NUMERICAL INTEGRATION OF STIFF SYSTEMS WITH ADAPTIVE STEP-SIZE CHANGE

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ABSTRACT

Many fields of application, notably nuclear, chemical engineering and control theory, yield initial value problems involving systems of ordinary differential equations with stiffness caused by eigenvalues close to the imaginary axis. The choice of a particular routine is governed by many factors. Certainly numerical integration errors due to numerical approximations and finite word length (round effects are important). Overall computing effort in terms of processor seconds, are also important, particularly in real-time analysis and large multi-run studies. Adaptive changes of integration step size h, especially for Explicit Routines, can ensure that at least local per step errors remain within specified bounds. The optimum step size is selected according to different states weighted time derivative. A lot of integration routines is used to test an approximate solution of four test Problems regarded to exact solution, and to checck the quality of adaptive step size change criterion.

INTRODUCTION

Mathematical simulation in thermo- and fluid dynamics are usually governed by system of Partial Differential Equation (PDE) in time and space. Their spatial semidiscretization generally leads to Initial Value Problem (IVP) in Ordinary Differential Equations (ODE).
An IVP

$$\frac{dY(t)}{dt} = A(Y(t)\ ,\ t)\ Y + \phi(t) \tag{1}$$

$$y(t) = \begin{bmatrix} y_1 \\ y_2 \\ y_m \end{bmatrix}, A = \begin{bmatrix} a_{11} & a_{12} & a_{1m} \\ a_{21} & \cdot\cdot & \cdot\cdot \\ a_{m1} & . a_{mm} & \end{bmatrix}, \phi(t) = \begin{bmatrix} \phi_1 \\ \Phi_1 \\ \phi_m \end{bmatrix}$$

with initial condition

$Y(0) = Y_o$; $\phi(t)$ = the source vector (2)

The system is said to be stiff if

(i) Re $\lambda < 0 i = 1,2,.., m$ (3)

(ii) Max $\lambda_i >>$ Min λ_i

where λ_i are the eigenvalues of a matrix A. The ratio is called Stiffness Ratio (SR). [1,2]

GENERAL FORM INTEGRATION FORMULAS

In the simulation of continuous-time systems, the primary numerical task is to approximate integration of a vector of a first order ODE.

$$\frac{dY}{dn} = G(Y, t)$$

We want to approximate, Y, for $t = 0, t_1, t_2, \ldots$

$$Y(t_{t+1}) = Y(t_k) + \int_{t_k}^{t_{k+1}} G(Y, t)\ .dt$$

For Multistep rules we utilize past values Y^{k-i} and G^{k-i} to approximate an updated solution Y^{k+1}

Table 1. Coefficients for Adames-Bashforth-Moulton Rules, Eq. (6).

Desionation	B_1	B_0	B_1	B_2	B_3	Common Name
P1	0	1	0	0	0	open or explicit Euler
P2	0	3/2	-1/2	0	0	open trapenzoidal
P3	0	23/12	-16/12	5/12	0	Adames 3-points predictor
P4	0	55/24	-59/24	37/24	-9/24	Adames 4-points predictor
C1	1	0	0	0	0	closed or implicit euler
C2	1/2	1/2	0	0	0	closed trapezoidal
C3	5/12	8/12	-1/12	0	0	Adames 3-points corrector
C4	9/24	19/24	-5/24	1/24	0	Adames 4-points corrector

$$Y^{k+1} = \sum_{i=0}^{P} A_i Yk-i+hY^{k-i} + h\sum_{i=-1}^{P} B_i G^{k-i} \qquad (6)$$

where $G^k = G(Y^k, k^t)$(7)

Ceofficients A_i, B_i for some Adams-Bashforth-Moulton Rules is shown in Table (1) [3]

EXPONENTIAL INTEGRATION METHOD [2]

Expanding the Eq. (4) in Taylor's series we get

$$\frac{dY}{dn} = G + (t-t_o)\times \hat{G} + F(Y-Y_o) \qquad (8)$$

where:

$\hat{G}$ is a vector has components $\partial G/\partial t$

and G is a matrix has elements $\partial G_j/\partial Y_t$

The solution of this equation with initial condition $Y(t\_o) = Y_o$ can be written in exponential difference from

$$Y_{n+1} = Y_n + hG + (e^{hF} - I - hF)(F^2 G + F^1 G) \qquad (9)$$

where I is the idensity matrix.

