

# Solution Algorithms for Nonlinear Problems

© Thomas J.R. Hughes

1

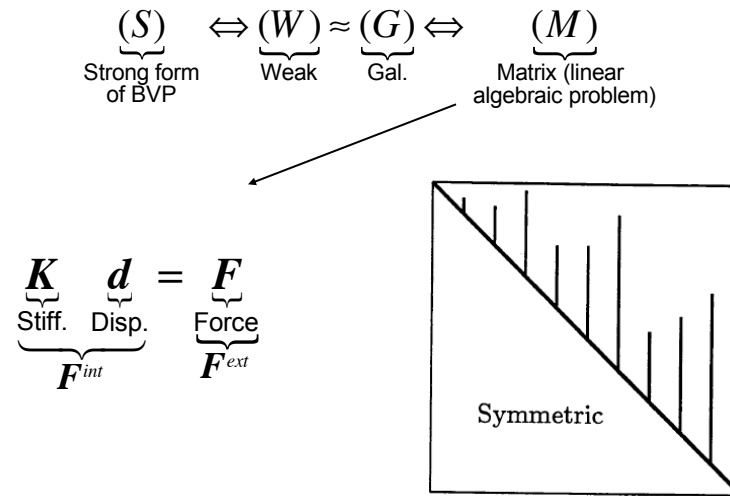
## Outline

- Consistent linearization
- Newton and modified Newton methods
- Line search
- Quasi-Newton methods (“BFGS”)
- Arc-length methods
- Convergence criteria

2

## Brief Overview of Linear Finite Element Analysis

### Statics



3

### Dynamics



$$\underbrace{\mathbf{M}^*}_{\text{Effective mass}} \underbrace{\Delta \mathbf{a}}_{\text{Acceleration increment}} = \underbrace{\mathbf{R}}_{\text{Residual or out-of-balance force}}$$

+ update formulas

In each case, a linear algebraic problem

$$\mathbf{Ax} = \mathbf{b}$$

4

## Nonlinear Finite Element Analysis

### Nonlinear statics

$$(S) \Leftrightarrow (W) \approx (G) \Leftrightarrow \text{Nonlinear problem}$$

$$\mathbf{F}^{int} = \underbrace{\mathbf{F}^{ext}}_{\text{known}}$$

e.g. elastostatics

$$\mathbf{F}^{int} = \mathbf{N}(\underbrace{\mathbf{d}}_{?}) = \text{Nonlin. algebraic ftn. of } \mathbf{d}$$

$$\mathbf{N} : \mathbb{R}^{n_{eq}} \rightarrow \mathbb{R}^{n_{eq}} \quad (\text{vect. valued ftn. of vect. } \mathbf{d})$$

$$\mathbf{N} = \{N_P\}, \quad 1 \leq P \leq n_{eq}$$

$\uparrow$   
 eq. no.

5

### Nonlinear dynamics

$$(S) \Leftrightarrow (W) \approx (G) \Leftrightarrow \begin{matrix} \text{Nonlin.} \\ \text{o.d.e.'s} \end{matrix} \approx \begin{matrix} \text{time-} \\ \text{stepping} \\ \text{algorithm} \end{matrix}$$

$$\mathbf{M}\ddot{\mathbf{d}} + \underbrace{\mathbf{F}^{int}}_{\substack{\mathbf{N}(\mathbf{d}) \\ \text{in elas.}}} = \mathbf{F}^{ext}$$

$$\mathbf{N}^*(\underbrace{\Delta \mathbf{a}}_{?}) = \mathbf{R}$$

We need to solve:

### nonlinear algebraic problems

Reduce to the solution of **linear** algebraic problems by way of incremental/iterative strategies

6

## Residual Methods

Assume the external load is parameterized by “time” (or equivalently, a load parameter).

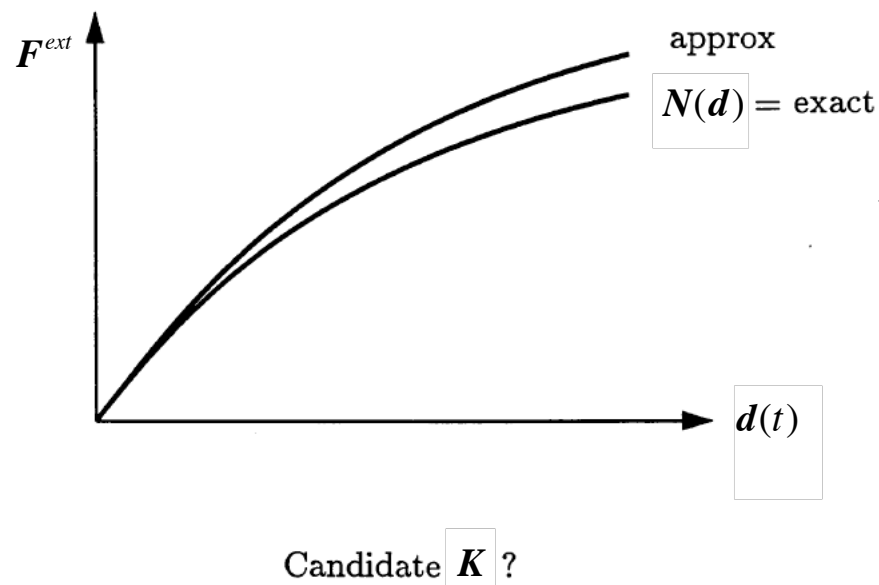
Try to achieve:

$$0 = \underbrace{\mathbf{F}^{ext}}_{\mathbf{F}^{ext}(t)} - \underbrace{\mathbf{F}^{int}}_{\text{e.g. } \mathbf{N}(\mathbf{d}(t))} \quad (\text{residual})$$

Example: **Incremental load method**

$$\begin{aligned} \left[ \begin{array}{l} \mathbf{K} \\ \text{matrix} \end{array} \right] \Delta \mathbf{d} &= \mathbf{R}^{n+1} \stackrel{\text{def}}{=} \underbrace{\mathbf{F}^{ext}}_{\mathbf{F}^{ext}(t_{n+1})} - \underbrace{\mathbf{F}^{int}}_{\mathbf{N}(\mathbf{d}_n)} \\ \mathbf{d}_{n+1} &= \mathbf{d}_n + \Delta \mathbf{d} \\ n &\leftarrow n + 1 \end{aligned}$$

7



8

## Consistent Tangents

Example 1. **Nonlinear elastostatics**

$$\begin{aligned}
 \mathbf{F}^{int} &= \mathbf{N}(\mathbf{d}) \\
 \mathbf{K}(\mathbf{d}) &\stackrel{\text{def}}{=} \frac{\partial \mathbf{N}(\mathbf{d})}{\partial \mathbf{d}} \quad (\text{tangent stiffness}) \\
 \mathbf{N} &= \{N_P\} \\
 \mathbf{K} &= \frac{\partial \mathbf{N}}{\partial \mathbf{d}} = \left[ \underbrace{\frac{\partial N_P}{\partial d_Q}}_{K_{PQ}} \right], \quad 1 \leq P, Q \leq n_{eq}
 \end{aligned}$$

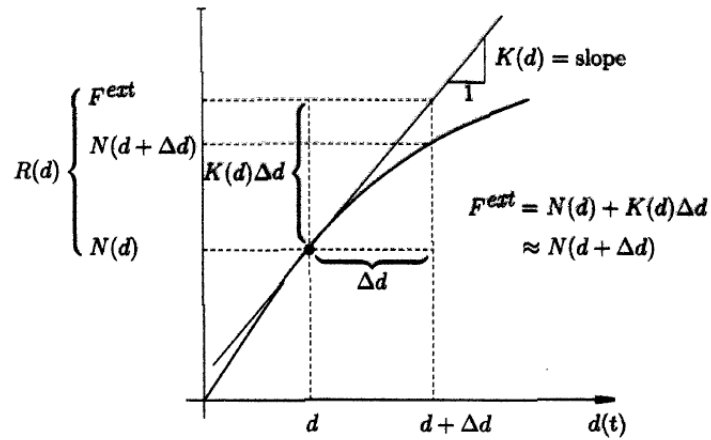
9

Example 1. **Nonlinear elastostatics** (cont.)

(hyper-) elasticity  $\Leftrightarrow \exists \overbrace{U(\mathbf{d})}^{\text{strain energy}}$  such that

$$\begin{aligned}
 \mathbf{N} &= \frac{\partial U}{\partial \mathbf{d}}, \quad \text{i.e.} \quad N_P = \frac{\partial U}{\partial d_P} \\
 \Rightarrow K_{PQ} &= \frac{\partial N_P}{\partial d_Q} = \frac{\partial^2 U}{\partial d_Q \partial d_P} = K_{QP} \\
 \mathbf{K} &= \mathbf{K}^\top \quad \text{symmetric}
 \end{aligned}$$

10



11

What's good about consistent tangents?

According to Taylor's theorem, the consistent tangent is the **best local approximation** in the sense that

$$\frac{\|K(d)\Delta d - (N(d + \Delta d) - N(d))\|}{\|\Delta d\|} \rightarrow 0 \quad \text{as} \quad \|\Delta d\| \rightarrow 0$$

$K(d)$  is the unique matrix achieving this property.

**Interpretation:**

$N(d) + K(d)\Delta d$  is a **good local** approximation of  $N(d + \Delta d)$ .

