Microstructure Mechanics

FEM: Introduction to the Method & Outlook on Applications

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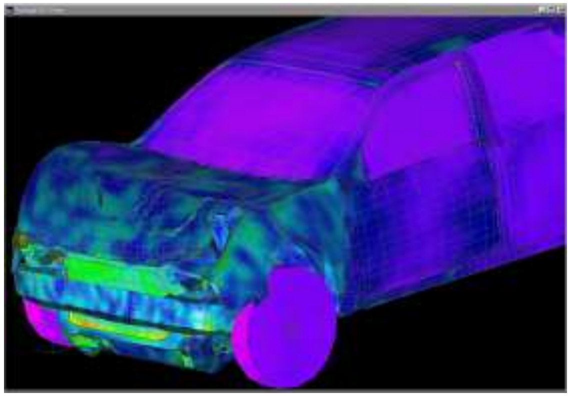
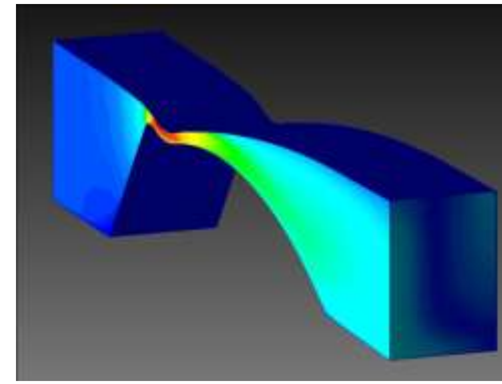
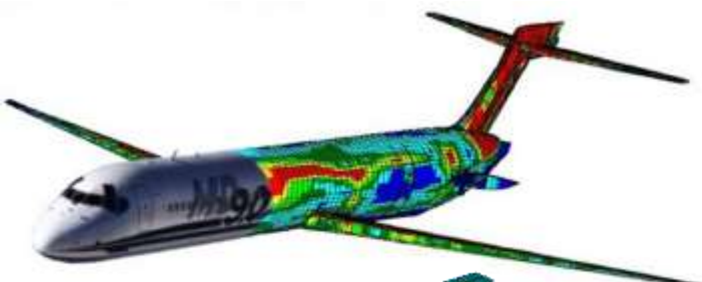
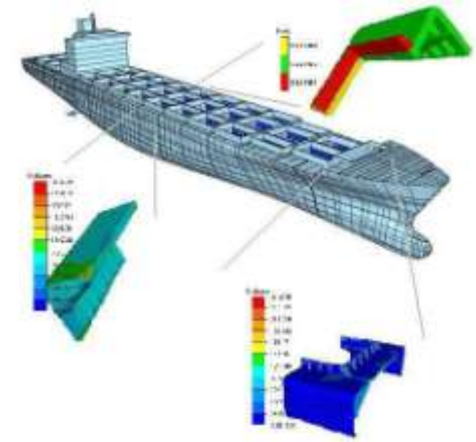
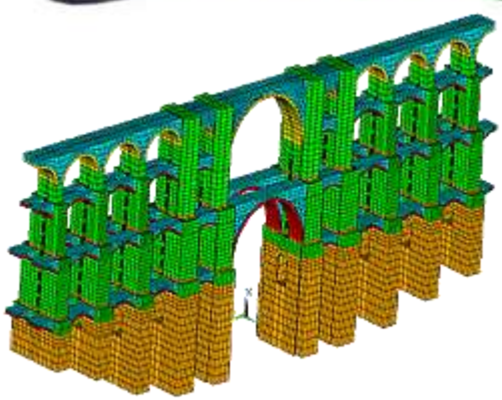
FEM: Finite Element Method

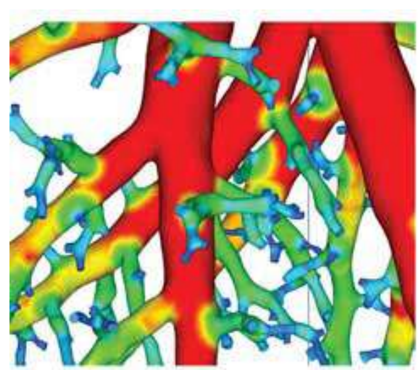












FEM – fields of application

- FEM can be applied to many different problems

Problem Type	DOF #1	DOF #2
Structures and solid mechanics	Displacement	Mechanical force
Heat conduction	Temperature	Heat flux
Acoustic fluid	Displacement potential	Particle velocity
Potential flows	Pressure	Particle velocity
General flows	Velocity	Fluxes
Electrostatics	Electric potential	Charge density
Magnetistatics	Magnetic potential	Magnetic intensity

- Going to use “Structures and solid mechanics” examples
- Easily apply other problem types by substituting appropriate variables and equations

Introduction

FEM is a mathematical tool to solve PDEs

Any physically meaningful output MUST result from physical input provided by you to FEM

Problem (usually partial differential equation) → **FEM** → **Solution**

Decompose problem into pieces

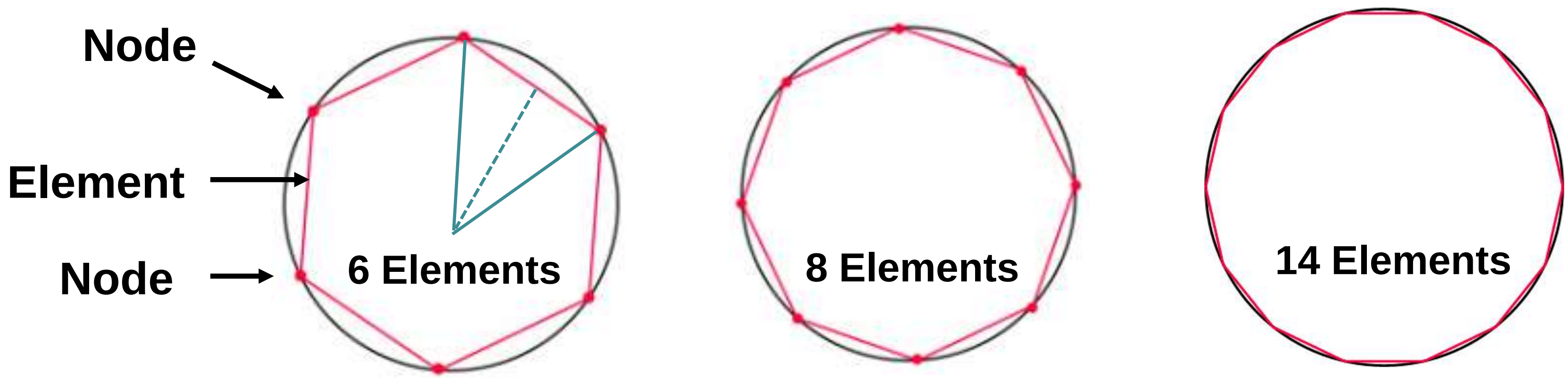
Make simple approximation of solution for each piece

Put the solution pieces together to form global solution

Introduction: discretization (this is NOT FEM)