In this case we are faced with the problem of evaluating the exponential of the matrix F. Using the series form for exponential of the matrix we get

$$Y_{n+1} = Y_n + \sum_{k=2}^{\infty} \frac{h^k f^{k-2}}{k!} [G+FG]$$

Even if the norm of F is moderately large, in general we are going to sum 20 to 30 terms of the series in Equation (10).

MODIFIED HANSEN's Method [4]

Let we use gain Equation (4), put

$$G = L + D + U \quad (11)$$

where L,D, and U are lower, diagonl and upper Matrices. then Eq. (4) take the form

$$\frac{dY}{dt} - Dy = (L + U)Y \quad (12)$$

After some matrix Algebric operation shown in [3] we get

$$Y_{n+1}=e^{Dh}Y_n+(\omega_o I-D)^{-1}[e^{w_o hI}-e^{Dh}][L+U]Yn \quad (13)$$

where:

ω_o is the largest eigenvalue of the matrix G.

CONTROL OF ERROR AND STEP SIZE

Reliable numerical ODE-Solves performs error control which is given by:

$$\epsilon_{max} = max_i \mid (y_i - \breve{y}_i)/y_i \mid \qquad i = 1,2,...,m \quad (14)$$

where $\breve{y}_1$ is the approximate numerical solution of state i.

Chossing an appropriate value for the step length is really difficult, the step size estimate in this work is given by:

$$h = max_i\ [\ y_i/(dy_i/dt),\ h_{min}\ ] \quad (15)$$

Evaluated for different time step and $h_{min} < h < h_{max}$

APPLICATION

Four typical test problem is tested using the criterion in Eq. (15), and is also study the maximum error between the exact analytical solution and the approximate numerical one.

Time step behaviour within the solution period is also shown aiming to increase the time step to minimize the computation effort.

Application (1)
Stiff System With Uncoupled States

In this test problem, for thr A-Matrix elements a_{ij}

$$a_{ij} = 0;\ a_{ij} \qquad i = 1,2,...,m \quad j = 1,2,...,m \quad (16)$$

$$\phi(t) = [\ \lambda_i\ y_{fi},\ ...\ ]^T \quad (17)$$

with initial condition

$$Y(0) = [\ y_{ii},\ ...\ ]^T \quad (18)$$

where y_{ii}, y_{fi} are the initial and final value of the state i respectively

For this problem we check two cases:

1st one for SR = 10 the system is non-stiff

2nd one for SR = 1000 the system is highly stiff.

The exact solution for the given system in Eqations (16) and (17) with the initial condition given by Eq. (18) takes the form:

$$Y_i(t) = Y_{fi} + (Y_{ii} - Y_{fi})e^{\lambda \cdot t}1 \quad (19)$$

Typical result for these two cases using either Exponential integration method or modified Hansen's method with adaptive step size control criterion listed in equation (15); is shown in Figure (1) with time step and maximum numerical error behaviour.

Application (2)
Stiff System With Coupled States

For this case

$$A = \begin{bmatrix} -21 & 19 & -20 \\ 19 & -21 & 20 \\ 40 & -40 & -40 \end{bmatrix} \quad (20)$$

$$\text{with } \phi(t) = 0;\ Y(0) = [1,0,-1]^T \quad (21)$$

its Analtytical solution [2]

