Numerical Solutions of Nonlinear Differential Equations for STEM College Education

M. Hafez,

Prof. Department of Mechanical & Aerospace Engineering

University of California, Davis

With

Faiza Alvi, Senior Undergraduate Student, UC Davis

Naijing Guo, Senior Undergraduate Student, UC Davis

Yash Taneja, Senior Undergraduate Student, UC Davis

UCDAVIS

Contents

UCDAVIS

Numerical Simulation Process

A. Physical Problem

B. Mathematical Formulation

C. Numerical Methods

D. Modular Programming

E. Data Analysis

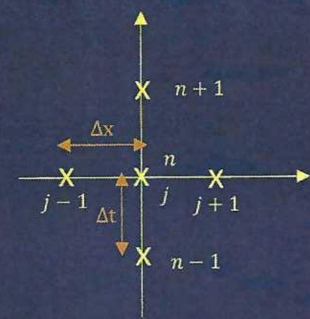
<u>Reference</u>:

Introduction to Computer Simulations for Integrated STEM College Education,
M.M. Hafez & W.E. Tavernetti, World Scientific 2019

UCDAVIS

Numerical Approximations

1. Discretization of the Domain (Space and/or time); Uniform Mesh



2. Discretization of Equations (Finite Differences)

a) First Derivatives

i. Central Difference $\left.\frac{dU}{dx}\right|_j = \frac{U(j+1) - U(j-1)}{2\Delta x} + O(\Delta x^2)$

ii. Backward Difference $\left.\frac{dU}{dx}\right|_j = \frac{U(j) - U(j-1)}{\Delta x} + O(\Delta x)$

iii. Forward Difference $\left.\frac{dU}{dx}\right|_j = \frac{U(j+1) - U(j)}{\Delta x} + O(\Delta x)$

b) Second Derivatives

Central Difference $\left.\frac{d^2U}{dx^2}\right|_j = \frac{U(j+1) - 2U(j) + U(j-1)}{2\Delta x^2} + O(\Delta x^2)$

c) Third Derivatives

Central Difference $\left.\frac{d^3U}{dx^3}\right|_j = \frac{U(j+2) - 2U(j+1) + 2U(j-1) + U(j-2)}{2\Delta x^3} + O(\Delta x^2)$

d) Fourth Derivatives

Central Difference $\left.\frac{d^4U}{dx^4}\right|_j = \frac{U(j+2) - 4U(j+1) + 6U(j) - 4U(j-1) + U(j-2)}{\Delta x^4} + O(\Delta x^2)$

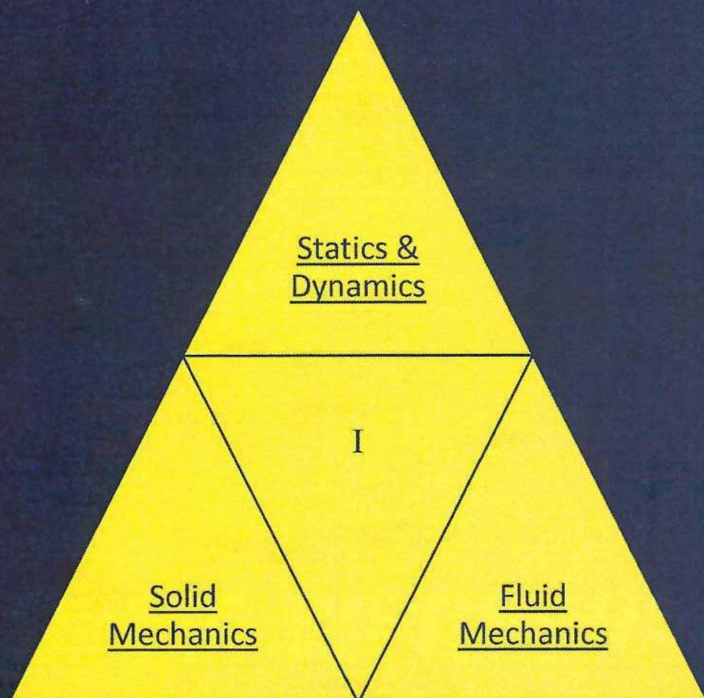
3. Solution of the discrete Equations

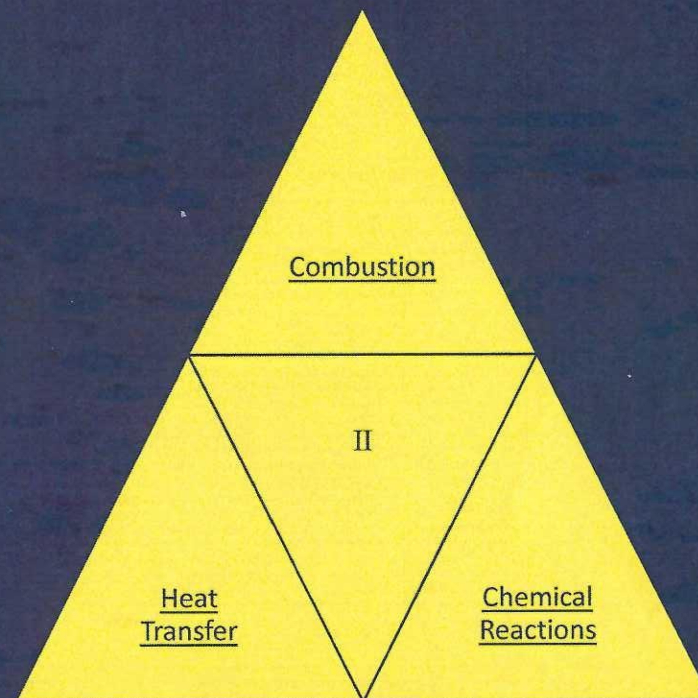
a) IVP (Point by Point)
- Explicit Scheme
- Implicit Scheme