12

### Example 2. Nonlinear heat conduction

$$\mathbf{F}^{int} = \underbrace{\hat{\mathbf{K}}(d)}_{\substack{\text{symm.} \\ \text{matrix}}} \underbrace{d}_{\substack{\text{temperature} \\ \text{vector}}}$$

consistent tangent:  $\frac{\partial \mathbf{F}^{int}}{\partial d} = \left[ \frac{\partial F_p^{int}}{\partial d_Q} \right]$

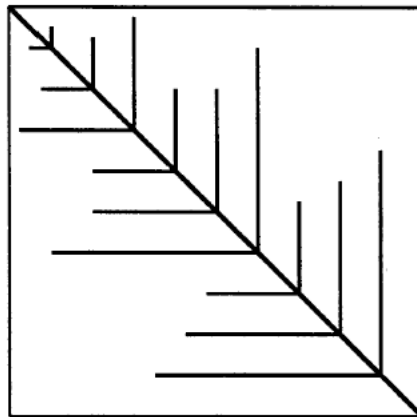
$$\frac{\partial (\overset{\text{sum}}{\hat{K}_{PR} d_R})}{\partial d_Q} = \underbrace{\hat{K}_{PQ}}_{\text{symm.}} + \frac{\partial \hat{K}_{PR}}{\partial d_Q} d_R$$

$$\frac{\partial \hat{K}_{PR}}{\partial d_Q} \stackrel{?}{=} \frac{\partial \hat{K}_{QR}}{\partial d_P} \quad \text{NO!}$$

**Consistent  
tangents are not  
always symmetric.**

13

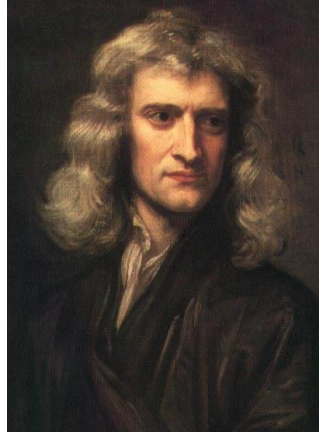
### Costs increase with the loss of symmetric matrices



$\Rightarrow$  Storage  $\times 2$   
Factor  $\times 2$

14


# Newton – Raphson Method



Isaac Newton

*I Joseph Raphson of London Gent.*  
do grant and agree to and with the President, Council,  
and Fellows of the Royal Society of London for improving  
Natural knowledge, That so long as I shall continue a Fel-  
low of the said Society, I will pay to the Treasurer  
of the said Society, for the time being, or to his Deputy, the  
sum of Fifty two shillings per annum; by four equal Quar-  
terly payments, at the four usual days of payment, that is  
to say, the Feast of the Nativity of our Lord; the Feast of  
the Annunciation of the Blessed Virgin Mary; the Feast of  
St. John Baptist; and the Feast of St. Michael the Archangel;  
the first payment to be made upon the *fourth day*  
*of December next being a feast-day*  
*hitherto of our Lord* — — — — —  
next ensuing the Date of these Presents; and I will pay in  
proportion, viz. One shilling per week, for any lesser  
time, after any the said days of payment, that I shall con-  
tinue Fellow of the said Society. For the true payment  
whereof I bind my Self and my Heirs in the penal sum  
of twenty pounds. In witness whereof I have hereunto set  
my Hand and Seal this *fourth day of December*  
One thousand six hundred *sixty nine* Joseph Raphson

Scaled and Delivered  
in the Presence of  
Em. H. B. G.  
sec. Hunt

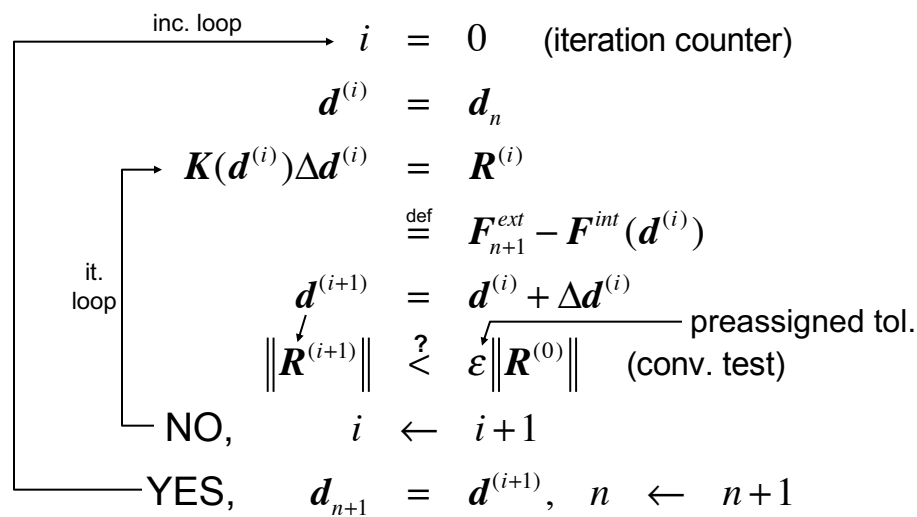


Joseph Raphson

15

A method based on the consistent tangent

## Newton-Raphson



16



where (strictly speaking)

$$\mathbf{K} = \frac{\partial \mathbf{F}^{int}}{\partial \mathbf{d}} = \text{consistent tangent}$$

In practice, frequently replace consistent tangent, e.g., **modified Newton**, etc.

17

### The order of convergence of an iterative scheme

Consider 1 d.o.f.

Let 
$$e^{(i)} = d^{(i)} - \underset{\text{exact}}{d}$$

Write 
$$|e^{(i+1)}| \leq c |e^{(i)}|^k$$

$k$  = **order of convergence**

18

Newton-Raphson is such that  $k = 2$ .

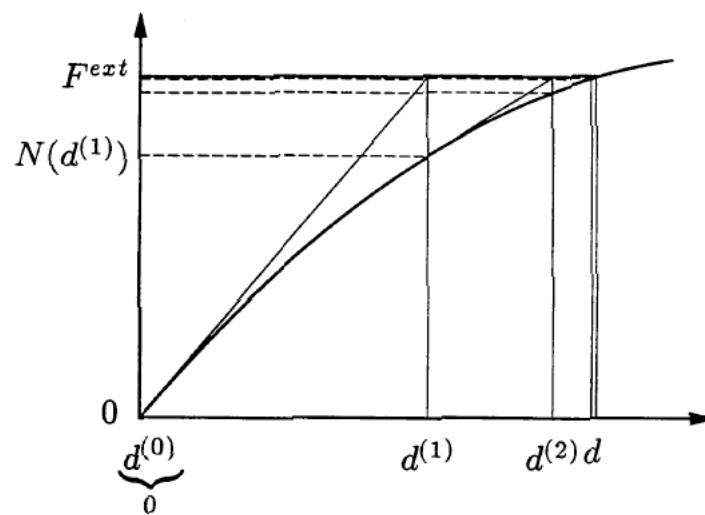
**Interpretation:**

Assume  $|e^{(0)}| = 0.9$ ,  $c = 1$ , then

$i$	$ e^{(i)} $ is $\leq$
1	.81
2	.66
3	.44
4	.19
5	<u>.036</u>
6	<u>.0013</u>
7	<u>.0000016</u>

quadratic convergence  
 $\Rightarrow$  the no. of 0's doubles  
 (at least) in each iteration

