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Introduction



FEM: Finite Element Method

A great picture generating tool!!!!



Introduction



My view: FEM is a mathematical tool.

Any physically meaningful output <u>MUST</u> result from physical input provided by you to FEM



Introduction



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

$$P_{c} = \sum_{N_{e}} L_{e} = \sum_{N_{e}} 2r \sin \frac{\theta}{2}$$

$$N_{e} = 6 P_{c} = 6.00 r$$

$$N_{e} = 8 P_{c} = 6.12 r$$

$$N_{e} = 14 P_{c} = 6.23 r$$

$$D_{e} = 14 P_{c} = 6.23 r$$

FEM



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

FEM – 1D Rod Example





2) Ensure compatibility (no formation of holes/voids)

Modeler

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

Model rods as elastic springs \implies F = kd $k = \frac{AE}{L}$

FEM – 1D Rod Example





For each element, write a force balance at each node



$$\frac{\text{Element 2}}{f_{E2}^{\text{Node-2}} + k_{E2} \left(u^{\text{Node-2}} - u^{\text{Node-3}} \right) = 0}$$
$$f_{E2}^{\text{Node-3}} + k_{E2} \left(u^{\text{Node-3}} - u^{\text{Node-2}} \right) = 0$$

FEM – 1D Rod Example



• Assemble the force balance equations for all 3 nodes

$$\begin{bmatrix} k_{E1} & -k_{E1} & 0 \\ k_{E1} & k_{E1} + k_{E2} & -k_{E2} \\ 0 & -k_{E2} & k_{E2} \end{bmatrix} \begin{bmatrix} u^{\text{Node-1}} \\ u^{\text{Node-2}} \\ u^{\text{Node-3}} \end{bmatrix} = \begin{bmatrix} -f_{E1}^{\text{Node-1}} \\ -f_{E1}^{\text{Node-2}} - f_{E2}^{\text{Node-2}} \\ -f_{E2}^{\text{Node-3}} \end{bmatrix}$$

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

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

Apply Boundary Conditions

$$\begin{bmatrix} k_{E1} & -k_{E1} & 0 \\ k_{E1} & k_{E1} + k_{E2} & -k_{E2} \\ 0 & -k_{E2} & k_{E2} \end{bmatrix} \begin{bmatrix} 0 \\ u^{Node-2} \\ u^{Node-3} \end{bmatrix} = \begin{bmatrix} -f_{E1}^{Node-1} \\ 0 \\ F \end{bmatrix}$$

3 equations and 3 unknowns

Easily solve with a matrix inversion









- Element can be displaced in 2 directions
- Element supports along axial direction

Element force balance equations





	<u>A(m²)</u>	E(MPa)	<u>L(m)</u>
Ele 1	0.01	10	5
Ele 2	0.01	10	8.66
Ele 3	0.01	10	10
	ŀ	_ AE	
	К	= <u> </u>	

 $k_1 = 2000$ $k_2 = 1154.73$ $k_3 = 1000$

$$\begin{bmatrix} T_1 \end{bmatrix} = \begin{bmatrix} c90 & s90 & 0 & 0 \\ -s90 & c90 & 0 & 0 \\ 0 & 0 & c90 & s90 \\ 0 & 0 & -s90 & c90 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad \begin{bmatrix} T_2 \end{bmatrix} = \begin{bmatrix} c0 & s0 & 0 & 0 \\ -s0 & c0 & 0 & 0 \\ 0 & 0 & c0 & s0 \\ 0 & 0 & -s0 & c0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} T_3 \end{bmatrix} = \begin{bmatrix} c150 & s150 & 0 & 0 \\ -s150 & c150 & 0 & 0 \\ 0 & 0 & c150 & s150 \\ 0 & 0 & -s150 & c150 \end{bmatrix} = \begin{bmatrix} -0.866 & -0.5 & 0 & 0 \\ 0.5 & -0.866 & 0 & 0 \\ 0 & 0 & -0.866 & -0.5 \\ 0 & 0 & 0.5 & -0.866 \end{bmatrix}$$



