPs derived in Eulerian and Lagrangian descriptions of the deforming continua. The assumption of isothermal physics reduces the mathematical models of the IVPs to the Balance of linear momenta (BLM) in Eulerian and Lagrangian descriptions. In the present work we consider a space-time decoupled finite element method in which the space-time approximations of the dependent variables use approximation functions in space while the degrees of freedom are functions of time. This assumption induces space-time decoupling. Galerkin method with Weak form (GM/WF) for spatial discretization of the spatial domain is the preferred method of constructing the integral form in space. Integration over the spatial discretization yields a first order or second order system of linear or nonlinear ODEs in time. Though decoupling of space and time may introduce irreversible damage, the benefits in terms of simplicity of implementation and the speed of the calculations outweigh the shortcomings, particularly for IVPs in $\mathbb{R}^3$ for which a space-time coupled approach is al-

most prohibitive. Discretization and p-level in space are based on converged solutions of the corresponding boundary value problems (BVPs). Integration time step, Δt, is based on smoothness of the evolution and consideration of the stationary state of the evolution being the same as the solution of the corresponding BVP. The work presented here needs to be augmented with stability analyses in order to realize its full potential as it is only then we have a criteria for the choices of Δx and Δt. A priori and a posteriori analyses in conjunction with stability analyses will enable optimal choices of discretization Δx, p-levels in space, and time integration step, Δt.

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Chapter 1

Introduction, Literature Review and Scope of Work

1.1 Introduction

The mathematical description of the state of matter in which quantities of interest change at spatial locations as time elapses often leads to partial differential equations (PDEs) in which the quantities of interest, dependent variables, exhibit simultaneous dependence on space and time. Mathematical models consisting of the PDEs are generally referred to as Initial Value Problem (IVPs). The most natural way to consider solutions of IVPs is to consider a space-time coupled method in which simultaneous dependence of the dependent variable on space and time is preserved. When considering methods of approximation for IVPs, space-time coupled finite element methods [1] are highly meritorious. In this approach one considers space-time finite elements to either discretize the entire space-time domain or to discretize a space-time strip or a slab for an increment of time followed by time-marching to compute the evolution up to the desired value of time. Benefits and shortcomings of these two approaches are discussed in [1]. It has been shown that using a space-time strip with time-marching is highly meritorious over a space-time mesh for the space-time domain in all aspects for IVPs. When space-time variationally consistent space-

time coupled finite element processes are constructed using space-time local approximations in higher order spaces, accurate a posteriori computation of the residual functional is possible which provides an absolute measure of the accuracy of the computed evolution without the knowledge of the theoretical solution of the IVP. This feature permits computations of time accurate evolution for all values of time desired. While space-time coupled FEM works exceptionally well and is highly meritorious in $\mathbb{R}^1$ and $\mathbb{R}^2$, use of this approach for IVPs in $\mathbb{R}^3$ becomes impractical due to three spatial coordinates and time. Local approximations, space-time discretizations, and computations become almost prohibitive.

Thus, for IVPs in $\mathbb{R}^3$ there is a need for an alternate computational strategy in which the complications using the space-time coupled approach in $\mathbb{R}^3$ can be avoided. This is the main incentive to undertake the investigations presented in this thesis. Approximation methods that are based on decoupling space and time have long been in use in context with with finite difference and finite volume methods. Ever since the advent of FEM in 1968, space-time decoupled finite element methods have been in use for obtaining solutions of IVPs. Even though all space-time decoupled methods are based on non-concurrent treatments in space and time which is contrary to the physics described by IVPs. These methods permit solutions of IVPs in $\mathbb{R}^3$ with greater simplicity and secondly offer a variety of methodologies for obtaining final time evolution. In the present work we only consider the space-time decoupled finite element method. In all space-time decoupled methods for IVPs the system of PDEs is converted into a system of ordinary differential equations (ODEs) in time. This approach of decoupling space and time in space-time decoupled finite element processes is highly meritorious over those that are considered in finite difference or finite volume methods. The solutions of the resulting system of linear or nonlinear ODEs in time can be obtained by

1. Finite Element Method in time

2. Direct time integration methods such as Runge-Kutta methods

3. Explicit time integration methods such as Euler's method

4. Implicit time integration methods such as Houbolt's method, Wilson's θ method, and Newmark's method, etc.

Choice of a stable and accurate time integration scheme is obviously crucial in obtaining solutions of ODEs in time. While the linear system of ODEs in time pose no particular difficulty in obtaining their solutions, nonlinear systems of ODEs in time require prudent use of iterative methods for each increment of time to obtain a converged solution [2–17].

1.2 Literature Review

Some of the common methods of time integration used for ODEs in time are discussed in the following. Newmark [3] presents a derivation and explanation of different parameters in his integration scheme. These two parameters γ and β decide how much of an influence the acceleration is going to have on the velocities and displacements at $t + \Delta t$. Different choices of γ and β permit different time integration formulations. Wilson's θ method [4], is very similar to Newmark's method. In this method equilibrium is considered at $t + \theta\Delta t$ followed by calculating the solution at $t + \theta\Delta t$ and then at $t + \Delta t$. For $\theta = 1.4$ this method is found to be unconditionally stable for second order linear systems of ODEs in time, and at a value of $\theta = 1.0$, Wilson's θ method reduces to Newmark's method.

Perhaps the earliest published work on numerical integration of ODEs in structural dynamics resulting from space-time decoupling using Galerkin method with Weak Form (GM/WF) in space is due to Hughes [2]. This paper considers Newmark's linear average acceleration method for time integrating nonlinear second order ODEs in time.

$$\boldsymbol{M} \cdot \ddot{\boldsymbol{u}} + \boldsymbol{C} \cdot \dot{\boldsymbol{u}} + \boldsymbol{K}(\boldsymbol{u})\boldsymbol{u} = \boldsymbol{f}$$

In which $\boldsymbol{M}$ and $\boldsymbol{C}$ have constant coefficients, but the coefficients of $\boldsymbol{K}$ are functions of $\boldsymbol{u}$. Integration schemes presented are intertwined with the energy functional, which is not a valid

concept for nonlinear systems. The numerical examples contain trivial cases of nonlinearities far removed form the nonlinearity in structural dynamics due to finite deformation and finite strain. In another paper [5], the authors consider multitudes of different physics leading to nonlinearities, without a clear and concise definition of the precise form of the ODEs addressed and the most meritorious integration technique for them. A host of different time integration methods are discussed for a first order system of ODEs in time derived using auxiliary variables(s) and auxiliary equations. Reference [6], considers second order ODEs in time for which finite element method in time is used in which the integral form is in time is constructed using GM/WF in time.

In Wood, Bossak, Zienkiewicz's (WBZ-α) work [7] authors propose modifications of Newmark's method as well as Hilber, Hughes, and Taylor (HHT-α) [8]. In both of these works a new parameter, α, is introduced. The α parameter introduces numerical dissipation to the integration scheme for the higher modes which was found to be desirable in both works. The WBZ-α method aims to add positive dissipation to the integration scheme and results from WBZ-α method show that there is less artificial dampening in the lower modes using their algorithm.

Chung and Hulbert considered the methods in [7, 8] and derived a generalized-α method that utilizes two damping parameters, α_f and α_m [9]. These parameters are determined based on the amount of dissipation wanted in integration of the higher modes. Erlicher [10] also proposed another variation of a generalized-α method for non-linear systems of ODEs in time by combining the WBZ-α and HHT-α methods. Results showed high overshoot in the computed solution and bad oscillations in energy.

There are other published papers that use variations of these methods for structural dynamics [11–17]. Many of these works discuss the use of different parameters to bias the integration schemes to yield desired solutions.

In the last two decades, there has been very little published work related to solutions of IVPs by decoupling space-time and, subsequently, integrating ODEs in time. The solutions of ODEs resulting from non-structural applications are almost exclusively obtained using Runge-Kutta methods of fourth or higher orders. Whereas in structural mechanics applications, (second order ODEs in

time) the solution of the ODEs are obtained using Wilson's θ method with $\theta = 1.4$ based on linear acceleration or Newmark's method based on constant average acceleration. We have found that for whatever reasons, Runge-Kutta methods are rarely or almost never used in structural applications. Likewise, Wilson's θ and Newmark's methods have not been used in non-structural applications such as solutions of ODEs in fluid mechanics and gas dynamics.

This observation is almost strange from the point of view that a single unified, general and robust integration scheme that is applicable to all ODEs in time, regardless of their origin, has never been pursued in the published works. This is the primary focus of this research, to investigate if such an integration scheme is possible for ODEs in time regardless of their origin or field of application.

1.3 Scope of Work

In Runge-Kutta methods of various orders, the sum of overlapping areas in the time interval with weighting coefficients are used to approximate the area under the curve between $t_n \leq t \leq t_{n+1}$. The expressions for these overlapping areas are derived using Taylor series expansion at points between $t_n \leq t \leq t_{n+1}$. In these methods there are many drawbacks.

1. Knowing the solution at t_n, one obtains a solution at t_{n+1}, but for any $t_n < t < t_{n+1}$ we don't know the solution. That is the method lacks a description of the situation as a function of t in the time interval $t_n \leq t \leq t_{n+1}$. This in itself is bad, but another serious limitation of this is that it prevents determination of norm of any kind (such as $L2$-norm).

2. In the case of nonlinear ODEs in time, when the solution is advanced from time t_n to t_{n+1} (solutions being known at t_n) the expressions for the area constants are nonlinear i.e. they are functions of unknown solution at t_{n+1}. In this case, an iterative method is necessary for the Runge-Kutta schemes in order to calculate a converged solution at time $t_n + \Delta t$. At present, in many cases, linearized expressions are used for the area constants. This is obviously not consistent mathematically and may lead to erroneous evolution.

On the other hand, in Wilson's θ method and Newmark's method that have been strictly developed for structural mechanics applications (have never been used in non-structural applications to our knowledge), there is a concept of a precise description of the solution as a function of time over each integration time interval. In Wilson's θ method based on linear acceleration in the time interval $[t_n, t_n + \theta\Delta t]$, the displacement is a cubic function of time in the interval $[t, t + \theta\Delta t]$. In Newmark's constant average acceleration method in the time interval $[t_n, t_n + \Delta t]$, the displacement is quadratic in the time interval $[t, t + \Delta t]$. Thus, we see that in both of these methods the solution is obviously known (after calculation) at t_n and t_{n+1} $(= t_n + \Delta t)$ but we also have an analytical expression in t for the solution at t_n and t_{n+1} that describes how the solution behaves for (t_n, t_{n+1}). This feature is extremely valuable in computing any described norms essential for error estimation or error computation.

In the case of linear structural mechanics, one could decouple space and time in the mathematical model of the IVP using GM/WF in space and then transform the resulting system of coupled second order ODEs in the modal basis. With the assumption of Rayleigh damping one could obtain a system of decoupled second order ODEs. This permits stability analyses [1] of the Wilson's θ method and Newmark's method using just a single ODE, as all of the ODEs are precisely similar and only differ in natural frequency ω_i and corresponding damping coefficient ζ_i. This allows us to establish the unconditional stability of Wilson's θ method and Newmark's method for linear structural dynamics.

Superiority of Wilson'n θ method and Newmark's method over Runge-Kutta methods is rather obvious from the discussion given above. When considering the use of Wilson's θ and Newmark's time integration methods for general non-structural applications requires further considerations. For a specific system of linear first order ODEs in time it is easier to derive the details of the methods, these can perhaps be generalized for a system of first order ODEs resulting from space-time decoupling of the IVPs in Eulerian descriptions. We first consider a general system of ODEs (first order or second order, linear or nonlinear) to describe some important steps involved in Wilson's θ method and Newmark's method.

1. Whether we choose Wilson's θ method or Newmark's method is irrelevant in the case of linear structural dynamics, but this is not the case for non-structural applications. Choice of $\theta = 1.4$ only holds for linear dynamics in the modal basis, thus using Wilson's θ method without the knowledge of θ can be detrimental. Determination of θ for the application at hand requires stability analysis. This limitation favors choosing Newmark's method in which stability is the issue for non-structural applications but there is no such requirement as θ in Wilson' θ method.

2. In structural mechanics applications for $t \leq \dfrac{t_{\text{critical}}}{10}$ (based on time period) both methods yield reasonable accuracy [1], however Wilson's θ method has base elongation, but Newmark's method does not. This feature also favors Newmark's method.

3. In the case of Newmark's method we have two choices:

   (a) Assumption of constant average value of the highest derivative of the dependent variable in the interval $[t_n, t_n + \Delta t]$.

   (b) Linear approximation of the highest derivative in the interval $[t_n, t_n + \Delta t]$. This is obviously superior over (a) as this is an approximation of one degree higher than in (a) in time t.

   Thus, Newmark's linear method is meritorious of consideration for systems of ODEs in time resulting from decoupling of space and time in the IVPs.

4. In the case of linear ODEs in time we must derive a recursive relationship based on the assumption of linear variation of the highest order time derivative in the time interval $[t_n, t_n + \Delta t]$ followed by satisfying ODEs at time $t_n + \Delta t$. This allows us to compute the solution for progressively increasing time with known initial conditions.

5. In the case of nonlinear ODEs in time we proceed as in (4). The recursive solution for time marching in this case is nonlinear, hence it must be dealt with iteratively. We propose

to use Newton's linear method for each time interval to obtain a converged solution before commencing to the next time step.

6. In decoupling space and time the choice of discretization in space and the choice of p-levels is important. In the present work we choose these based on the converged solutions of the corresponding BVPs.

7. The choice of Δt is primarily based on oscillation free evolution and comparison of the stationary state with the solution of the corresponding BVP.

In this thesis we consider IVPs in Lagrangian (Solid mechanics) as well as Eulerian (Fluid mechanics) descriptions. For small strain-small deformation mathematical models (IVPs) in solid mechanics, are primarily BLM. These are linear second order PDEs in space and time when expressed in terms of displacements. When the deformation and strain are finite the BLM results in second order nonlinear PDEs in space and time for isothermal physics). In the present work we consider both linear and nonlinear systems of second order PDEs in space and time resulting from BLM in the Lagrangian description.

In the case of the Eulerian description, the IVPs as used in fluid mechanics, also results primarily in BLM which are naturally a system of nonlinear PDEs in space and time. In the present work we consider a variety of representative mathematical models in the Eulerian description. Convection Diffusion equation, Burgers equation, Pure Advection, and the Energy equation representing transient heat conduction in the presence of a diverging-converging velocity field.

In all IVPs a space-time decoupled formulation is constructed using GM/WF in space. Solutions of the resulting linear or nonlinear ODEs in time are obtained using Newmark's linear method, linear acceleration or linear velocity, for second order systems and first order systems of ODEs in time respectively. In many cases the solutions obtained by the space-time decoupled method are compared with solutions from space-time coupled methods to demonstrate accuracy of the evolution obtained from the space-time coupled methods.

Stability analysis of the system of coupled linear ODEs resulting from decoupling of space

and time in the IVPs using GM/WF in space can not be based on the approach used in Wilson's θ method and Newmark's method as these ODEs can not be transformed into modal basis. Thus, decoupling of the ODEs in time appears not feasible (at least at this stage). Investigation of the stability of Newmark's linear method for coupled linear systems of ODEs requires further work and is beyond the scope of work undertaken in this thesis.