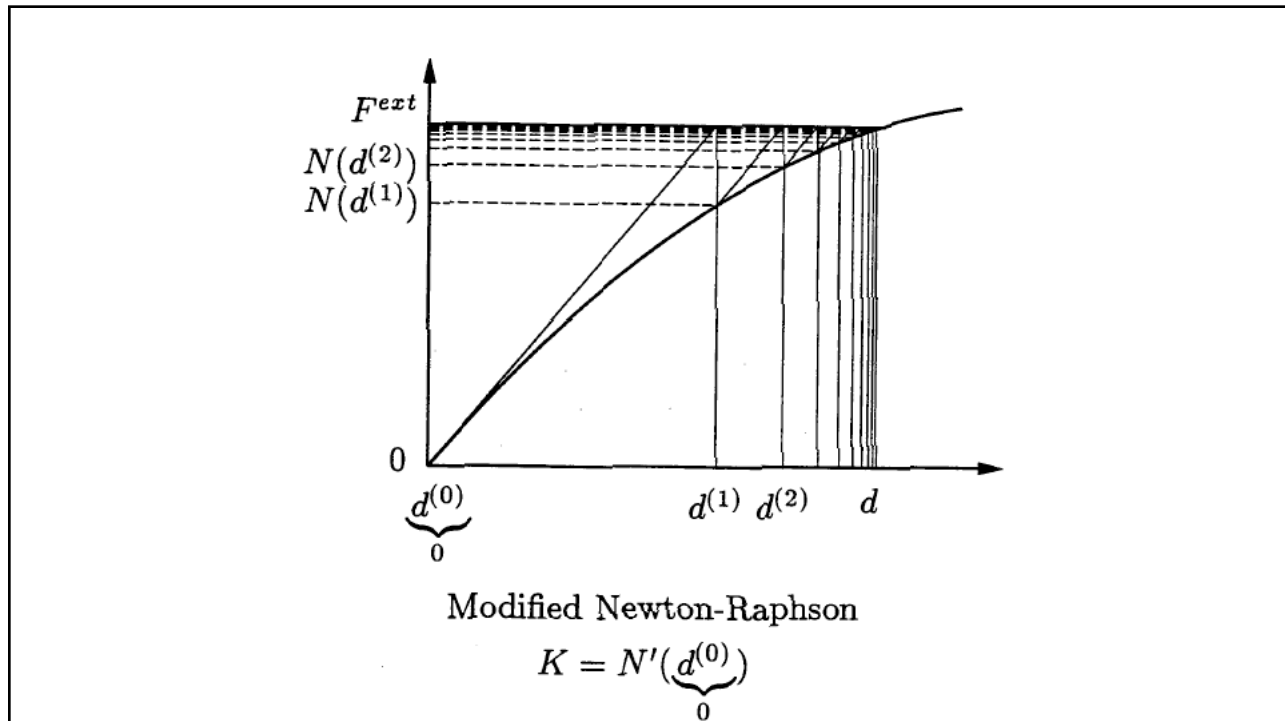
19



Newton-Raphson

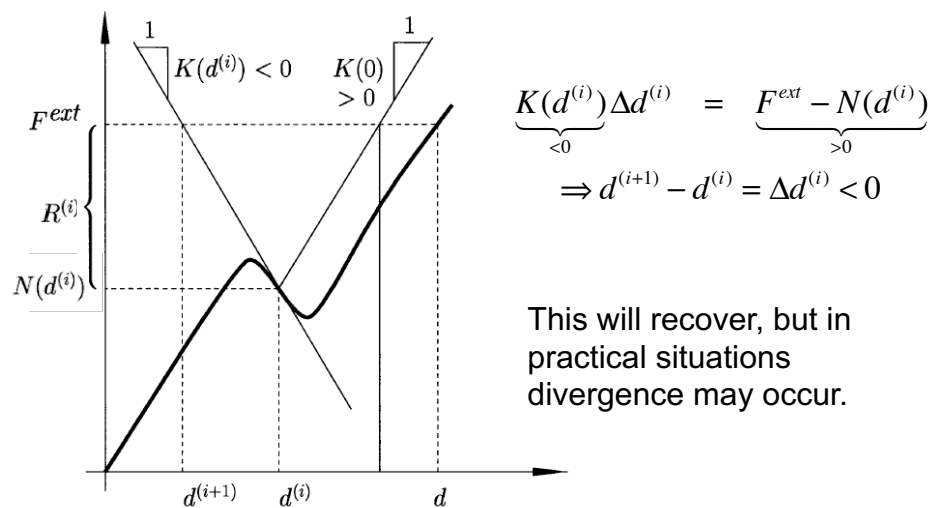
$$K = N'(d^{(i)})$$

20



21

Globally, or far away from the solution, consistent tangents are frequently very poor.



23

Developing an understanding of some aspects of nonlinear equation solving:

1. **Soft/stiff tangent behavior**

1 d.o.f. linear model problem:  $Kd = F$ ,  $K > 0$

Newton-Raphson-type algorithm

$$\underbrace{\tilde{K}}_{\alpha K} \Delta d^{(i)} = F - Kd^{(i)} \quad (= R^{(i)})$$

$$\alpha < 1, \quad \text{soft}$$

$$\alpha > 1, \quad \text{stiff}$$

$$\alpha K(d^{(i+1)} - d^{(i)}) = F - Kd^{(i)}$$

$$-\alpha K(\underbrace{d - d}_0) = -(\underbrace{F - Kd}_0)$$

---


$$\alpha K(e^{(i+1)} - e^{(i)}) = -Ke^{(i)}$$

24

where  $e^{(i)} = d^{(i)} - d$

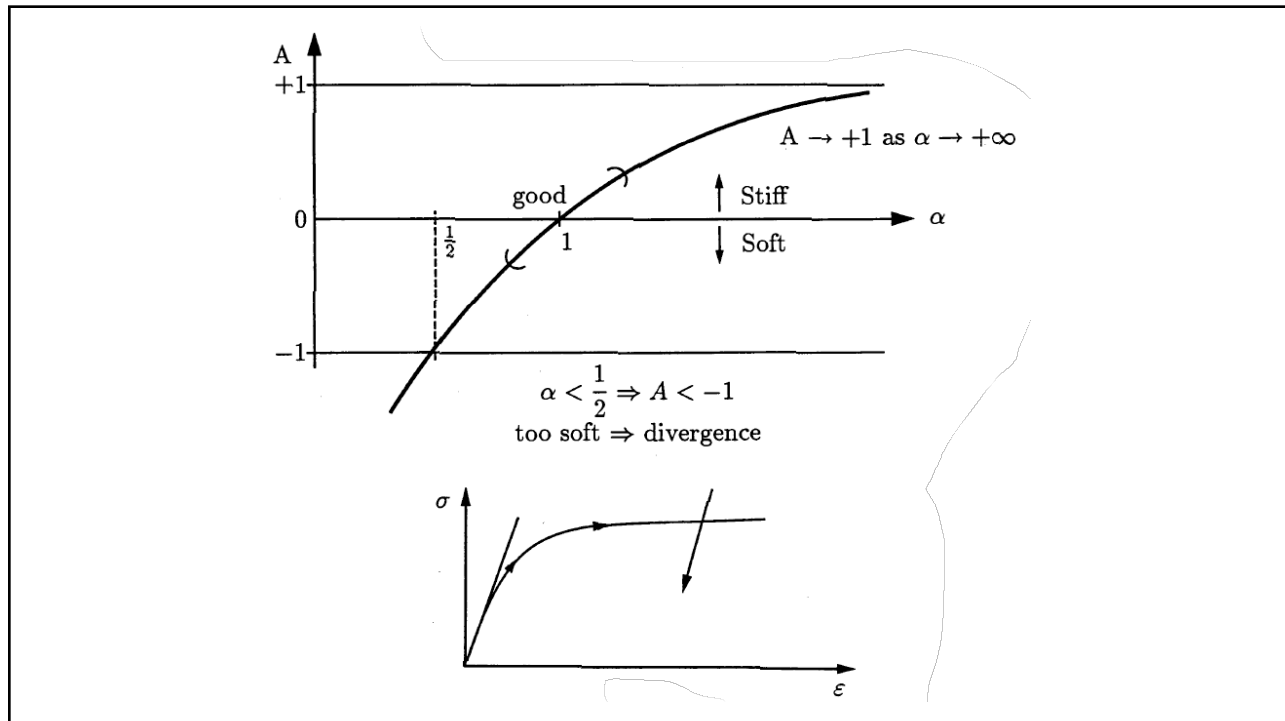
$$e^{(i+1)} = Ae^{(i)}$$

$$A = \frac{\alpha - 1}{\alpha} = 1 - \frac{1}{\alpha}$$

$$\text{convergence} \Leftrightarrow |A| < 1$$

$$\text{divergence} \Leftrightarrow |A| > 1$$

25



26

## 2. Linear systems reduce to 1 d.o.f. model problem

Consider

$$\tilde{K} \Delta d^{(i)} = F - K d^{(i)} \quad (*)$$

$$d^{(i+1)} = d^{(i)} + \Delta d^{(i)}$$

Assume  $K = K^T > 0$

$$\tilde{K} = \tilde{K}^T > 0$$

The associated eigenproblem:

$$(K - \lambda \tilde{K}) \psi = 0$$

Solve for  $\{\lambda, \psi\}_1^{n_{eq}}$ ; leads to uncoupled scalar versions

of (\*):

$$\Delta d_l^{(i)} = F_l - \lambda_l d_l^{(i)}, \quad l = 1, \dots, n_{eq}$$

$\downarrow$   
 no sum

27

Drop “ $l$ ” subscript, proceed as before:

$$\begin{aligned}
 d^{(i+1)} - d^{(i)} &= F - \lambda d^{(i)} \\
 -(d^{(i+1)} - d^{(i)}) &= -(F - \lambda d^{(i)}) \equiv 0
 \end{aligned}$$

↑  
defines  $d$

---


$$e^{(i+1)} = \underbrace{(1 - \lambda)}_A e^{(i)}$$

### Remarks

1.  $\lambda = \frac{1}{\alpha}$  (cf. previous analysis)  $\Rightarrow$  each "mode" reduces to previous analysis.
2. A good  $\tilde{K}$  is such that  $\lambda$ 's are as close to unity as possible.
3. Soft modal components of  $\tilde{K}$  will cause the iteration to **diverge**.

28

## Line Search

### I. Linear case

$$\begin{aligned}
 \tilde{K} \underbrace{\Delta d^{(i)}}_{\substack{\text{search} \\ \text{dir. (vect.)}}} &= F - K d^{(i)} = R^{(i)} \\
 d^{(i+1)} &= d^{(i)} + \underbrace{s^{(i)}}_{\substack{\text{search} \\ \text{param. (scalar)}}} \Delta d^{(i)}
 \end{aligned}$$

What is the proper  $s^{(i)}$  ?

29

### Two derivations

1. Select  $s^{(i)}$  such that the potential energy is minimized

$$p(s^{(i)}) = P(\mathbf{d}^{(i)} + s^{(i)} \Delta \mathbf{d}^{(i)})$$

$$\text{where } P(\mathbf{d}) = \frac{1}{2} \mathbf{d}^\top \mathbf{K} \mathbf{d} - \mathbf{d}^\top \mathbf{F}$$

$$\frac{dp}{ds} = 0 \Rightarrow$$

$$s^{(i)} = \frac{\Delta \mathbf{d}^{(i)} \cdot \mathbf{R}^{(i)}}{\Delta \mathbf{d}^{(i)} \cdot \mathbf{K} \Delta \mathbf{d}^{(i)}}$$

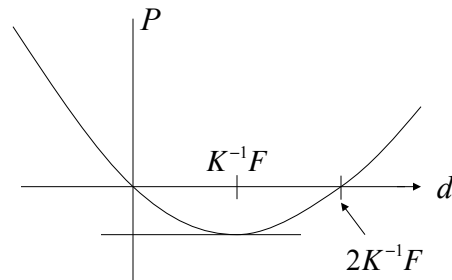
$$> 0, \text{ if } \Delta \mathbf{d} \neq 0$$

30

$$\mathbf{K} \mathbf{d} = \mathbf{F}$$

$$P(\mathbf{d}) = \frac{1}{2} \mathbf{d}^\top \mathbf{K} \mathbf{d} - \mathbf{d}^\top \mathbf{F}$$

$$P'(\mathbf{d}) = 0 \Rightarrow \mathbf{K} \mathbf{d} = \mathbf{F}$$



1 d.o.f. :

$$s^{(i)} = \frac{\cancel{\Delta \mathbf{d}^{(i)\top} \tilde{\mathbf{K}} \Delta \mathbf{d}^{(i)}}}{\cancel{\Delta \mathbf{d}^{(i)\top} \mathbf{K} \Delta \mathbf{d}^{(i)}}}$$

$$= \alpha \frac{K}{K} = \alpha$$

31

### Two derivations (cont.)

2. Select  $s^{(i)}$  such that  $\mathbf{R}^{(i+1)} = \mathbf{F} - \mathbf{K}\mathbf{d}^{(i+1)}$  has zero component in the direction of  $\Delta\mathbf{d}^{(i)}$ , viz.

$$0 = \Delta\mathbf{d}^{(i)} \cdot \mathbf{R}^{(i+1)} \Rightarrow s^{(i)} \text{ above}$$

This criterion is very general and may be applied when no potential exists.

