Topic 10

Solution of the Nonlinear Finite Element Equations in Static Analysis—Part I

Contents:

- **Short review of Newton-Raphson iteration for the root of a single equation**
- **Newton-Raphson iteration for multiple degree of freedom systems**
- **Derivation of governing equations by Taylor series expansion**
- **Initial stress, modified Newton-Raphson and full Newton-Raphson methods**
- **Demonstrative simple example**
- **Line searches**
- **The Broyden-Fletcher-Goldfarb-Shanno (BFGS) method**
- **Computations in the BFGS method as an effective scheme**
- **Flow charts of modified Newton-Raphson, BFGS, and full Newton-Raphson methods**
- **Convergence criteria and tolerances**

Textbook: Sections 6.1, 8.6, 8.6.1, 8.6.2, 8.6.3

Examples: 6.4, 8.25, 8.26

- WE DERIVED IN THE PREVIOUS LECTURES THE F.E. EQUATIONS

$$ {}^{t}\underline{K}\,\Delta\underline{U}^{(i)} = {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)} $$

$$ {}^{t+\Delta t}\underline{U}^{(i)} = {}^{t+\Delta t}\underline{U}^{(i-1)} + \Delta\underline{U}^{(i)} $$

$$ i = 1, 2, 3, \ldots $$

- IN THIS LECTURE WE CONSIDER VARIOUS TECHNIQUES OF ITERATION AND CONVERGENCE CRITERIA

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SOLUTION OF NONLINEAR EQUATIONS

We want to solve

$$\underbrace{{}^{t+\Delta t}\underline{R}}_{\text{externally applied loads}} - \underbrace{{}^{t+\Delta t}\underline{F}}_{\text{nodal point forces corresponding to internal element stresses}} = \underline{0}$$

- Loading is deformation-independent

- $${}^{t+\Delta t}\underline{F} = \underbrace{\int_{{}^0V} {}^{t+\Delta t}_{\ 0}\underline{B}_L^T \ {}^{t+\Delta t}_{\ 0}\hat{\underline{S}} \ {}^0dV}_{\text{T.L. formulation}} = \underbrace{\int_{{}^{t+\Delta t}V} {}^{t+\Delta t}_{t+\Delta t}\underline{B}_L^T \ {}^{t+\Delta t}\hat{\underline{\tau}} \ {}^{t+\Delta t}dV}_{\text{U.L. formulation}}$$

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The procedures used are based on the Newton-Raphson method (commonly used to find the roots of an equation).

A historical note:

- Newton gave a version of the method in 1669.
- Raphson generalized and presented the method in 1690.

Both mathematicians used the same concept, and both algorithms gave the same numerical results.

Consider a single Newton-Raphson iteration. We seek a root of f(x), given an estimate to the root, say x_{i-1}, by

$$x_i = x_{i-1} - \frac{f(x_{i-1})}{f'(x_{i-1})}$$

Once x_i is obtained, x_{i+1} may be computed using

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

The process is repeated until the root is obtained.

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The formula used for a Newton-Raphson iteration may be derived using a Taylor series expansion.

We can write, for any point x_i and neighboring point x_{i-1},

$$f(x_i) = f(x_{i-1}) + f'(x_{i-1})(x_i - x_{i-1}) + \text{higher order terms}$$

$$\doteq f(x_{i-1}) + f'(x_{i-1})(x_i - x_{i-1})$$

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Since we want a root of f(x), we set the Taylor series approximation of $f(x_i)$ to zero, and solve for x_i:

$$0 = f(x_{i-1}) + f'(x_{i-1})(x_i - x_{i-1})$$

$$\downarrow$$

$$x_i = x_{i-1} - \frac{f(x_{i-1})}{f'(x_{i-1})}$$

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Mathematical example, given merely to demonstrate the Newton-Raphson iteration algorithm:

Let $f(x) = \sin x$, $x_0 = 2$

Using Newton-Raphson iterations, we obtain

i	x_i	error = $\lvert\pi - x_i\rvert$	
0	2.0	1.14	
1	4.185039863	1.04	
2	2.467893675	.67	
3	3.266186277	.12	
4	3.140943912	6.5×10^{-4}	quadratic convergence is observed
5	3.141592654	$< 10^{-9}$	

The approximations obtained using Newton-Raphson iterations exhibit quadratic convergence, if the approximations are "close" to the root.