Example: Computing the circumference of a circle with radius r

- Decompose (or Discretize) the problem



- Approximate solution for each piece (or element)

$$L_e = 2r\sin\frac{\theta}{2}$$

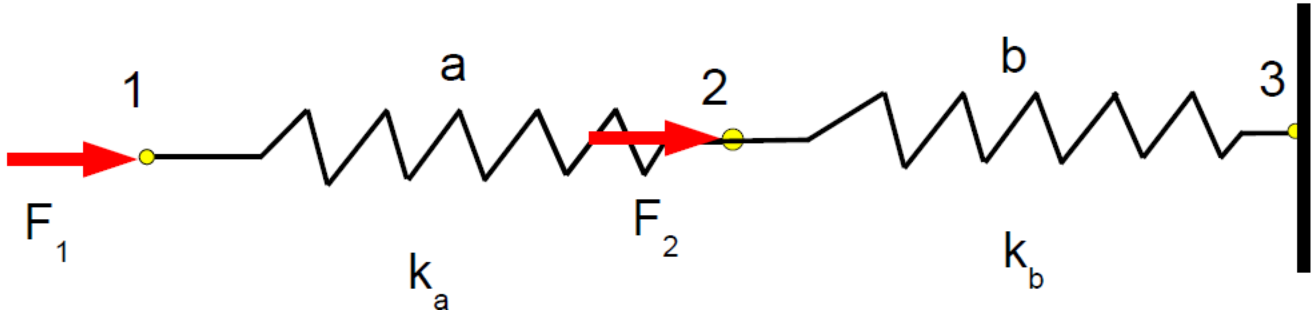
- Assemble the Element Equations and Solve

$$P_c = \sum_{N_e} L_e = \sum_{N_e} 2r\sin\frac{\theta}{2}$$

$N_e = 6$ $P_c = 6.00$ r
$N_e = 8$ $P_c = 6.12$ r
$N_e = 14$ $P_c = 6.23$ r

→ **$2\pi r$**

FEM – example of coupled spring problem



F: force
u: displacement
k: spring constant
1,2: point number
a,b: identifier for discretization

FEM

- Discretize
- Enforce Equilibrium → $\sum F = 0$
- Ensure compatibility (no formation of holes/voids)

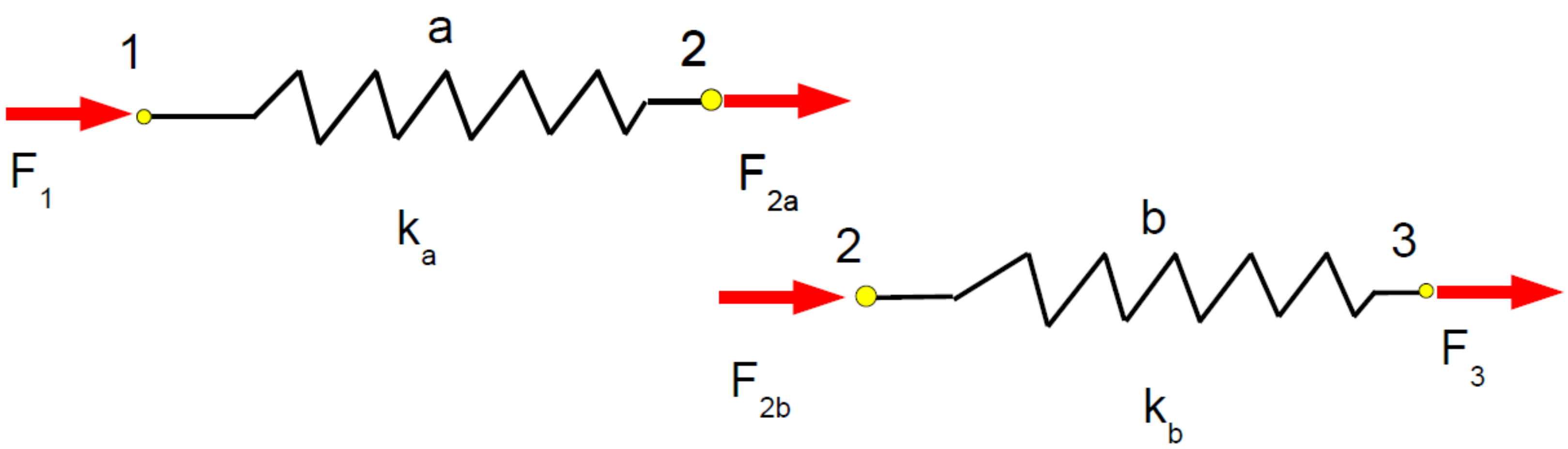
Material Modeling

Provide constitutive equation for each spring
(i.e. what is the relationship between force and displacement)

Model rods as elastic springs → $F = k\,u$

FEM – example of coupled spring problem

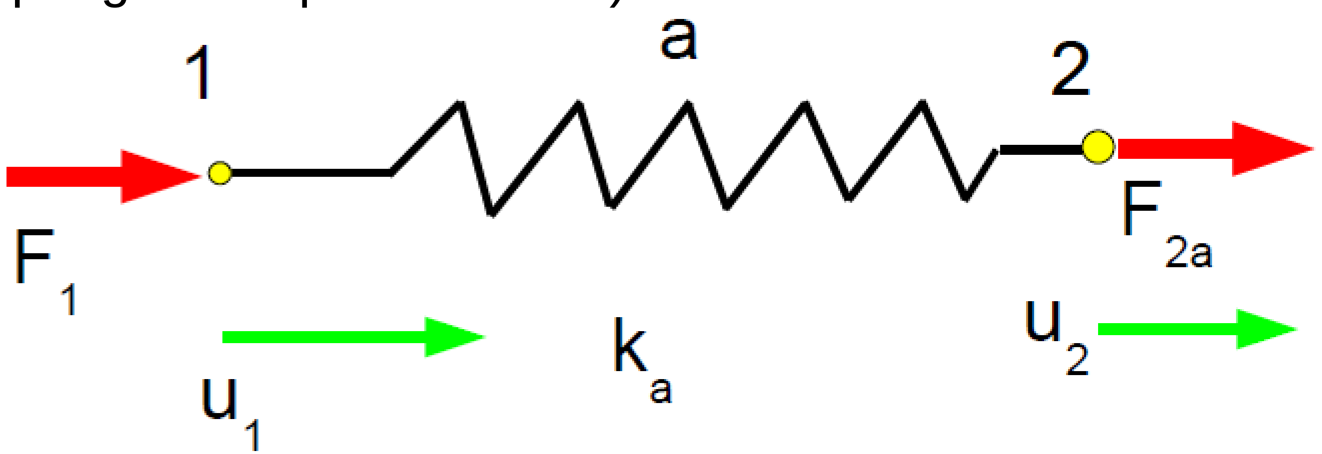
Discretize



FEM – example of coupled spring problem

For each element, write a force balance at each node

Part a, (spring is compressed here)