b) BVP (Coupled Equation)
- Iterative Method
  - Point Jacobi
  - Point Gauss-Seidel
  - Point SOR
- Direct Method
  - Scale Tridiagonal solver or Block for second order equation
  - Pentadiagonal solver for fourth order equation

UCDAVIS

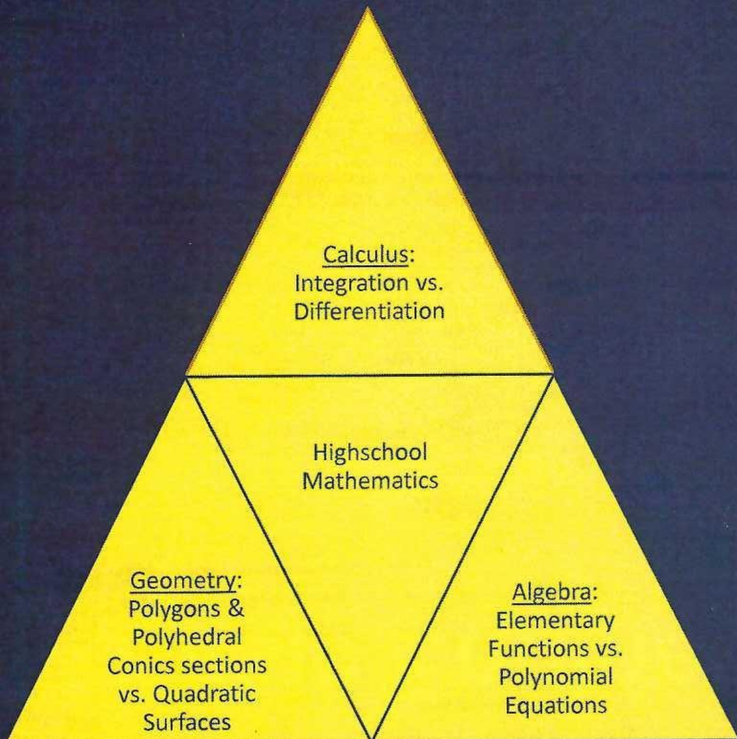
Basic Engineering Mechanics

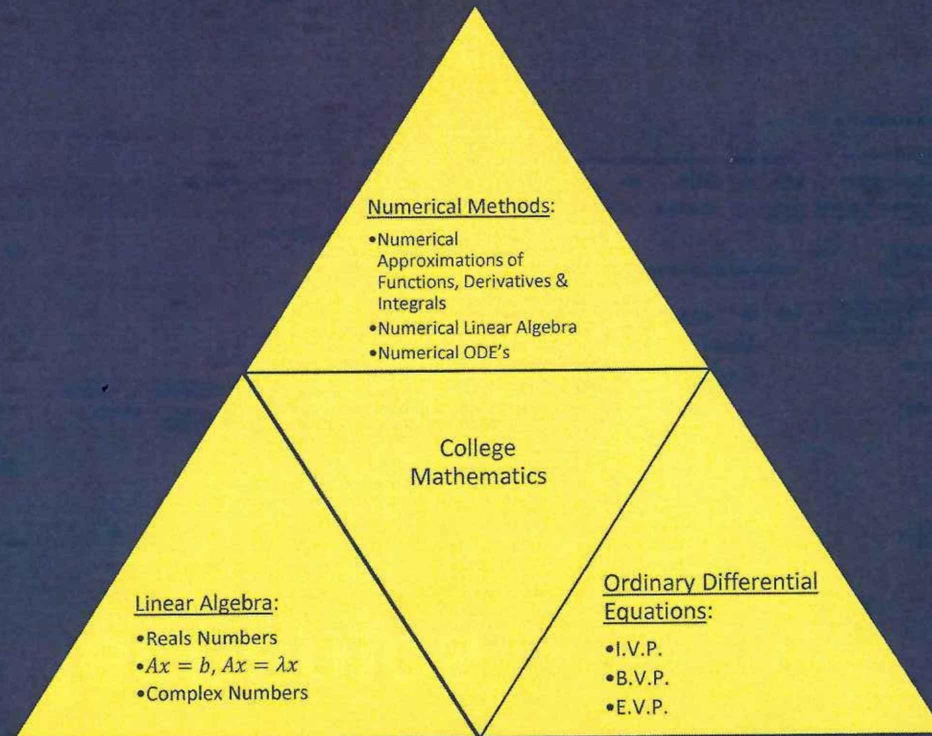




UCDAVIS

Basic Mathematics





UCDAVIS

Initial Value Problem (I.V.P.)