Mathematically, if $|E_{i-1}| \doteq 10^{-m}$

then $|E_i| \doteq 10^{-2m}$

where E_i is the error in the approximation x_i.

The convergence rate is seen to be quite rapid, once quadratic convergence is obtained.

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However, if the first approximation x_0 is "far" from the root, Newton-Raphson iterations may not converge to the desired value.

Example: $f(x) = \sin x$, $x_0 = 1.58$

i	x_i
0	1.58
1	110.2292036
2	109.9487161
3	109.9557430
4	109.9557429] not the desired root

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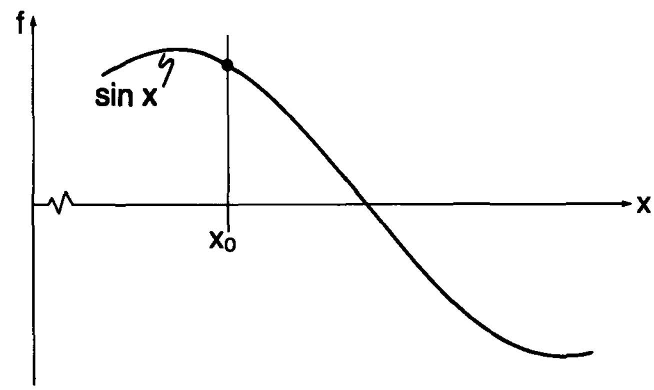
Pictorially:



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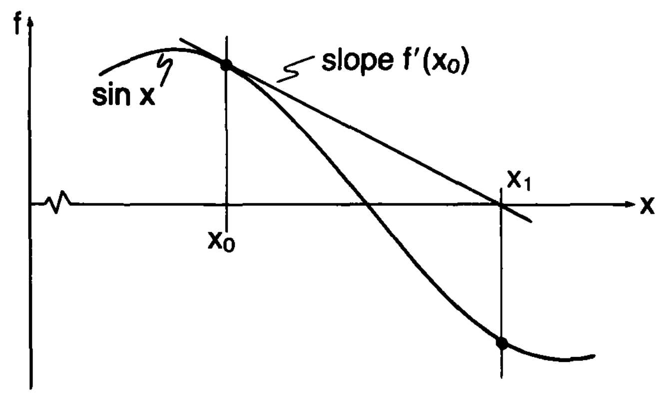
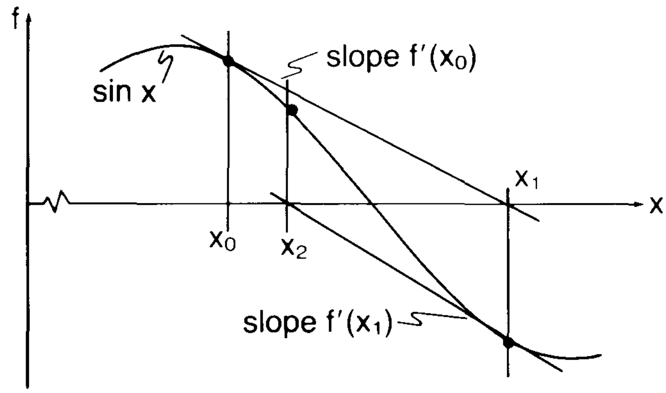
Pictorially: Iteration 1