 Calculate the element stiffness matrixes For example Element 3: 	[T]	$\begin{bmatrix} k_{\rm E} \\ 0 \\ -k_{\rm E} \\ 0 \end{bmatrix}$	$ \begin{array}{ccc} 0 & -k_{\rm E} \\ 0 & 0 \\ 0 & k_{\rm E} \\ 0 & 0 \end{array} $	$\begin{bmatrix} 0\\0\\0\\0\end{bmatrix} \begin{bmatrix} T \end{bmatrix}$
$\begin{bmatrix} -0.866 & -0.5 & 0 & 0 \\ 0.5 & -0.866 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1000 & 0 & -1000 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} -0.866\\ 0.5 \end{bmatrix}$	-0.5 -0.866	0	$\begin{bmatrix} 0 \\ 0 \end{bmatrix}$
0 0 -0.866 -0.5 -1000 0 1000 0	0	0	- 0.866	- 0.5
	0	0	0.5	-0.866
$ \begin{bmatrix} \mathbf{k}'_{\text{E3}} \end{bmatrix} = \begin{bmatrix} 750 & -433.2 & -750 \\ -433.2 & 250 & 433.2 \\ -750 & 433.2 & 750 \\ 433.2 & -250 & -433.2 \end{bmatrix} $	433.2 - 250 - 433 2 250	$\begin{bmatrix} 2 \\ 0 \\ .2 \end{bmatrix}$		
$\begin{bmatrix} \mathbf{k}'_{E1} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 2000 & 0 & -2000 \\ 0 & 0 & 0 & 0 \\ 0 & -2000 & 0 & 2000 \end{bmatrix} \begin{bmatrix} \mathbf{k}'_{E2} \end{bmatrix} =$	$= \begin{bmatrix} 1154.' \\ 0 \\ -1154. \\ 0 \end{bmatrix}$	73 0 0 .73 0 0	-1154.73 0 1154.73 0	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$



Assemble the element stiffness matrixes

[1	154.73 + 750	-433.2	-750	433.2	-1154.73	0	$\left \left[u_x^{N-2} \right] \right $]	f_x^{N-2}	
	-433.2	250	433.2	- 250	0	0	u _y ^{N-2}		$f_y^{N\text{-}2}$	
	-750	433.2	750	-433.2	0	0	u_x^{N-3}		f_x^{N-3}	
	433.2	-250	-433.2	250 + 2000	0	-2000	u _y ^{N-3}	=	f_y^{N-3}	
	-1154.73	0	0	0	1154.73	0	u _x ^{N-1}		$f_x^{N\text{-}1}$	
	0	0	0	- 2000	0	2000	u _y ^{N-1}		f_y^{N-1}	

Apply boundary conditions

[1154.73 + 750	-433.2	-750	433.2	-1154.73	0]	$\left[u_{x}^{N-2}\right]$		0	
-433.2	250	433.2	-250	0	0	u _y ^{N-2}		-10	
- 750	433.2	750	-433.2	0	0	0		0	
433.2	-250	-433.2	250 + 2000	0	- 2000	u _y ^{N-3}	=	0	
-1154.73	0	0	0	1154.73	0	0		0	
0	0	0	- 2000	0	2000	0		0	

Solve 3 equations with 3 unknowns

$$u_x^{N-2} = -0.015$$
 $u_y^{N-2} = -0.071$ $u_y^{N-3} = -0.005$



- Governing equations are usually complex differential equations
- Often these equations cannot be solved over an element





Weak Form is based on <u>Potential Energy (Π)</u> Π = Strain Energy – Energy from applied loads Π = U – W









Exact solution, u(x) is unknown

FEM "guesses" an admissible displacement field, w(x)





FEM works w(x) \longrightarrow $\Pi(w) = \frac{1}{2} \int_{0}^{L} EA\left(\frac{dw}{dx}\right)^{2} dx - \int_{0}^{L} bw dx - Fw(x = L)$



How are w(x) and u(x) related?