For Initial Value Problem:

$$\frac{dU}{dt} = f(U,t), U(0) = U_0$$

Use Multistage or Multistep Methods

I. Improved Euler (or Runge Kutta)

$$\frac{\overline{U}_{n+1} - U_n}{\Delta t} = f(U_n, t_n)$$

$$\frac{U_{n+1} - U_n}{\Delta t} = \frac{1}{2}(f(U_n, t_n)) + \frac{1}{2}(f(\overline{U}_{n+1}, t_{n+1}))$$

II. Predictor/Corrector 2nd order (3 level)

$$\frac{\overline{U}_{n+1} - U_n}{\Delta t} = \frac{3}{2}(f(U_n, t_n)) - \frac{1}{2}(f(U_{n-1}, t_{n-1}))$$

$$\frac{3}{2}\left(\frac{U_{n+1} - U_n}{\Delta t}\right) - \frac{1}{2}\left(\frac{U_n - U_{n-1}}{\Delta t}\right) = f(\overline{U}_{n+1}, t_{n+1})$$

or

$$\frac{3U_{n+1} - 4U_n + U_{n-1}}{2\Delta t} = f(\overline{U}_{n+1}, t_{n+1})$$

UCDAVIS

Boundary Value Problem (B.V.P.)

Tri and Penta –diagonal systems (latter can be reformed as tridiagonal system)

Consider the system:

$$a_i u_{j-1} + b_j u_j + c_j u_{j+1} = d_j$$

Jacobi Method

$$b_j u_j^{new} = d_j - a_j u_{j-1}^{old} - c_j u_{j+1}^{old}$$

Gauss Seidel Method

$$b_j u_j^{new} = d_j - a_j u_{j-1}^{n+1} - c_j u_{j+1}^{old}$$

S.O.R.

$$u_j^{new} = u_j^{old} + \omega(u_j(Gauss\ Sedel) - u_j^{old})$$

<u>Other Methods:</u>

Use I.V.P. methods to solve problem

a. Shooting & Double Shooting methods

b. Transformations

UCDAVIS

Stability of Simple Schemes for I.V.P.s

i. $\frac{dU}{dt} = -\alpha U$, Let $U = A\eta^n$

$$\frac{U(n+1) - U(n)}{\Delta t} = -\alpha U(n)$$

$$\eta^{n+1} = \eta^n - \alpha \Delta t \eta^n = (1 - \alpha \Delta t)\eta^n$$

$$|\eta| < 1, |1 - \alpha \Delta t| < 1$$

ii. $\frac{d^2U}{dt^2} + \omega^2 U = 0$, Let $U = A\eta^n$

$$\frac{\eta^{n+1} - 2\eta^n + \eta^{n-1}}{\Delta t^2} + \omega \eta^n = 0$$

$$\eta^{n+1} - (2 - \omega^2 \Delta t^2)\eta^n + \eta^{n-1} = 0$$

$$\omega^2 \Delta t^2 < 2$$

UCDAVIS

Treatment of Initial Conditions

$$\frac{d^2U}{dt^2} = f(U,t)$$

$$U(0) = U_0$$

$$\frac{dU}{dt} = V_0$$

Second Order Central Difference

$$\frac{U(n+1) - 2U(n) + U(n-1)}{\Delta t^2} = f(U_n, t_n)$$

$f_n = 3,4, \ldots$

$f_n = 2$

Taylor Series expansion about $j = const., n = 2$

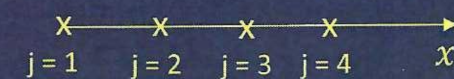
$$U(j,2) = U(j,1) + \left.\frac{dU}{dt}\right|_{j,n=1} \Delta t + \frac{1}{2}\left.\frac{d^2U}{dt^2}\right|_{j,n=1} \Delta t^2$$

Treatment of Boundary Conditions

$$\frac{d^2U}{dx^2} = f(U,x)$$

$$U_x(0) = U_0$$

$$U(l) = U_l$$



Second Order Central Difference

$$\frac{U(j+1) - 2U(j) + U(j-1)}{\Delta x^2} = f(U_j, t_j)$$

$f_j = 3,4, \ldots$

$f_j = 2$

Taylor Series expansion about $j = 2, n = const.$

$$U(2,n) = U(1,n) + \left.\frac{dU}{dx}\right|_{j=1,n} \Delta x + \frac{1}{2}\left.\frac{d^2U}{dx^2}\right|_{j=1,n} \Delta x^2$$

UCDAVIS

Cont.

Apply Neumann Boundary Condition at $\boldsymbol{j = 1}$

$$\frac{U(2) - U_{fictious}}{2\Delta x} = V_0$$

Hence:

$$U_{fictious} = U(2) - 2V_0$$

Use $U_{fictious}$ in the previous discrete equation

Use $U(n+1) = U_l$

Solve n equations for $U_1, U_2, \dots . U_n$ coupled using Gaussian Elimination or Damper Iterative method

UCDAVIS