Pictorially: Iteration 1
Iteration 2



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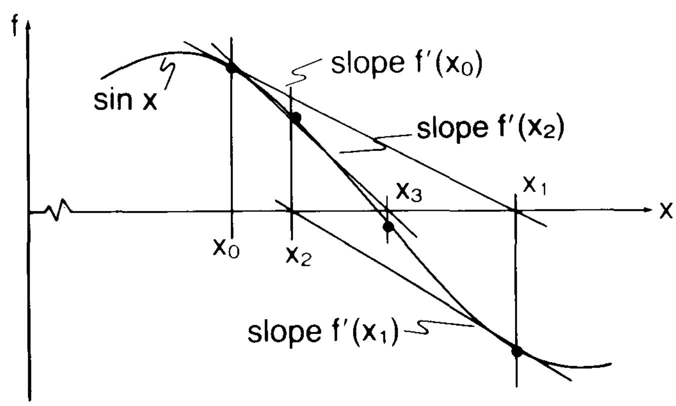
Pictorially: Iteration 1
Iteration 2
Iteration 3



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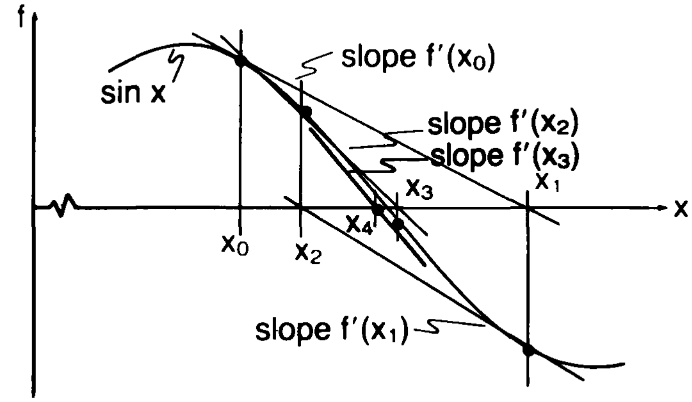
Pictorially: Iteration 1
Iteration 2
Iteration 3
Iteration 4



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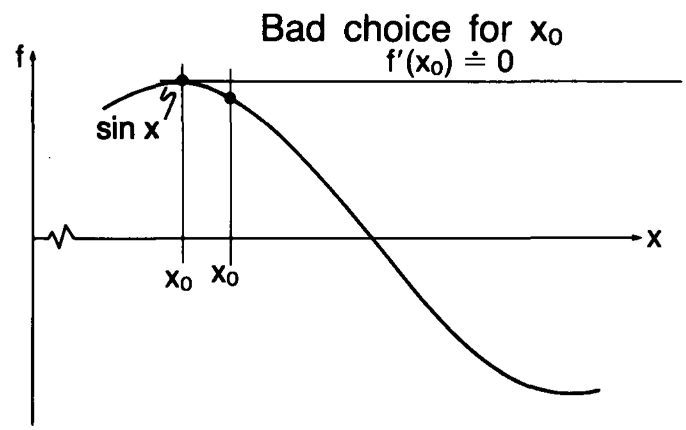
Pictorially:



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Newton-Raphson iterations for multiple degrees of freedom

We would like to solve

$$\underline{f}(\underline{U}) = {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F} = \underline{0}$$

where now $\underline{f}$ is a vector (one row for each degree of freedom). For equilibrium, each row in $\underline{f}$ must equal zero.

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To derive the iteration formula, we generalize our earlier derivation.

We write

$$\underline{f}({}^{t+\Delta t}\underline{U}^{(i)}) = \underline{f}({}^{t+\Delta t}\underline{U}^{(i-1)}) + \left[\frac{\partial \underline{f}}{\partial \underline{U}}\right]\Bigg|_{{}^{t+\Delta t}\underline{U}^{(i-1)}} ({}^{t+\Delta t}\underline{U}^{(i)} - {}^{t+\Delta t}\underline{U}^{(i-1)}) + \underbrace{\text{higher order terms}}_{\substack{\text{neglected to obtain a} \\ \text{Taylor series approximation}}}$$

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Since we want a root of $\underline{f}(\underline{U})$, we set the Taylor series approximation of $\underline{f}({}^{t+\Delta t}\underline{U}^{(i)})$ to zero.