A priori error estimation and a posteriori error computation procedures for Wilson's θ method and Newmark's method have been developed by Surana and Surana et al [1,18] and can be extended for the time integration using Newmark's method used for the ODEs considered in this thesis arising from non-standard applications. This requires further consideration and is also beyond the scope of work considered here.

Chapter 2

Decoupling space and time in IVPs

2.1 Introduction

As discussed in Chapter 1, there are many approaches of decoupling space and time in IVPs. The space-time decoupled finite element method is highly meritorious over all others as it enjoys the benefits of the mathematical foundation of the calculus of variations. In this chapter we first present a general treatment of decoupling space and time for linear and nonlinear IVPs.

2.2 Decoupling of space and time in space-time decoupled finite element processes

Consider an initial value problem

$$A\phi - f = 0 \quad \forall (x,t) \in \Omega_{xt} = \Omega_x \times \Omega_t \tag{2.1}$$

with some boundary conditions and initial conditions. In space-time decoupled finite element methods we discretize the spatial domain $\bar{\Omega}_x$ such that the discretization $\bar{\Omega}_x^T = \bigcup_e \bar{\Omega}_x^e(x,t)$ in which $\bar{\Omega}_x^e$ is the spatial domain of element Ω^e. Let $\phi_h(x,t)$ be the approximation of ϕ over $\bar{\Omega}_x^T$ such that $\phi_h(x,t) = \bigcup_e \phi_h^e(x,t)$ in which $\phi_h^e(x,t)$ is the local approximation of ϕ over $\bar{\Omega}_x^e$. Based on

fundamental lemma [1] we can construct the integral form of (2.1) over $\bar{\Omega}_x^T$.

$$(A\phi_h - f, v)_{\bar{\Omega}_x^T} = 0 \tag{2.2}$$

$$(A\phi_h - f, v)_{\bar{\Omega}_x^T} = \sum_e (A\phi_h^e - f, v) = 0 \tag{2.3}$$

We generally consider GM/WF in space (see [1]) in which case $v = \delta\phi_h$ in (2.2) and $v = \delta\phi_h^e$ in (2.3). Consider the following local approximation $\phi_h^e(x,t)$

$$\phi_h^e(x,t) = \sum_{i=1}^{n} N_i(x)\delta_i^e(t) = [N(x)]\{\delta^e\} \tag{2.4}$$

In (2.4), $N_i(x)$ are approximation functions in space and $\delta_i^e(t)$ are nodal degrees of freedom that change as time elapses, hence they are functions of time. Equation (2.4) decouples space and time. Consider $(A\phi_h^e - f, v)_{\bar{\Omega}_x^e}$ for an element e and substitute (2.4) and $v = N_j(x); \quad j = 1, 2, ..., n.$

$$(A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = \left(A\left(\sum_{i=1}^{n} N_i(x)\delta_i^e \right) - f, N_j(x) \right)_{\bar{\Omega}_x^e} \tag{2.5}$$

In (2.5), we let A act on the local approximation then integrate over $\bar{\Omega}_x^e$. When the space-time operator A is linear, then (2.5) reduces to

$$(A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = [H_1^e]\{\delta^e\} + [H_2^e]\{\dot{\delta}^e\} + \ ... \ - \{P^e\} - \{f^e\} \tag{2.6}$$

Substituting (2.6) in (2.3) gives,

$$[H_1]\{\delta\} + [H_2]\{\dot{\delta}\} + [H_3]\{\ddot{\delta}\} + \ ... \ = \{P\} + \{F\} \tag{2.7}$$

in which,

$$[H_1] = \sum_e [H_1^e] \ , \ [H_2] = \sum_e [H_2^e] \ , \ [H_3] = \sum_e [H_3^e] \tag{2.8}$$

$$\text{and} \quad \{P\} = \sum_e \{P^e\} \ , \ \{F\} = \sum \{f^e\} \tag{2.9}$$

$$\{\delta\} = \bigcup_e \{\delta^e\} \ , \ \{\dot{\delta}\} = \bigcup_e \{\dot{\delta}^e\} \ , \ \{\ddot{\delta}\} = \bigcup_e \{\ddot{\delta}^e\} \tag{2.10}$$

Since the space-time operator A is linear, then all matrices in (2.7) contain constant coefficients.

When A is a nonlinear differential operator, the nonlinearity is generally in the spatial derivatives, the time derivative terms are linear. For example, BLM in the Eulerian description. In such cases, we shall find that the coefficients of $[H_1]$ are linear or nonlinear functions of $\{\delta\}$, but the coefficients of $[H_2]$ and $[H_3]$ are constants. In this case, (2.7) represents a nonlinear system of ODEs in time. The linear or nonlinear ODEs in time (2.7) resulting from the decoupling of space and time are integrated using Newmark's linear method [1]. We consider the details in the following.

2.3 First order system of linear ODEs

When the mathematical models for IVPs contain a linear space-time differential operator A with only first order time derivatives, then GM/WF in space yield the following system of ODEs for discretization $\bar{\Omega}_x^T$ of spatial domain $\bar{\Omega}_x$.

$$\boldsymbol{C} \cdot \dot{\boldsymbol{\delta}} + \boldsymbol{K} \cdot \boldsymbol{\delta} = \boldsymbol{F} + \boldsymbol{P} \tag{2.11}$$

We consider Newmark's method [1] with linear approximation of $\dot{\boldsymbol{\delta}}$ between time $[t, t + \Delta t]$

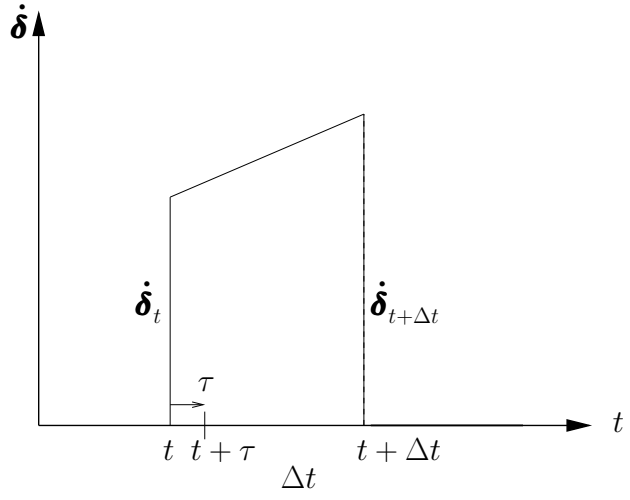


Figure 2.1: Newmark's linear method: Linear velocity for first order systems

Referring to figure 2.1,

$$\dot{\boldsymbol{\delta}}_{t+\tau} = \dot{\boldsymbol{\delta}}_t + \frac{\tau}{\Delta t}(\dot{\boldsymbol{\delta}}_{t+\Delta t} - \dot{\boldsymbol{\delta}}_t) \tag{2.12}$$

then integrating with respect to τ,

$$\boldsymbol{\delta}_{t+\tau} = \tau\dot{\boldsymbol{\delta}}_t + \frac{\tau^2}{2\Delta t}(\dot{\boldsymbol{\delta}}_{t+\Delta t} - \dot{\boldsymbol{\delta}}_t) + \boldsymbol{C} \tag{2.13}$$

$$\text{at} \quad \tau = 0 \ , \ \boldsymbol{\delta}_{t+\tau} = \boldsymbol{\delta}_t \tag{2.14}$$

Using (2.14) in (2.13), we can evaluate $\boldsymbol{C}$ and then obtain the following from (2.13) after substituting $\boldsymbol{C}$.

$$\boldsymbol{\delta}_{t+\tau} = \boldsymbol{\delta}_t + \tau\dot{\boldsymbol{\delta}}_t + \frac{\tau^2}{2\Delta t}(\dot{\boldsymbol{\delta}}_{t+\Delta t} - \dot{\boldsymbol{\delta}}_t) \tag{2.15}$$

Using $\tau = \Delta t$ in (2.12) and (2.15) we obtain,

$$\dot{\boldsymbol{\delta}}_{t+\Delta t} = \dot{\boldsymbol{\delta}}_{t+\Delta t} \tag{2.16}$$

$$\boldsymbol{\delta}_{t+\Delta t} = \boldsymbol{\delta}_t + \Delta t\dot{\boldsymbol{\delta}}_t + \frac{\Delta t}{2}(\dot{\boldsymbol{\delta}}_{t+\Delta t} - \dot{\boldsymbol{\delta}}_t) \tag{2.17}$$

from (2.17)

$$\dot{\boldsymbol{\delta}}_{t+\Delta t} = \frac{2}{\Delta t}(\boldsymbol{\delta}_{t+\Delta t} - \boldsymbol{\delta}_t - \Delta t\dot{\boldsymbol{\delta}}_t) + \dot{\boldsymbol{\delta}}_t \tag{2.18}$$

Consider (2.11) at $t + \Delta t$,

$$\boldsymbol{C} \cdot \dot{\boldsymbol{\delta}}_{t+\Delta t} + \boldsymbol{K} \cdot \boldsymbol{\delta}_{t+\Delta t} = \boldsymbol{F}_{t+\Delta t} + \boldsymbol{P}_{t+\Delta t} \tag{2.19}$$

substituting for $\dot{\boldsymbol{\delta}}_{t+\Delta t}$ from (2.18) in (2.19),

$$\boldsymbol{C} \cdot \left(\frac{2}{\Delta t}(\boldsymbol{\delta}_{t+\Delta t} - \boldsymbol{\delta}_t - \Delta t\dot{\boldsymbol{\delta}}_t) + \dot{\boldsymbol{\delta}}_t \right) + \boldsymbol{K} \cdot \boldsymbol{\delta}_{t+\Delta t} = \boldsymbol{F}_{t+\Delta t} + \boldsymbol{P}_{t+\Delta t} \tag{2.20}$$

rearranging terms,

$$\left(\frac{2}{\Delta t}\boldsymbol{C}+\boldsymbol{K}\right)\cdot\boldsymbol{\delta}_{t+\Delta t}=\boldsymbol{F}_{t+\Delta t}+\boldsymbol{P}_{t+\Delta t}-\boldsymbol{C}\cdot\left(\frac{2}{\Delta t}\boldsymbol{\delta}_t+\dot{\boldsymbol{\delta}}_t\right) \tag{2.21}$$

and from (2.18),

$$\dot{\boldsymbol{\delta}}_{t+\Delta t}=\frac{2}{\Delta t}(\boldsymbol{\delta}_{t+\Delta t}-\boldsymbol{\delta}_t)-\dot{\boldsymbol{\delta}}_t \tag{2.22}$$

Initial conditions for (1) consists of

$$\boldsymbol{\delta}_{t=0}=\boldsymbol{\delta}_0 \tag{2.23}$$

Using (2.23) in (2.11), we can obtain $\dot{\boldsymbol{\delta}}_0$:

$$\dot{\boldsymbol{\delta}}_0=\boldsymbol{C}^{-1}\cdot(\boldsymbol{P}_{t=0}+\boldsymbol{F}_{t=0}-\boldsymbol{K}\delta_0) \tag{2.24}$$

Thus, $\boldsymbol{\delta}_0$ and $\dot{\boldsymbol{\delta}}_0$ are known at $t=0$, hence solutions can now be completed at $t+\Delta t$ i.e $\boldsymbol{\delta}_{t+\Delta t}=\boldsymbol{\delta}_{\Delta t}$ and $\dot{\boldsymbol{\delta}}_{t+\Delta t}=\dot{\boldsymbol{\delta}}_{\Delta t}$ using (2.21) and (2.22). This process is continued until the desired time $t=\tau$ is reached.

2.4 First order system of nonlinear ODEs

When the space-time differential operator has first order time derivatives but is nonlinear in space, then the use of GM/WF for spatial discretization of $\bar{\Omega}_x^T$ yields a system of nonlinear first order ODEs in time. Consider,

$$\boldsymbol{C}\cdot\dot{\boldsymbol{\delta}}+\boldsymbol{K}(\boldsymbol{\delta})\cdot\boldsymbol{\delta}=\boldsymbol{F}+\boldsymbol{P} \tag{2.25}$$

Application of Newmark linear method described in section 2.3 will yield,

$$\left(\frac{2}{\Delta t}\boldsymbol{C}+\boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\boldsymbol{\delta}_{t+\Delta t}=\boldsymbol{F}_{t+\Delta t}+\boldsymbol{P}_{t+\Delta t}-\boldsymbol{C}\cdot\left(\frac{2}{\Delta t}\boldsymbol{\delta}_t+\dot{\boldsymbol{\delta}}_t\right) \tag{2.26}$$

Since $\boldsymbol{K}$ is a function of unknown $\boldsymbol{\delta}_{t+\Delta t}$, (2.26) is a system of nonlinear algebraic equations in $\boldsymbol{\delta}_{t+\Delta t}$. Thus, we must calculate $\boldsymbol{\delta}_{t+\Delta t}$ iteratively to satisfy (2.26). First we rewrite (2.26) as,

$$\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t}) = \left(\frac{2}{\Delta t}\boldsymbol{C} + \boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t})\right) \cdot \boldsymbol{\delta}_{t+\Delta t} - \boldsymbol{F}_{t+\Delta t} - \boldsymbol{P}_{t+\Delta t} + \boldsymbol{C} \cdot \left(\frac{2}{\Delta t}\boldsymbol{\delta}_t + \dot{\boldsymbol{\delta}}_t\right) \tag{2.27}$$

We must find a $\boldsymbol{\delta}_{t+\Delta t}$ iteratively that satisfies (2.27)

Let $\boldsymbol{\delta}^0_{t+\Delta t}$ be an assumed solution of $\boldsymbol{\delta}_{t+\Delta t}$ Then,

$$\boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t}) \neq 0 \tag{2.28}$$

and let $\Delta\boldsymbol{\delta}_{t+\Delta t}$ be a correction to $\boldsymbol{\delta}^0_{t+\Delta t}$ such that

$$\boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t} + \Delta\boldsymbol{\delta}_{t+\Delta t}) = 0 \tag{2.29}$$

Expanding (2.29) in Taylor series about $\boldsymbol{\delta}^0_{t+\Delta t}$ and retaining only up to linear terms in $\Delta\boldsymbol{\delta}_{t+\Delta t}$:

$$\boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t} + \Delta\boldsymbol{\delta}_{t+\Delta t}) = \boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t}) + \frac{\partial \boldsymbol{g}()}{\partial \boldsymbol{\delta}^0_{t+\Delta t}}|_{\boldsymbol{\delta}^0_{t+\Delta t}} \cdot \Delta\boldsymbol{\delta}_{t+\Delta t} = 0 \tag{2.30}$$

$$\Delta\boldsymbol{\delta}_{t+\Delta t} = -(\delta\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})|_{\boldsymbol{\delta}^0_{t+\Delta t}})^{-1} \cdot \boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t}) \tag{2.31}$$

$$\text{and} \quad \boldsymbol{\delta}_{t+\Delta t} = \boldsymbol{\delta}^0_{t+\Delta t} + \Delta\boldsymbol{\delta}_{t+\Delta t} \tag{2.32}$$

The solution is considered converged for the time step Δt when

$$\begin{aligned} |\boldsymbol{g}_i(\boldsymbol{\delta}_{t+\Delta t})| &\leq \Delta \text{ , a preset tolerance for zero} \\ \max_i |\Delta\boldsymbol{\delta}_{t+\Delta t}| &\leq \Delta \text{ , a preset tolerance for zero} \end{aligned} \tag{2.33}$$

This is Newton's linear method for nonlinear algebraic equations. $\delta\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})$ can be obtained using (2.27).

$$\delta\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t}) = \delta(\boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t}) \cdot \boldsymbol{\delta}_{t+\Delta t}) = \delta\boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t}) \cdot \boldsymbol{\delta}_{t+\Delta t} + \boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t}) \tag{2.34}$$

using (2.34) in (2.31), $\Delta\boldsymbol{\delta}_{t+\Delta t}$ can be calculated.