$y_1(t) = 1/2^{e-2t} + 1/2e^{-40}*(\cos 40t + \sin 40t)$

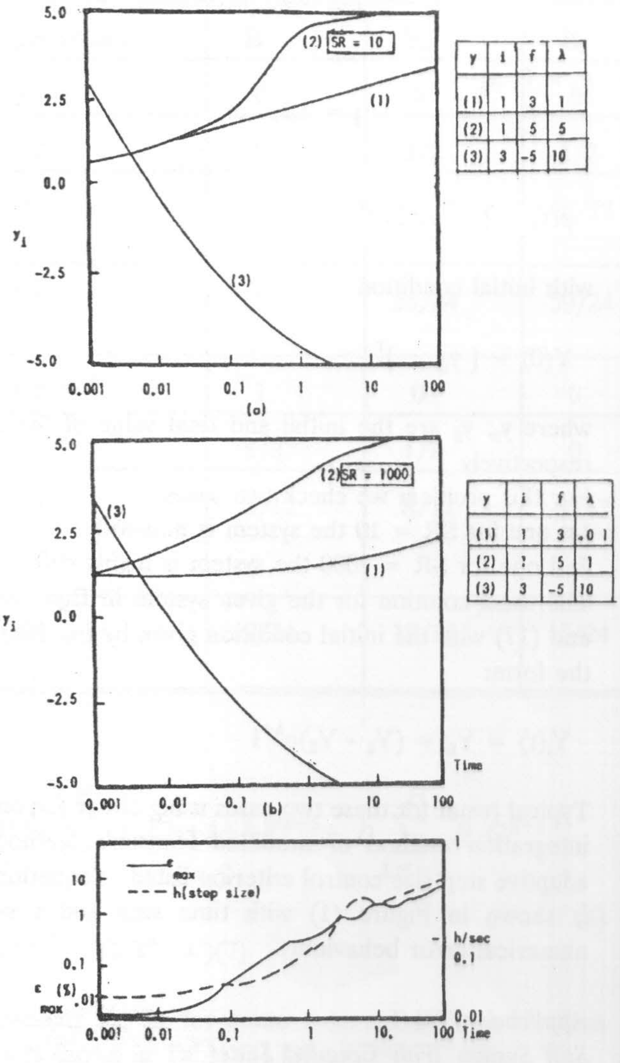

Figure 1. Time behaviour for uncoupled stiff-system.
(a) Non stiff system.
(b) Stiff system.
(c) Step error behaviour.

$$y_2(t) = 1/2^{e-2t} - 1/2e^{-40}*(\cos 40t + \sin 40t) \quad (22)$$

$$y_3(t) = -e^{-40t}(\cos 40t - \sin 40t)$$

Typical result for this case is shown in Figure (2) with time step and maximum numerical error behaviour.

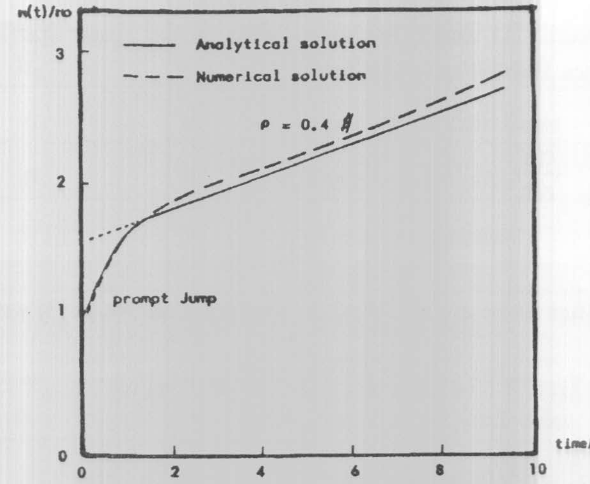

Figure 2. Neutron level behaviour to step reactivity change.

Application (3)

Numerical Solution of The Reactor Kinetics Equations

The Kinetics Equations are relatively difficult to be solved both analytically and numerically due to the large difference in the time constants in the equations.

For one effective delayed neutron group, these equations take the form

$$Y = \begin{bmatrix} n(t) \\ c(t) \end{bmatrix}; A = \begin{bmatrix} \frac{\rho(t)-\beta}{\Lambda} & \lambda \\ \frac{\beta}{\Lambda} & -\lambda \end{bmatrix}; \ \phi(t) = \quad (23)$$

with initial condition

$$Y(0) = [\, n_o, C_o]^T \quad (24)$$

For step reactivety input $\rho(t) = \rho_o$, $\beta = 0.0064$, $\lambda = 0.0719$ sec^{-1} and $\Lambda = 1.0E\text{-}5$ sec

The Eaxact Solution for this case [4]

$$n(t) = n_o\left[\frac{\beta}{\beta-\rho_o} e^{\lambda\rho_o t/\beta-\rho_o} - \frac{\rho_o}{\beta-\rho_o}\, \bar{e}^{\frac{(\rho_o-\beta)t}{\Lambda}}\right] \quad (25)$$

Comparison between analytical and numerical solution is shown in Figure (3).

