FEM and X-FEM in Continuum Mechanics

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1 Finite Element Method

The Finite Element Method (FEM) is a very well known method for the numerical solution of partial differential equations. First the FEM was mainly applied to elliptic PDE's, but hyperbolic PDE's which describe dynamic behavior in continuum mechanics can be solved as well.

1.1 Problem Definition

The most important equation that has to be solved in continuum mechanics is the equation of linear momentum

$$\rho(x,t)u_{,tt}(x,t) - \sigma_{,x}(x,t) = 0 \qquad in \;\; \Omega, \tag{1}$$

where $u(x,t)$ denotes the displacement, $\rho(x,t)$ the density and $\sigma(x,t)$ the stress. For simplicity only the one-dimensional case is considered.
The material properties are stated in a constitutive law that relates stress and strain. The constitutive law for linear elasticity in one dimension is written as follows:

$$\sigma(x,t) = E\epsilon(x,t) = Eu_{,x}(x,t) \tag{2}$$

The Young's modulus E represents the material constant and $\epsilon(x,t)$ expresses the strain. The strain $\epsilon(x,t)$ can be linearly approximated by the gradient of the displacement $u_{,x}(x,t)$.
Inserting (2) in (1) leads to a well known hyperbolic partial differential equation: the linear wave equation:

$$\rho(x,t)\, u_{,tt}(x,t) - E\, u_{,xx}(x,t) = 0 \qquad in \;\; \Omega \tag{3}$$

The boundary conditions can be defined as Neumann boundary conditions (traction in continuum mechanics), or as Dirichlet boundary conditions (displacements):

$$\sigma = \bar{t} \quad\; on \;\; \Gamma_t \tag{4}$$

$$u = \bar{u} \quad\; on \; \Gamma_u \tag{5}$$

Initial conditions have to be stated as well:

$$u(0,t) = u_0 \tag{6}$$

$$u_{,t}(0,t) = v_0 \tag{7}$$

1.2 Weak formulation - Principle of Virtual Work

The partial differential equation cannot be discretized directly by using the FEM. Instead a so called weak form is developed by multiplying the linear momentum equation with a test function δu and by integrating over the whole domain Ω:

$$\int_\Omega \delta u \Big(\rho\, u_{,tt} - E\, u_{,xx}\Big) d\Omega = 0 \tag{8}$$

Applying Gauss's theorem and integration by parts leads to:

$$\int_\Omega \delta u\, \rho\, u_{,tt}\; d\Omega + \int_{\bar{\Omega}} \frac{\partial(\delta u)}{\partial x}\, E\, u_{,x}\; d\Omega - \int_{\Gamma_t} \sum \delta u\, \bar{t}\, d\Gamma = 0 \tag{9}$$

In continuum mechanics this equation is equivalent to the Principle of Virtual Work:

$$\delta\mathcal{W}_{tot} = \delta\mathcal{W}_{kin} + \delta\mathcal{W}_{int} - \delta\mathcal{W}_{ext} = 0 \tag{10}$$

The total work (or energy) consisting of the external work, the internal work and the kinetic work equals zero.
Now, the function spaces for the trial functions u and the test function δu can be defined:

$$\mathcal{U} = \{u(x,t) | u(x,t) \in H^1, u(x,t) = \bar{u}(t) \;\; on \; \Gamma_u\} \tag{11}$$

$$\mathcal{U}_0 = \{\delta u(x) | \delta u(x) \in H^1, \delta u(x) = 0 \;\; on \; \Gamma_u\} \tag{12}$$

Since we developed a weak form, trial and test functions can be taken from the Sobolev space H^1.