2.5 Second order system of linear ODEs in time

For small deformation, small strain, isothermal deformation of solids, BLM in displacements is a system of linear second order PDEs in space and time. If we consider dissipation to be a function of strain rate, then the integral form based on GM/WF for a spatial discretization $\bar{\Omega}_x^T$ yields (assuming entropy production due to dissipation is negligible) the following at time t.

$$\boldsymbol{M} \cdot \ddot{\boldsymbol{\delta}} + \boldsymbol{C} \cdot \dot{\boldsymbol{\delta}} + \boldsymbol{K} \cdot \boldsymbol{\delta} = \boldsymbol{F} + \boldsymbol{P} \tag{2.35}$$

In this case $\boldsymbol{M}$, $\boldsymbol{C}$, and $\boldsymbol{K}$ have constant coefficients, hence (2.35) is a system of linear second order ODEs in time. It has been shown that Newmark's linear method [1] is unconditionally stable and has the best accuracy for integrating (2.35) in time. The derivation presented in reference [1] is given in the following.

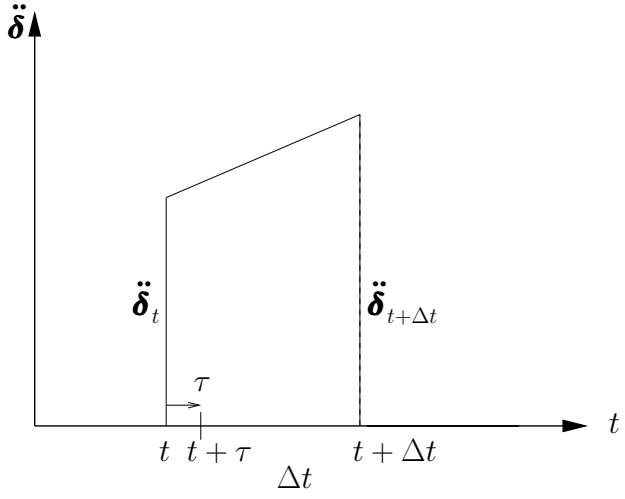


Figure 2.2: Newmark's linear method: Linear acceleration for second order systems

Based on a linear $\ddot{\boldsymbol{\delta}}$ over the interval $[t, t+\Delta t]$ we can write,

$$\ddot{\boldsymbol{\delta}}_{t+\tau} = \ddot{\boldsymbol{\delta}}_t + \frac{\tau}{\Delta t}(\ddot{\boldsymbol{\delta}}_{t+\Delta t} - \ddot{\boldsymbol{\delta}}_t) \tag{2.36}$$

integrating with respect to τ and evaluating constant of integration at $\tau = 0$.

$$\ddot{\boldsymbol{\delta}}_{t+\tau} = \dot{\boldsymbol{\delta}}_t + \tau\ddot{\boldsymbol{\delta}}_t + \frac{\tau^2}{2\Delta t}(\ddot{\boldsymbol{\delta}}_{t+\Delta t} - \ddot{\boldsymbol{\delta}}_t) \tag{2.37}$$

Integrating (2.37) with respect to τ and evaluating constant of integration at $\tau = 0$.

$$\boldsymbol{\delta}_{t+\tau} = \boldsymbol{\delta}_t + \tau\dot{\boldsymbol{\delta}}_t + \frac{\tau^2}{2}\ddot{\boldsymbol{\delta}}_t + \frac{\tau^3}{6\Delta t}(\ddot{\boldsymbol{\delta}}_{t+\Delta t} - \ddot{\boldsymbol{\delta}}_t) \tag{2.38}$$

Using $\tau = \Delta t$ in (2.36)-(2.38) we obtain,

$$\ddot{\boldsymbol{\delta}}_{t+\Delta t} = \ddot{\boldsymbol{\delta}}_{t+\Delta t} \tag{2.39}$$

$$\dot{\boldsymbol{\delta}}_{t+\Delta t} = \dot{\boldsymbol{\delta}}_t + \frac{\Delta t}{2}\ddot{\boldsymbol{\delta}}_t + \frac{\Delta t}{2}\dot{\boldsymbol{\delta}}_{t+\Delta t} \tag{2.40}$$

$$\boldsymbol{\delta}_{t+\Delta t} = \dot{\boldsymbol{\delta}}_t + \Delta t\dot{\boldsymbol{\delta}}_t + \frac{(\Delta t)^2}{3}\ddot{\boldsymbol{\delta}}_t + \frac{(\Delta t)^2}{6}\ddot{\boldsymbol{\delta}}_{t+\Delta t} \tag{2.41}$$

using (2.41) we can solve for $\ddot{\boldsymbol{\delta}}_{t+\Delta t}$.

$$\ddot{\boldsymbol{\delta}}_{t+\Delta t} = \frac{6}{(\Delta t)^2}(\boldsymbol{\delta}_{t+\Delta t} - \boldsymbol{\delta}_t) - \frac{6}{(\Delta t)^2}\dot{\boldsymbol{\delta}}_t - 2\ddot{\boldsymbol{\delta}}_t \tag{2.42}$$

substituting $\ddot{\boldsymbol{\delta}}_{t+\Delta t}$ in (2.40) we obtain,

$$\dot{\boldsymbol{\delta}}_{t+\Delta t} = \frac{3}{\Delta t}(\boldsymbol{\delta}_{t+\Delta t} - \boldsymbol{\delta}_t) - 2\dot{\boldsymbol{\delta}}_t - \frac{\Delta t}{2}\ddot{\boldsymbol{\delta}}_t \tag{2.43}$$

Consider (2.35) at $t + \Delta t$:

$$\boldsymbol{M} \cdot \boldsymbol{\delta}_{t+\Delta t} + \boldsymbol{C} \cdot \dot{\boldsymbol{\delta}}_{t+\Delta t} + \boldsymbol{K} \cdot \ddot{\boldsymbol{\delta}}_{t+\Delta t} = \boldsymbol{F}_{t+\Delta t} + \boldsymbol{P}_{t+\Delta t} \tag{2.44}$$

substituting for (2.42) and (2.43) in (2.44) and rearranging terms we can obtain the following,

$$\left(\frac{6}{(\Delta t)^2}\boldsymbol{M}+\frac{3}{\Delta t}\boldsymbol{C}+\boldsymbol{K}\right)\cdot\boldsymbol{\delta}_{t+\Delta t}=\boldsymbol{F}_{t+\Delta t}+\boldsymbol{P}_{t+\Delta t}+\left(\frac{6}{(\Delta t)^2}\boldsymbol{M}+\frac{3}{\Delta t}\boldsymbol{C}\right)\cdot\boldsymbol{\delta}_{t}+\left(\frac{6}{\Delta t}\boldsymbol{M}+2\boldsymbol{C}\right)\cdot\dot{\boldsymbol{\delta}}_{t}+\left(2\boldsymbol{M}+\frac{\Delta t}{2}\boldsymbol{C}\right)\cdot\ddot{\boldsymbol{\delta}}_{t} \tag{2.45}$$

using initial conditions at $t=0$ for $\boldsymbol{\delta}_{t=0}$ and $\dot{\boldsymbol{\delta}}_{t=0}$, we can calculate $\ddot{\boldsymbol{\delta}}_{t=0}$ using (2.35) at $t=0$.

$$\ddot{\boldsymbol{\delta}}_{t=0}=\boldsymbol{M}^{-1}(\boldsymbol{P}_{t=0}+\boldsymbol{F}_{t=0}-\boldsymbol{C}\dot{\boldsymbol{\delta}}_{t=0}-\boldsymbol{K}\boldsymbol{\delta}_{t=0}) \tag{2.46}$$

Then $\boldsymbol{\delta}_{t=0}$, $\dot{\boldsymbol{\delta}}_{t=0}$, and $\ddot{\boldsymbol{\delta}}_{t=0}$ are known at $t=0$. using these ICs and (2.45), the solution at $t+\Delta t$ i.e $\boldsymbol{\delta}_{t+\Delta t}$ can calculated followed by the calculation of $\dot{\boldsymbol{\delta}}_{t+\Delta t}$ and $\ddot{\boldsymbol{\delta}}_{t+\Delta t}$ using (2.43) and (2.42). The solution at $t+\Delta t$ is used as ICs to calculate the solution at $t+2\Delta t$. This is continued until the desired time is reached.

2.6 Second order systems of nonlinear ODEs in time

For finite deformation, finite strain but no isothermal deformation physics, Green's strain measure and rate of Green's strain measure are used in the constitutive theory for contravariant second Piola-Kirchhoff stress tensor. This leads to nonlinear PDEs in displacements from from BLM. Use of GM/WF in space yields the following system of nonlinear ODEs in time,

$$\boldsymbol{M}\cdot\ddot{\boldsymbol{\delta}}+\boldsymbol{C}(\boldsymbol{\delta})\cdot\dot{\boldsymbol{\delta}}+\boldsymbol{K}(\boldsymbol{\delta})\cdot\boldsymbol{\delta}=\boldsymbol{F}+\boldsymbol{P} \tag{2.47}$$

in which the mass matrix $\boldsymbol{M}$ has constant coefficients but the coefficients of $\boldsymbol{C}$ and $\boldsymbol{K}$ are at least up to quadratic functions of $\boldsymbol{\delta}$.

Application of Newmark's linear acceleration method to (2.47) (following section 2.5), yields

the following for (2.47) for time marching the solution of the ODEs.

$$\left(\frac{6}{(\Delta t)^2}\boldsymbol{M}+\frac{3}{\Delta t}\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})+\boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\boldsymbol{\delta}_{t+\Delta t}=\boldsymbol{F}_{t+\Delta t}+\boldsymbol{P}_{t+\Delta t}+ \left(\frac{6}{(\Delta t)^2}\boldsymbol{M}+\frac{3}{\Delta t}\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\boldsymbol{\delta}_t+\left(\frac{6}{\Delta t}\boldsymbol{M}+2\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\dot{\boldsymbol{\delta}}_t+ \left(2\boldsymbol{M}+\frac{\Delta t}{2}\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\ddot{\boldsymbol{\delta}}_t \tag{2.48}$$

Since $\boldsymbol{C}$ and $\boldsymbol{K}$ are functions of unknown $\boldsymbol{\delta}_{t+\Delta t}$, (2.48) is a system of nonlinear algebraic equations in $\boldsymbol{\delta}_{t+\Delta t}$, thus we must calculate a solution for $\boldsymbol{\delta}_{t+\Delta t}$ iteratively that satisfies (2.48). By transferring all terms to the LHS.

$$\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})=\left(\frac{6}{(\Delta t)^2}\boldsymbol{M}+\frac{3}{\Delta t}\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})+\boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\boldsymbol{\delta}_{t+\Delta t}-\boldsymbol{F}_{t+\Delta t}-\boldsymbol{P}_{t+\Delta t}- \left(\frac{6}{(\Delta t)^2}\boldsymbol{M}+\frac{3}{\Delta t}\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\boldsymbol{\delta}_t-\left(\frac{6}{\Delta t}\boldsymbol{M}+2\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\dot{\boldsymbol{\delta}}_t- \left(2\boldsymbol{M}+\frac{\Delta t}{2}\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\ddot{\boldsymbol{\delta}}_t=0 \tag{2.49}$$

Since $\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})$ is a nonlinear function of unknown solution $\boldsymbol{\delta}_{t+\Delta t}$, we must now find $\boldsymbol{\delta}_{t+\Delta t}$ iteratively that satisfies (2.49). Let $\boldsymbol{\delta}^0_{t+\Delta t}$ be an assumed solution of $\boldsymbol{\delta}_{t+\Delta t}$ then,

$$\boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t})\neq 0 \tag{2.50}$$

Let $\Delta t\boldsymbol{\delta}_{t+\Delta t}$ be a correction to $\dot{\boldsymbol{\delta}}_{t+\Delta t}$ such that,

$$\boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t}+\Delta t\boldsymbol{\delta}_{t+\Delta t})=0 \tag{2.51}$$

following the details in section 2.4, we can obtain,

$$\Delta\boldsymbol{\delta}_{t+\Delta t}=-(\delta\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})|_{\boldsymbol{\delta}^0_{t+\Delta t}})^{-1}\cdot\boldsymbol{g}(\boldsymbol{\delta}^0_{t+\Delta t}) \tag{2.52}$$

and an improved solution of $\boldsymbol{\delta}_{t+\Delta t}$ is given by,

$$\boldsymbol{\delta}_{t+\Delta t}=\boldsymbol{\delta}^0_{t+\Delta t}+\Delta\boldsymbol{\delta}_{t+\Delta t} \tag{2.53}$$

This is Newton's linear method for these nonlinear algebraic equations. Convergence criteria and

other details follow section 2.4. The variation of $\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})$ can be obtained using (2.49):

$$\begin{aligned}\delta(\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})) = \left(\frac{6}{(\Delta t)^2}\boldsymbol{M} + \frac{3}{\Delta t}\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t}) + \boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t})\right) + \\ \left(\frac{3}{\Delta t}\delta\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t}) + \delta\boldsymbol{K}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\boldsymbol{\delta}_{t+\Delta t} - \\ \left(\frac{3}{\Delta t}\delta\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\boldsymbol{\delta}_t - \left(2\delta\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\dot{\boldsymbol{\delta}}_t - \\ \left(\frac{\Delta t}{2}\delta\boldsymbol{C}(\boldsymbol{\delta}_{t+\Delta t})\right)\cdot\ddot{\boldsymbol{\delta}}_t\end{aligned} \tag{2.54}$$

using $\delta\boldsymbol{g}(\boldsymbol{\delta}_{t+\Delta t})$ from (2.54) in (2.52), we can calculate $\Delta\boldsymbol{\delta}_{t+\Delta t}$.

Remarks

1. The time integration schemes presented here for linear and nonlinear first and second order ODEs in time are applied to various model problems in Chapter 3.

2. In most cases, the solutions obtained from the space-time decoupled approach are compared with these obtained using space-time coupled finite element method based on residual functional [1].

Chapter 3

Model Problem Studies

3.1 Introduction

In this chapter we consider numerical solutions of model IVPs that lead to first order and second order systems of linear and nonlinear ODEs in time due to space-time decoupling by using GM/WF in space to construct the integral form over the spatial discretization of $\bar{\Omega}_x^T$ of the spatial domain $\bar{\Omega}_x$. Solutions of ODEs in time are calculated using Newmark's linear method described in Chapter 2. These solutions are also compared with the solutions obtained using a space-time coupled finite element method with a space-time strip or space-time slab and then time marching (see [1] for details).

3.2 First order system of ODEs in time

In this section we consider IVPs in which space-time decoupling leads to a first order system of linear or nonlinear ODEs in time. These IVPs naturally result from the conservation and the balance laws (CBL) in Eulerian descriptions such as fluid mechanics.

