

Time-Integration and Related Solution Techniques

Tayfun E. Tezduyar
Rice University

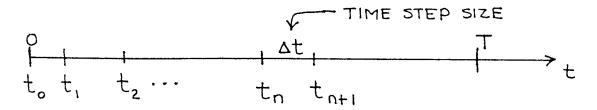
Kenji Takizawa Waseda University

TIME-INTEGRATION

CONSIDER THE FOLLOWING LINEAR, ORDINARY

DIFFERENTIAL EQUATION SYSTEM:

TIME-DISCRETIZATION:



Nts : TOTAL NUMBER OF TIME STEPS

$$d_n \doteq d(t_n)$$

 $\Delta t = t_{n+1} - t_n : CAN BE VARIABLE$

GIVEN: dn, HOW DO WE CALCULATE dn+1

THERE ARE MANY WAYS. WE DESCRIBE 3 OF THEM ...

1)
$$M\left(\frac{d_{n+1}-d_n}{\Delta t}\right) + K\left(d_n\right) = F_n$$

(FORWARD DIFFERENCES)

(FORWARD EULER)

1) $+ K\left(d_{n+1}\right) = F_{n+1}$

(BACKWARD DIFFERENCES)

(BACKWARD EULER)

1) $+ K\left(\frac{d_{n+1}+d_n}{2}\right) = \frac{1}{2}\left(F_{n+1}+F_n\right)$

(CENTRAL DIFFERENCES)

(TRAPEZOIDAL RULE)

IN 1), IF WE APPROXIMATE M WITH A

DIAGONAL MATRIX, THEN TIME-MARCHING

CAN BE DONE WITHOUT SOLVING A

MATRIX SYSTEM.

DEFINITION:

EXPLICIT METHOD

A TIME-MARCHING METHOD THAT DOES NOT REQUIRE SOLUTION OF A MATRIX SYSTEM.

IMPLICIT METHOD

A TIME-MARCHING METHOD THAT

REQUIRES SOLUTION OF A MATRIX SYSTEM.

NOTE THAT 2) AND 3) ARE IMPLICIT METHODS, and, WITH $M \leftarrow M_L$, 1) IS AN EXPLICIT METHOD.

GENERALIZED TRAPEZOIDAL FAMILY:
$$(0 \leqslant \alpha \leqslant 1)$$

$$M\left(\frac{d_{n+1}-d_n}{\Delta t}\right) + K\left(\alpha d_{n+1} + (1-\alpha)d_n\right) = \alpha F_{n+1} + (1-\alpha)F_n$$

$$def d_{n+\alpha} = F_{n+\alpha}$$

$$\Rightarrow M\left(\frac{d_{n+1}-d_n}{\Delta t}\right) + Kd_{n+\alpha} = F_{n+\alpha}$$

$$\alpha = 0 \Rightarrow 1 \qquad \alpha = 1 \Rightarrow 2 \qquad \alpha = 1/2 \Rightarrow 3 \qquad (M \leftarrow M_L)$$

RE-ARRANGE THE EQUATION TO COLLECT THE UNKNOWN TERMS ON THE LEFT-HAND-SIDE:

$$(M + \alpha \Delta t K) \bowtie_{n+1} = (M - (I - \alpha) \Delta t K) \bowtie_{n} + \Delta t F_{n+\alpha}$$

$$NEEDS TO BE \qquad THESE MATRICES$$

$$FORMED AND \qquad DO NOT NEED$$

$$FACTORIZED \qquad TO BE FORMED.$$

$$IF \alpha > 0 \qquad BECAUSE$$

$$M \bowtie_{n} = \bigcap_{e=1}^{nel} (M \vee)_{n}$$

$$IMPLICIT METHOD$$

$$K \bowtie_{n} = \bigcap_{e=1}^{nel} (K \vee)_{n}^{e}$$

IF Δt is <u>small</u> enough, then there could be a justification to approximate $(M + \alpha \Delta t K)$ by M_L .