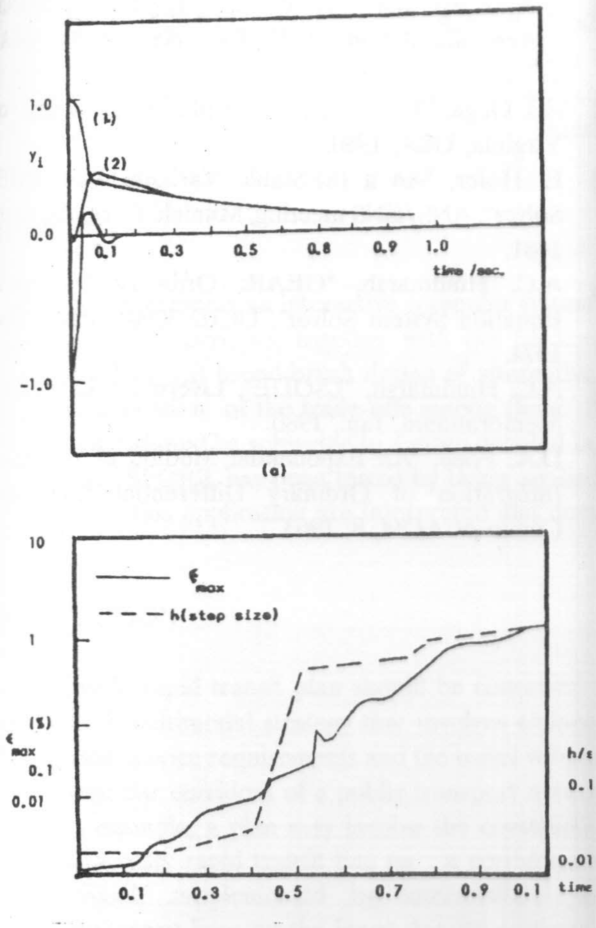

Figure 3. Time behaviour for coupled stiff system.
(a) State variable behaviour
(b) lime step and maximum error behaviour.

Application (4)

Solution of Stiff PDE

For one-dimensional unsteady heat conduction equation. Let us define [1]

$$X_j = j\Delta x$$

$$t_m = m\Delta t \qquad (26)$$

$$u^m{}_j(m) = u(x_j, t_m)$$

By discretize the space x

$$\frac{du_j^{(m)}}{dt} = \frac{u_{j+1}^{(m)} - 2u_j^{(m)} + u_{j-1}^{(m)}}{(\Delta x)^2/K} \qquad (27)$$

with initial condition

$$u_j^{(0)} = u(x,0) = f(x) = f(x_j) \qquad (28)$$

and boundary condition

$$u_0^{(m)} = u(0,t) = 0 \qquad (29)$$

$$u_N^{(m)} = u(L,t) = 0$$

The exact solution for this problem is given by:

$$u(x,t) = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi x}{L} e^{-k(n\pi)/L)}$$

$$a_n = \frac{2}{L}\int_0^{I_d} f(x)\sin\frac{n\pi x}{L}dx$$

Integration of system given by Equation (27) and its comparison with results drawn from finite difference solution [1] for this test problem is shown in Figure (4).

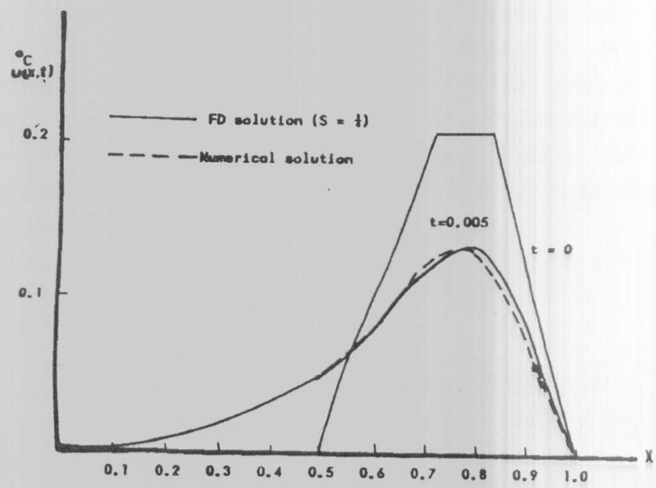

Figure 4. Comparison between FD and numerica integration solutions.

CONCLUTIONS

Simulation in thermo-dluidynamics often require the numerical solution of IVPs with stiffness caused by large Stiff-Ratio due to large difference in system eigenvalues. Therefore suitable ODE-Solvers is highly require for minimum computation time, this is done by maximizing the time step during the time marching.

Chossing appropriate criterion for time step selection [6,7,8] must take large consideration in the next study.

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