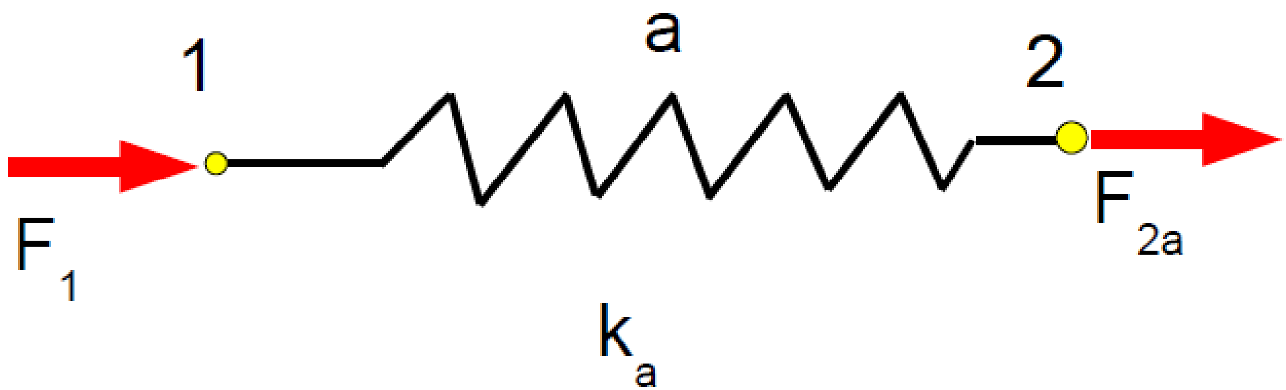
$$F_1 = k_a \cdot (u_1 - u_2);$$

$$F_1 + F_{2a} = 0; \quad \rightarrow \quad F_{2a} = -F_1;$$

$$F_{2a} = k_a \cdot (-u_1 + u_2);$$

FEM – example of coupled spring problem

Part a
(stiffness matrix)



$$F_1 = k_a \cdot (u_1 - u_2);$$

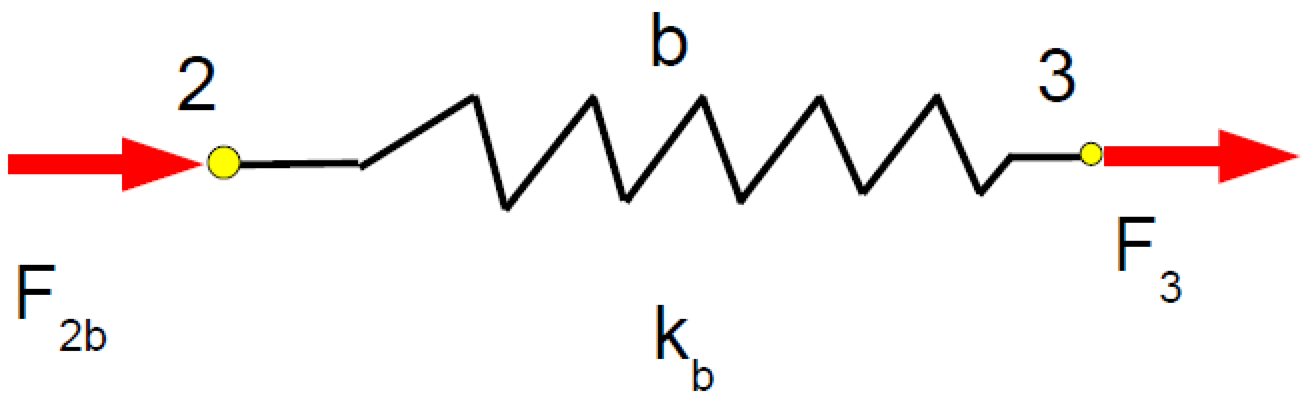
$$F_{2a} = k_a \cdot (-u_1 + u_2);$$

$$\rightarrow \quad \begin{bmatrix} F_1 \\ F_{2a} \end{bmatrix} = \begin{bmatrix} k_a & -k_a \\ -k_a & k_a \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

stiffness matrix part a

FEM – example of coupled spring problem

Part b



$$F_{2b}=k_b\cdot(u_2-u_3);$$

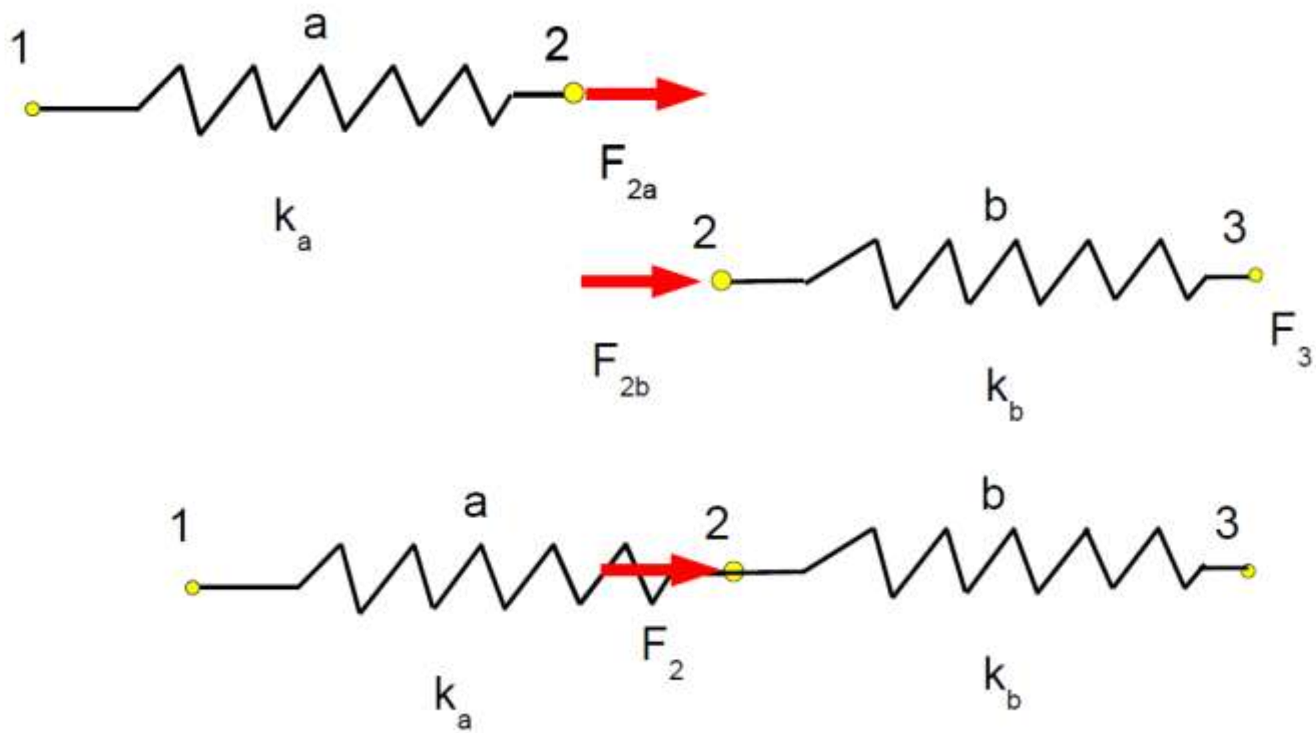
$$F_3=k_b\cdot(-u_2+u_3);$$

$$\begin{bmatrix} F_{2b} \\ F_3 \end{bmatrix}=\begin{bmatrix} k_b & -k_b \\ -k_b & k_b \end{bmatrix}\cdot\begin{bmatrix} u_2 \\ u_3 \end{bmatrix}$$

