

Material forces in Computational Mechanics : Variational ALE Method

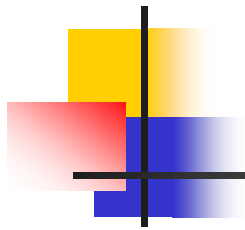
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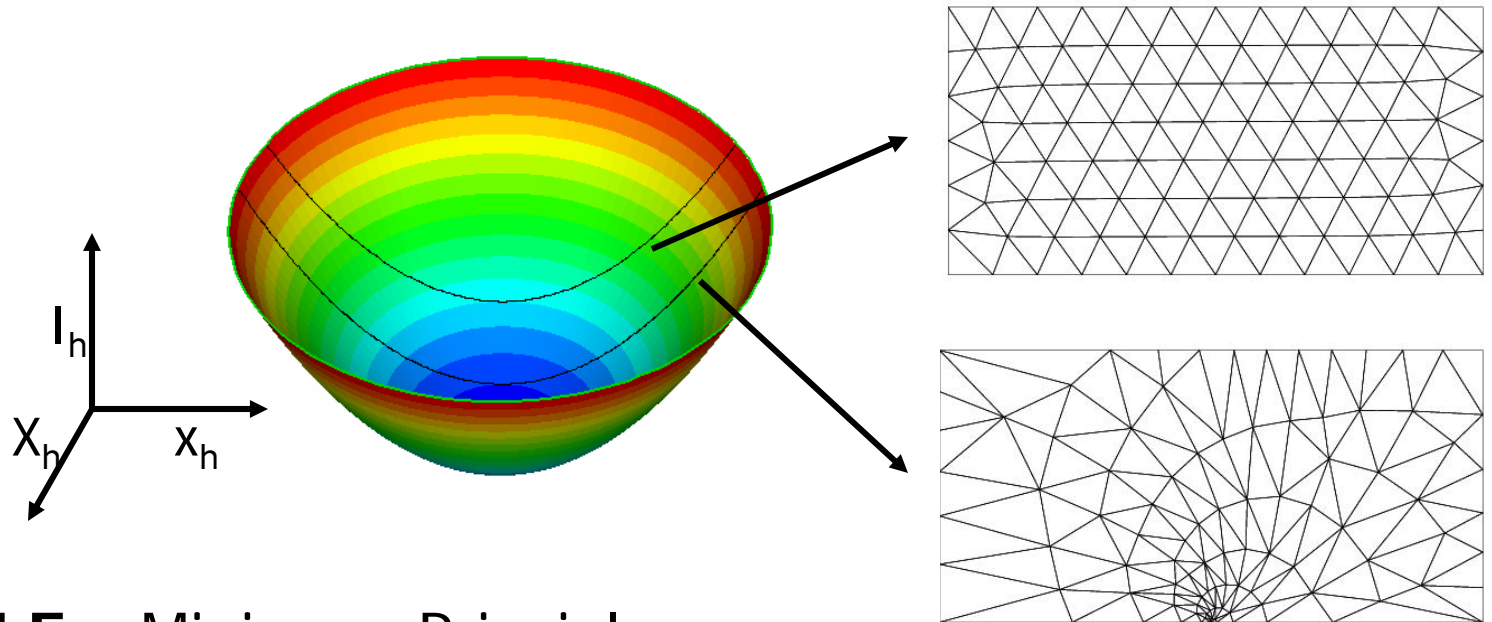


Organization

- VALE – description
- Static mesh adaption
- Shape optimization
- Variational Integrator with horizontal variations
- Conclusions

Introduction

Variational ALE (VALE) method is finite element method for PDE's generalized to account for **horizontal variations**



Static **VALE** – Minimum Principle:

- Find the solution

$$\mathbf{x}_h^*, \mathbf{X}_h^* : \text{Min } I[\mathbf{x}_h, \mathbf{X}_h] \quad \forall \text{ admissible } \mathbf{x}_h, \mathbf{X}_h$$



VALE method

Dynamic **VALE** – Hamilton's Stationarity Principle :