THEN, THERE IS NO MATRIX FORMATION OR FACTORIZATION. \Rightarrow Explicit METHOD \Rightarrow ECONOMICAL

STABILITY : CONDITIONAL (WILL CONVERGE IF $\Delta t < (\Delta t)_{CRITICAL}$)

ACCURACY : 1ST-ORDER

(IF YOU HALVE At, THE ERROR WILL BE HALVED)

 $(NOTE: IN A 2ND-ORDER METHOD: HALVE <math>\Delta t \implies ERROR HALVED)$ TWICE

PROPERTIES OF THE GENERALIZED TRAPEZOIDAL FAMILY

α =	0	I	1/2
NAME OF METHOD	FORWARD DIFF FORWARD EULER	BACKWARD DIFF BACKWARD EULER	CENTRAL DIFF TRAPEZOIDAL RULE
COST OF MATRIX FORMATION & FACTORIZATION	NO	YES	YES
IMPLICIT OR EXPLICIT	EXPLICIT	IMPLICIT	IMPLICIT
STABILITY	CONDITIONAL	UNCONDITIONAL	UNCONDITIONAL
ACCURACY	1 ST ORDER	1st order	2ND ORDER

PREDICTOR / MULTI-CORRECTOR METHOD

$$(M + \alpha \Delta t K) \qquad d_{n+1} = (M - (1 - \alpha) \Delta t K) d_n + \Delta t F_{n+\alpha}$$

$$d_{n+1}^{(0)} + \Delta d_{n+1}^{(0)}$$

$$(N) = (M - (1 - \alpha) \Delta t K) d_n + \Delta t F_{n+\alpha}$$

$$d_{n+1}^{(0)} + \Delta d_{n+1}^{(0)}$$

$$(N) = (M - (1 - \alpha) \Delta t K) d_n + \Delta t F_{n+\alpha}$$

$$d_{n+1}^{(0)} + \Delta d_{n+1}^{(0)}$$

$$(N) = (M - (1 - \alpha) \Delta t K) d_n + \Delta t F_{n+\alpha}$$

$$(M + \alpha \Delta t K) d_n + \Delta t F_{n+\alpha}$$

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$$(M +$$

(0) ← ZEROTH

TERATION START WITH AN INITIAL GUESS:

GIVEN:
$$d_{n+1}^{(i)}$$
 FIND: $\Delta d_{n+1}^{(i)}$

FROM:

$$\left(\underbrace{\mathbb{M}} + \alpha \Delta t \underbrace{\mathbb{K}} \right) \Delta \underbrace{\mathbb{M}}_{n+1}^{(i)} = \left(\underbrace{\mathbb{M}} - (I - \alpha) \Delta t \underbrace{\mathbb{K}} \right) \underbrace{\mathbb{M}}_{n+1}^{(i)}$$

$$- \left(\underbrace{\mathbb{M}} + \alpha \Delta t \underbrace{\mathbb{K}} \right) \underbrace{\mathbb{M}}_{n+1}^{(i)}$$

CALCULATE THE CORRECTION, AND UPDATE :

$$\mathcal{A}_{n+l}^{(i+1)} = \mathcal{A}_{n+l}^{(i)} + \Delta \mathcal{A}_{n+l}^{(i)}$$

WHEN THIS RESIDUAL BECOMES SUFFICIENTLY CLOSE TO ZERO, OUR ITERATIONS ARE ASSUMED TO HAYE CONVERGED

REMARKS:

- I. IF $(M + \alpha \Delta t K)$ is left as it is, then

 IT TAKES ONLY ONE ITERATION TO CONVERGE.
- 2. WE CAN APPROXIMATE $(M + \alpha \Delta t K)$ ANYWAY

 WE WISH, PROVIDED THAT THE ITERATIONS CONVERGE.
- 3. THE OBJECTIVE IS TO APPROXIMATE (M+ & At K)

 WITH SOMETHING SUFFICIENTLY SIMPLE, BUT

 NOT TOO SIMPLE TO CONVERGE WITHIN REASONABLE

 NUMBER OF ITERATIONS.
- 4. EXAMPLE: (M+ XA+ K) ← ML
 - · LIMIT ON At
 - · CONVERGES SLOWLY
- 5. EXAMPLES: $(M + \alpha \Delta t K) \leftarrow (M_t + \alpha \Delta t Diag(K))$ $(M + \alpha \Delta t K) \leftarrow Diag(M + \alpha \Delta t K)$