stiffness matrix part b

FEM – example of coupled spring problem

Total force at point 2 from parts a and b



FEM – example of coupled spring problem

Assemble the force balance equations for all 3 nodes, get total stiffness matrix

$$F_1 = k_a \cdot (u_1 - u_2);$$

$$F_2 = F_{2a} + F_{2b}$$

$$F_2 = F_{2a} + F_{2b} = \quad k_a \cdot (-u_1 + u_2) + k_b \cdot (u_2 - u_3)$$

$$-k_a \cdot u_1 + (k_a + k_b) \cdot u_2 - k_b \cdot u_3$$

$$F_3 = k_b \cdot (-u_2 + u_3);$$

$$\begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = \begin{bmatrix} k_a & -k_a & 0 \\ -k_a & k_a + k_b & -k_b \\ 0 & -k_b & k_b \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

FEM – example of coupled spring problem

$$[K][u]=[f]$$

K = Stiffness Matrix u = displacement vector f = force vector

Apply Boundary Conditions

$$\begin{bmatrix} F_1 \\ F_2 \\ F_3 \end{bmatrix} = \begin{bmatrix} k_a & -k_a & 0 \\ -k_a & k_a+k_b & -k_b \\ 0 & -k_b & k_b \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \\ 0 \end{bmatrix}$$

3 equations and 3 unknowns

Easily solve with a matrix inversion

NOT FEM ! only simple matrix assembly

FEM: Strong Form vs. Weak Form

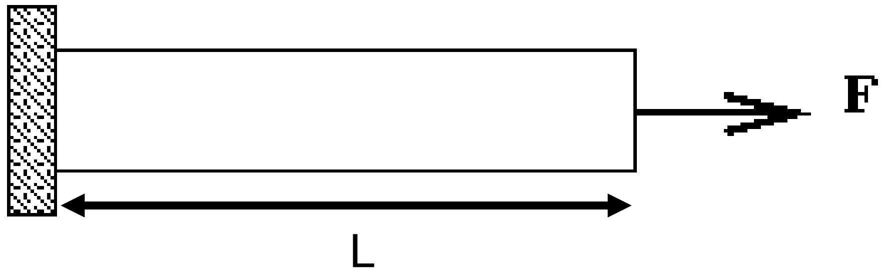
- Governing equations are usually complex differential equations
- Often these equations cannot be solved exactly

PROBLEM
Equations do not permit the exact solution

TOOL
Variational Approach

SOLUTION
Instead of finding an exact solution at every point, we find a solution that satisfies the strong form on average over the domain

FEM: Strong Form vs. Weak Form



Strong Form

- Governing PDE's with boundary conditions

PDE: $$EA\frac{d^2u}{dx^2} = F$$

BC: $$u(0) = 0$$

$$EA\left.\frac{du}{dx}\right|_{x=L} = 0$$

FEM →

Weak Form

- *Variational statement* of the problem

Strong: $$EA\frac{d^2u}{dx^2} = F$$

$$EA\frac{d^2u}{dx^2} - F = 0$$

Weak: $$\int_0^L \left(EA\frac{d^2u}{dx^2} - F\right) v\,dx = 0$$

FEM: Strong Form vs. Weak Form

Strong Form vs. Weak Form

$$EA\frac{d^2u}{dx^2} = F$$

$$\int_0^L \left(EA\frac{d^2u}{dx^2} - F \right) v\,dx = 0$$

v = arbitrary test function

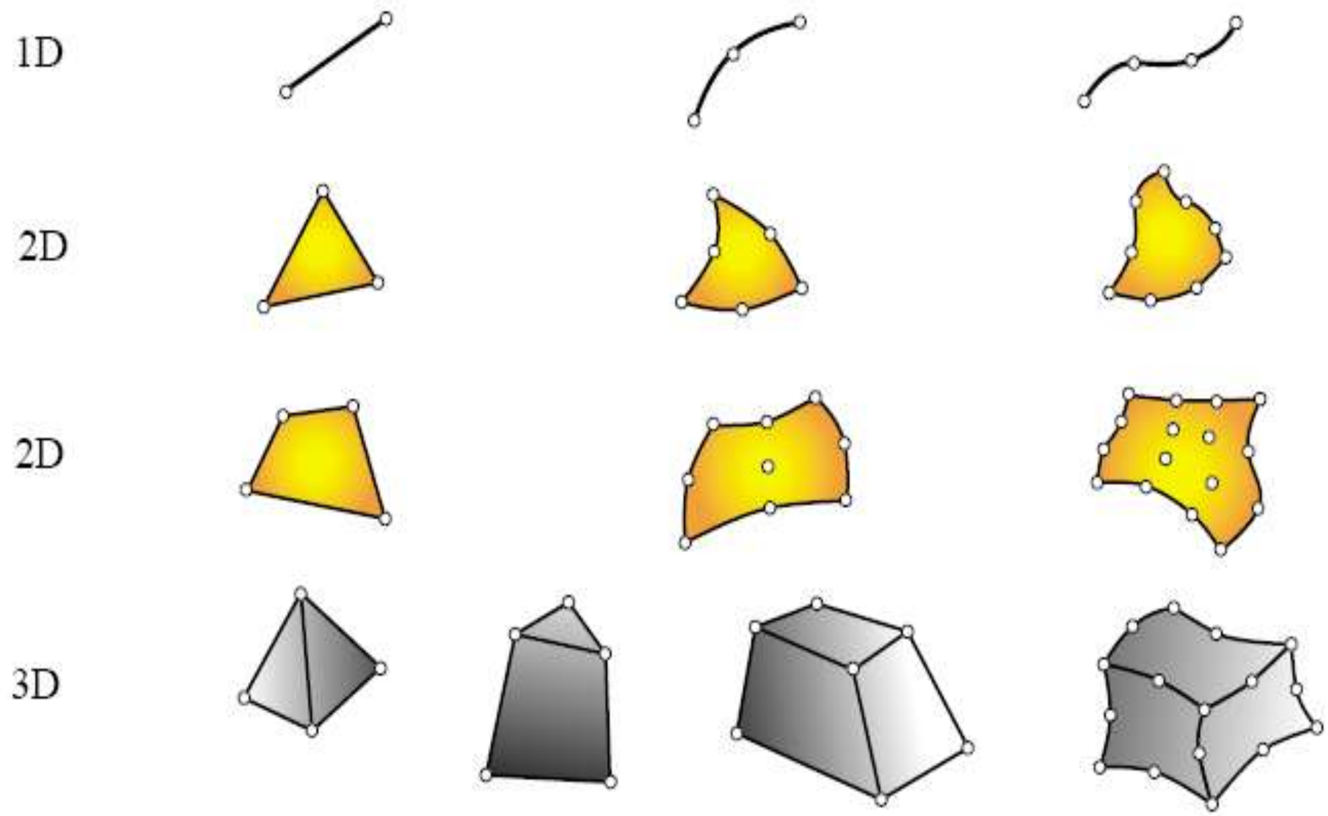
- Weak Form ➡ weaker statement of the problem
  - Has the effect of relaxing the problem
  - “Average” solution over the domain
  - A solution of the strong form will also satisfy the weak form, but not vice versa.