3.2.1 Convection diffusion equation

Consider the time dependent convection diffusion equation (simplified form of the energy equation).

$$\frac{\partial \phi}{\partial t} + \frac{\partial \phi}{\partial x} - \frac{1}{Pe}\frac{\partial^2 \phi}{\partial x^2} = f(x,t) \quad \forall (x,t) \in \Omega_{xt} = \Omega_x \times \Omega_t = (0,1) \times (0,\tau) \tag{3.1}$$

$$\begin{aligned} &\text{BCs: } \phi(0,t) = 1, \phi(1,t) = 0 \quad \forall t \in (0,\tau) \\ &\text{ICs: } \phi(x,0) = 0 \quad \forall x \in (0,1) \end{aligned} \tag{3.2}$$

Consider a three node 25 element uniform discretization of $\bar{\Omega}_x = [0,1]$ with element local-nodes treated at 1, 2, and 3. Based on the fundamental lemma, we can write the following using approximation ϕ_h of ϕ over $\bar{\Omega}_x^T$.

$$(A\phi_h - f, v)_{\bar{\Omega}_x^T} = \sum_e (A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = 0 \tag{3.3}$$

$$\text{using,} \quad \phi_h^e(x,t) = \sum_{i=1}^{n} N_i(x)\delta_i^e(t) = [N(x)]\{\delta^e(t)\} \tag{3.4}$$

in (3.3) in GM/WF over $\bar{\Omega}_x^e$ we can obtain,

$$(A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = [C^e]\{\dot{\delta}^e\} + [K^e]\{\delta^e\} - \{f^e\} - \{P^e\} \tag{3.5}$$

in which,

$$C_{ij}^e = \int_{\bar{\Omega}_x^e} N_i(x) N_j(x) dx \tag{3.6}$$

$$K_{ij}^e = \int_{\bar{\Omega}_x^e} (N_i \frac{\partial N_j}{dx} + \frac{1}{Pe}\frac{\partial N_i}{dx}\frac{\partial N_j}{dx}) dx \tag{3.7}$$

$$f_i^e = \int_{\bar{\Omega}_x^e} f N_i dx \tag{3.8}$$

$$\{P^e\} = \begin{Bmatrix} P_1^e \\ \vdots \\ P_n^e \end{Bmatrix} \tag{3.9}$$

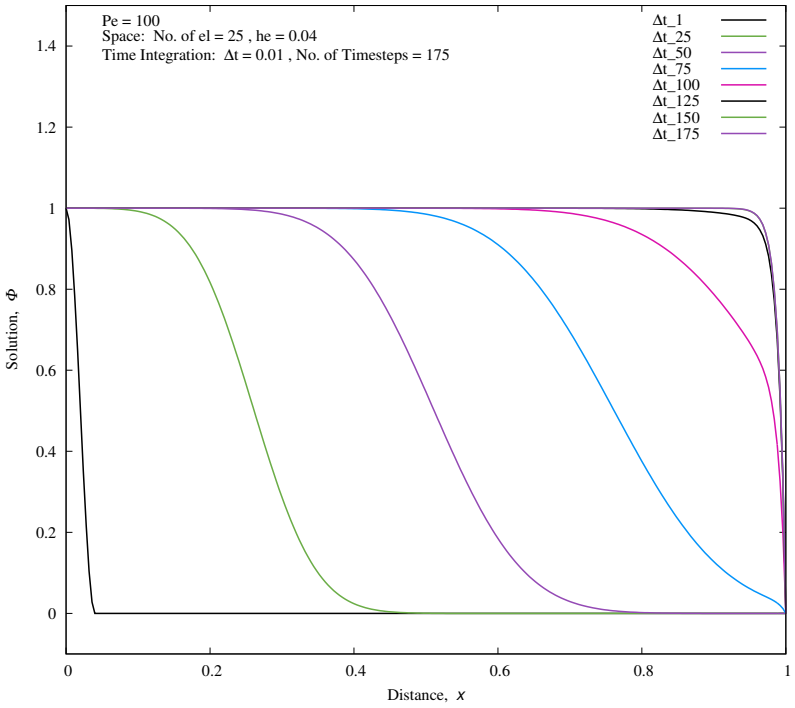
using (3.5) in (3.3) we obtain,

$$[C]\{\dot{\delta}(t)\} + [K]\{\delta(t)\} = \{F(t)\} + \{P(t)\} \tag{3.10}$$

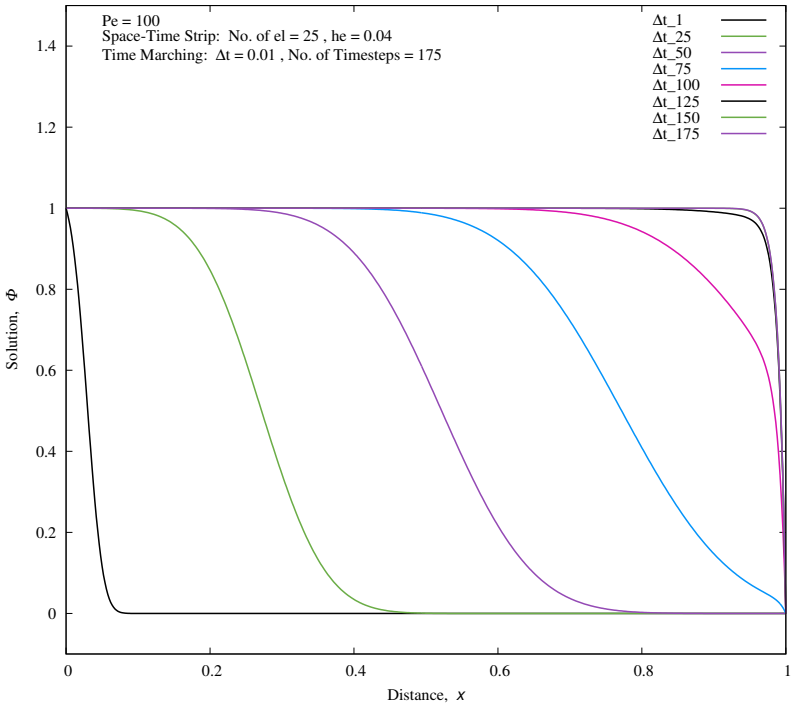
in which,

$$\begin{aligned} [C] &= \sum_e [C^e] \\ [K] &= \sum_e [K^e] \\ \{F\} &= \sum_e \{F^e\} \\ \{P\} &= \sum_e \{P^e\} \end{aligned} \tag{3.11}$$

Equation (3.10) with BCs and ICs (3.2) are integrated using Newmark's linear method using a p-level of 15 in space and integration time step Δt = 0.01, 0.005, and 0.001 for Pe = 100, 1000, and 10000. Figures 3.1-3.3 show the evolution of ϕ versus x for various values of time t. As Pe is increased steepened fronts of ϕ are accurately simulated. Solutions compared from the space-time coupled finite element method based on a space-time strip with a 25 element, 9 node uniform discretization with $p_\xi = p_\eta = 9$ and a time marching step of Δt = 0.01, 0.005, and 0.001 for Pe = 100, 1000, and 10000 are in perfect agreement with the evolutions reported in figures 3.1-3.3.

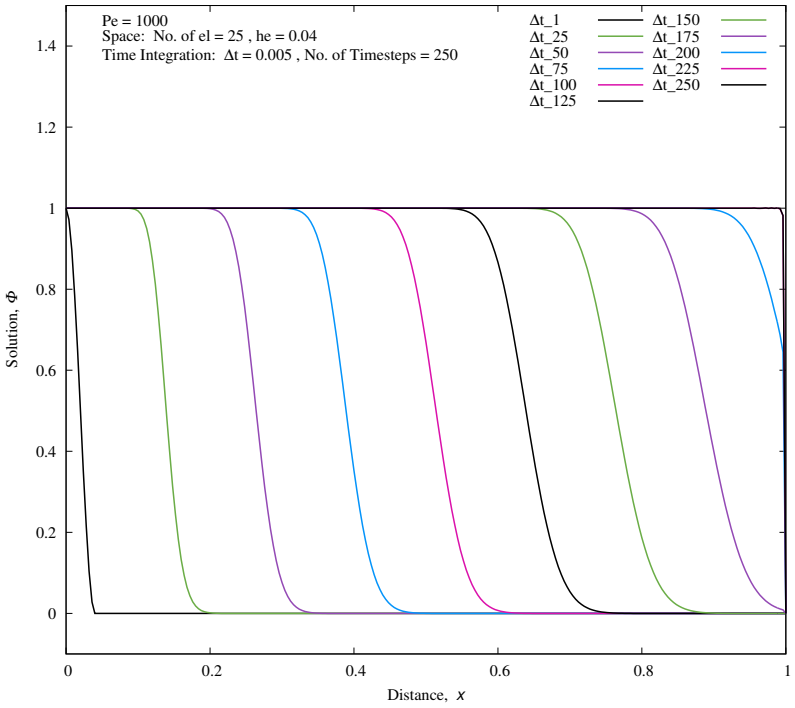


(a) Convection diffusion equation (space-time decoupled)

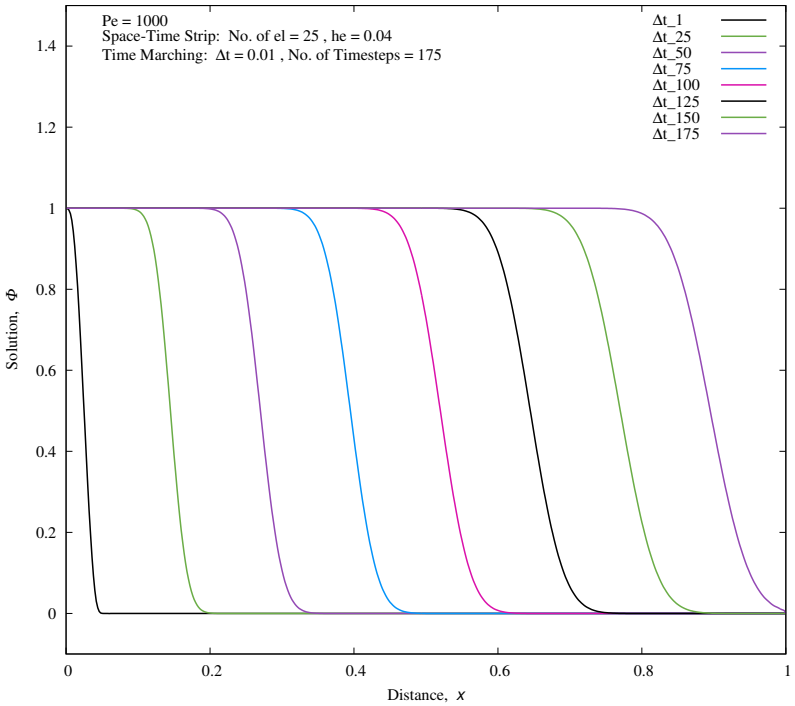


(b) Convection diffusion equation (space-time coupled)

Figure 3.1: Convection diffusion equation: Pe = 100 (STDC vs. STC)

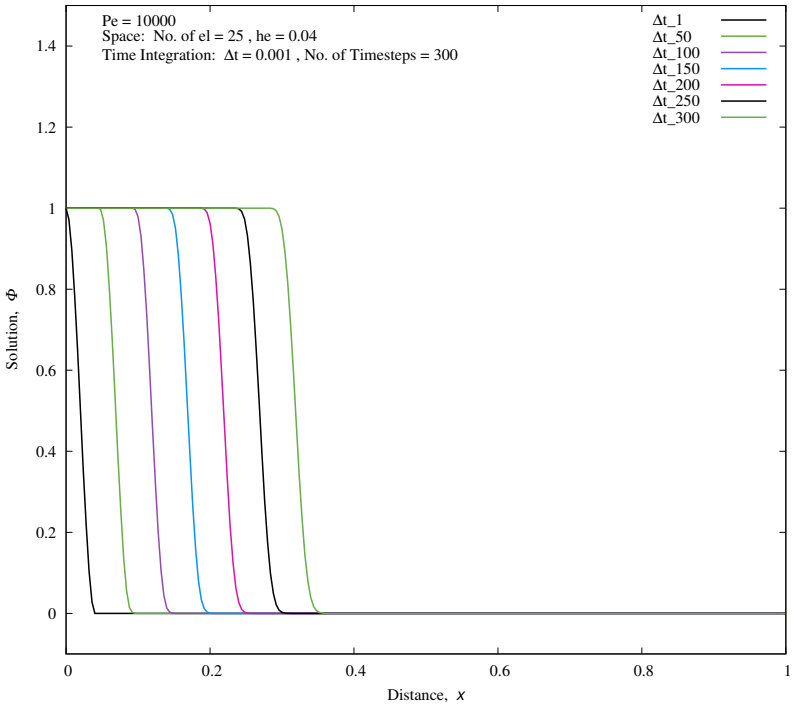


(a) Convection diffusion equation (space-time decoupled)

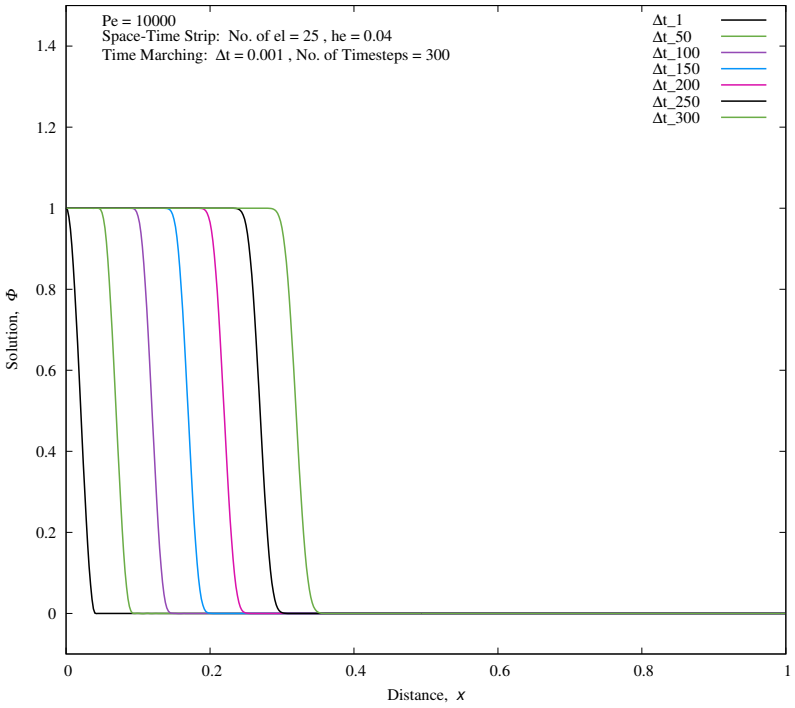


(b) Convection diffusion equation (space-time coupled)

Figure 3.2: Convection diffusion equation: Pe = 1000 (space-time decoupled)



(a) Convection diffusion equation (space-time decoupled)



(b) Convection diffusion equation (space-time coupled)

Figure 3.3: Convection diffusion equation: Pe = 10000 (space-time decoupled)

3.2.2 Pure advection

Consider the following initial value problem, referred to as pure advection, due to absence of diffusion. Initial conditions propagate spatially without any change. This model problem is a good test of the presence of numerical dispersion in the computational process.