SOLUTION TECHNIQUES FOR NONLINEAR EQUATIONS

CONSIDER THE FOLLOWING SYSTEM OF NONLINEAR ORDINARY DIFFERENTIAL EQUATIONS IN TIME:

$$M\dot{U} + N(U) + KU = F$$

$$M(0) = U_0$$

THIS CAN BE DISCRETIZED AS FOLLOWS:

$$\underbrace{M\left(\frac{U_{n+1}-U_n}{\Delta t}\right)}_{\text{At}} + \underbrace{N\left(\alpha\,U_{n+1} + (1-\alpha)\,U_n\right)}_{\text{NONLINEAR VECTUR FUNCTION}} \\
+ \underbrace{K\left(\alpha\,U_{n+1} + (1-\alpha)\,U_n\right)}_{\text{En+}} = \underbrace{F_{n+}}_{\text{n}} + \underbrace{K\left(\alpha\,U_{n+1} + (1-\alpha)\,U_n\right)}_{\text{en}} = \underbrace{F_{n+}}_{\text{n}} + \underbrace{K\left(\alpha\,U_{n+1} + (1-\alpha)\,U_n\right)}_{\text{en}} = \underbrace{F_{n+}}_{\text{en}} + \underbrace{K\left(\alpha\,U_{n+1} + (1-\alpha)\,U_n\right)}_{\text{en}} = \underbrace{K_{n+}}_{\text{en}} + \underbrace$$

THIS MEANS THAT IN NONLINEAR PROBLEMS,

INSTEAD OF A LINEAR EQUATION SYSTEM

$$(M + \alpha \Delta t K) d_{n+1} = \dots,$$

WE NEED TO SOLVE AT EVERY TIME STEP

A NONLINEAR EQUATION SYSTEM $N(d_{n+1}) = \dots$

FOR NOTATIONAL CONVENIENCE, DROP THE SUBSCRIP n+1 AND CALL THE R.H.S. \digamma . THEN,

$$N(d) = F$$

IS WHAT NEEDS TO BE SOLVED AT EVERY TIME STEP.

NEWTON-RAPHSON METHOD
IN SOLVING

START WITH AN INITIAL GUESS d° , ZEROTH ITERATION and AT EACH ITERATION, GIVEN d^{i} , CALCULATE A CORRECTION Δd^{i} , Such that

$$N \left(d + \Delta d^{i} \right) \doteq E$$
.

TO CALCULATE Δd^i , CONSIDER THE FOLLOWING TRUNCATED TAYLOR SERIES EXPANSION AROUND d^i : $N(d^i + \Delta d^i) = N(d^i) + \frac{\partial N}{\partial d^i} \Delta d^i$ THEN SOLVE

 $\frac{\partial N}{\partial d} \Big|_{d^{i}} \Delta d^{i} = F - N(d^{i}),$ $K_{T}(d^{i}) : \text{"TANGENT STIFFNESS" MATRIX}$

AND UPDATE: $d^{i+1} = d^{i} + \Delta d^{i}$

NEWTON-RAPHSON METHOD CONVERGES QUADRATICALLY,
PROVIDED THAT

- 1) THE INITIAL GUESS & IS SUFFICIENTLY CLOSE TO THE SOLUTION, AND
- 2) INVERSE OF $\frac{\partial N}{\partial d}$ EXISTS.

HOW DO WE DECIDE WHEN TO STOP ITERATIONS?

ANSWER: WHEN

- a) $E N(d^i)$ is sufficiently close to 0, or
- b) A PREDETERMINED NUMBER OF ITERATIONS HAVE BEEN PERFORMED.