- Integrate the weak form against a *test function* (v)
- The choice of test function is up to the user

FEM: Elements

- Wide range of element types and shapes

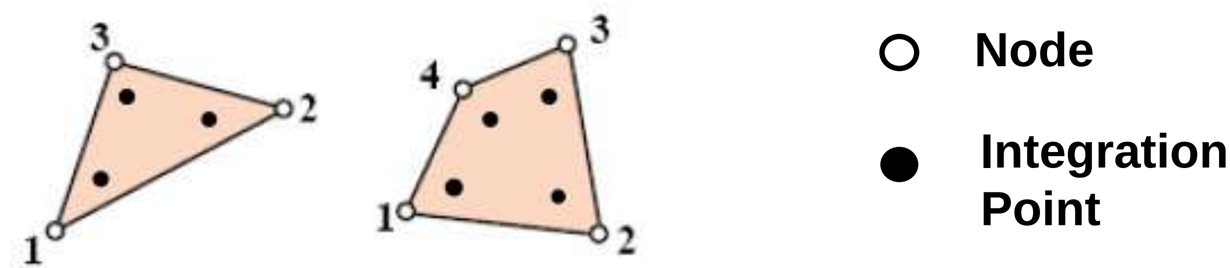
Sample Elements



- Main difference ➡ Solution form within the element

FEM: Elements

- Three important parts that make up an element
  - Nodes
  - Integration Points
  - Shape Function (Internal interpolation function)



$$\#\text{Nodes} \neq \#\text{Integration Points}$$

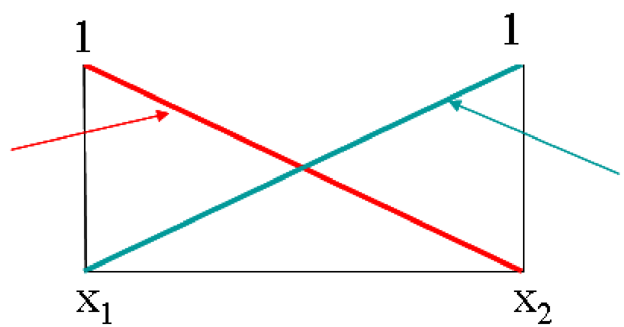
- Forces & displacements are defined at Nodes
- Stresses & Strains are defined at the Integration Points
- Nodes and Integration Points are linked via the shape functions

FEM: Elements

- Shape function describes how much each node affects the rest of the element
  - Internal interpolation functions
- 1 shape function per node
- Shape function can have various forms
  - Most common are linear & quadratic

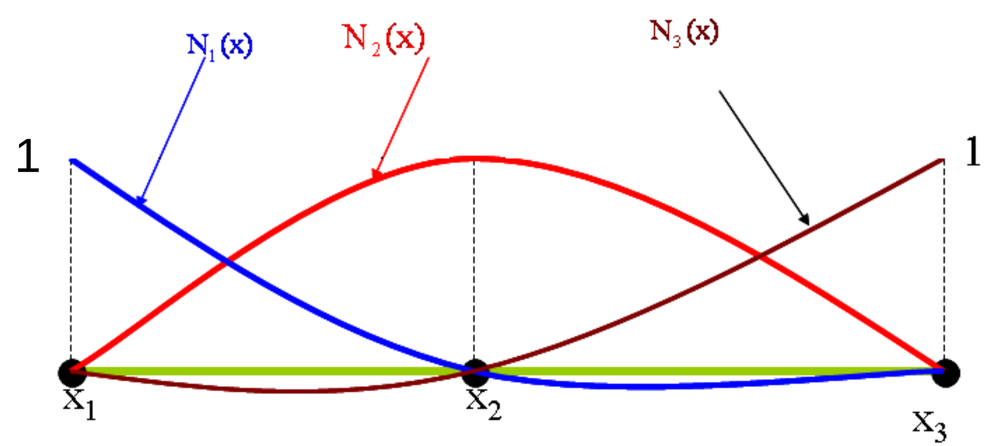
1D – Linear:

$$N_1(x) = \frac{x_2 - x}{x_2 - x_1}$$



$$N_2(x) = \frac{x - x_1}{x_2 - x_1}$$

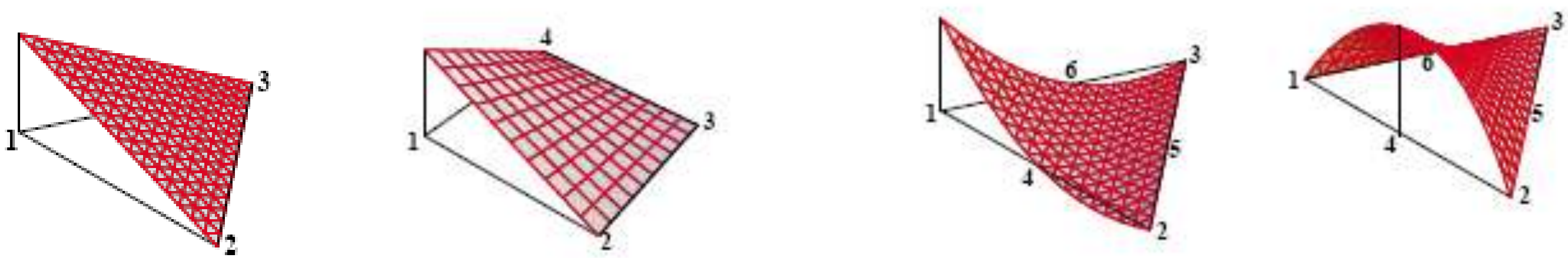
1D – Quad:



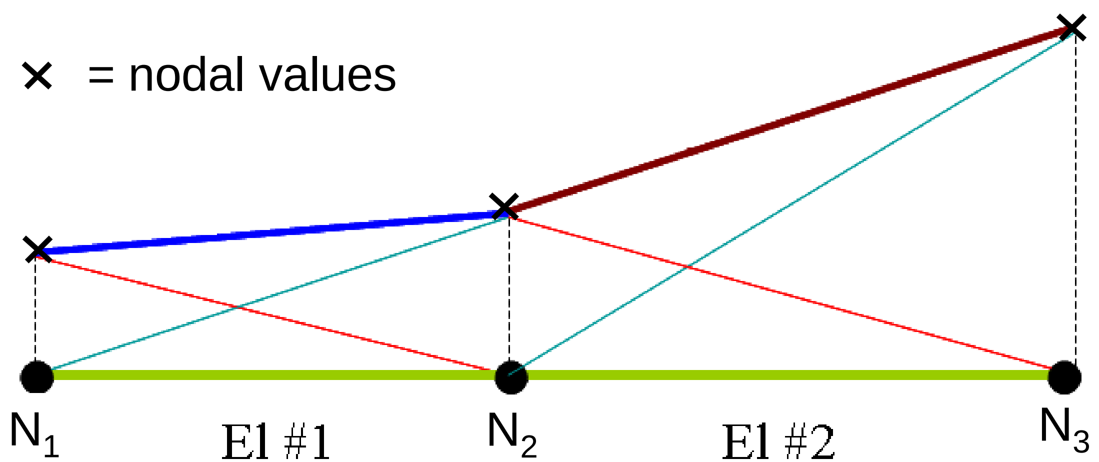
FEM: Elements

- 2D Shape functions are planes rather than lines

Linear Shape functions | **Quad. Shape Functions**

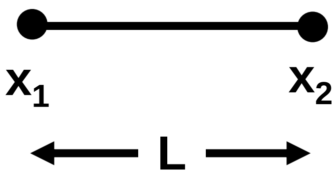


- Shape functions guarantee nodal based quantities (like force and displacement) are CONTINUOUS across element boundaries
- Shape function derivatives are NOT CONTINUOUS across element boundaries



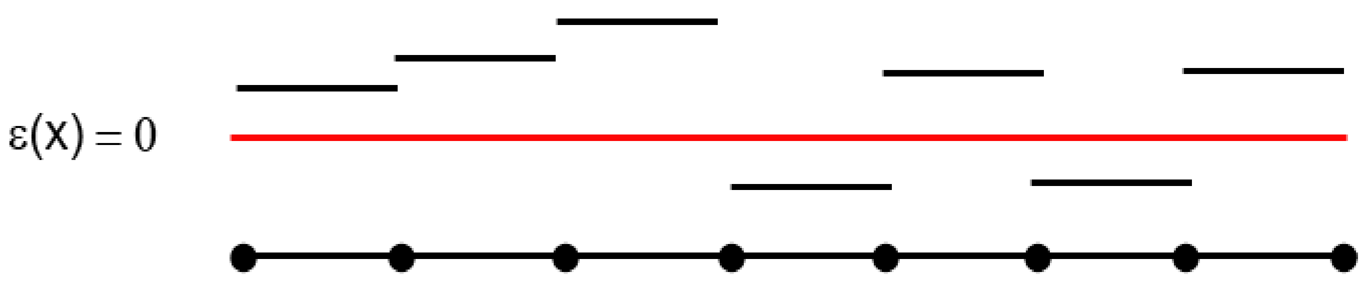
FEM: Elements

1D Element with Linear Shape Functions



Linear Shape Functions

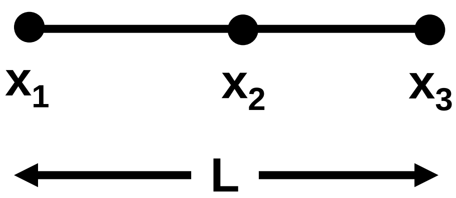
$$N_1(x) = \frac{x_2 - x}{x_2 - x_1} = \frac{x_2 - x}{L} \qquad N_2(x) = \frac{x - x_1}{x_2 - x_1} = \frac{x - x_1}{L}$$



Linear shape functions lead to elements that have a constant strain profile

FEM: Elements

1D Element with Quadratic Shape Functions

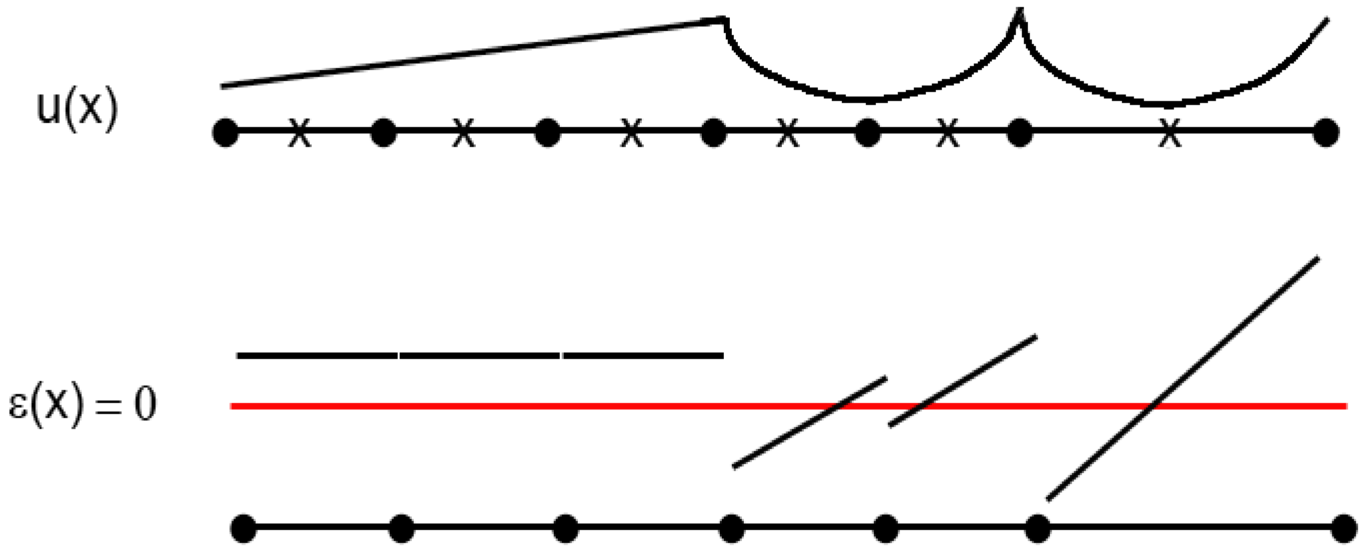


Quad. Shape Functions

$$N_1(x) = \frac{(x_2 - x)(x_3 - x)}{(x_2 - x_1)(x_3 - x_1)}$$

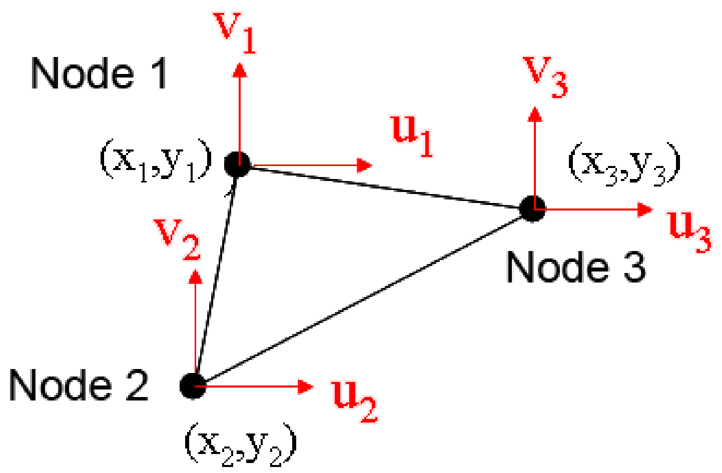
$$N_2(x) = \frac{(x_1 - x)(x_3 - x)}{(x_1 - x_2)(x_3 - x_2)}$$