1.3 Finite Element Discretization

The entire domain is separated into finite elements (1D: rods, 2D: triangles, rectangles, 3D: tetrahydrons,...). Since we only consider one dimension, one-dimensional rod elements are chosen. The solution is now approximated in the element coordinate system, where $\xi_1 = -1$ and $\xi_2 = 1$ are the end points of the rod. The shape functions N_I build the base and the nodal degrees of freedom $d_I(t)$ are the coefficients. The subscript I denotes the nodal degrees of freedom per element:

$$u(\xi, t) = \sum_I N_I(\xi) d_I(t) \tag{13}$$

$$\delta u(\xi) = \sum_I N_I(\xi) \delta d_I \tag{14}$$

Linear shape functions are described here for each node per element:

$$N_1 = \frac{1}{2}(1 - \xi) \tag{15}$$

$$N_2 = \frac{1}{2}(1 + \xi) \tag{16}$$

1.4 Nonlinear system of equations

Transforming (13) and (14) in the x-coordinate system and inserting them in the weak form (9) leads to the following equation:

$$\int_\Omega \rho N_I N_J \, d\Omega \, \ddot{d}_J + \int_{\bar{\Omega}} N_{I,x} \, \sigma \, d\Omega - \int_{\Gamma_t} N_I \, \bar{t} \, d\Gamma \tag{17}$$

In continuum mechanics this refers to Newton's first law:

$$M_{IJ} a_J + f_I^{int} - f_I^{ext} = 0 \tag{18}$$

1.5 Linearization with the Newton-Raphson-Method

The resulting equation that has to be solved is nonlinear and hence has to be linearized by the Newton-Raphson-method:

$$\begin{aligned} & r_I(\boldsymbol{d}^{t+1}, t^{t+1}) = \\ & M_{IJ} a_J^{t+1} + f_I^{int}(\boldsymbol{d}^{t+1}, t^{t+1}) - f_I^{ext}(\boldsymbol{d}^{t+1}, t^{t+1}) = 0 \end{aligned} \tag{19}$$

The residual is expanded in a Taylor-series up to first order.

$$r_I(\boldsymbol{d}^n) = \frac{\partial r_I(\boldsymbol{d}^n)}{\partial d_J} \Delta d_J + O(\Delta \boldsymbol{d})^2 = r_I + A_{IJ} \Delta d_J = 0 \tag{20}$$

The first derivative of the residual with respect to the displacement is called Jacobian matrix A_{IJ}:

$$A_{IJ} = \frac{M_{IJ}}{\beta \Delta t^2} + \frac{\partial f_I^{int}}{\partial d_J} - \frac{\partial f_I^{ext}}{\partial d_J} = \frac{M_{IJ}}{\beta \Delta t^2} + K_{IJ}^{int} - K_{IJ}^{ext} \tag{21}$$

The damping factor β is determined in section 1.7.. With help of the Jacobian A_{IJ} the update of the approximated solution can be determined in an iteration:

$$d_I^{n+1} = d_I^n + \Delta d_I = d_I^n - A_{IJ}^{-1} r_J^n \tag{22}$$

An appropriate stopping criterion has to be implemented to break the iteration.

1.6 Numerical Integration

For the determination of the Jacobian A_{IJ} several integrals have to be evaluated numerically. First a transformation in the element coordinate system is done by $J_\xi = det(\boldsymbol{x}_{,\boldsymbol{\xi}})$, the determinant of an appropriate transformation matrix. Then the integral can be evaluated by Gauss quadrature.

$$\begin{aligned} M_{IJ} &= \int_\Omega \rho N_I N_J \, d\Omega = \int_{-1}^{1} \rho N_I N_J J_\xi A \, d\xi \\ &= \sum_{Q=1}^{n_Q} \bar{w}_Q \rho N_I(\xi_Q) N_J(\xi_Q) J_\xi A \end{aligned} \tag{23}$$

The external stiffness matrix K_{IJ}^{ext} and the internal stiffness matrix K_{IJ}^{int} are obtained analogously.

1.7 Time Integration with the Newmark-β-method

Since the Gauss quadrature only considers the integration over the domain, the time integration has to be conducted separately. A popular time integrator is the Newmark-β-method, that updates displacement, velocity and acceleration:

$$\bar{d_I}^{t+1} = d_I^t + \Delta t v_I^t + \frac{\Delta t^2}{2}(1-2\beta)a_I^t \tag{24}$$

$$\bar{v_I}^{t+1} = v_I^t + (1-\gamma)\Delta t\, a_I^t \tag{25}$$

$$v_I^{t+1} = \bar{v_I}^{t+1} + \gamma \Delta t\, a_I^{t+1} \tag{26}$$

$$a_I^{t+1} = \frac{1}{\beta \Delta t^2}(d_I^{t+1} - \bar{d_I}^{t+1}) \tag{27}$$

The time integration is unconditionally stable for $\beta \geq \frac{\gamma}{2} \geq \frac{1}{4}$.