32

### II. Nonlinear cases

$$\tilde{\mathbf{K}}\Delta\mathbf{d}^{(i)} = \mathbf{F}^{ext} - \mathbf{F}^{int}(\mathbf{d}^{(i)})$$

$$\mathbf{d}^{(i+1)} = \mathbf{d}^{(i)} + s^{(i)}\Delta\mathbf{d}^{(i)}$$

Derivation 2 may be used:

$$(*) \quad \underbrace{0 = G(s^{(i)})}_{\substack{\text{Nonlin. scalar} \\ \text{eq. for } s^{(i)}}} = \Delta\mathbf{d}^{(i)} \cdot (\mathbf{F}^{ext} - \mathbf{F}^{int}(\mathbf{d}^{(i)} + s^{(i)}\Delta\mathbf{d}^{(i)}))$$

Strang-Matthies suggest accepting  $s^{(i)}$  if

$$|G(s^{(i)})| \leq \frac{1}{2}|G(0)|$$

For details see H. Matthies and G. Strang, "The solution of Nonlinear F.E. Equations," *IJNME*, Vol. 14, 1613-1626 (1979).

33



**Remarks**

1. If  $\exists$  a potential  $U(\mathbf{d})$  such that

$$\mathbf{F}^{int} = \mathbf{N} = \frac{\partial U}{\partial \mathbf{d}},$$

then derivation 1 also results in (\*). This is the case for nonlinear elastostatics where

$$P(\mathbf{d}) = U(\mathbf{d}) - \mathbf{d}^\top \mathbf{F}$$

2. For situations in which the consistent tangent is not symmetric, positive definite, a minimization of the residual is frequently used to define  $s$  :

$$\min_s \mathbf{R}(\mathbf{d} + s\Delta\mathbf{d}) \cdot \mathbf{R}(\mathbf{d} + s\Delta\mathbf{d})$$

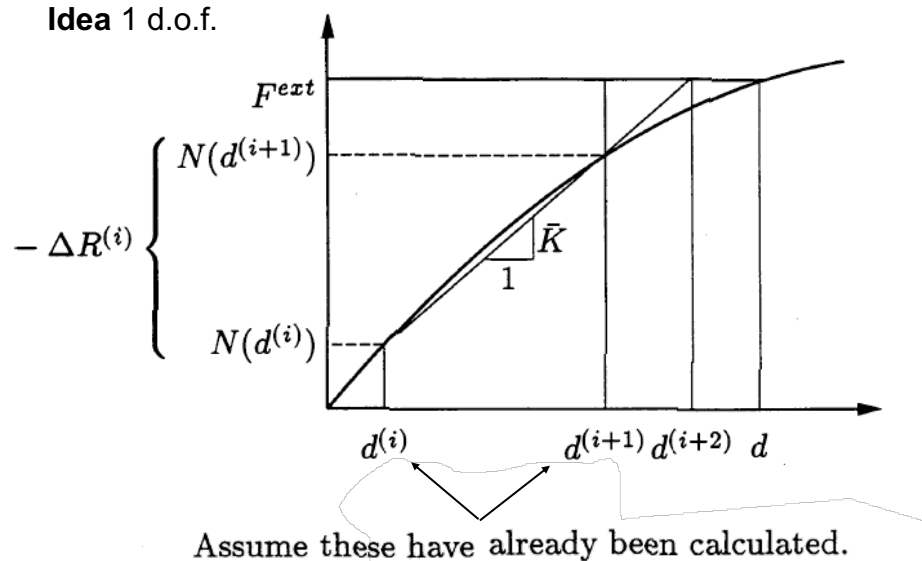
**Caution:** Structural bending elements, multiphysics, etc.

34

**Quasi-Newton Updates**

(Also referred to as **secant updates**)

Idea 1 d.o.f.



35

$$\begin{aligned}
\Delta R^{(i)} &= R^{(i+1)} - R^{(i)} \\
&= \left( \mathcal{K}^{ext} - N(d^{(i+1)}) - \left( \mathcal{K}^{ext} - N(d^{(i)}) \right) \right) \\
&= - \left( N(d^{(i+1)}) - N(d^{(i)}) \right)
\end{aligned}$$

The **secant**  $\bar{K}$  would suffice as a good approximate l.h.s. matrix

$$\bar{K} \equiv \frac{-\Delta R^{(i)}}{(d^{(i+1)} - d^{(i)})} \quad (*)$$

$$\begin{aligned}
\bar{K}(d^{(i+2)} - d^{(i+1)}) &= R^{(i+1)} \equiv F^{ext} - N(d^{(i+1)}) \\
&\text{defines } d^{(i+2)}
\end{aligned}$$

36

For  $n_{eq} = 1$ , (\*) uniquely defines  $\bar{K}$ . The generalization of (\*) for  $n_{eq} > 1$  is

$$\bar{K}(\underbrace{d^{(i+1)} - d^{(i)}}_{\text{known}}) = - \underbrace{\Delta R^{(i)}}_{\text{known}}$$

This is called the **quasi - Newton equation**. It does not uniquely define  $\bar{K}$  for  $n_{eq} > 1$ , but places a restriction on its definition.

Quasi-Newton updates provide definitions for  $\bar{K}$  such that the quasi-Newton equation is satisfied.

37

Quasi-Newton updates are often used with **line searches**.

The quasi-Newton equation becomes

$$\mathbf{d}^{(i+1)} = \mathbf{d}^{(i)} + s^{(i)} \Delta \mathbf{d}^{(i)}$$

$$\bar{\mathbf{K}} s^{(i)} \Delta \mathbf{d}^{(i)} = -\Delta \mathbf{R}^{(i)}$$

38

Perhaps the most widely used in F. E. analysis is BFGS, which we shall describe.

### **BFGS (inverse) update**

Broyden-Fletcher-Goldfarb-Shanno

$$\bar{\mathbf{K}}^{-1} = (\mathbf{I} + \mathbf{v}\mathbf{w}^T) \tilde{\mathbf{K}}^{-1} (\mathbf{I} + \mathbf{w}\mathbf{v}^T)$$

$\mathbf{v}, \mathbf{w}$  are vectors

### **Properties**

1.  $\tilde{\mathbf{K}}^{-1}$  symmetric  $\Rightarrow \bar{\mathbf{K}}^{-1}$  symmetric
2.  $\tilde{\mathbf{K}}^{-1} > 0$  (and  $\mathbf{v} \cdot \mathbf{w} \neq -1$ ), then  $\bar{\mathbf{K}}^{-1} > 0$
3. "Rank-2 update"

39

### Calculations (from right to left)

$$\begin{aligned}
 \Delta d^{(i+1)} &= \bar{K}^{-1} R^{(i+1)} \\
 &= (I + v w^T) \tilde{K}^{-1} \underbrace{(I + w v^T) R^{(i+1)}}_{\underbrace{R^{(i+1)} + (v \cdot R^{(i+1)}) w}_{\tilde{R}}} \\
 &\quad \underbrace{\text{fwd. red./back sub.}}_{=\Delta \bar{d}} \\
 &= \Delta \bar{d} + (w \cdot \Delta \bar{d}) v
 \end{aligned}$$

The factored  $\tilde{K}$  is never altered during the calculations

40

### Series of updates ( $i$ updates)

$\tilde{K}^{-1}$  represents the last formed and factored stiffness.

$$\begin{aligned}
 \bar{K}^{-1} &= (I + v^{(i)} w^{(i)T}) (I + v^{(i-1)} w^{(i-1)T}) \dots \\
 &\quad (I + v^{(1)} w^{(1)T}) \tilde{K}^{-1} (I + w^{(1)} v^{(1)T}) \times \\
 &\quad (I + w^{(2)} v^{(2)T}) \dots (I + w^{(i)} v^{(i)T})
 \end{aligned}$$

41

$$\begin{aligned}
\Delta \mathbf{d}^{(i+1)} &= \tilde{\mathbf{K}}^{-1} \mathbf{R}^{(i+1)} \\
&= \underbrace{\begin{pmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{pmatrix}}_{\substack{i \quad i-1 \quad 1}} \tilde{\mathbf{K}}^{-1} \underbrace{\begin{pmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{pmatrix}}_{\substack{1 \quad 2 \quad i}} \mathbf{R}^{(i+1)} \\
&\quad \left\{ \begin{array}{l} 1. \quad \bar{\mathbf{R}}^{(1)} = \mathbf{R}^{(i+1)} + (\mathbf{v}^{(i)} \cdot \mathbf{R}^{(i+1)}) \mathbf{w}^{(i)} \\ 2. \quad \bar{\mathbf{R}}^{(2)} = \bar{\mathbf{R}}^{(1)} + (\mathbf{v}^{(i-1)} \cdot \bar{\mathbf{R}}^{(1)}) \mathbf{w}^{(i-1)} \\ \vdots \\ i. \quad \bar{\mathbf{R}}^{(i)} = \bar{\mathbf{R}}^{(i-1)} + (\mathbf{v}^{(1)} \cdot \bar{\mathbf{R}}^{(i-1)}) \mathbf{w}^{(1)} \end{array} \right. \\
&\quad \left\{ \begin{array}{l} \text{summary: do } k = 1, \dots, i \\ \bar{\mathbf{R}}^{(k)} = \bar{\mathbf{R}}^{(k-1)} + (\mathbf{v}^{(i-k+1)} \cdot \bar{\mathbf{R}}^{(k-1)}) \mathbf{w}^{(i-k+1)} \\ \text{where } \bar{\mathbf{R}}^{(0)} \equiv \mathbf{R}^{(i+1)} \end{array} \right. \\
&\quad \xrightarrow{\text{Solve}} \Delta \bar{\mathbf{d}}^{(0)} = \tilde{\mathbf{K}}^{-1} \bar{\mathbf{R}}^{(i)} \\
&\quad \Delta \mathbf{d}^{(i+1)} = \underbrace{\begin{pmatrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{pmatrix}}_{\substack{i \quad i-1 \quad 1}} \Delta \bar{\mathbf{d}}^{(0)}
\end{aligned}$$