$$N_3(x) = \frac{(x_1 - x)(x_2 - x)}{(x_1 - x_3)(x_2 - x_3)}$$



Quadratic shape functions lead to elements that have a linear strain profile

FEM: Elements



Linear Shape Functions

$$N_1 = \frac{a_1 + b_1 x + c_1 y}{2A}$$

$$N_2 = \frac{a_2 + b_2 x + c_2 y}{2A}$$

$$N_3 = \frac{a_3 + b_3 x + c_3 y}{2A}$$

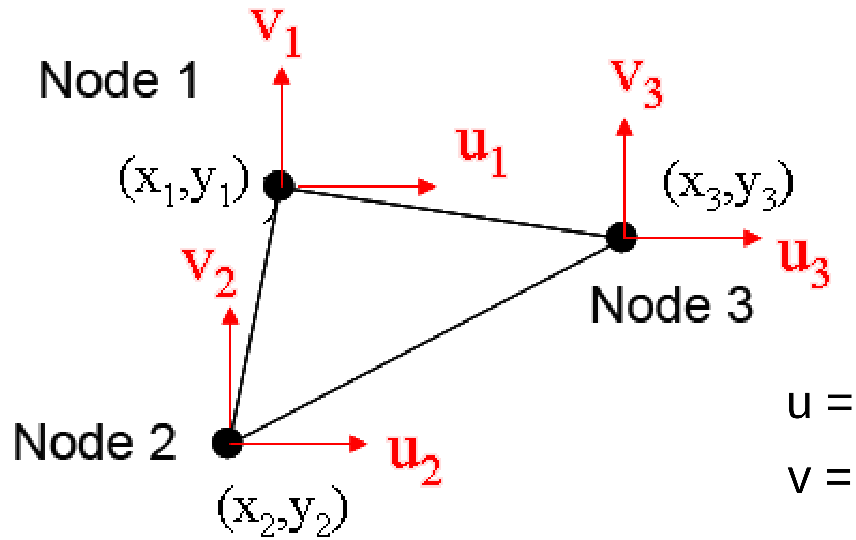
$$[B] = \frac{1}{2A}\begin{bmatrix} b_1 & 0 & b_2 & 0 & b_3 & 0 \\ 0 & c_1 & 0 & c_2 & 0 & c_3 \\ b_1 & c_1 & b_2 & c_2 & b_3 & c_3 \end{bmatrix} \Rightarrow \begin{aligned} \varepsilon_x &= u_1 b_1 + u_2 b_2 + u_3 b_3 \\ \varepsilon_y &= u_1 c_1 + u_2 c_2 + u_3 c_3 \end{aligned}$$

Note: No dependence on x and y

Linear shape functions lead to elements that have a constant strain profile

FEM: Elements

2D Linear Element:



u = displacement in x

v = displacement in y

A displacement *approximation*

$$u(x,y) \approx N_1 u_1 + N_2 u_2 + N_3 u_3 \qquad v(x,y) \approx N_1 v_1 + N_2 v_2 + N_3 v_3$$

$$\begin{Bmatrix} u(x,y) \\ v(x,y) \end{Bmatrix} = \begin{bmatrix} N_1 & 0 & N_2 & 0 & N_3 & 0 \\ 0 & N_1 & 0 & N_2 & 0 & N_3 \end{bmatrix} \begin{bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \end{bmatrix}$$

FEM: Elements

FEM calculates strain from the nodal displacements

Definition of Strain

$$\varepsilon = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{bmatrix} = \begin{bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial y} \\ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \end{bmatrix}$$

FEM Strain Calculation

Based on the derivative of the shape functions

$$\varepsilon_x \approx \frac{\partial N_1(x,y)}{\partial x} u(x,y) + \frac{\partial N_2(x,y)}{\partial x} u(x,y) + \frac{\partial N_3(x,y)}{\partial x} u(x,y)$$

$$\varepsilon_y \approx \frac{\partial N_1(x,y)}{\partial y} v(x,y) + \frac{\partial N_2(x,y)}{\partial y} v(x,y) + \frac{\partial N_3(x,y)}{\partial y} v(x,y)$$

$$\varepsilon \approx \begin{bmatrix} \frac{\partial N_1(x,y)}{\partial x} & 0 & \frac{\partial N_2(x,y)}{\partial x} & 0 & \frac{\partial N_3(x,y)}{\partial x} & 0 \\ 0 & \frac{\partial N_1(x,y)}{\partial y} & 0 & \frac{\partial N_2(x,y)}{\partial y} & 0 & \frac{\partial N_3(x,y)}{\partial y} \\ \frac{\partial N_1(x,y)}{\partial y} & \frac{\partial N_1(x,y)}{\partial x} & \frac{\partial N_2(x,y)}{\partial y} & \frac{\partial N_2(x,y)}{\partial x} & \frac{\partial N_3(x,y)}{\partial y} & \frac{\partial N_3(x,y)}{\partial x} \end{bmatrix} \begin{bmatrix} u_1 \\ v_1 \\ v_2 \\ u_2 \\ v_3 \\ u_3 \end{bmatrix}$$

- Because shape function derivatives are NOT CONTINUOUS across element boundaries, calculating ε at nodes could be a problem.
- ε is always calculated at integration points (inside the element)

FEM: Elements

Stress at each integration point

$$\sigma = [D][\varepsilon] = [D][B][u]$$

D = appropriate elasticity matrix (user input)

B = element dependent

Summary: For a 1D linear element

- **Approximate displacement**

$$u(x) = \frac{1}{L}\begin{bmatrix} x_2 - x & x - x_1 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

- **Approximate Strain**

$$\varepsilon = \frac{1}{L}\begin{bmatrix} -1 & 1 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

- **Approximate Stress**

$$\sigma = \frac{E}{L}\begin{bmatrix} -1 & 1 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

FEM: Elements

FEM Method with Elements

- **Assemble individual element stiffness matrix**

$$[K_e] = \int_{V^e} [B_e]^T [D_e][B_e] \, dV$$

- **Assemble global stiffness matrix**

$$[K] = \sum_{\#\,Ele} [K_e]$$

- **Apply Boundary Conditions**

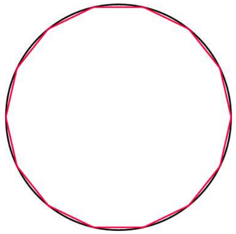
$$[K][u] = [f]$$

FEM ERROR

There are three general sources of error in a finite-element solution

#1: Errors due to the approximation of the domain

vs.



#2: Errors due to the approximation of the solution

$$EA\frac{d^2u}{dx^2} = F \quad \text{vs.} \quad \int_0^L \left(EA\frac{d^2u}{dx^2} - F \right) v\,dx = 0$$

#3: Errors due to numerical computation
(like numerical integration and round-off errors in a computer)

The estimation of these errors, in general, is not a simple matter.