$$\frac{\partial \phi}{\partial t} + \frac{\partial \phi}{\partial x} = f(x,t) \quad \forall x,t \in \Omega_{xt} = \Omega_x \times \Omega_t = (0,1) \times (0,\tau) \tag{3.12}$$

$$\text{BC: } \phi(0) = 0 \tag{3.13}$$

Initial conditions consist of a Gaussian distribution for $\phi(x,0)$ given by

$$\begin{aligned} \phi(x,0) = \exp(\frac{-(x-x_0)^2}{2\sigma_0^2}) \quad \forall x \in [0,1] \\ x_0 = 0.2; \quad \sigma_0 = 0.03 \end{aligned} \tag{3.14}$$

We note that ICs (3.14) does yield BC $\phi(0) = 0$ at $x = 0$. We consider a 20 element uniform discretization $\bar{\Omega}_x^T = \bigcup_e \bar{\Omega}_x^e$ of spatial domain $\bar{\Omega}_x = [0,1]$ using three node p-version hierarchical finite elements with nodes located at 1, 2, and 3. Based on fundamental lemma, we can write the following using (3.12) and approximation ϕ_h of ϕ over $\bar{\Omega}_x^T$ such that $\phi_h(x,t) = \bigcup_e \phi_h^e(x,t)$.

$$(A\phi_h - f, v)_{\bar{\Omega}_x^T} = \sum_e (A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = 0 \tag{3.15}$$

Let

$$\phi_h^e(x,t) = \sum_{i=1}^{n} N_i(x)\delta_i^e(t) = [N(x)]\{\delta^e(t)\} \tag{3.16}$$

using (3.12) in (3.13) and GM/WF over $\bar{\Omega}_x^e$ we can obtain,

$$(A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = [C^e]\{\dot{\delta}^e(t)\} + [K^e]\{\delta^e(t)\} - \{f^e(t)\} \tag{3.17}$$

in which

$$C_{ij}^e = \int_{\bar{\Omega}_x^e} N_i N_j dx \tag{3.18}$$

$$K_{ij}^e = \int_{\bar{\Omega}_x^e} (N_i \frac{\partial N_i}{dx}) dx \tag{3.19}$$

$$f_i^e = \int_{\bar{\Omega}_x^e} f N_i dx \tag{3.20}$$

Using (3.17) in (3.15) we can obtain the following assembled equations for $\bar{\Omega}_x^T$.

$$[C]\{\dot{\delta}(t)\} + [K]\{\delta(t)\} = \{F\} \tag{3.21}$$

in which

$$\begin{aligned} [C] &= \sum_e [C^e] \\ [K] &= \sum_e [K^e] \\ \{F\} &= \sum_e \{f^e\} \\ \{\delta\} &= \bigcup_e \{\delta^e\} \end{aligned} \tag{3.22}$$

Equations (3.21) with BCs (3.13) and ICs (3.14) are integrated using Newmark's linear method using a p-level of 15 in space and Δt= 0.001. The solution is calculated for 300 time steps. Figure 3.4 shows the evolution of ϕ, i.e ϕ versus x, for various values of time. We clearly observe there is virtually no amplitude reduction and base elongation of the applied Gaussian distribution at $t = 0$, confirming the absence of numerical dispersion. Solutions are also computed using space-time coupled finite element formulation based on the residual functional using a space-time strip with uniform discretization containing 20 space-time p-version finite elements and time marching. The two solutions show excellent agreement.

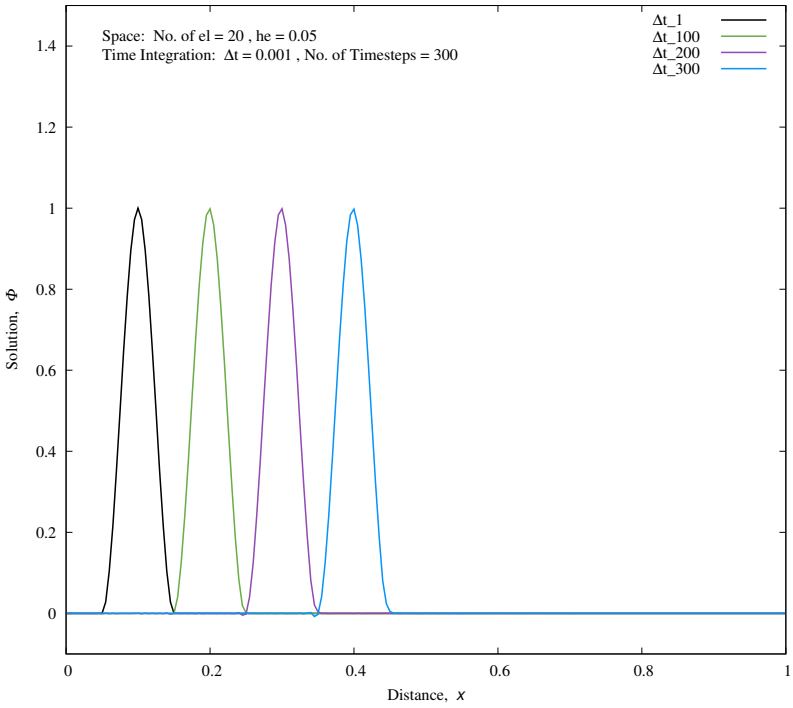


Figure 3.4: Pure advection: Gaussian Distribution (space-time decoupled)

3.2.3 Transient heat conduction in Eulerian description

In this model problem we consider the simplified form of the energy equation (in the absence dissipation, sources, and sinks).

$$\frac{\partial \phi}{\partial t} + v(x)\frac{\partial \phi}{\partial x} - \frac{k}{RePr}\frac{\partial^2 \phi}{\partial x^2} = f(x,t) \quad \forall (x,t) \in \Omega_{xt} = \Omega_x \times \Omega_t = (0,1) \times (0,\tau) \tag{3.23}$$

$$\begin{aligned} &\text{BCs: } \phi(0,t) = 1, \phi(1,t) = 0 \quad \forall t \in (0,\tau) \\ &\text{ICs: } \phi(x,0) = 0 \quad \forall x \in (0,1) \end{aligned} \tag{3.24}$$

In which ϕ is dimensionless temperature, $v(x)$ is a known velocity field, k is thermal conductivity, Pe is Peclet number, and Pr is Prandtl number. We consider a 25 element uniform discretization $\bar{\Omega}_x^T = \bigcup_e \bar{\Omega}_x^e$ of $\bar{\Omega}_x$ using three node hierarchical elements. Let ϕ_h be approximation of ϕ over $\bar{\Omega}_x^T$ and ϕ_h^e be local approximation over an element $\bar{\Omega}_x^e$. Then based on the fundamental lemma [1] we

can write,

$$(A\phi_h - f, v)_{\bar{\Omega}_x^T} = \sum_e (A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = 0 \tag{3.25}$$

$$\text{in which,} \quad \phi_h(x,t) = \bigcup_e \phi_h^e(x,t) \tag{3.26}$$

$$\text{and} \quad \phi_h^e(x,t) = \sum_{i=1}^{n} N_i(x)\delta_i^e(t) = [N(x)]\{\delta^e(t)\} \tag{3.27}$$

Substituting (3.26) in (3.25) for an element $\bar{\Omega}_x^e$ and using GM/WF we obtain,

$$(A\phi_h^e - f, v)_{\bar{\Omega}_x^e} = [C^e]\{\dot{\delta}^e(t)\} + [K^e]\{\delta^e(t)\} - \{f^e(t)\} \tag{3.28}$$

In (3.28), we have performed integration by parts once in the term with a second derivative of ϕ with respect to x. In (3.28), the coefficient matrix and vectors are given by,

$$C_{ij}^e = \int_{\bar{\Omega}_x^e} N_i N_j dx \tag{3.29}$$

$$K_{ij}^e = \int_{\bar{\Omega}_x^e} (v(x) N_i \frac{\partial N_j}{dx}) dx + \frac{k}{PePr} \int_{\bar{\Omega}_x^e} \frac{\partial N_i}{dx} \frac{\partial N_j}{dx} dx \tag{3.30}$$

$$f_i^e = \int_{\bar{\Omega}_x^e} f N_i dx \tag{3.31}$$

$$\{P^e\} = \begin{Bmatrix} P_1^e \\ \vdots \\ P_n^e \end{Bmatrix} \tag{3.32}$$

Substituting (3.28) in (3.25) we obtain,

$$[C]\{\dot{\delta}(t)\} + [K]\{\delta(t)\} = \{F(t)\} + \{P(t)\} \tag{3.33}$$

Matrix $[K]$ contains known velocity field $v(x)$. We choose the following for $v(x)$ (figure 3.5).

$$v(x) = \frac{(v_1 - v_2)}{0.25}(x - 0.5)^2 + v_2 \quad \forall x \in [0, 1]$$
$$\text{in which,} \quad v_1 = v|_{x=0} = v|_{x=1} \tag{3.34}$$
$$v_2 = v|_{x=0.5}$$

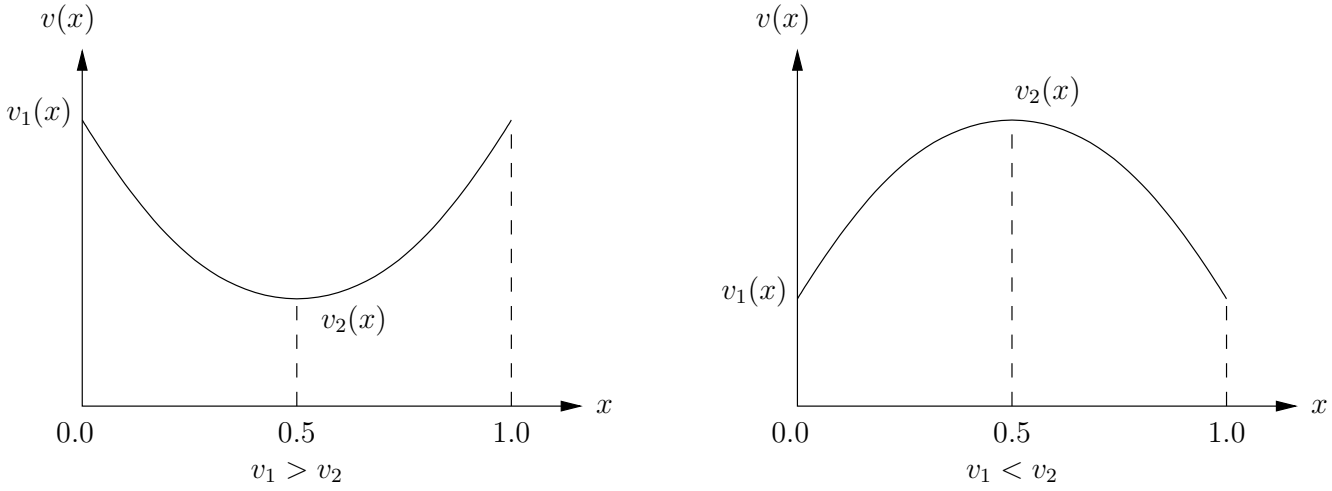


Figure 3.5: Plots of $v(x)$ versus x

Evolution is completed using (3.33) and (3.24) using Newmark's linear method with time step Δt = 0.01 in all computations. We present the following numerical studies in which we have used k = 1, Pr = 1, but vary Re.

Case (a): In this study we choose Re = 100 and

1. $v_1 = 0.25, v_2 = 1.00 \quad (v_1 < v_2)$
2. $v_1 = 1.00, v_2 = 0.25 \quad (v_1 > v_2)$

Case (b): In this study we choose Re = 1000 and

1. $v_1 = 0.25, v_2 = 1.00 \quad (v_1 < v_2)$
2. $v_1 = 1.00, v_2 = 0.25 \quad (v_1 > v_2)$

Case (c): In this study we choose Re = 1000 and

1. $v_1 = v_2 = 0.25$
2. $v_1 = v_2 = 0.50$
3. $v_1 = v_2 = 1.00$

Calculated solutions are presented and discussed in the following.

Case (a): Figures 3.6 and 3.7 show plots of ϕ versus x for various values of time for $v_1 = 0.25, v_2 = 1.00$ and $v_1 = 1.00, v_2 = 0.25$ respectively. Influence of the velocity field is clearly observed on the evolution of ϕ.

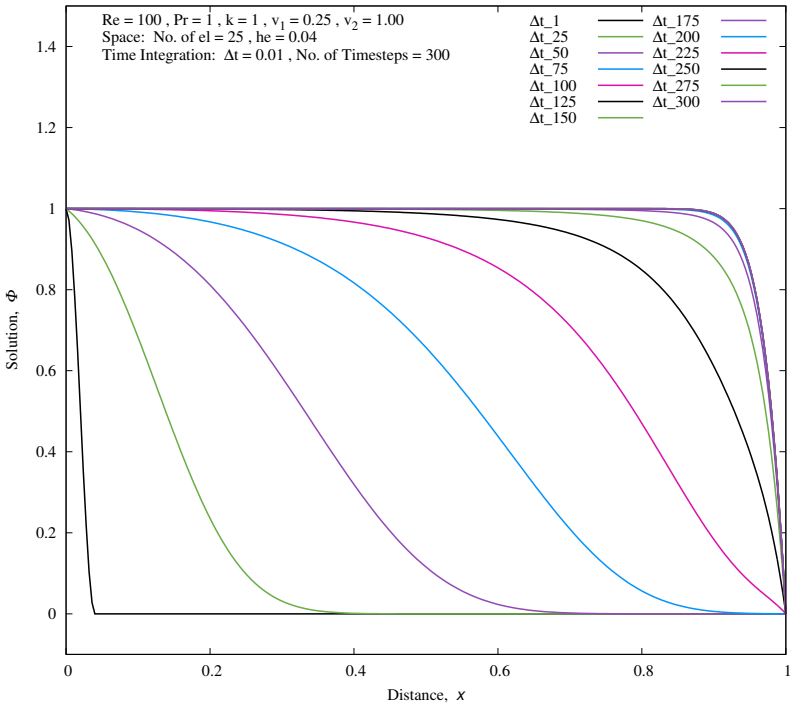


Figure 3.6: Energy equation Eulerian description Re = 100, $v_1 = 0.25$, $v_2 = 1.00$

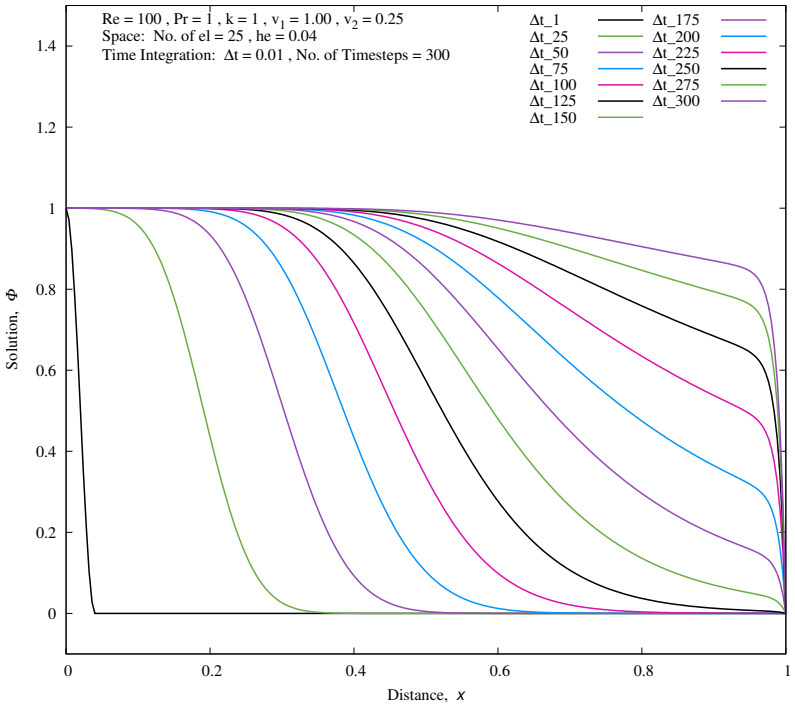


Figure 3.7: Energy equation Eulerian description Re = 100, $v_1 = 1.00$, $v_2 = 0.25$

Case (b): In this case the studies presented in Case (a) are repeated for Re = 1000. Figures 3.8 and 3.9 show the evolution of ϕ for $v_1 = 0.25, v_2 = 1.00$ and $v_1 = 1.00, v_2 = 0.25$ respectively. We note steepening of the evolution compared to Case (a) due to a higher Reynolds number. The influence of the velocity field is clearly seen in figures (3.8) and (3.9).