42

$$\begin{aligned}
&\left\{ \begin{array}{l} 1. \quad \Delta \bar{\mathbf{d}}^{(1)} = \Delta \bar{\mathbf{d}}^{(0)} + (\mathbf{w}^{(1)} \cdot \Delta \bar{\mathbf{d}}^{(0)}) \mathbf{v}^{(1)} \\ 2. \quad \Delta \bar{\mathbf{d}}^{(2)} = \Delta \bar{\mathbf{d}}^{(1)} + (\mathbf{w}^{(2)} \cdot \Delta \bar{\mathbf{d}}^{(1)}) \mathbf{v}^{(2)} \\ \vdots \\ i. \quad \Delta \bar{\mathbf{d}}^{(i)} = \Delta \bar{\mathbf{d}}^{(i-1)} + (\mathbf{w}^{(i)} \cdot \Delta \bar{\mathbf{d}}^{(i-1)}) \mathbf{v}^{(i)} \end{array} \right. \\
&\left\{ \begin{array}{l} \text{summary: do } k = 1, \dots, i \\ \Delta \bar{\mathbf{d}}^{(k)} = \Delta \bar{\mathbf{d}}^{(k-1)} + (\mathbf{w}^{(k)} \cdot \Delta \bar{\mathbf{d}}^{(k-1)}) \mathbf{v}^{(k)} \\ \text{define } \Delta \mathbf{d}^{(i+1)} = \Delta \bar{\mathbf{d}}^{(i)} \end{array} \right.
\end{aligned}$$

43

$$\begin{aligned}\text{Storage} &= \text{no. of BFGS updates} \times 2 \times n_{eq} \\ &= \{\mathbf{v}^{(i)}, \mathbf{w}^{(i)}\}_{i=1}^{\text{no. updates}}\end{aligned}$$

**Definitions of BFGS vectors:**

$$\begin{aligned}\mathbf{v}^{(k)} &= \frac{\Delta \mathbf{d}^{(k)}}{(\Delta \mathbf{d}^{(k)} \cdot \Delta \mathbf{R}^{(k)})} \\ \mathbf{w}^{(k)} &= -\Delta \mathbf{R}^{(k)} + \alpha^{(k)} \mathbf{R}^{(k)} \\ \text{where } \alpha^{(k)} &= \sqrt{\frac{-s^{(k)} \Delta \mathbf{R}^{(k)} \cdot \Delta \mathbf{d}^{(k)}}{\mathbf{R}^{(k)} \cdot \Delta \mathbf{d}^{(k)}}}\end{aligned}$$

44

**Alternative definitions of BFGS vectors commonly used in practice.**

$$\text{Recall: } G^{(k)}(s^{(k)}) = \Delta \mathbf{d}^{(k)} \cdot (\mathbf{R}(\mathbf{d}^{(k)} + s^{(k)} \Delta \mathbf{d}^{(k)}))$$

$$G^{(k)}(0) = \Delta \mathbf{d}^{(k)} \cdot (\mathbf{R}(\mathbf{d}^{(k)}))$$

$$G^{(k)}(s^{(k)}) - G^{(k)}(0) = \Delta \mathbf{d}^{(k)} \cdot \Delta \mathbf{R}^{(k)}$$

---

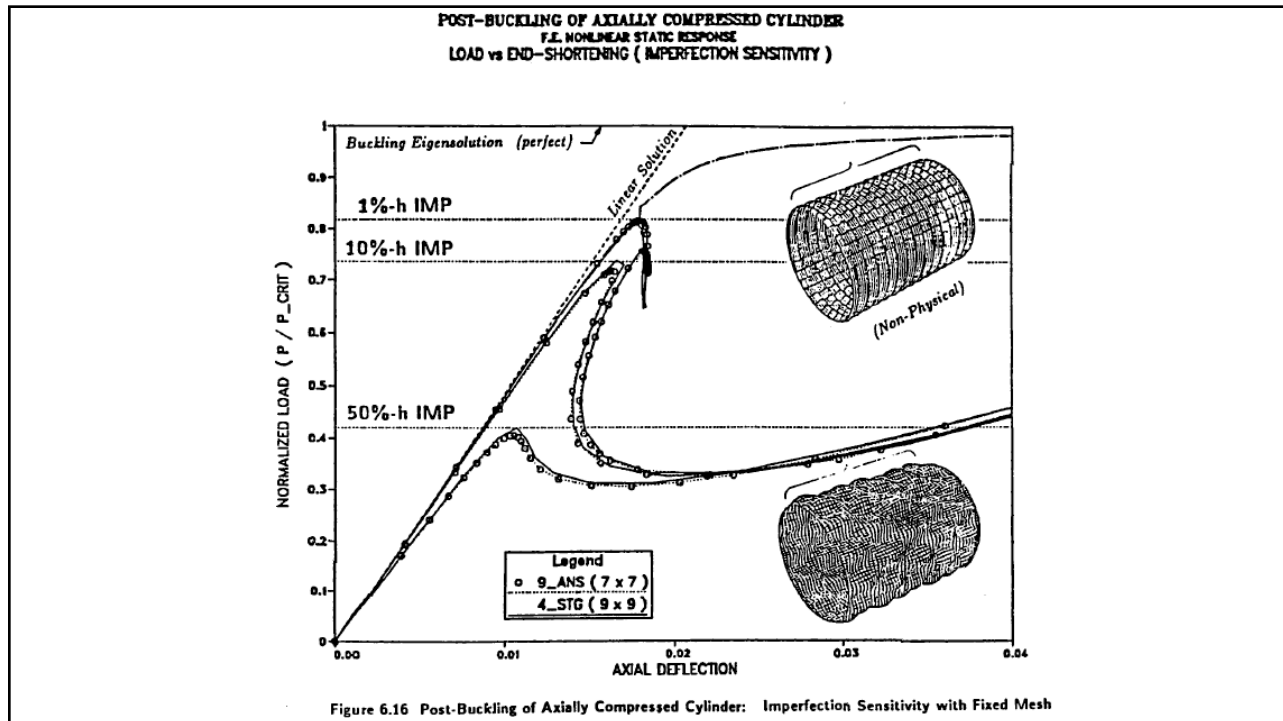

$$\mathbf{v}^{(k)} = \frac{\Delta \mathbf{d}^{(k)}}{(G^{(k)}(s^{(k)}) - G^{(k)}(0))}$$

$$\mathbf{w}^{(k)} = -\Delta \mathbf{R}^{(k)} + \alpha^{(k)} \mathbf{R}^{(k)}$$

$$\text{where } \alpha^{(k)} = \sqrt{\frac{-s^{(k)} (G^{(k)}(s^{(k)}) - G^{(k)}(0))}{G^{(k)}(0)}}$$

(See Strang and Matthies for further details.)

45



46

### Arc-length strategies (written in collaboration with R.M. Ferencz)

So far in this lecture external loading has been assumed to be a **given** function of time. Now we wish to trace load-displacement processes in which there is no **a priori** knowledge of the load-time function.

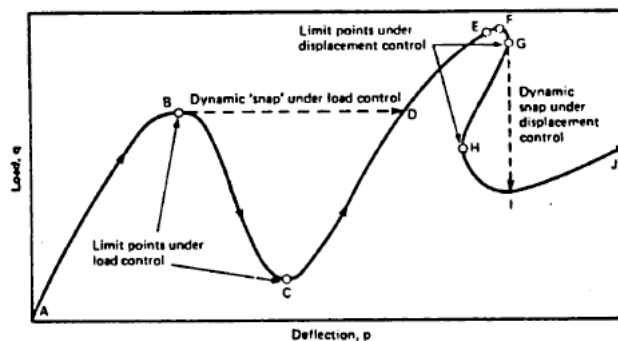


Fig. 1. "Snap buckling". (Crisfield 1981)

47

Better methods are clearly needed. In structures, the basic ideas are due to Riks, Wempner, Ramm, Bergan and Crisfield. Some useful references follow. In the mathematical literature, these techniques are referred to as **continuation methods**, in structures they are called **arc-length methods**.

### References

- M.A. Crisfield, "A Fast Incremental/Iterative Solution Procedure that Handles 'Snap-through' ," *Computers and Structures*, Vol. 13, 55-62, (1981).
- M.A. Crisfield, "An Arc-length Method Including Line Searches and Accelerations," *IJNME*, Vol. 19, 1269-1289, (1983).

48

### References (cont.)

- K.H. Schweizerhof and P. Wriggers, "Consistent Linearization for Path Following Methods in Nonlinear F.E. Analysis," *CMAME*, Vol. 59, 261-279, (1986)
- C.A. Felippa, "Solution of Nonlinear Static Equations," *Handbook Series on Computer Methods in Mechanics*, Volume on Large Deflection and Stability of Structures.