$$\underline{0} = \underline{f}({}^{t+\Delta t}\underline{U}^{(i-1)}) + \left[\frac{\partial \underline{f}}{\partial \underline{U}}\right]_{{}^{t+\Delta t}\underline{U}^{(i-1)}} \overbrace{\Delta \underline{U}^{(i)}}^{{}^{t+\Delta t}\underline{U}^{(i)} - {}^{t+\Delta t}\underline{U}^{(i-1)}}$$

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or

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}_{{}^{t+\Delta t}\underline{U}^{(i-1)}} + \underbrace{\begin{bmatrix} \frac{\partial f_1}{\partial U_1} & \cdots & \frac{\partial f_1}{\partial U_n} \\ \vdots & & \vdots \\ \frac{\partial f_n}{\partial U_1} & \cdots & \frac{\partial f_n}{\partial U_n} \end{bmatrix}_{{}^{t+\Delta t}\underline{U}^{(i-1)}}}_{\text{a square matrix}} \begin{bmatrix} \Delta U_1^{(i)} \\ \vdots \\ \Delta U_n^{(i)} \end{bmatrix}$$

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We now use

$$\underline{f}({}^{t+\Delta t}\underline{U}^{(i-1)}) = {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)},$$

$$\left.\frac{\partial \underline{f}}{\partial \underline{U}}\right|_{{}^{t+\Delta t}\underline{U}^{(i-1)}} = \underbrace{\left.\left[\frac{\partial\, {}^{t+\Delta t}\underline{R}}{\partial \underline{U}}\right]\right|_{{}^{t+\Delta t}\underline{U}^{(i-1)}}}_{\rightarrow 0} - \left.\left[\frac{\partial\, {}^{t+\Delta t}\underline{F}^{(i-1)}}{\partial \underline{U}}\right]\right|_{{}^{t+\Delta t}\underline{U}^{(i-1)}}$$

because the loads are deformation-independent

$$= -{}^{t+\Delta t}\underline{K}^{(i-1)}$$

the tangent stiffness matrix

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Important: ${}^{t+\Delta t}\underline{K}^{(i-1)}$ is symmetric because

- We used symmetric stress and strain measures in our governing equation.
- We interpolated the real displacements and the virtual displacements with exactly the same functions.
- We assumed that the loading was deformation-independent.

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Our final result is

$$^{t+\Delta t}\underline{K}^{(i-1)}\ \Delta\underline{U}^{(i)} = {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)}$$

This is a set of simultaneous linear equations, which can be solved for $\Delta\underline{U}^{(i)}$. Then

$$^{t+\Delta t}\underline{U}^{(i)} = {}^{t+\Delta t}\underline{U}^{(i-1)} + \Delta\underline{U}^{(i)}$$

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This iteration scheme is referred to as the full Newton-Raphson method (we update the stiffness matrix in each iteration).

The full Newton-Raphson iteration shows mathematically quadratic convergence when solving for the root of an algebraic equation. In finite element analysis, a number of requirements must be fulfilled (for example, the updating of stresses, rotations need careful attention) to actually achieve quadratic convergence.

We can depict the iteration process in two equivalent ways:

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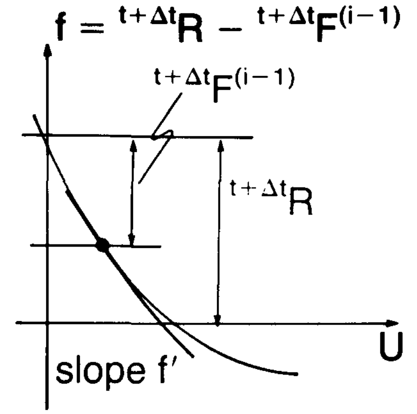

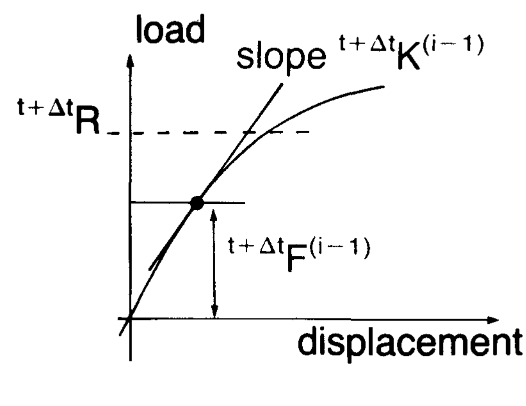

This is like a force-deflection curve. We use this representation henceforth.