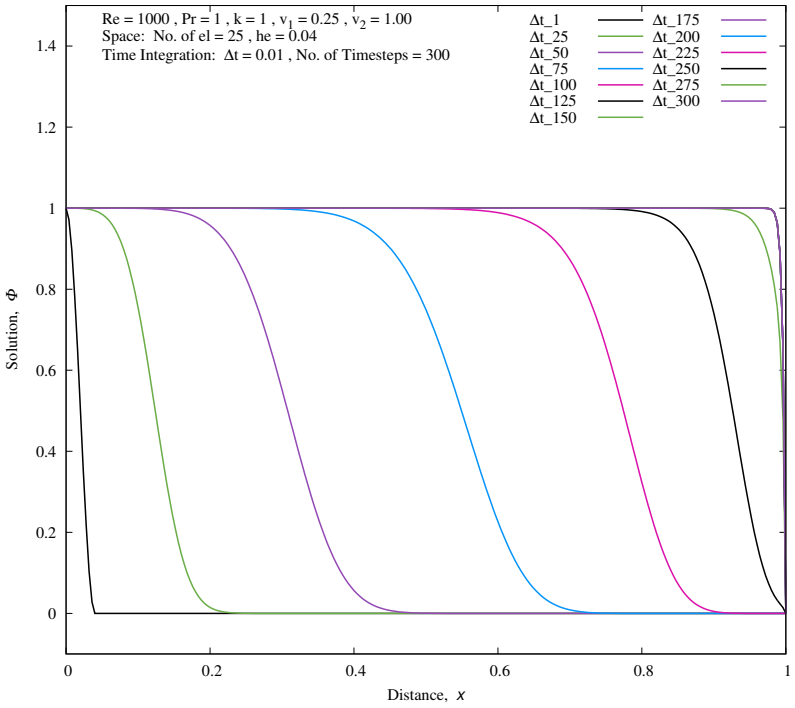


Figure 3.8: Energy equation Eulerian description Re = 1000, $v_1 = 0.25$, $v_2 = 1.00$

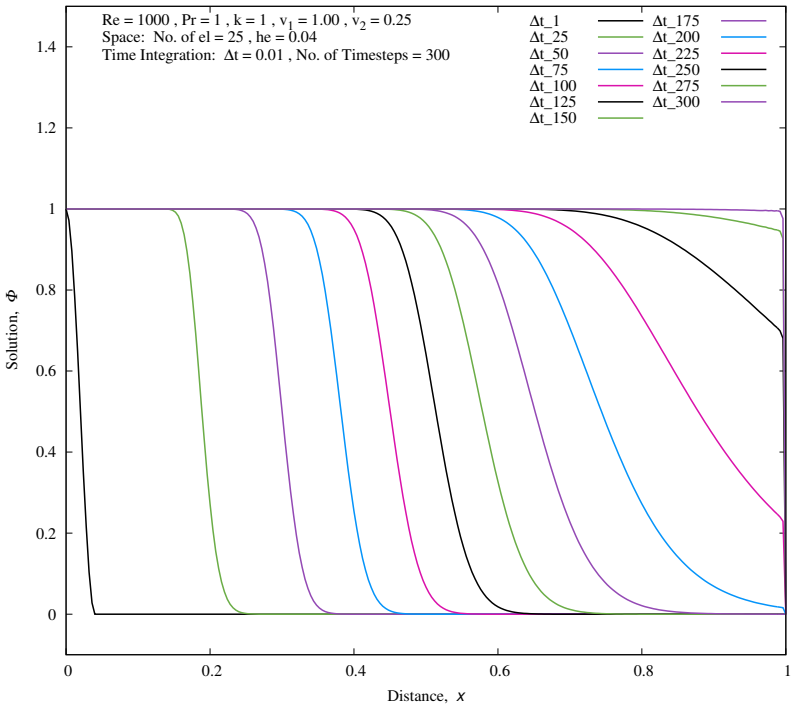


Figure 3.9: Energy equation Eulerian description Re = 1000, $v_1 = 1.00$, $v_2 = 0.25$

Case (c): In these studies Re = 1000 is kept fixed and the influence of constant (independent of x) but progressively increasing velcity field is studied. Figures 3.10-3.12 show evolutions of ϕ for $v_1 = v_2$ =0.25, 0.50, and 1.00 respectively. We observe steepening of the temperature front as well as faster propagation of the fronts with progressively increasing velocity field.

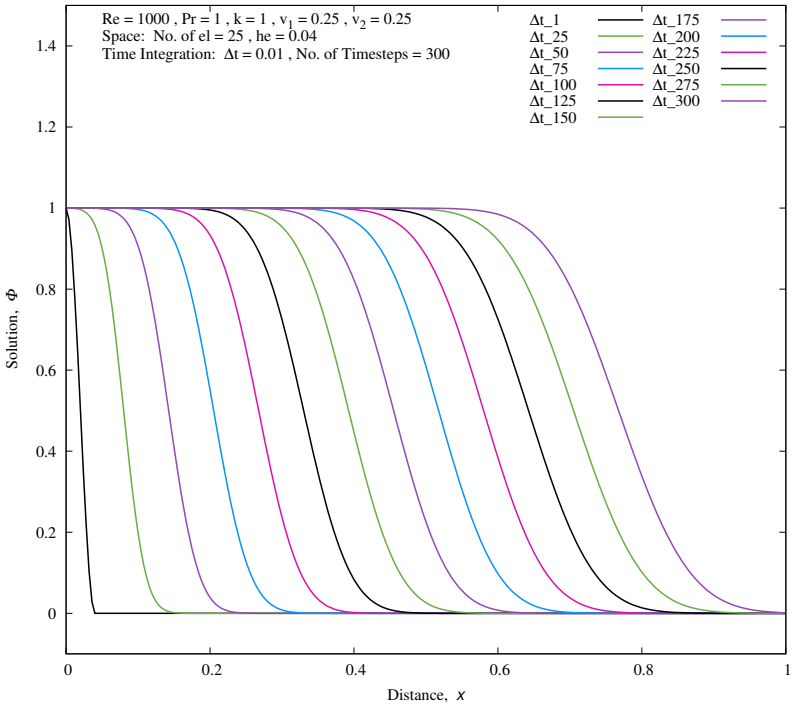


Figure 3.10: Energy equation Eulerian description Re = 1000, $v_1 = v_2 = 0.25$

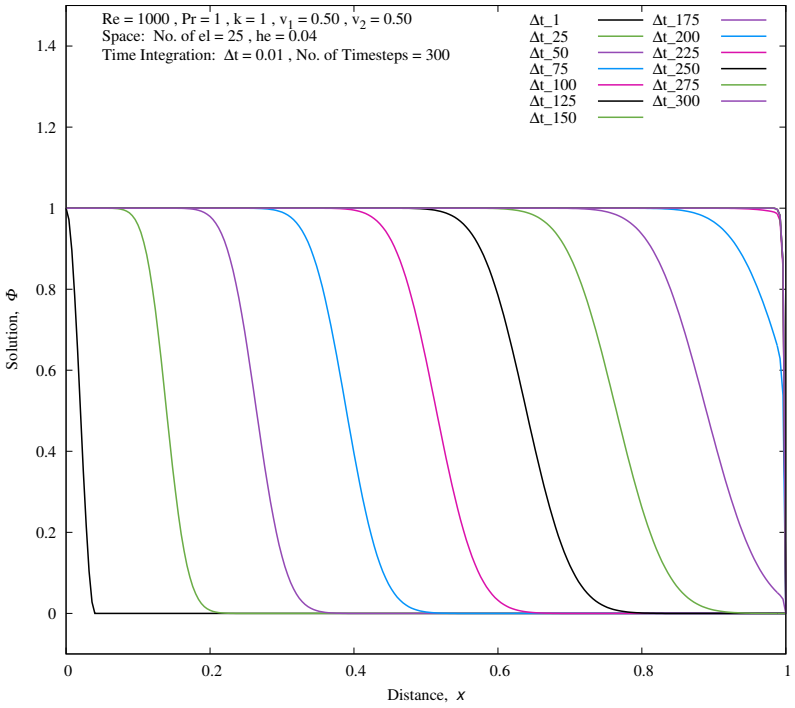


Figure 3.11: Energy equation Eulerian description Re = 1000, $v_1 = v_2 = 0.50$

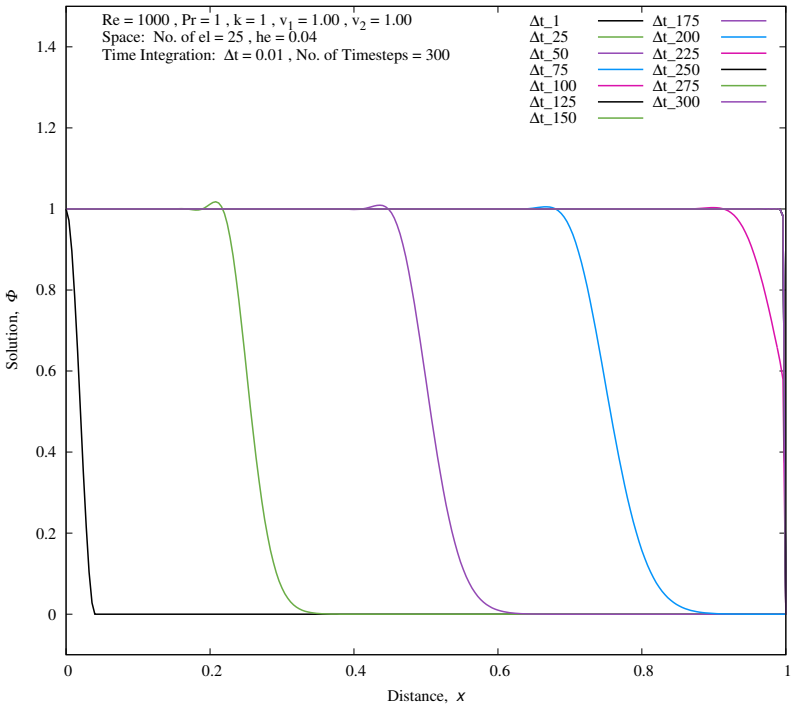


Figure 3.12: Energy equation Eulerian description Re = 1000, $v_1 = v_2 = 1.00$

Computations remain stable in all cases presented here. Evolutions are small and oscillation free.

3.2.4 First order nonlinear ODE in time

In this study we consider a single first order nonlinear ODE giaven in the following.

$$c_1\frac{\partial\phi}{\partial t} + (c_2 + c_3 q(\phi))\phi = f(t) \quad \forall t \in \Omega_t \in (0,\tau) \tag{3.35}$$

$$\begin{aligned} \text{IC:} \quad & \phi(0) = 1.0 \\ \text{and} \quad & q(\phi) = 1, \phi, \phi^2, \phi^3 \end{aligned} \tag{3.36}$$

This model problem is considered to provide proof of concept for time integrating nonlinear ODEs in time using Newmark's linear method in conjunction with Newton's linear method. If we choose $c_1 = c$ and $c_2 + c_3 q(\phi) = k$, then (3.35) reduces to,

$$c\frac{\partial\phi}{\partial t} + k(\phi)\phi = f(t) \tag{3.37}$$

(3.37) is exactly the same as (2.25), except that (3.37) is a single ODE, thus the derivations presented in 2.4 are applicable here. Based on section 2.4, we need $\delta(k(\phi_{t+\Delta t})\phi_{t+\Delta t})$, which is given by

$$\delta(k(\phi_{t+\Delta t})\phi_{t+\Delta t}) = (\delta k(\phi_{t+\Delta t}))\phi_{t+\Delta t} + k(\phi_{t+\Delta t}) \tag{3.38}$$

Since $k = c_2 + c_3 q(\phi)$,

$$\begin{aligned} \delta k &= c_3 \delta q(\phi) \\ \delta q(\phi) &= 0, 1, 2\phi, 3\phi^2 \end{aligned} \tag{3.39}$$

We compute evolution described by (3.35) using Newmark's linear method with Newton's linear method (derived in section 2.4).

Case (a): $c_1 = 1.0, c_2 = 0.1, c_3 = 0.1$

and $q(\phi) = 1, \phi, \phi^2, \phi^3$

Case (b): $c_1 = 1.0, c_2 = 0.5, c_3 = 0.5$

and $q(\phi) = 1, \phi, \phi^2, \phi^3$

Figures 3.13 and 3.14 show plots of ϕ versus t for different choices of $q(\phi)$ for Case (a) and Case (b). We observe steepening of ϕ versus t for increasing values of c_2 and c_3 for all choices of $q(\phi)$. Influence of the choice of $q(\phi)$ is clearly observed also. Dependence of $q(\phi)$ on progressively increasing degree of ϕ results in progressively higher values of ϕ. However, the difference diminishes with increasing power of ϕ in $q(\phi)$. Newton's linear method converges between 3-5 iterations for each time step. Evolutions are oscillation free and the computation remain stable for all choices of parameters used.