49



The essential idea in arc-length strategies is to control the arc-length of the solution curve in force-displacement space. This will accommodate automatic unloading as is needed to trace the solution curves in the above fig. A scalar arc-length function (i.e. constraint equation) is introduced along with an additional unknown, the loading parameter, to automatically control the amplitude of applied loading. The continuous version of the problem may be stated as follows:

<p>Find <math>\mathbf{d}(t)</math> and <math>\lambda(t)</math> such that</p> $(*) \quad \begin{cases} \mathbf{F}^{int}(\mathbf{d}(t)) = \lambda(t) \mathbf{F}^{ext} \\ f(\dot{\mathbf{d}}, \dot{\lambda}) = \dot{a} = \text{given} \end{cases}$	<p>where</p> <p><math>a =</math> arc-length</p> <p><math>f =</math> arc-length function</p> <p><math>(\dot{\phantom{x}}) = \frac{\partial(\phantom{x})}{\partial t}</math></p>
---	--

50

$f$  should satisfy the definition of a norm on the  $n_{eq} + 1$  dimensional space consisting of pairs  $\dot{\mathbf{d}}, \dot{\lambda}$ .

The discrete form of (\*) is seen more frequently in the literature:

$$\left. \begin{aligned} \mathbf{F}^{int}(\underbrace{\mathbf{d}_{n+1}}_{\text{unknown}}) &= \underbrace{\lambda_{n+1}}_{\text{unknown}} \mathbf{F}^{ext} \\ f(\delta \mathbf{d}, \delta \lambda) &\equiv f(\mathbf{d}_{n+1} - \mathbf{d}_n, \lambda_{n+1} - \lambda_n) \\ &= \delta a = \text{given} \end{aligned} \right\} \quad (**)$$

51

As a candidate  $f$  consider:

$$f(\delta \mathbf{d}, \delta \lambda) = \sqrt{(c \delta \mathbf{d}^T \text{diag} \tilde{\mathbf{K}}_0 \delta \mathbf{d} + b \delta \lambda^2}$$

where

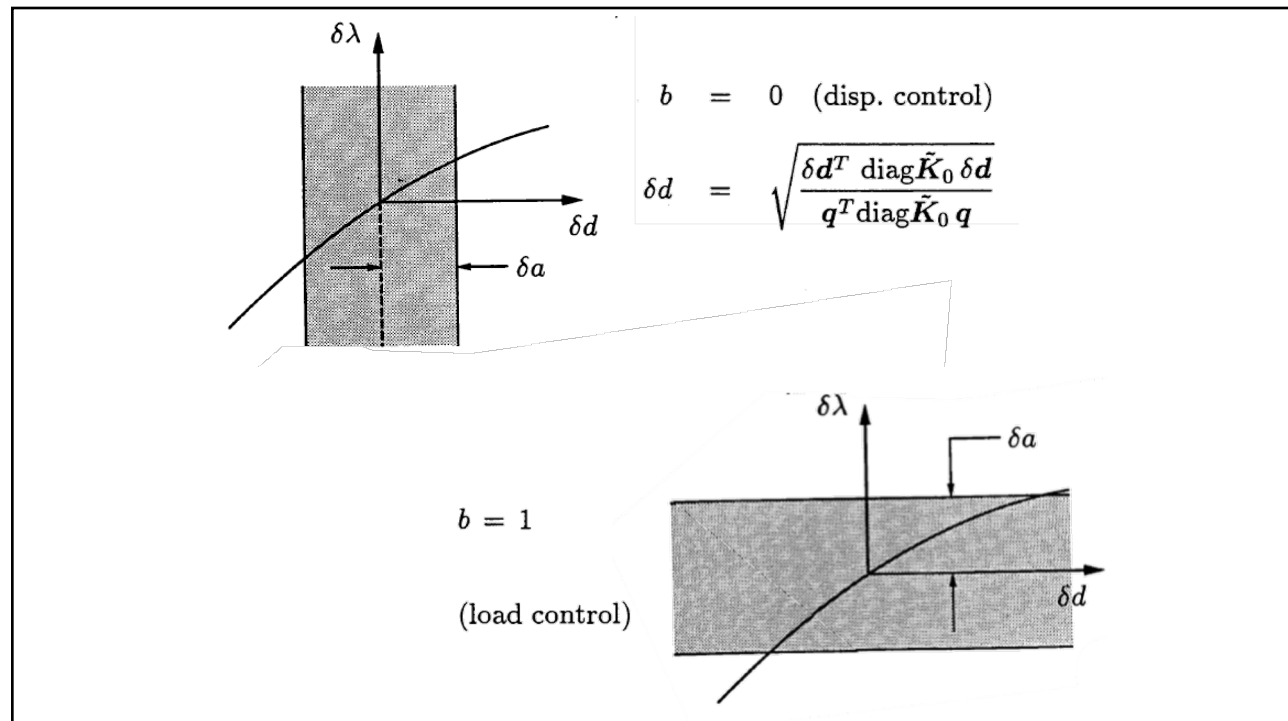
$$c = \frac{(1-b)}{(\mathbf{q}^T \text{diag} \tilde{\mathbf{K}}_0 \mathbf{q})}$$

$$\mathbf{q} = \tilde{\mathbf{K}}_0^{-1} \mathbf{F}^{ext}$$

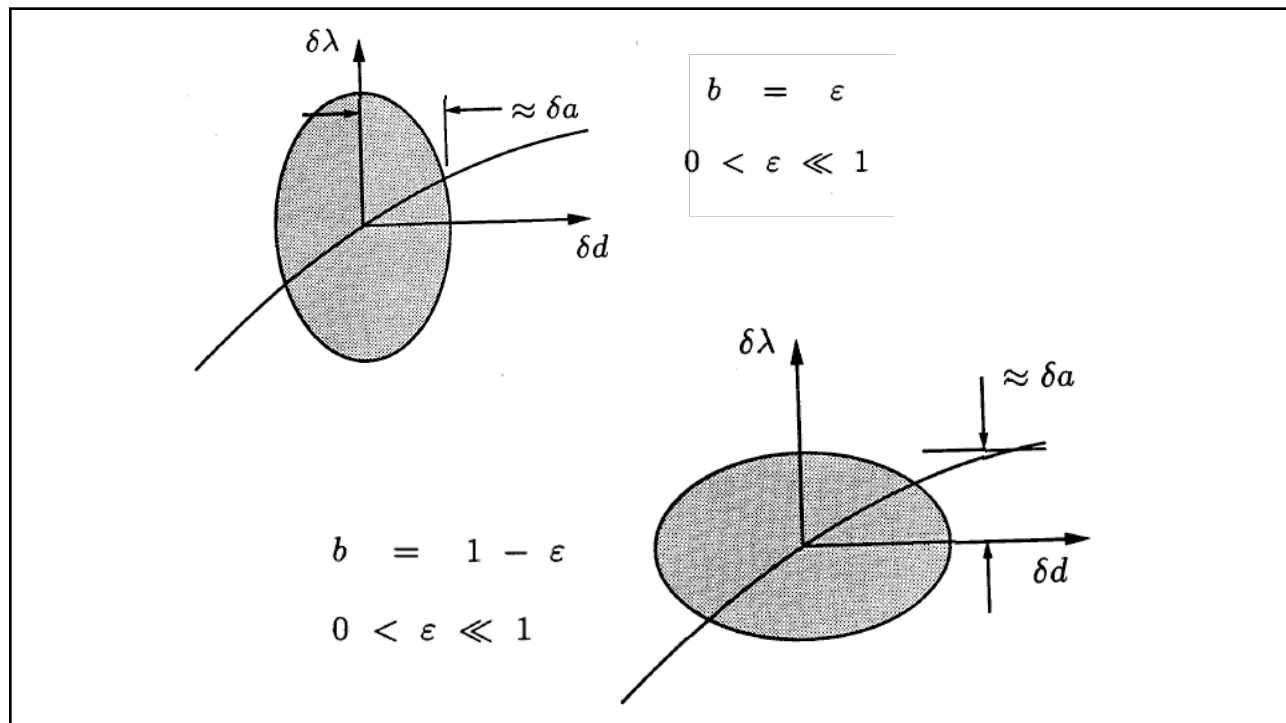
$$b \in [0,1]$$

and  $\tilde{\mathbf{K}}_0$  is the first formed/factorized l.h.s. matrix.