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Modifications:

$$ {}^{\tau}\underline{K}\, \Delta \underline{U}^{(i)} = {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)} $$

- $\tau = 0$: Initial stress method
- $\tau = t$: Modified Newton method
- Or, more effectively, we update the stiffness matrix at certain times only.

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We note:

- The initial stress method and the modified Newton method are much less expensive than the full Newton method per iteration.
- However, many more iterations are necessary to achieve the same accuracy.
- The initial stress method and the modified Newton method "cannot" exhibit quadratic convergence.

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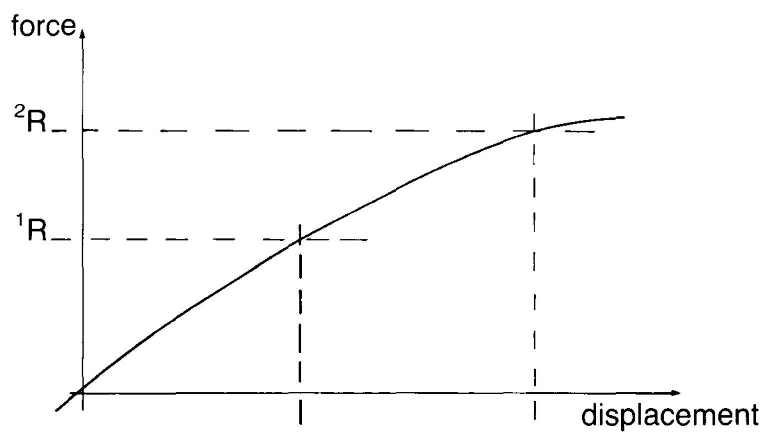
Example: One degree of freedom, two load steps



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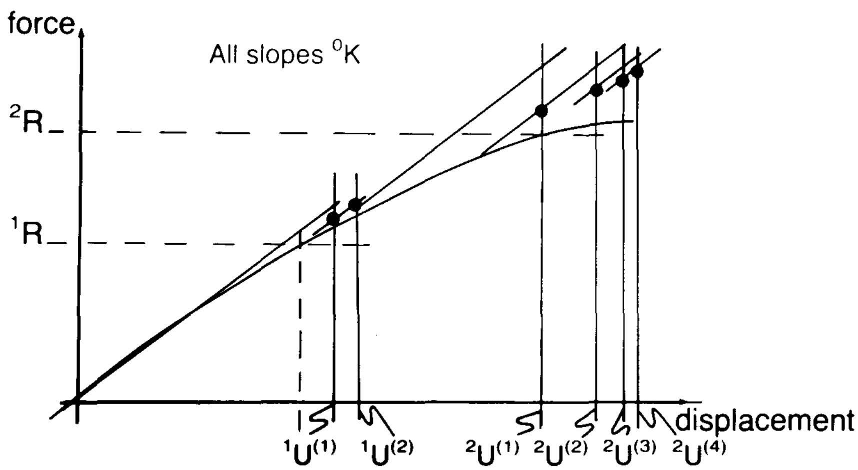
Initial stress method: $\tau = 0$

Example: One degree of freedom, two load steps



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Line searches:

We solve

$$ {}^{\tau}\underline{K}\,\Delta\bar{\underline{U}} = {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)} $$

and consider forming ${}^{t+\Delta t}\underline{F}^{(i)}$ using

$$ {}^{t+\Delta t}\underline{U}^{(i)} = {}^{t+\Delta t}\underline{U}^{(i-1)} + \beta\,\Delta\bar{\underline{U}} $$

where we choose β so as to make ${}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i)}$ small "in some sense".