Principle of Minimum Potential Energy

Among all admissible displacements (w(x)'s), the one that MINIMIZES the total potential energy (II) is u(x) $\Pi(u) < \Pi(w)$

FEM











- Weak Form \rightarrow weaker statement of the problem
 - Based on potential energy
 - 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.
 - Principle of Minimum Potential Energy
 - w(x) that minimizes Π , equals u(x)



How does FEM determine w(x) function?

w(x) must be 1st order continuous and satisfy BC

Generally, polynomials and sine/cosine functions are simple enough to be practical.

$$w(x) = w_0 + w_1 x$$

 $w(x) = w_0 + w_1 x + w_2 x^2$

w_i's are to be determined

$$\frac{\partial \Pi}{\partial w_i} = 0$$

Numerical Methodology used to determine w_i's



Galerkin's Method/ Rayleigh-Ritz













Reformulate equations in a more general form

$$w(x) = \sum_{j=1}^{N} c_j \varphi_j(x)$$

solve for $\mathbf{c}_{\mathbf{j}}$

$$\sum_{j=1}^{N} c_j \int_0^L \frac{d\varphi_j}{dx} \frac{d\varphi_i}{dx} dx = \int_0^L b\varphi_i dx$$

$$K_{ij} = \int_0^L \frac{d\varphi_j}{dx} \frac{d\varphi_i}{dx} dx$$

 $f_i = \int_0^L p_0 \varphi_i dx$

Stiffness Matrix

Force vector



Wide range of element types and shapes





Main difference
 Solution form within the element



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



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



- 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





2D Shape functions are planes rather than lines



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







A displacement *approximation*

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



FEM calculates strain from the nodal displacements





- 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)



1D Element with Linear Shape Functions





1D Element with Quadratic Shape Functions









$$\begin{bmatrix} B \end{bmatrix} = \frac{1}{2A} \begin{bmatrix} b_1 & 0 & b_2 & 0 & b_3 & 0 \\ 0 & c_1 & 0 & c_2 & 0 & c_3 \\ b_1 & c_1 & b_2 & c_2 & b_3 & c_3 \end{bmatrix} \implies \begin{array}{l} \boldsymbol{\epsilon}_x = u_1 b_1 + u_2 b_2 + u_3 b_3 \\ \boldsymbol{\epsilon}_y = u_1 c_1 + u_2 c_2 + u_3 c_3 \end{array}$$

Note: No dependence on x and y

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

Stress at each integration point

$$\sigma = \begin{bmatrix} D \\ \epsilon \end{bmatrix} = \begin{bmatrix} D \\ B \end{bmatrix} \begin{bmatrix} u \\ u \end{bmatrix}$$
 D = appropriate elasticity matrix (user input)

B = element dependent

Summary: For a 1D linear element

Approximate displacement

$$u(\mathbf{x}) = \frac{1}{L} \begin{bmatrix} \mathbf{x}_2 - \mathbf{x} & \mathbf{x} - \mathbf{x}_1 \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix}$$

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 Method with Elements

Assemble individual element stiffness matrix

 $\begin{bmatrix} K_e \end{bmatrix} = \int_{V^e} \begin{bmatrix} B_e \end{bmatrix}^T \begin{bmatrix} D_e \end{bmatrix} \begin{bmatrix} B_e \end{bmatrix} dV$

Assemble global stiffness matrix

 $\left[\mathbf{K}\right] = \sum_{\# \text{ Ele}} \left[\mathbf{K}_{e}\right]$

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



#2: Errors due to the approximation of the solution

$$EA\frac{d^{2}u}{dx^{2}} = F \qquad \text{vs.} \qquad \Pi(w) = \frac{1}{2}\int_{0}^{L} EA\left(\frac{dw}{dx}\right)^{2} dx - \int_{0}^{L} bw \, dx - Fw(x = L)$$

#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: Accuracy vs. Convergence

- The accuracy and convergence of the finite-element solution depends on a number of factors
 - Like the differential equation solved (or the variational form used) and the type of element.
- Accuracy

А

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- Difference between the exact solution and the finite-element solution
- Convergence
 - The accuracy of the solution as the number of elements in the mesh is increased





FEM: Overview



- 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 <u>MUST</u> result from physical input provided by you to FEM

FEM: Cases where it works well



Examples:



Coupled temperature and deformation problems



FEM: Cases where it works well





Complex deformations

Elastic spring-back

FEM: Cases where it works well



Multiple components/complex geometries







FEM: Cases where it does not work as well



- 2 Material Science examples
 - FEM "works"
 - ⇒ Converges to a solution
 - ⇒ Solution is not correct
- Length scale issues
- Inhomogeneous Materials