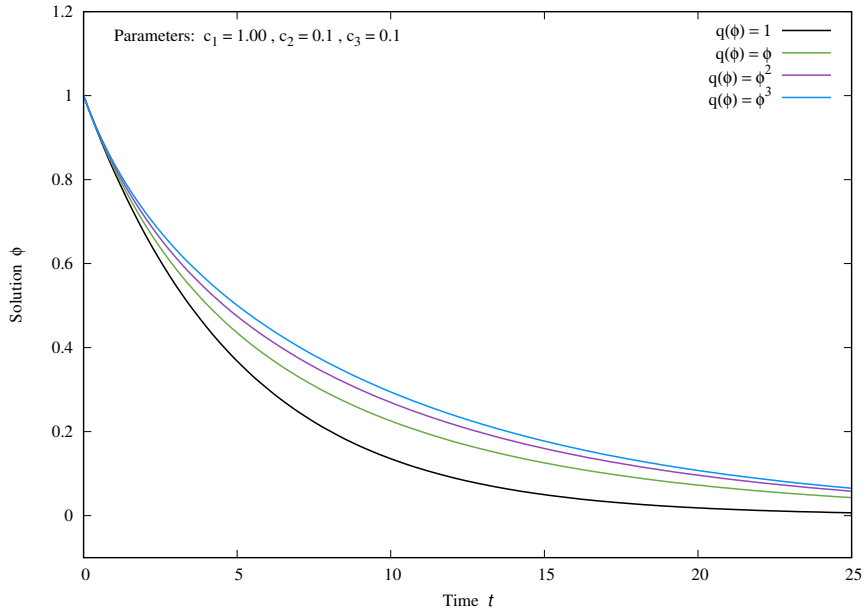


Figure 3.13: First order nonlinear ODE: $c_1 = 1.0, c_2 = 0.1, c_3 = 0.1$

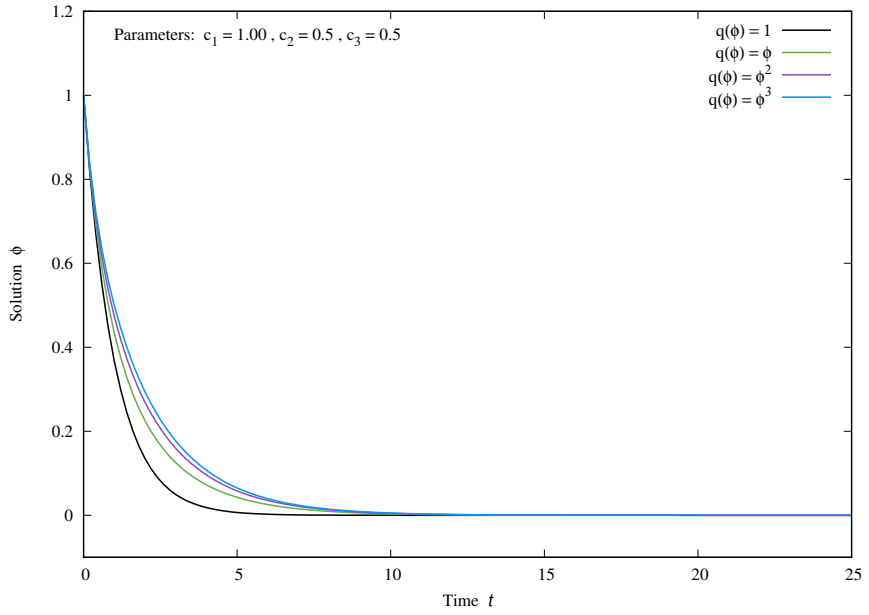


Figure 3.14: First order nonlinear ODE: $c_1 = 1.0$, $c_2 = 0.5$, $c_3 = 0.5$

3.2.5 Second order linear and nonlinear ODE in time

Mathematical descriptions of deforming solids in Lagrangian description for isothermal physics, small deformation, and small strain leads to BLM in displacements that are a system of second order linear PDEs in space and time. Use of GM/WF in space for a spatial discretization $\bar{\Omega}_x^T = \bigcup_e \bar{\Omega}_x^e$ yields a system of linear second order ODEs in time. When the deformation and strain are finite, BLM yields second order nonlinear PDEs in space but linear in time. Use of GM/WF in space to decouple space and time yields a system of second order nonlinear ODEs in time. Newmark's linear acceleration method for these two systems of ODEs in time have been presented in Chapter 2 (Sections 2.5, 2.6).

In the studies presented here, we consider only one second order ODE in time, linear as well as nonlinear, to demonstrate proof of concept of Newmark's linear method with Newton's linear method. We consider the constitutive theory for deviatoric stress tensor in terms of strain as well as strain rate, thus permitting a dissipation mechanism.

In the case of finite deformation, finite strain both damping as well as stiffness matrices are

nonlinear functions of displacements, hence after decoupling space and time using GM/WF in space, the damping and stiffness matrices are matrices up to quadratic functions of the degrees of freedom $\{\delta\}$.

Consider the following second order nonlinear ODE in time,

$$m\frac{\partial^2 u}{\partial t^2} + cp(u)\frac{\partial u}{\partial t} + kq(u)u = f(t) \quad \forall t \in (0, \tau) \tag{3.40}$$

in which,

$$\begin{aligned} p(u) &= c_1 + c_2 u + c_3 u^2 \\ q(u) &= d_1 + d_2 u + d_3 u^2 \end{aligned} \tag{3.41}$$

$$\begin{aligned} \text{ICs:} \quad & u(0,t) = 1.0 \\ & \frac{du(0,t)}{dt} = 0.0 \end{aligned} \tag{3.42}$$

We note that when $c_2 = c_3 = 0$ and $d_2 = d_3 = 0$, (3.40) is a linear second order ODE in time. Numerical solutions for ϕ are obtained using Newmark's linear method for the linear case and Newmark's linear method with Newton's linear method for the nonlinear case. We consider the following studies. In all studies we consider $m = 1$, $c = 1$, $k = 1$.

Case (a): $c_1 = 0.01, 0.10, 0.50$ and 1.00

$c_2 = c_3 = 0$

$d_1 = 1, d_2 = d_3 = 0$

This is a linear case in which the damping coefficient is varied from 0.01 to 1.00

Case (b): $c_1 = 0.50$ and 1.00

$c_2 = c_3 = 0.10$

$d_1 = d_2 = d_3 = 1$

This is a nonlinear case in which stiffness and damping are both nonlinear. Choice of $d_1 = d_2 = d_3 = 1$ keeps nonlinearity in k to be up to quadratic in u. Fixed values of c_2 and c_3 keep nonlinearity in damping fixed as well. Variable c_1 (0.10, 0.50, 1.00) allows us to study

the influence of varying the linear part of damping.

Case (c): $c_2 = c_3 = 0.10$ and 0.50

$c_1 = 1.00$

$d_1 = d_2 = d_3 = 1$

In this case the linear part of damping is kept fixed and the coefficients for nonlinear terms are varied keeping the nonlinear stiffness terms the same in each study.

Case (d): $c_1 = c_2 = c_3 = 0.01, 0.10$, and 0.50

$d_1 = d_2 = d_3 = 1$

In this case for fixed nonlinearity in stiffness, we study the influence of nonlinear damping by choosing all damping coefficients c_1, c_2, c_3 to be the same.

We discuss the results in the following. Figures 3.15-3.18 show u versus t for $c_1 = 0.01, 0.10, 0.50$ and 1.00 respectively. In this study the stiffness is constant and dissipation is independent of u but the dissipation coefficient c_1 is increased progressively. As c_1 increases amplitude decay and base elongation is clearly observed.

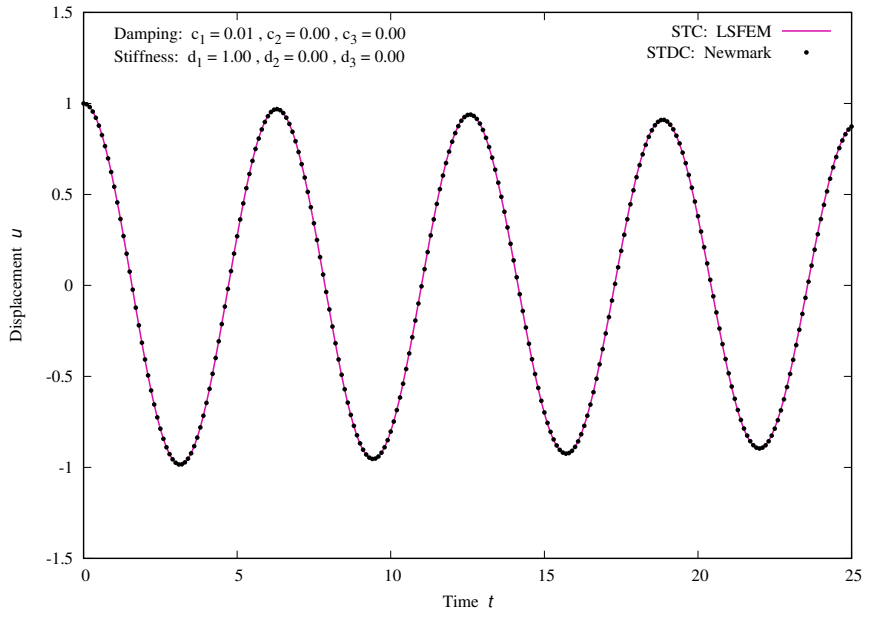


Figure 3.15: u versus t: Second order linear ODE ($c_1 = 0.01$)

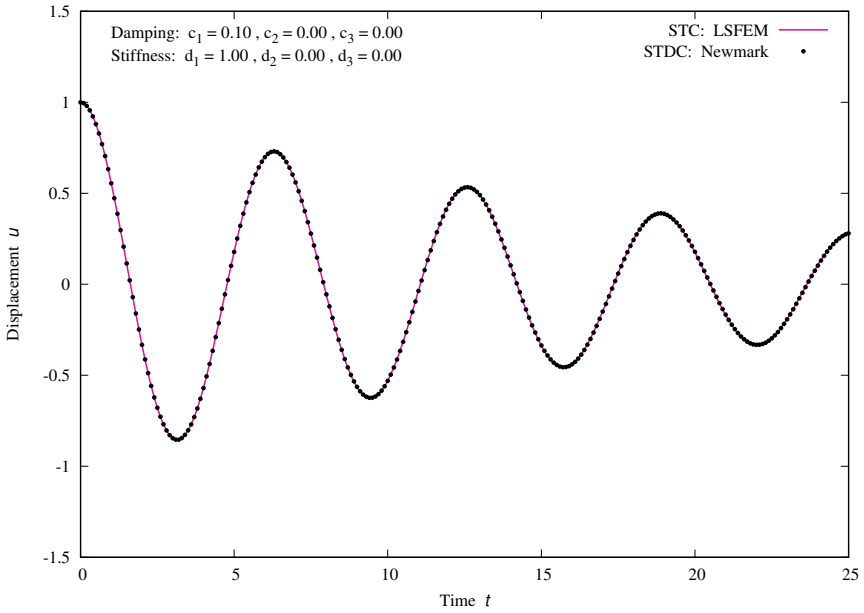


Figure 3.16: u versus t: Second order linear ODE ($c_1 = 0.10$)

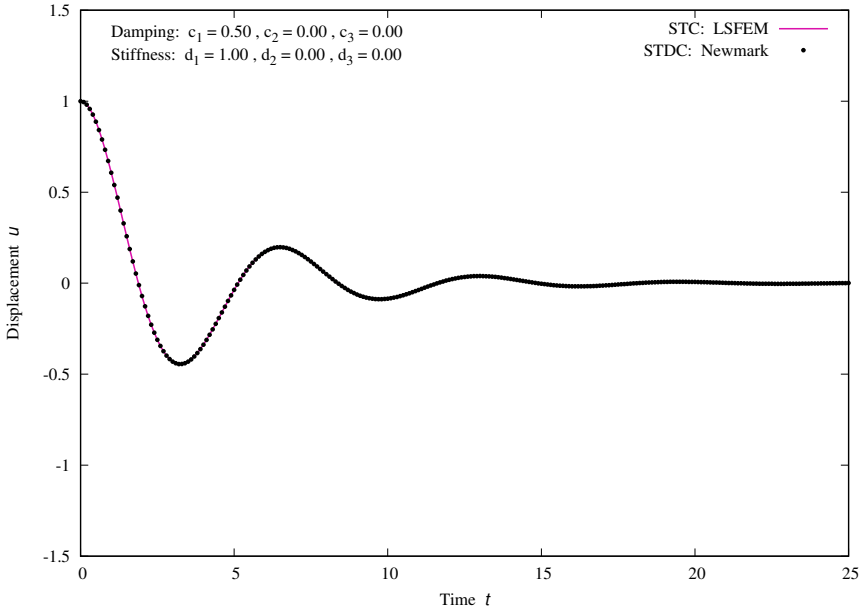


Figure 3.17: u versus t: Second order linear ODE ($c_1 = 0.50$)

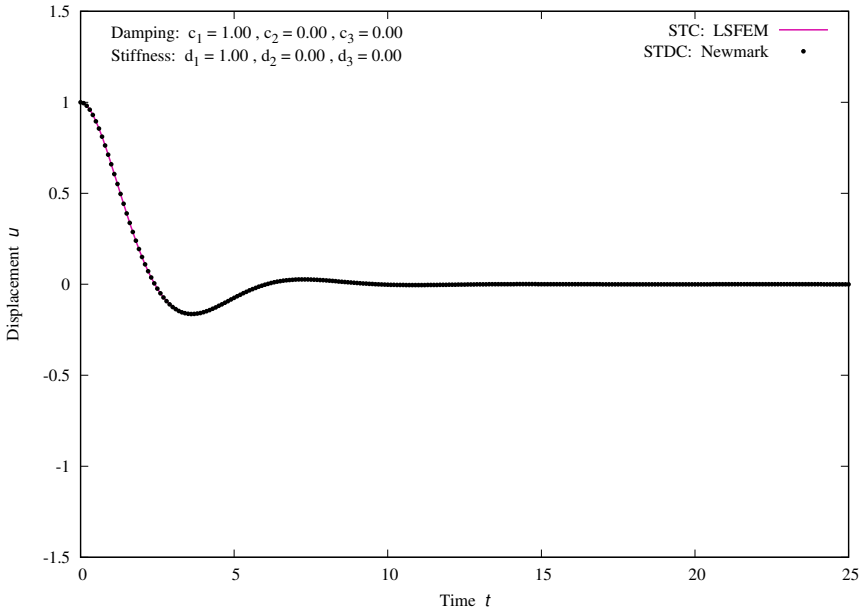


Figure 3.18: u versus t: Second order linear ODE ($c_1 = 1.00$)

Figures 3.19 and 3.20 show u versus t plot for Case (b). For fixed nonlinearity in k and c and increasing the coefficient c_1 shows the usual affect of progressively more amplitude decay and base elongation with increasing c_1.