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Aside:

If, for all possible $\underline{U}$, the number

$$\underline{U}^T \left({}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i)} \right) = 0$$

then $\quad {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i)} = \underline{0}$

Reason: consider

$$\underline{U}^T = [0 \quad 0 \quad 0 \quad \cdots \quad \underbrace{1}_{\text{any row of } \underline{U}} \quad \cdots \quad 0 \quad 0]$$

This isolates one row of ${}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i)}$

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During the line search, we choose $\underline{U} = \Delta\bar{\underline{U}}$ and seek β such that

$$\Delta\bar{\underline{U}}^T \left({}^{t+\Delta t}\underline{R} - \underbrace{{}^{t+\Delta t}\underline{F}^{(i)}}_{\text{a function of } \beta} \right) = 0$$

since ${}^{t+\Delta t}\underline{U}^{(i)} = {}^{t+\Delta t}\underline{U}^{(i-1)} + \beta\, \Delta\bar{\underline{U}}$

In practice, we use

$$\frac{\Delta\bar{\underline{U}}^T \left({}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i)} \right)}{\Delta\bar{\underline{U}}^T \left({}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)} \right)} \leq \underbrace{\text{STOL}}_{\text{a convergence tolerance}}$$

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BFGS (Broyden-Fletcher-Goldfarb-Shanno) method:

We define

$$\underline{\delta}^{(i)} = {}^{t+\Delta t}\underline{U}^{(i)} - {}^{t+\Delta t}\underline{U}^{(i-1)}$$

$$\underline{\gamma}^{(i)} = {}^{t+\Delta t}\underline{F}^{(i)} - {}^{t+\Delta t}\underline{F}^{(i-1)}$$

and want a coefficient matrix such that

$$({}^{t+\Delta t}\underline{K}^{(i)})\,\underline{\delta}^{(i)} = \underline{\gamma}^{(i)}$$

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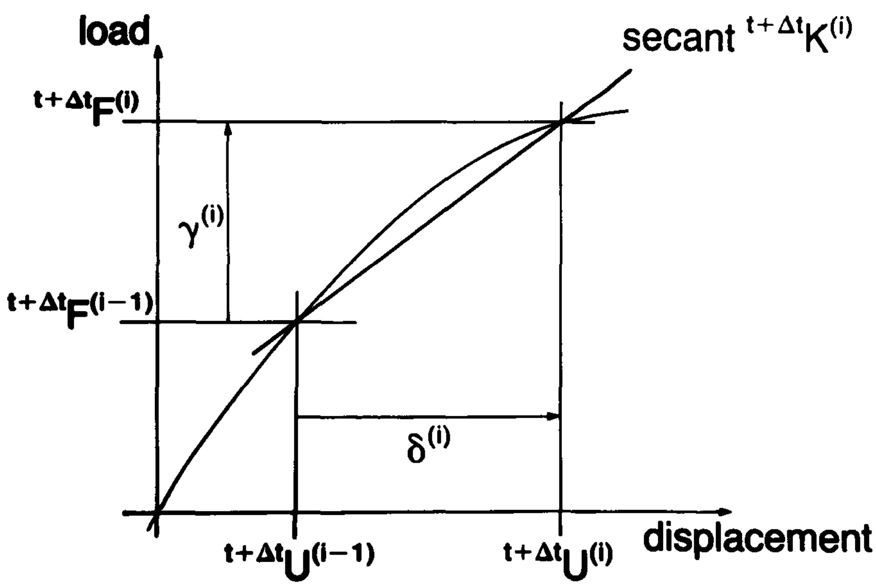
Pictorially, for one degree of freedom,



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- The BFGS method is an iterative algorithm which produces successive approximations to an effective stiffness matrix (actually, to its inverse).
- A compromise between the full Newton method and the modified Newton method

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Step 1: Calculate direction of displacement increment

$$\Delta \bar{\underline{U}}^{(i)} = ({}^{t+\Delta t}\underline{K}^{-1})^{(i-1)} \, ({}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)})$$

(Note: We do not calculate the inverse of the coefficient matrix; we use the usual $\underline{L}\,\underline{D}\,\underline{L}^T$ factorization)

Step 2: Line search

$$^{t+\Delta t}\underline{U}^{(i)} = {}^{t+\Delta t}\underline{U}^{(i-1)} + \beta\, \Delta\bar{\underline{U}}^{(i)}$$

a function of β

$$\frac{\Delta\bar{\underline{U}}^{(i)T}\,(^{t+\Delta t}\underline{R} - \overbrace{^{t+\Delta t}\underline{F}^{(i)}})}{\Delta\bar{\underline{U}}^{(i)T}\,(^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)})} \leq \text{STOL}$$

Hence we can now calculate $\underline{\delta}^{(i)}$ and $\underline{\gamma}^{(i)}$.