FEM Example: Length Scales



 Structural finite element codes are continuum based

 Finite element mesh has dimensions

Local models:
dimensions do not
effect the σ-ε result

Predicted σ-ε results
from two different
grain sizes are similar





150 um

3.4 um



FEM Example: Overview



Motivation

- Accounting for microstructure heterogeneity within a material computationally expensive.
- At the microscopic scale, strain and stress path are complex.
- Generally, it is not possible to exactly mesh and simulate the material's microstructure

Problem Statement

To investigate the effect of element type and mesh resolution on the σ - ϵ response of a two phase material. (Hard Phase: Martensite) (Soft Phase: Ferrite)

FEM Example: Mesh Refinement





482xx482cettermeentss(2BQ44 ttottal eltermeentss))



FEM Example: Element Types

- Element Types
 - 2D Linear (4 nodes)





- 2D Quadratic (9 nodes)



Full Integration



Reduced Integration



FEM Example: Results



2D Plane Strain Rolling

- Prescribe displacements
- Volume conserving $(\epsilon_x = \epsilon_y)$

- 30 % thickness reduction
- Elastic-plastic constitutive equations



Study the effect of element type & mesh resolution on the $\sigma\text{-}\epsilon$ response

FEM Example: σ-ε Results





FEM Example: Effect of Mesh Refinement





FEM Example: Effect of Element Type





FEM Example: Strain Maps





Strain state appears reasonable

- Linear elements $\implies \varepsilon$ is relatively flat
- Quad elements $\implies \varepsilon$ flows around the martensite







Use of linear elements **GREATLY** reduces computation time

FEM Example: Conclusions



- Mesh dimensions do not enter into σ - ϵ constitutive relationship
- Element type and mesh resolution do affect the overall σ - ϵ response
 - Δσ = 100 MPa
- Increasing the mesh resolution leads to a softer $\sigma\text{-}\epsilon$ response
- Use of quadratic elements leads to a softer σ - ϵ response
- Linear elements predict a relatively flat e profile
- Quadratic elements predict a much more contoured e profile
- Use of linear elements GREATLY reduces computation time

PART IV

Polycrystal Plasticity Models

micro-macro homogenization

motivation



• orientation, **g**, of crystallite can be specified by a set of three Euler angles

$$\mathbf{g} = \{\varphi_1, \phi, \varphi_2\}$$

 crystallite orientation distribution function (codf) defines probability, *f*(g), that a volume fraction, dV/V, of the polycrystaline aggregate is taken up by crystals of orientation between g and g+dg

$$\upsilon \equiv \frac{\mathrm{d}V}{V} = f(\mathbf{g})\mathrm{d}\mathbf{g}$$

 codf values typically available on a discrete grid in orientation space, or continuously from coefficients of a harmonic series expansion





• select N^* from all those N orientations having non-zero v_i in discrete codf representation





- add randomly selected orientation if random number $r \in [0,1] \leq v_i$
- continue until N^* orientations collected



L.S. Tóth, P. Van Houtte, Textures Microstruct. 19 (1992) 229–244.

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L.S. Tóth, P. Van Houtte, Textures Microstruct. 19 (1992) 229–244.











T. Leffers, D. Juul Jensen, Textures Microstruct. 6 (1986) 231–263.

strong

- N = 6048 (monoclinic)
- N = 1512 (orthotropic)

intermediate

- *N* = 6048
- N = 1512

random

- N = 186624
- *N* = 27000
- *N* = 5832



$$\text{RMSD} = \sqrt{\sum_{i=1}^{N} (v_i - v_i^*)^2}$$










J. Tarasiuk and K. Wierzbanowski, Phil. Mag. A 73 (1996) 1083–1091

















select each orientation

$$n_i^* = \operatorname{round} \left(C \, v_i \right)$$

times

• vary C to ensure population size $\sum_{i=1}^{N} n_i^* \stackrel{!}{=} \max(N^*, N)$

 select N* orientations from this population at random





 select N* orientations from this population at random





 select N* orientations from this population at random











 $N^*/N = 1$