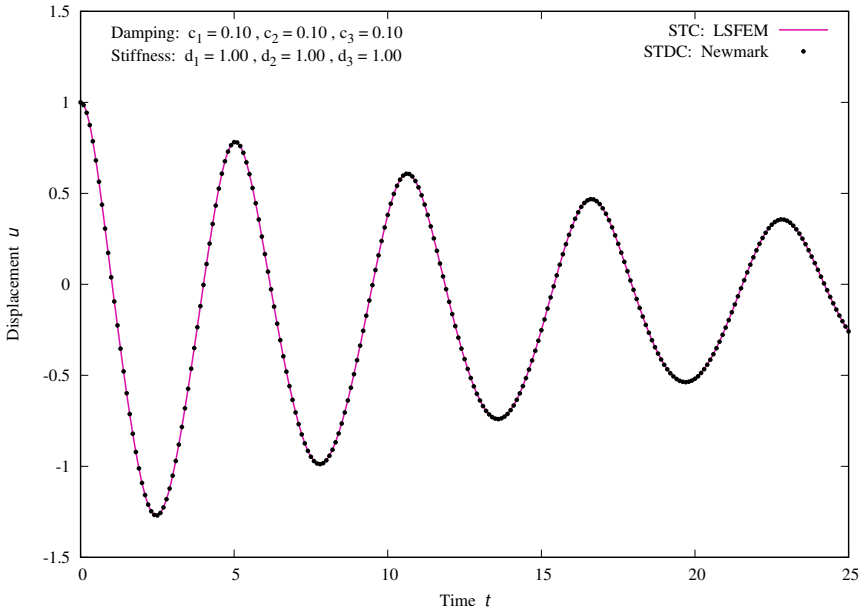


Figure 3.19: u versus t: Second order nonlinear ODE ($c_1 = c_2 = c_3 = 0.10$)

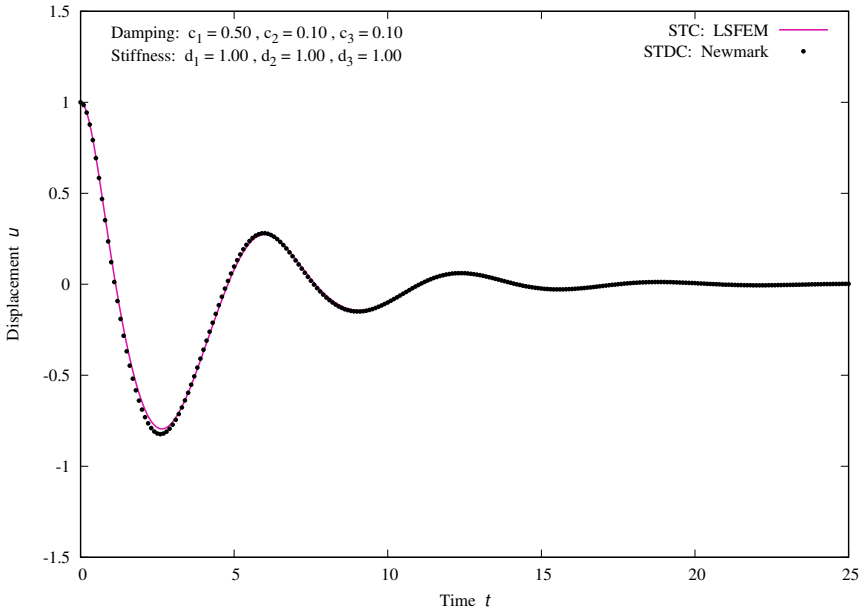


Figure 3.20: u versus t: Second order nonlinear ODE ($c_1 = 0.50, c_2 = c_3 = 0.10$)

In Case (c), with fixed linear damping (relatively high, $c_1 = 1.00$), the influence of nonlinear damping terms is not very significant. In this study k is nonlinear but the coefficients d_1, d_2, d_3 are kept fixed.

In the last study, Case (d), $c_1 = c_2 = c_3 = 0.01, 0.10,$ and 0.50 are used. As shown in Case (c), since c_1 dominates the response, the contribution of c_2 and c_3 is not expected to be significant. This can be confirmed by comparing results in figure (3.23) and figure (3.17).

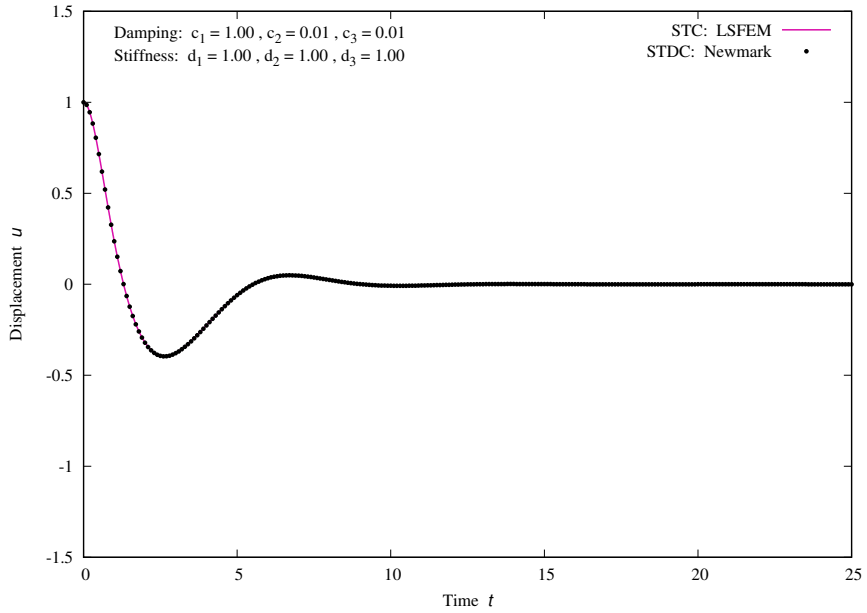


Figure 3.21: u versus t: Second order nonlinear ODE ($c_1 = 1.00, c_2 = c_3 = 0.01$)

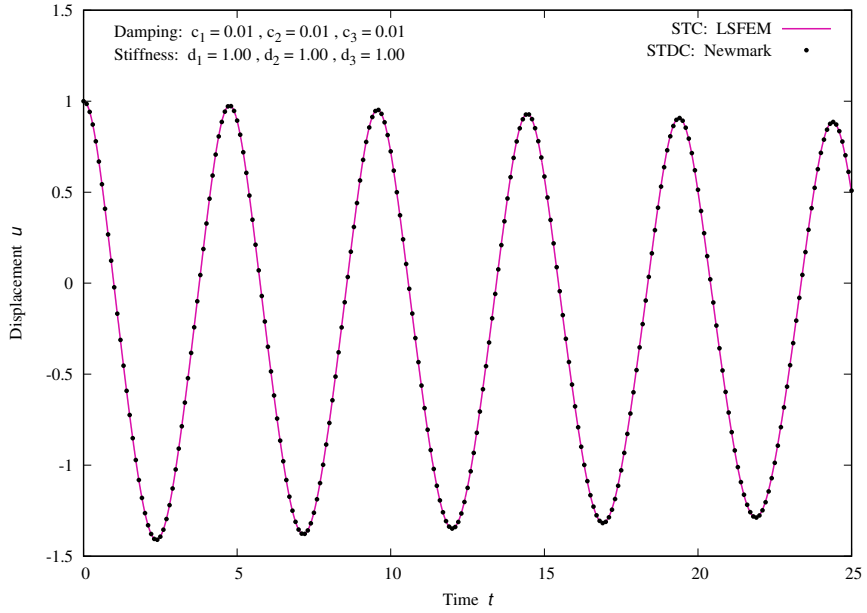


Figure 3.22: u versus t: Second order nonlinear ODE ($c_1 = c_2 = c_3 = 0.01$)

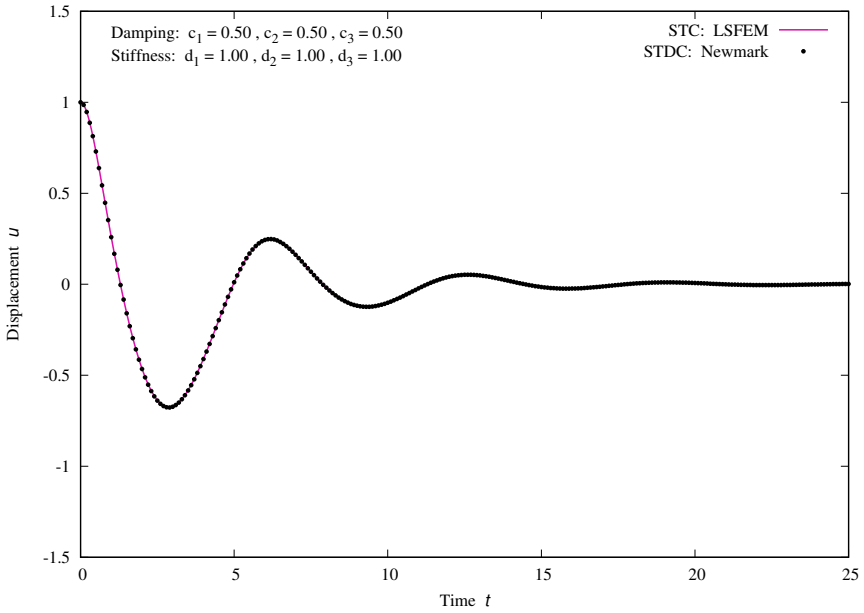


Figure 3.23: u versus t: Second order nonlinear ODE ($c_1 = c_2 = c_3 = 0.50$)

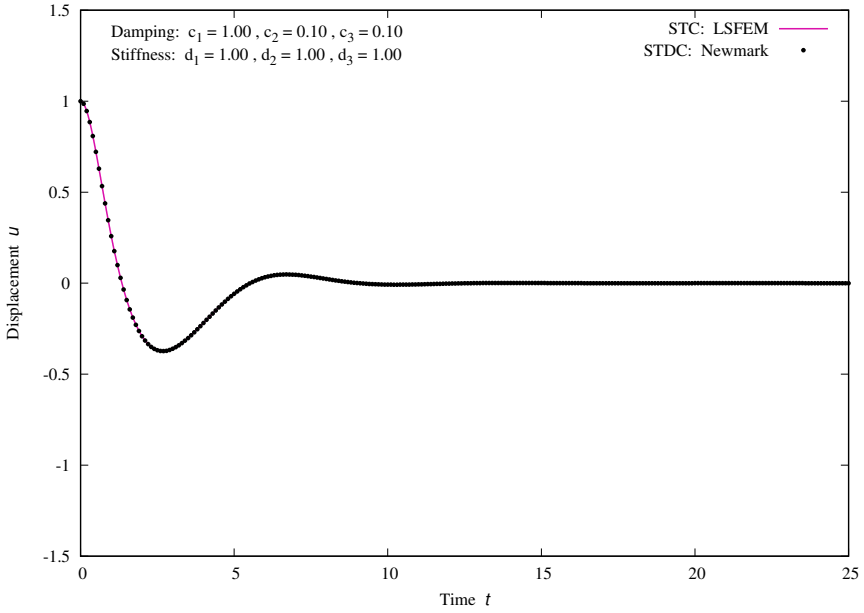


Figure 3.24: u versus t: Second order nonlinear ODE ($c_1 = 1.00, c_2 = c_3 = 0.10$)

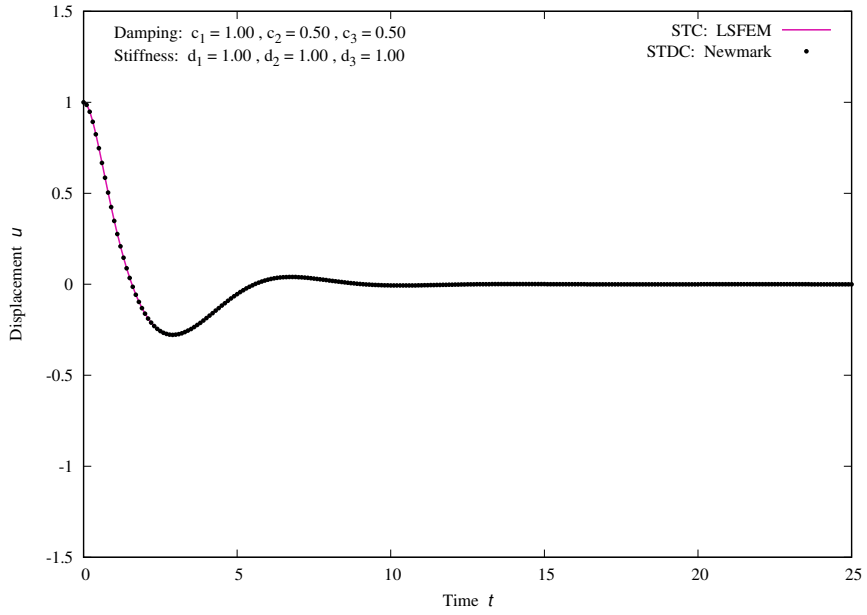


Figure 3.25: u versus t: Second order nonlinear ODE ($c_1 = 1.00, c_2 = c_3 = 0.50$)

Remarks

1. A number of linear and nonlinear second order ODEs are considered.

2. Newmark's linear method with Newton's linear method works well. Newton's linear method converges in 3-5 iterations for each time step.

3. Space-time coupled finite element solutions presented for selected model problems are naturally the same as those from the space-time decoupled method.

4. Extension of this work to a system of second order linear and nonlinear ODEs should present no problems.

Chapter 4

Summary and Conclusions

Rationale has been presented for choosing Newmark's linear method as a preferred time integration method for linear and nonlinear ODEs in time resulting from decoupling space and time in IVPs using GM/WF for discretization in space. Newmark's linear method has been applied for integrating linear and nonlinear first order and second order ODEs in time resulting from the decoupling of space and time in IVPs.

1. GM/WF is meritorious in space if the IVPs description contains second or higher order even derivatives of the dependent variable(s) in space. The symmetric nature of the coefficient matrices resulting from these terms after integration by parts has a stabilizing effect on the time integration schemes.

2. It has been shown that Wilson's θ method and Newmark's linear method are worthy of consideration as general time integration strategies for ODEs in time. Furthermore, Newmark's linear method is superior over Wilson's θ-method [1] in terms of spectral radius, hence in stability as well as in accuracy. This method does not require determination of a parameter like θ which can not be done without stability analysis.

3. In the case of nonlinear ODEs in time resulting from the nonlinear IVPs, Newton's linear method is utilized to obtain a converged solution for each increment of time. Newton's linear

method is highly meritorious as has quadratic convergence. Only 3-5 iterations were needed for convergence of each time step.

4. Convection diffusion, pure advection, and the energy equation in Eulerian description are first order linear systems considered as model problems to investigate Newmark's linear method for integrating the resulting ODEs after decoupling space and time using GM/WF in space.

5. The second order linear and nonlinear ODEs considered in the present work are representative of ODEs in time that result from decoupling space and time in IVPs for deforming solid continua with small deformation, small strain, and finite deformation, finite strain.

6. The solutions obtained from the space-time decoupled method presented here are also compared with space-time coupled finite element method, The agreement between the two is good.

7. Stability analysis for a single linear ODE is quite straight forward [1]. However, in the case of a system of linear ODEs or nonlinear ODEs, the stability analysis is not that straight forward. It requires determination of the spectral radius of a large matrix in the case of a linear system and in the case of a nonlinear system the determination of the spectral radius is not possible unless the matrix is linearized.

8. In all numerical studies presented in this thesis, no issues of stability are encountered when using Newmark's linear method.

9. Attempts made using Wilson's linear θ-method showed that Wilson's linear θ-method was only stable for $\theta = 1.0$. In which case Wilson's linear θ-method is the same as Newmark's linear method.

10. Comparisons of the space-time decoupled evolution with the space-time coupled finite element method evolution confirm good accuracy of the solutions presented here.

11. Computations of the space-time decoupled finite element formulations are significantly faster than the computations for space-time coupled finite element formulations.

12. For IVPs in $\mathbb{R}^3$, this approach is vastly superior in terms of practicality and usefulness. What is prohibitive for IVPs in $\mathbb{R}^3$ when using the space-time coupled finite element method becomes relatively straight forward when space and time are decoupled, preferably using GM/WF in space.

13. The full impact of this work can only be realized after the associated stability analyses are developed as these would shed light on the possible prudent choices of Δx in space an integration time step Δt.

14. In the present work, spatial discretization and p-levels are based on converged solutions of the corresponding BVPs.

15. Choice of Δt is based on obtaining smooth evolutions in which the stationary state of the evolution is same as the solution of the corresponding BVPs.

16. Thus, Δx and Δt used in the present work by no means are unique or optimal. There may be many other choices of Δx and Δt that may yield accurate evolutions. Stability analyses in conjunction with a priori error estimate and a posteriori error computation are essential to determine prudent and optimal choices of Δx and Δt for stability as well as accuracy.

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