IN BOTH CASES, THE RESIDUAL $F-N(d^i)$ NEED TO BE MONITORED. THE RESIDUAL AT ITERATION i:

$$\mathbb{R}^{i} = \mathcal{F} - \mathcal{N}(\mathbf{g}^{i}).$$

CHECK TO SEE IF

 $\| \mathcal{R}^{i} \| \leqslant \mathcal{E} \leftarrow A$ PREDETERMINED, SMALL VALUE EXAMPLE FOR THE NORM $\| \cdot \| :$ $\| \mathbf{x} \| = \left(\mathbf{x}_{1}^{2} + \mathbf{x}_{2}^{2} + \ldots + \mathbf{x}_{n}^{2} \right)^{1/2}$.

TO CHECK CONVERGENCE IN A WAY THAT MAKES SENSE, WE NEED TO SCALE $\|R^i\|$. ONE WAY IS TO SCALE IT WITH $\|R^0\|$.

1 INITIAL RESIDUAL

THEREFORE, THE CONVERGENCE CHECK TAKET

THE FORM :

$$\frac{\parallel \mathcal{R}^{i} \parallel}{\parallel \mathcal{R}^{\circ} \parallel} \leqslant \varepsilon$$

QUITE OFTEN, IT IS MORE PRACTICAL, ESPECIALLY
IN SOLVING TIME-DEPENDENT PROBLEMS, TO PERFORM
A PREDETERMINED NUMBER OF ITERATIONS AT EACH
TIME STEP, BUT AT THE SAME TIME KEEP AN
EYE ON

$$\frac{\parallel \mathbb{R}^{i}\parallel}{\parallel \mathbb{R}^{\circ}\parallel},$$

TO MAKE SURF THAT IT DOES NOT EXCEED A CERTAIN LEVEL.

MODIFIED NEWTON-RAPHSON METHOD

 $\underbrace{K_{T}(\underline{d}^{i})} \Delta \underline{d}^{i} = \underbrace{F} - \underbrace{N(\underline{d}^{i})}_{IN \ THE} \quad FULL'' \ NEWTON-RAPHSON METHOD$ THIS GETS UPDATED AT EVERY ITERATION $BY \quad \underbrace{K_{T}(\underline{d}^{i})}_{\partial \underline{d}} = \frac{\partial \underline{N}}{\partial \underline{d}} \Big|_{\underline{d}^{i}}$

IN THE MODIFIED NEWTON-RAPHSON METHOD K_T is <u>Not</u> updated every iteration. At some of the iterations, old values of K_T are used.

THIS APPROACH

- · CUTS COST OF COMPUTATION
- · BUT MAY REDUCE THE CONVERGENCE RATE.

INCREMENTAL NEWTON-RAPHSON METHOD

THE NEWTON-RAPHSON METHOD MAY HAVE CONVERGENCE

DIFFICULTIES IF THE INITIAL GUESS do is too "FAR"

FROM THE SOLUTION.

ONE APPROACH: INCREMANTAL "LOADING" (i.e. LOAD RAMPING)

$$N(d) = E$$

START WITH A FRACTION OF

THIS. THIS MEANS A "LOAD"

SMALLER THAN THE ACTUAL ONE.

- 2) GET A CONVERGED SOLUTION FOR THIS LOAD LEVEL
- 3) USE THAT SOLUTION AS THE INITIAL GUESS FOR THE NEXT LEVEL.
- 4) REPAT 2) AND 3) UNTIL THE FULL LOAD LEVEL IS REACHED.

EXAMPLE: START WITH
$$\frac{1}{10} \stackrel{\text{GET}}{\sim} \stackrel{\text{J}}{\sim} \frac{1}{10} \stackrel{\text{GET}}{\sim} \stackrel{\text{J}}{\sim} \frac{1}{10} \stackrel{\text{GET}}{\sim} \frac{1}{10} \stackrel{\text{GET}}{\sim}$$

RAMPING UP THE REYNOLDS NUMBER

IN FLUID DYNAMICS PROBLEMS, TYPICALLY, THE NONLINEAR TERMS ARE PROPORTIONAL TO THE REYNOLDS NUMBER.

ONE CAN START WITH A FRACTION OF THE ACTUAL REYNOLDS NUMBER,

- 2) GET A CONVERGED SOLUTION FOR THAT REYNOLDS NUMBER
- 3) USE THAT SOLUTION AS THE INITIAL GUESS FOR THE NEXT LEVEL OF THE REYNOLDS NUMBER
- 4) REPEAT 2) AND 3) UNTIL THE FULL REYNOLDS NUMBER IS REACHED.