FEM ERROR

- FEM Partial Differential Equation Solver
  - Solves PDE by
    1) Breaking solution space into pieces (elements)
    2) Approximating the solution on each element
    3) Solving a force balance (equilibrium) equation

$$[K][u]=[f]$$

K = stiffness matrix (composed of element and material properties)

- FEM solves the weak form of the equilibrium equation
  - "Average" solution over the domain NOT the exact solution
- Three primary parts of an element
  - Nodes
  - Integration Points
  - Shape Functions

FEM: Overview

- Large number of element types and shapes
  - Element choice will affect your results

Linear elements → Constant strain

Quadratic elements → Linear strain

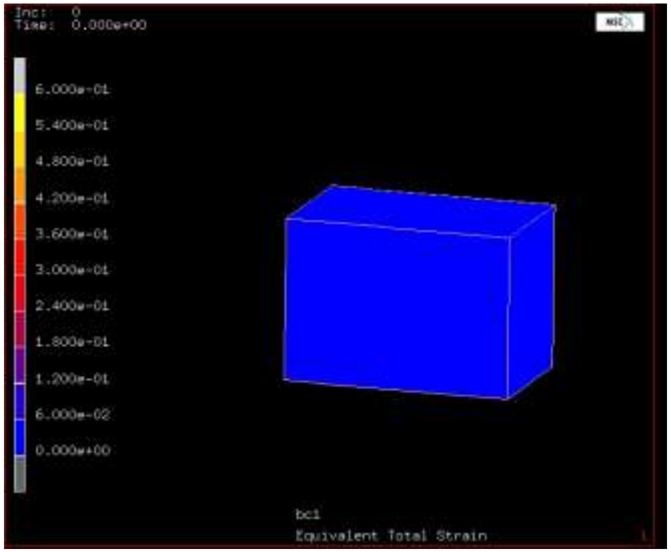
- FEM Error
  - Domain Approximation
  - Solution Approximation
  - Numerical Computations

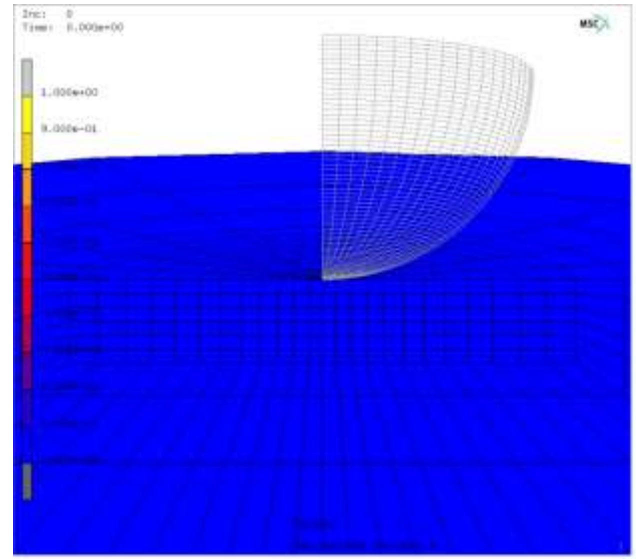
FEM error is difficult to quantify

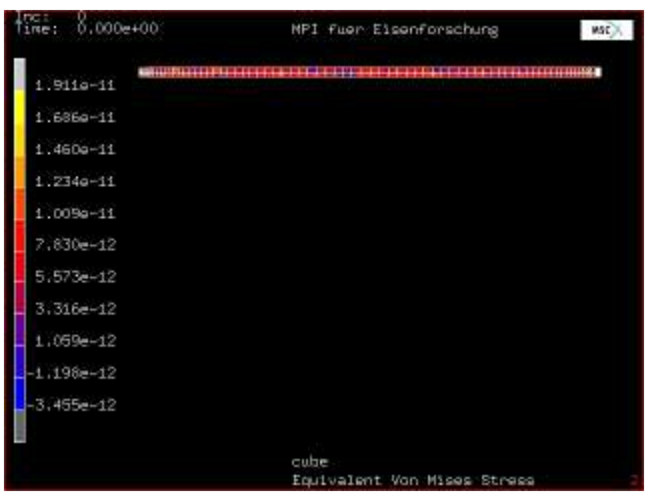
- Convergence vs. Accuracy
  - A converged result is NOT necessarily an accurate result

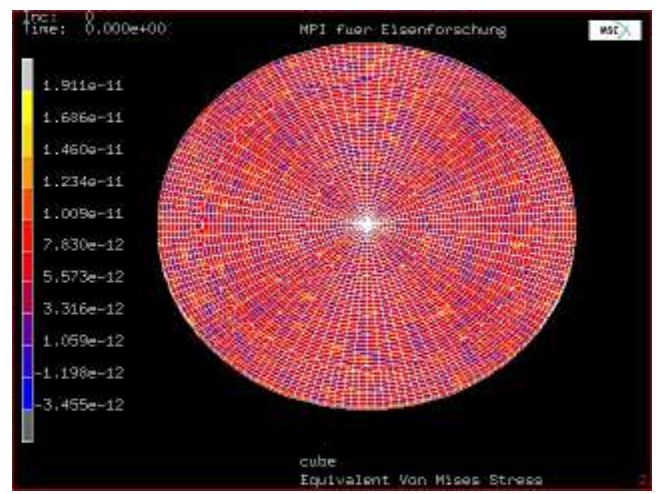
Any physically meaningful output MUST result from physical input provided by you to FEM

FEM: Examples





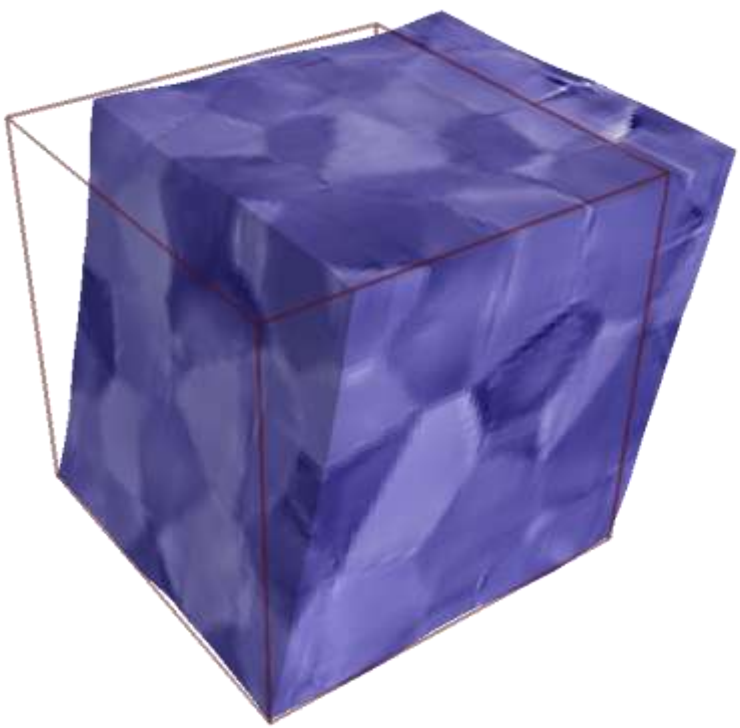




FEM: Examples

- **VE with 50 randomly oiented grains**
- **Simple shear**

FEM 64x64x64



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