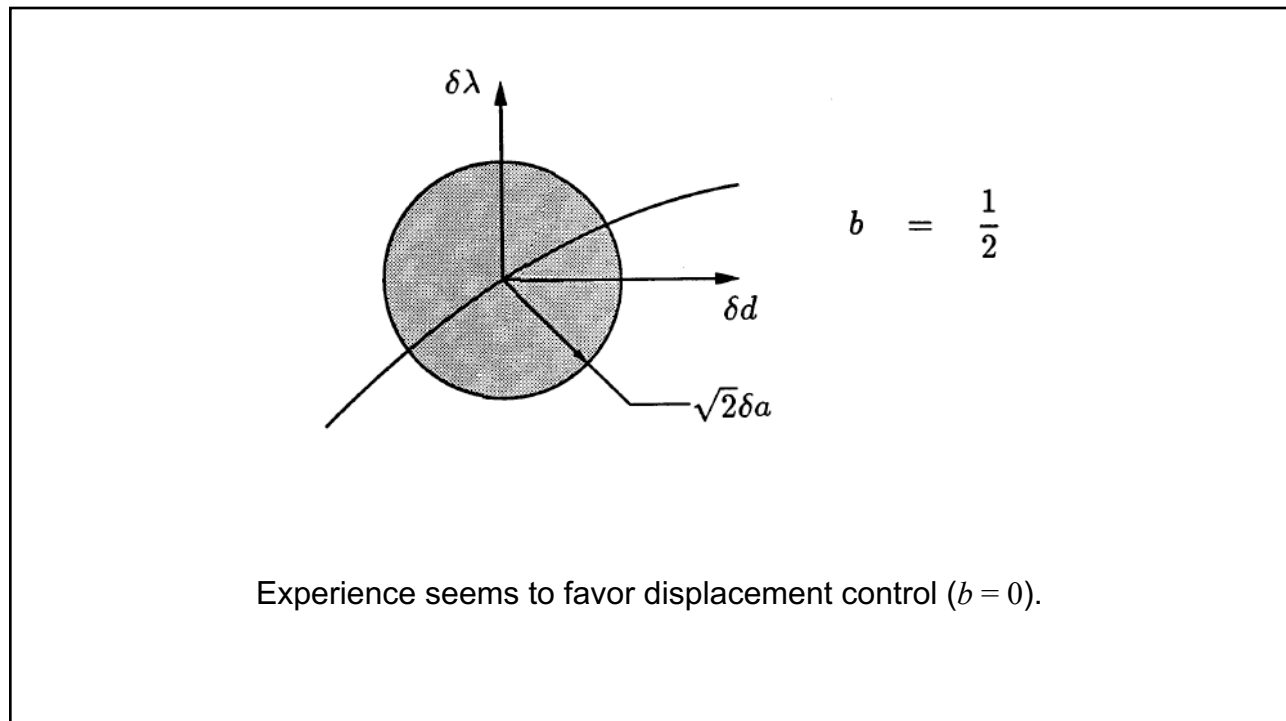
52



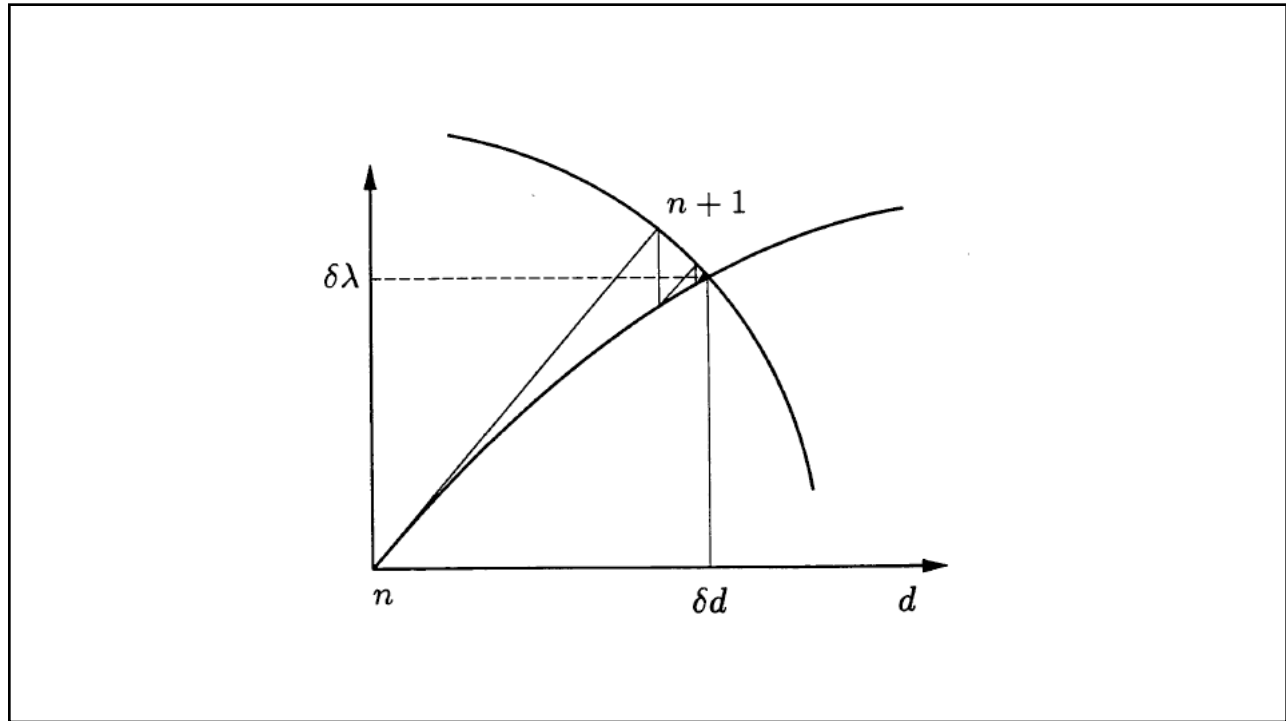
53



54



55



56

### Solution of (\*\*)

Consistently linearize (\*\*) w.r.t.  $d_{n+1}$  and  $\lambda_{n+1}$ . That is

$$d_{n+1} \leftarrow d_{n+1}^{(i)} + \Delta d^{(i)}$$

$$\lambda_{n+1} \leftarrow \lambda_{n+1}^{(i)} + \Delta \lambda^{(i)}$$

in (\*\*) and linearize w.r.t.  $\Delta d^{(i)}$  and  $\Delta \lambda^{(i)}$ . Using Taylor's formula:

$$\begin{aligned} F^{int}(d_{n+1}^{(i)}) + K(d_{n+1}^{(i)})\Delta d^{(i)} &\cong F^{int}(d_{n+1}^{(i)} + \Delta d^{(i)}) \\ &= (\lambda_{n+1}^{(i)} + \Delta \lambda^{(i)})F^{ext} \end{aligned}$$

57

$$\begin{aligned}
& f_{n+1}^{(i)} + \left( \frac{\partial f}{\partial \delta \mathbf{d}} \right)_{n+1}^{(i)} \cdot \Delta \mathbf{d}^{(i)} + \left( \frac{\partial f}{\partial \delta \lambda} \right)_{n+1}^{(i)} \cdot \Delta \lambda^{(i)} \\
& \cong f(\mathbf{d}_{n+1}^{(i)} + \Delta \mathbf{d}^{(i)} - \mathbf{d}_n, \lambda_{n+1}^{(i)} + \Delta \lambda^{(i)} - \lambda_n) \\
& = \delta a
\end{aligned}$$

where

$$\begin{aligned}
f_{n+1}^{(i)} &= f(\delta \mathbf{d}^{(i)}, \delta \lambda^{(i)}) \\
\left( \frac{\partial f}{\partial \delta \mathbf{d}} \right)_{n+1}^{(i)} &= \frac{\partial f}{\partial \delta \mathbf{d}}(\delta \mathbf{d}^{(i)}, \delta \lambda^{(i)}) \\
\left( \frac{\partial f}{\partial \delta \lambda} \right)_{n+1}^{(i)} &= \frac{\partial f}{\partial \delta \lambda}(\delta \mathbf{d}^{(i)}, \delta \lambda^{(i)}) \\
\delta \mathbf{d}^{(i)} &= \mathbf{d}_{n+1}^{(i)} - \mathbf{d}_n \\
\delta \lambda^{(i)} &= \lambda_{n+1}^{(i)} - \lambda_n
\end{aligned}$$

58

$n_{eq} + 1$  equation matrix problem :

$$\begin{bmatrix} \mathbf{K} & -\mathbf{F}^{ext} \\ \frac{\partial f}{\partial \delta \mathbf{d}} & \frac{\partial f}{\partial \delta \lambda} \end{bmatrix} \begin{Bmatrix} \Delta \mathbf{d}^{(i)} \\ \Delta \lambda^{(i)} \end{Bmatrix} = \begin{Bmatrix} \overbrace{\lambda_{n+1}^{(i)} \mathbf{F}^{ext} - \mathbf{F}^{int}(\mathbf{d}_{n+1}^{(i)})}^{\mathbf{R}_{n+1}^{(i)}} \\ \delta a - f_{n+1}^{(i)} \end{Bmatrix}$$

### Remarks

1.  $\mathbf{K}$  can be replaced by any convenient l.h.s. matrix, say  $\bar{\mathbf{K}}$ , accounting, e.g., for quasi-Newton updates.
2. Line searches may also be accounted for by updating

$$\mathbf{d}_{n+1}^{(i+1)} = \mathbf{d}_{n+1}^{(i)} + s^{(i)} \Delta \mathbf{d}^{(i)}$$

59

where  $s^{(i)}$  is defined by

$$\begin{aligned} 0 &= G(s^{(i)}) \\ &\equiv \Delta \mathbf{d}^{(i)} \cdot \left( \lambda_{n+1}^{(i)} \mathbf{F}^{ext} - \mathbf{F}^{int}(\mathbf{d}_{n+1}^{(i)} + s^{(i)} \Delta \mathbf{d}^{(i)}) \right) \end{aligned}$$

3. It is not expensive to calculate  $\frac{\partial f}{\partial \delta \mathbf{d}}$  and  $\frac{\partial f}{\partial \delta \lambda}$ , so normally

the latest updated values are used.