EXAMPLE: START WITH $Re \times 10^{-5} \xrightarrow{66T} d_{\times 10^{-5}}$ USE $d_{\times 10^{-5}}$ AS INITIAL GUESS FOR $Re \times 10^{-4} \xrightarrow{66T} d_{\times 10^{-4}}$ USE $d_{\times 10^{-4}}$ " " Re $d_{\times 10^{-3}}$ derivation of the second s

NOTE: IN A TIME-DEPENDENT PROBLEM, RAMPING THE REYNOLDS NUMBER NEEDS TO BE EXERCISED ONLY IN THE INITIAL STAGES OF THE TIME-MARCHING.

ITERATIVE SOLUTION TECQNIQUES FOR LINEAR EQUATION SYSTEMS

$$A \times = b$$

EXAMPLE :

WHERE DO THESE SYSTEMS COME FROM?

NONLINEAR $X_{T}(\underline{d}^{i})\Delta\underline{d}^{i} = \underline{F} - N(\underline{d}^{i})$ A $X_{T} = \underline{b}$ LINEAR $X_{T}(\underline{d}^{i})\Delta\underline{d}^{i} = \underline{F} - N(\underline{d}^{i})$ PROBLEMS $X_{T}(\underline{d}^{i})\Delta\underline{d}^{i} = \underline{F} - N(\underline{d}^{i})$

IN MOST CASES, ESPECIALLY THOSE IN 3D,

THE MATRIX A IS TOO LARGE, AND THEREFORE

WE CANNOT USE A "DIRECT" SOLUTION METHOD

SUCH AS THE GAUSSIAN ELIMINATION METHOD OR

OTHER FACTORIZATION TECQNIQUES, BECASE WE

CANNOT AFFORD TO

- a) FACTORIZE A
- b) STORE THE FACTORIZED A.

IN ITERATIVE SOLUTION OF

START WITH AN INITIAL GUESS X - ZEROTH ITERATION AND AT EACH ITERATION, GIVEN Xm, CALCULATE A CORRECTION $\Delta \times_m$, SUCH THAT

$$\overset{\triangle}{\approx} \left(\underset{\approx}{\times}_{m} + \Delta \underset{\approx}{\times}_{m} \right) = \overset{\triangle}{\approx}$$

OR

$$\stackrel{A}{\widetilde{\uparrow}} \Delta \times_{m} = \stackrel{b}{\widetilde{\smile}} - \stackrel{A}{\widetilde{\smile}} \times_{m}$$

AND UPDATE
$$X_{m+1} = X_m + \Delta X_m .$$

IF WE LEAVE A AS IT IS, THIS PROCEDURE IS ESSENTIALLY NO DIFFERENT THAN SOLVING AX=b, IT CONVERGES IN ONE ITERATION TO THE SOLUTION OF AX = b. FOR EXAMPLE, IF WE START WITH $X_0 = Q$, THEN $\Delta X_1 = X$. BUT....

IN MOST CASES, WE CANNOT AFFORD LEAVING

A AS IT IS. THEREFORE WE APPROXIMATE

A WITH A "PRECONDITIONING" MATRIX P, AND

SOLVE AT EVERY ITERATION

$$P \Delta y_m = b - A \times_m$$

AND UPDATE X_m BY USING AN UPDATE METHOD MORE SOPHISTICATED THAN SIMPLY ADDING Δy_m δX_m .

THERE ARE 3 MAIN ISSUES HERE.

- I) HOW TO COMPUTE $b-A \times_m$ IN THE MOST EFFICIENT WAY.
- 2) HOW TO DESIGN P IN A WAY THAT KEEPS IT SIMPLE WITHOUT SLOWING THE CONVERGENCE TOO MUCH.
- 3) HOW TO UPDATE & M IN A WAY THAT IS ECONOMICAL BUT ALSO HELPS CONVERGENCE.