2 Extended Finite Element Method

Treating discontinuities (i.e. interfaces, cracks,...) is still a big challenge in continuum mechanics. Since the FEM only solves continuous problems, the EXtended Finite Element Method (X-FEM) was developed by Belytschko[2] et. alter[3],[4] to deal with these difficulties.

2.1 Problem Definition

The same partial differential equation (3) from section 1.1 is intended to be solved. Only additional boundary conditions have to be stated for the interface boundary Γ_c.

$$\sigma^- = \sigma^+ = \bar{\tau} \quad on\ \ \Gamma_{c,t} \tag{28}$$

$$[\![\boldsymbol{u}_N]\!] \geq 0 \quad on\ \ \Gamma_{c,u} \tag{29}$$

2.2 Weak Formulation

Considering the additional boundary conditions we obtain the following weak form:

$$\begin{aligned}\int_{\Gamma_t} \delta u\, \bar{t}\, d\Gamma + \int_{\Gamma_c,t} \delta u\, \bar{\tau}\, d\Gamma - \int_{\bar{\Omega}} \frac{\partial(\delta u)}{\partial x} E\, u_{,x}\ d\Omega \\ - \int_{\Omega} \delta u\, \rho\, u_{,tt}\ d\Omega = 0\end{aligned}, \tag{30}$$

where a new term occurs, that represents the external work caused by the Neumann boundary condition $\bar{\tau}$ at the interface surface.

The function spaces for the trial functions u and the test function δu are defined as follows:

$$\begin{aligned}\mathcal{U} = \{u(x,t) | u(x,t) \in H^1, u(x,t) = \bar{u}(t)\ \ on\ \Gamma_u, \\ u(x,t) \text{ discontinuous on } \ \Gamma_c\}\end{aligned} \tag{31}$$

$$\begin{aligned}\mathcal{U}_0 = \{\delta u(x) | \delta u(x) \in H^1, \delta u(x) = 0\ \ on\ \Gamma_u, \\ \delta u(x) \text{ discontinuous on } \ \Gamma_c\}\end{aligned} \tag{32}$$

2.3 Extended Finite Element Discretization

A discontinuous term to describe the behavior of the discontinuity is added to the well-known approximation of the solution $u(\xi,t)$, but only for cracked elements or elements, where interfaces occur:

$$u(\xi,t) = u_{cont}(\xi,t) + u_{disc}(\xi,t) \tag{33}$$

This approach is called enrichment, because we "enrich" the nodes of an element by additional degrees of freedom $q_I(t)$:

$$u(\xi,t) = \sum_{I=1}^{n} N_I(\xi) u_I(t) + \sum_{I \in \mathcal{L}} \Psi_I(\xi) q_I(t) \tag{34}$$

$$\delta u(\xi) = \sum_{I} N_I(\xi) \delta u_I + \sum_{I \in \mathcal{L}} \Psi_I(\xi) \delta q_I \tag{35}$$

The enrichment functionΨ_I is defined as:

$$\Psi_I(\xi) = N_I(\xi)\Phi_I(\xi), \tag{36}$$

where $N_I(\xi)$ are the shape functions, and $\Phi_I(\xi)$ can be obtained by:

$$\Phi_I(\xi) = \text{sign}(\phi(\xi)) - \text{sign}(\phi_I) \tag{37}$$

The value $\phi_I = \phi(\xi_I)$ describes the location of the I-th node. The signum function is defined by:

$$\text{sign}(\xi) = \begin{cases} -1 & \text{for} \quad \xi < \xi_c \\ +1 & \text{for} \quad \xi > \xi_c \end{cases} \tag{38}$$

where ξ_c describes the location of the crack.

The enrichment leads to a partitioning of the element where the crack occurred, since the separated parts are kinematically decoupled. Thus, the element-wise integrals are evaluated in each part and then they are summed up over the whole element. Partitioning must not be confused with remeshing, since only the integration is done over parts of the element, but no further elements are created.