4. Explicit formulae:

$$\begin{aligned} \left( \frac{\partial f}{\partial \delta \mathbf{d}} \right)_{n+1}^{(i)} &= \frac{c}{f_{n+1}^{(i)}} \text{diag} \tilde{\mathbf{K}}_0 \delta \mathbf{d}^{(i)} \\ \left( \frac{\partial f}{\partial \delta \lambda} \right)_{n+1}^{(i)} &= \frac{b}{f_{n+1}^{(i)}} \delta \lambda^{(i)} \end{aligned}$$

60

**Solution** (Note:  $\frac{\partial f}{\partial \delta \lambda}$  may be zero!)

1. Solve first eq. for  $\Delta \mathbf{d}^{(i)}$  as a function of  $\Delta \lambda^{(i)}$  (unknown).

2. Substitute this result into second eq. and solve for  $\Delta \lambda^{(i)}$ .

**Results**

$$\begin{aligned} \Delta \lambda^{(i)} &= \frac{(\delta a - f_{n+1}^{(i)}) - \left( \frac{\partial f}{\partial \delta \mathbf{d}} \right)_{n+1}^{(i)} \cdot \Delta \bar{\mathbf{d}}}{\left( \left( \frac{\partial f}{\partial \delta \mathbf{d}} \right)_{n+1}^{(i)} \cdot \bar{\mathbf{q}} + \left( \frac{\partial f}{\partial \delta \lambda} \right)_{n+1}^{(i)} \right)} \\ \Delta \mathbf{d}_{n+1}^{(i)} &= \Delta \lambda^{(i)} \bar{\mathbf{q}} + \Delta \bar{\mathbf{d}} \\ \Delta \bar{\mathbf{d}} &= \bar{\mathbf{K}}^{-1} \mathbf{R}_{n+1}^{(i)} \\ \bar{\mathbf{q}} &= \bar{\mathbf{K}}^{-1} \mathbf{F}^{ext} \end{aligned}$$

61

### Initialization

To get the arc-length method started in each step requires **specification** of  $\delta\lambda^{(0)}$  and  $\delta\mathbf{d}^{(0)}$ .

Let

$$\begin{aligned}\tilde{\mathbf{q}} &= \tilde{\mathbf{K}}^{-1}(\mathbf{d}_n)\mathbf{F}^{ext} \\ \delta\mathbf{d}^{(0)} &= \delta\lambda^{(0)}\tilde{\mathbf{q}}\end{aligned}$$

Thus all that is required is to define  $\delta\lambda^{(0)}$ . The arc-length constraint determines the **magnitude** of  $\delta\lambda^{(0)}$ .

62

$$\begin{aligned}\delta a &= f(\delta\mathbf{d}^{(0)}, \delta\lambda^{(0)}) \\ &= f(\delta\lambda^{(0)}\tilde{\mathbf{q}}, \delta\lambda^{(0)}) \\ &= |\delta\lambda^{(0)}|f(\tilde{\mathbf{q}}, 1)\end{aligned}$$

$$\Rightarrow |\delta\lambda^{(0)}| = \frac{\delta a}{f(\tilde{\mathbf{q}}, 1)}$$

To determine the **sign** of  $\delta\lambda^{(0)} = \delta\lambda_{n+1}^{(0)}$ , we proceed as follows:

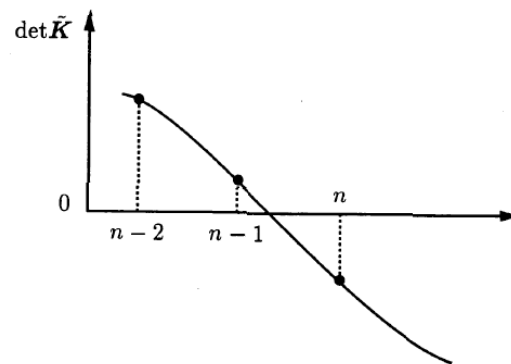
63

If the following two conditions are true we set

$$\text{sign } \delta\lambda^{(0)} = -\text{sign } \delta\lambda_n^{(0)} :$$

(i)  $\det \tilde{\mathbf{K}}(d_n) = -\det \tilde{\mathbf{K}}(d_{n-1})$

(ii) The determinant has passed through **zero**; for example:



64

If **either** of the above is **not** true we set

$$\text{sign } \delta\lambda^{(0)} = \text{sign } \delta\lambda_n^{(0)}$$

#### Remarks

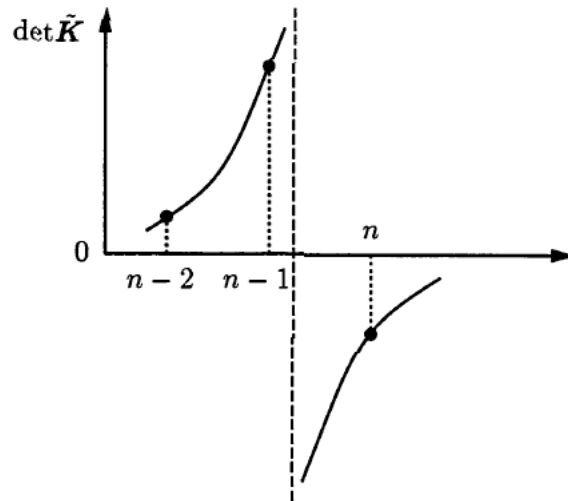
To understand the rationale behind the strategy, consider the scalar case. The condition that the determinant passed through zero corresponds to a **maximum** or a **minimum** in the load-displacement diagram:



65



Note that the determinant can change signs by passing through **infinity**; for example:



66

This corresponds to **turning points** in the load-deflection curve:



#### Remarks

1. An adaptive strategy for increasing/decreasing the size of  $\delta a$  is essential for good performance of the algorithm.
2. Arc-length strategies have not yet progressed to the point where they are 100% reliable.

67

### Convergence

def.  $\|R\|^2 = R^\top (\text{diag } \tilde{K}_0)^{-1} R$

(i) Insist  $\|R_{n+1}^{(i)}\| \leq \varepsilon_R \|R^{(0)}\|$

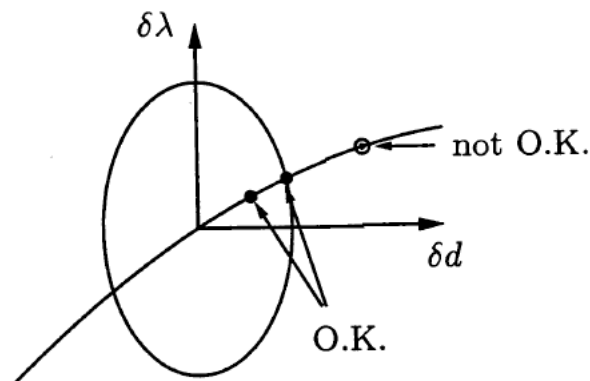
where  $\varepsilon_R$  is a user-specified tolerance.

(ii) In addition, we must ensure arc-length constraint is maintained:

$$f_{n+1}^{(i)} - \delta a \leq \varepsilon_f \delta a$$

68

**Interpretation:**  $d_{n+1}^{(i)}, \lambda_{n+1}^{(i)}$  is inside the ellipse.



69

Some codes also employ a displacement criterion:

$$\text{Let } \|d\|^2 = d^T \text{diag} \tilde{K}_0 d$$

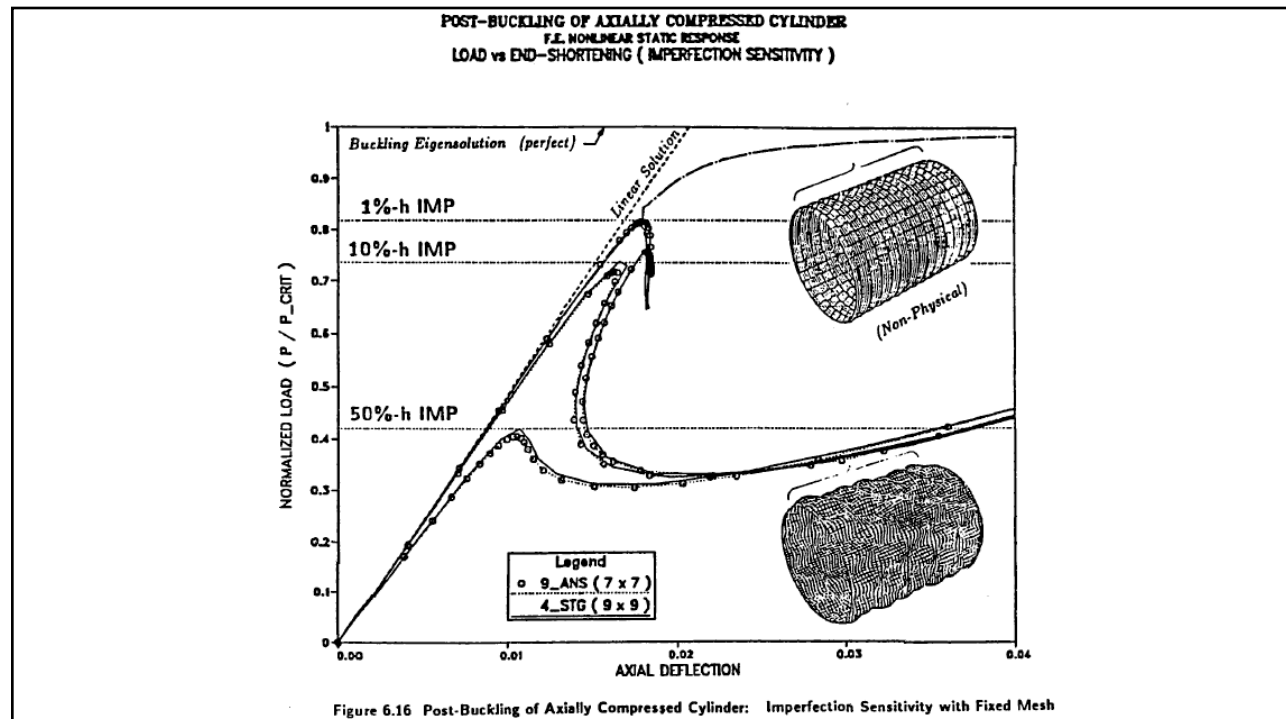
Insist,

$$\|\Delta d^{(i)}\| \leq \varepsilon_d \|\delta d^{(i)}\| = \varepsilon_d \|d_{n+1}^{(i)} - d_n\|$$

As long as  $b \neq 1$  (i.e., not load control), the displacement criterion is redundant with the arc-length constraint. In other situation (e.g., Newton-like methods), the displacement criterion should generally be used.

The next slide shows an application of the arc-length method to a shell buckling problem. From G. Stanley, Ph.D. Thesis, Stanford, 1985.

70



71