C ELEMENT VECTOR

- 1) HOW TO COMPUTE $b A \times m$
 - a) SPARSE-MATRIX-BASED :

STORE A BY USING A SPAPSE-MATRIX STORAGE TECHNIQUE, AND PERFORM THE COMPUTATION WITH GLOBAL MATRIX-VECTOR PRODUCTS.

b) ELEMENT-MATRIX-BASED :

C) ELEMENT- VECTOR -BASED :

$$\overset{\triangle}{\sim} \overset{\times}{\sim} m = \frac{\partial \overset{\triangle}{\mathcal{N}}}{\partial \overset{\triangle}{\mathcal{Q}}} \overset{\times}{\sim} m = \lim_{\varepsilon \to 0} \frac{\overset{\triangle}{\mathcal{N}} (\overset{\triangle}{\mathcal{Q}} + \varepsilon \overset{\times}{\times}_m) - \overset{\triangle}{\mathcal{N}} (\overset{\triangle}{\mathcal{Q}})}{\varepsilon}$$

$$\stackrel{\text{nel}}{\underset{\varepsilon}{\wedge}} \times_{m} \doteq \frac{\bigcap_{e=1}^{nel} N^{e}(\cancel{d} + \varepsilon \times_{m}) - \bigcap_{e=1}^{nel} N^{e}(\cancel{d})}{\varepsilon}$$

WHERE E IS A SMALL NUMBER.

2) HOW TO DESIGN P

P = DIAG (A) IS THE SIMPLEST CHOICE.

DIAGONAL OR NODAL-BLOCK-DIAGONAL

CONVERGES SLOWLY, ESPECIALLY FOR

- OTHER POSSIBILITIES: CLUSTERED ELEMENT-BY-ELEMENT

 PRECONDITIONING
 - · MIXED PRECONDITIONING
- 3) HOW TO UPDATE Xm

AS A WAY JUST ONE STEP MORE SOPHISTICATED THAN SIMPLY ADDING Δy_m to χ_m ,

WE UPDATE Xm BY USING THE EXPRESSION

WE DETERMINE THE "BEST" S" BY MINIMIZING

THE UPDATED RESIDUAL $\Gamma_{m+1} = b - A \times_{m+1}$

WITH RESPECT TO "S".

 $\mathcal{L}_{m+1} = \mathcal{L} - \mathcal{A} \left(\mathcal{X}_m + s \Delta \mathcal{Y}_m \right) = \mathcal{L} - \mathcal{A} \mathcal{X}_m - s \mathcal{A} \Delta \mathcal{Y}_m$

MINIMIZE
$$\| \Gamma_{m+1} \|$$
 WITH RESPECT TO "S". \Leftrightarrow

MINIMIZE $\| \Gamma_{m+1} \|^2$ WITH RESPECT TO "S". \Leftrightarrow

$$\frac{d}{ds} \| \Gamma_{m+1} \|^2 = 0 \Leftrightarrow \frac{d}{ds} (\Gamma_{m+1} \cdot \Gamma_{m+1}) = 0$$

$$\Rightarrow \quad \mathcal{L}_{m+1} \cdot \frac{d}{ds} \left(\mathcal{L}_{m+1} \right) = 0$$

$$\Rightarrow \qquad \stackrel{r}{\sim}_{m+1} \quad \cdot \left(- \underset{\sim}{A} \Delta \underset{\sim}{y}_{m} \right) = 0$$

$$\Rightarrow \left(\mathcal{L}_m - 5 \overset{A}{\sim} \Delta y_m \right) \cdot \left(\overset{A}{\sim} \Delta y_m \right) = 0$$

$$\Rightarrow s = \frac{\mathcal{L}_m \cdot (\underline{A} \Delta \underline{y}_m)}{(\underline{A} \Delta \underline{y}_m) \cdot (\underline{A} \Delta \underline{y}_m)}$$

$$= \frac{\sum_{m} \cdot (A \Delta y_{m})}{\|A \Delta y_{m}\|^{2}}$$

THERE ARE MANY OTHER WAYS, INCLUDING METHODS WITH MULTIPLE "SEARCH" PARAMETERS AND DIRECTIONS.