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Step 3: Calculation of the new "secant" matrix

$$(^{t+\Delta t}\underline{K}^{-1})^{(i)} = \underline{A}^{(i)T}\,(^{t+\Delta t}\underline{K}^{-1})^{(i-1)}\,\underline{A}^{(i)}$$

where

$\underline{A}^{(i)} = \underline{I} + \underline{v}^{(i)}\ \underline{w}^{(i)T}$

$\underline{v}^{(i)}$ = vector, function of $\underline{\delta}^{(i)}, \underline{\gamma}^{(i)}, {}^{t+\Delta t}\underline{K}^{(i-1)}$

$\underline{w}^{(i)}$ = vector, function of $\underline{\delta}^{(i)}, \underline{\gamma}^{(i)}$

See the textbook.

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Transparency 10-37

Important:

- Only vector products are needed to obtain $\underline{v}^{(i)}$ and $\underline{w}^{(i)}$.
- Only vector products are used to calculate $\Delta\bar{\underline{U}}^{(i)}$.

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Reason:

$$\Delta\bar{\underline{U}}^{(i)} = \{(\underline{I} + \underline{w}^{(i-1)}\,\underline{v}^{(i-1)T}) \cdots (\underline{I} + \underline{w}^{(1)}\,\underline{v}^{(1)T})\ {}^{\tau}\underline{K}^{-1}\ (\underline{I} + \underline{v}^{(1)}\,\underline{w}^{(1)T}) \cdots (\underline{I} + \underline{v}^{(i-1)}\,\underline{w}^{(i-1)T})\} \times [{}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)}]$$

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In summary

The following solution procedures are most effective, depending on the application.

1) Modified Newton-Raphson iteration with line searches

$$ {}^{t}\underline{K}\,\Delta\bar{\underline{U}}^{(i)} = {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)} $$

$$ {}^{t+\Delta t}\underline{U}^{(i)} = {}^{t+\Delta t}\underline{U}^{(i-1)} + \underbrace{\beta}_{\text{determined by the line search}}\,\Delta\bar{\underline{U}}^{(i)} $$

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2) BFGS method with line searches

3) Full Newton-Raphson iteration with or without line searches
(full Newton-Raphson iteration with line searches is most powerful)

But, these methods cannot directly be used for post-buckling analyses.

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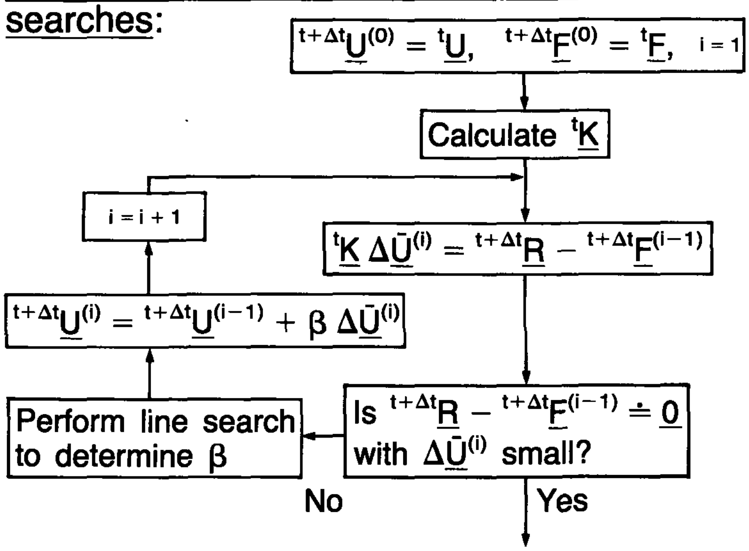
Modified Newton iteration with line searches:



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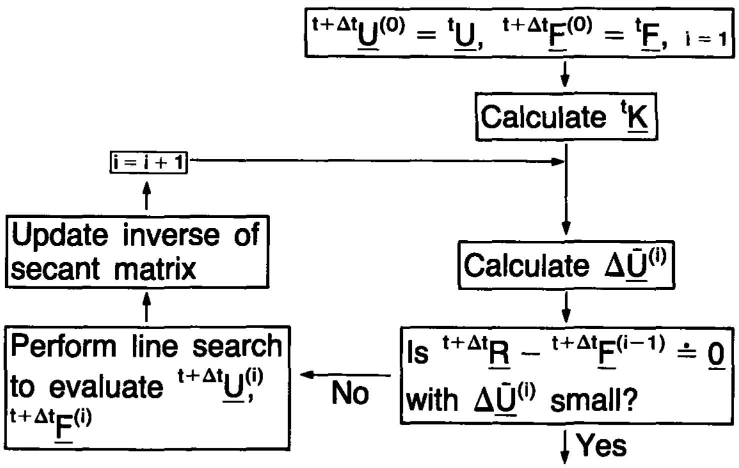
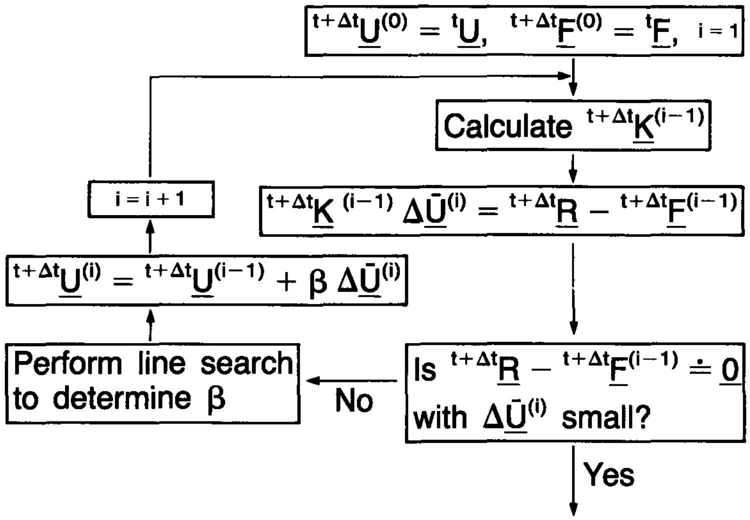
BFGS method:



Full Newton iteration with line searches:



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Convergence criteria:

- These measure how well the obtained solution satisfies equilibrium.
- We use
    1) Energy
    2) Force (or moment)
    3) Displacement

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On energy:

$$\frac{\Delta \underline{\bar{U}}^{(i)T} \left({}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)} \right)}{\Delta \underline{\bar{U}}^{(1)T} \left({}^{t+\Delta t}\underline{R} - {}^{t}\underline{F} \right)} \leq \text{ETOL}$$

(Note: applied prior to line searching)

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On forces:

$$\frac{\left\| {}^{t+\Delta t}\underline{R} - {}^{t+\Delta t}\underline{F}^{(i-1)} \right\|_2}{\underbrace{\text{RNORM}}_{\text{reference force}}} \leq \text{RTOL}$$

reference force
(for moments, use RMNORM)

Typically, RTOL = 0.01
RNORM = $\max \| \underbrace{{}^{t}\underline{R}} \|_2$

considering only translational degrees of freedom

Note: $\|\underline{a}\|_2 = \sqrt{\sum_k (a_k)^2}$

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On displacements:

$$\frac{\|\Delta \underline{\bar{U}}^{(i)}\|_2}{\text{DNORM}} \leq \text{DTOL}$$

reference displacement
(for rotations, use DMNORM)