2.4 Nonlinear System of Equations

We insert again the trial functions (34) and the test function (35) in the weak form (30) and obtain the following nonlinear system of equations:

$$\begin{bmatrix} M^{d}_{IJ} & M^{dq}_{IJ} \\ M^{qd}_{IJ} & M^{q}_{IJ} \end{bmatrix} \begin{Bmatrix} \ddot{d}_J \\ \ddot{q}_J \end{Bmatrix} = \begin{bmatrix} f^{ext}_I - f^{int}_I \\ Q^{ext}_I - Q^{int}_I \end{bmatrix} \tag{39}$$

2.5 Linearization

The nonlinear system has to be linearized as well by the Newton-Raphson method and we have to determine the Jacobian matrix A_{IJ} by numerical integration (i.e. Gauss quadrature):

$$\begin{bmatrix} A^{d}_{IJ} & A^{dq}_{IJ} \\ A^{qd}_{IJ} & A^{q}_{IJ} \end{bmatrix} = \frac{1}{\beta \Delta t^2} \begin{bmatrix} M^{d}_{IJ} & M^{dq}_{IJ} \\ M^{qd}_{IJ} & M^{q}_{IJ} \end{bmatrix} + \begin{bmatrix} K^{i,d}_{IJ} & K^{i,dq}_{IJ} \\ K^{i,qd}_{IJ} & K^{i,q}_{IJ} \end{bmatrix} - \begin{bmatrix} K^{e,d}_{IJ} & K^{e,dq}_{IJ} \\ K^{e,qd}_{IJ} & K^{e,q}_{IJ} \end{bmatrix} \tag{40}$$

2.6 Numerical Integration

Here we will experience the biggest differences in contrast to the FEM. It shows that M^{d}_{IJ} is the only well-known block in the mass matrix. Due the discontinuous part in the approximated solution, we obtained three additional blocks in the mass matrix containing the enrichment function Ψ:

$$M^{d}_{IJ} = \int_{\Omega} \rho N_I N_J \, d\Omega \tag{41}$$

$$M^{dq}_{IJ} = \int_{\Omega} \rho N_I \Psi_J \, d\Omega \tag{42}$$

$$M^{qd}_{IJ} = \int_{\Omega} \rho \Psi_I N_J \, d\Omega \tag{43}$$

$$M^{q}_{IJ} = \int_{\Omega} \rho \Psi_I \Psi_J \, d\Omega \tag{44}$$

Since we have a discontinuity in the element, we cannot simply integrate over the entire element. Instead the element is partitioned and each partition is integrated separately and then the results of all partitions per element are summed up:

$$\begin{aligned} M^{dq}_{IJ} &= \int_{\Omega} \rho N_I \Psi_J \, d\Omega \\ &= \int_{-1}^{\xi_c} \rho N_I \Psi^b_J J^b_\xi A \, d\xi + \int_{\xi_c}^{1} \rho N_I \Psi^a_J J^a_\xi A \, d\xi \end{aligned} \tag{45}$$

The external and internal stiffness matrices are again determined analogously. For the time integration the Newmark-β-method can be applied identically.

2.7 Application of the X_FEM

The X_FEM can be used to compute problems in solid and fluid mechanics with interfaces i.e. between different materials or different phases. The interfaces can be defined within the element. The complexity of meshes can be therefore dramatically reduced, and no remeshing has to be carried out.

Dynamical problems involving cracks can be solved in solid mechanics if the crack is already predefined in the input data and does not occur during run-time. In the quasi-static case cracks can even evolve and propagate during run-time.

Thus the X_FEM was found to be applicable for a variety of problems and still shows a big potential for further development.

References

[1] Belytschko T.; *Nonlinear finite elements for continua and structures*; Wiley; 2000

[2] Belytschko T., Chen H., Xu J., Zi G.; *Dynamic crack propagation based on loss of hyperbolicity and a new discontinuous enrichment*; International Journal for Numerical Methods in Engineering, 58, p.1873-1905; 2003

[3] Belytschko T., Moes N., Usui S., Parimi C.; *Arbitrary discontinuities in finite elements*; International Journal for Numerical Methods in Engineering, 50, p.993-1013; 2001

[4] Zi G.; Belytschko T.; *New crack-tip elements for XFEM and applications to cohesive cracks*; International Journal for Numerical Methods in Engineering, 57, p.2221-2240; 2003