- Find the solution

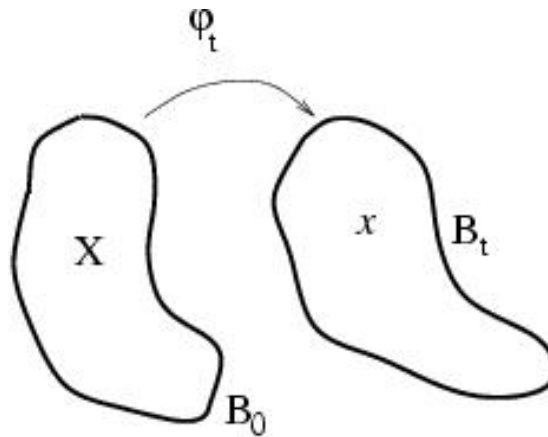
$\mathbf{x}_h^{i*}, \mathbf{X}_h^{i*}$: Stationarity of $S_d[\cup \mathbf{x}_h^i, \cup \mathbf{X}_h^i]$ **w.r.t** $\mathbf{x}_h^i, \mathbf{X}_h^i$

- Variational Integrator with horizontal variations

Salient Features :

- Mesh (nodal coordinates) itself is the solution, in addition to nodal variable solution
- Furnishes precise mesh optimality criterion
- Devoid of error estimates and mesh-to-mesh transfer
- Enables solution for optimal material configuration

Variational Formulation - Static



Variational Formulation :

- Consider solid with strain energy density $W(\mathbf{F})$, then functional

$$I[\varphi] = \int_{B_0} W(\nabla_0 \varphi) dV_0$$

$$\mathbf{x} = \varphi(\mathbf{X})$$



Variational Formulation - Static

Discrete Mechanics:

- Introducing Discretization

$$\mathbf{x}_h(\mathbf{X}) = \sum_{a=1}^N \mathbf{x}_a N_a(\mathbf{X}) = \sum_{a=1}^n \mathbf{x}_a^e N_a^e(\mathbf{X}), \quad \mathbf{X} \in \Omega^e$$

- Discrete Functional

$$I_h[\mathbf{x}_h, \mathbf{X}_h] = \sum_{e=1}^E \int_{\Omega_0^e(\mathbf{X}_h)} W(\nabla_0 \mathbf{x}_h) dV_0$$

Variational Formulation – Static

Discrete Equations – Stationarity condition:

$$\langle DI_h, \delta \mathbf{x}_h \rangle \cdot \delta \mathbf{x}_h + \langle DI_h, \delta \mathbf{X}_h \rangle \cdot \delta \mathbf{X}_h = 0$$

for δx_h and δX_h independent everywhere except on dirichlet boundary

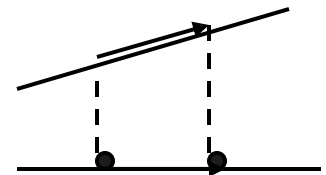
$$\langle DI_h, \delta \mathbf{x}_h \rangle = 0 \Rightarrow \mathbf{r} = \frac{\partial I_h}{\partial \mathbf{x}_h} = \mathbf{0} : \text{Nodal force equilibrium}$$

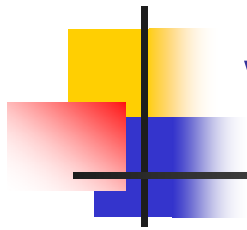
$$\langle DI_h, \delta \mathbf{X}_h \rangle = 0 \Rightarrow \mathbf{R} = \frac{\partial I_h}{\partial \mathbf{X}_h} = \mathbf{0} : \text{Configurational force equilibrium}$$

Optimal mesh criterion : Configurational force equilibrium

• On the Dirichlet boundary :

$$\delta x_{ia} = \frac{\partial \bar{x}_i}{\partial X_I} \delta X_{Ia} \Rightarrow R_{Kb} = \frac{\partial I_h}{\partial X_{Kb}} + \frac{\partial \bar{x}_k}{\partial X_K} \frac{\partial I_h}{\partial x_{kb}} = 0$$





Variational Formulation – Static

Model Problem – Elastic solid

First Piola-Kirchhoff stress : $\mathbf{P} = \frac{\partial W}{\partial \mathbf{F}}$

Nodal and Configurational forces

$$\frac{\partial I_h}{\partial x_{kb}} = \sum_{e=1}^E \int_{\Omega_0^e} P_{kJ} N_{b,J} V_0,$$

$$\frac{\partial I_h}{\partial X_{Kb}} = \sum_{e=1}^E \int_{\Omega_0^e} M_{KJ} N_{b,J} dV_0$$

Eshelby energy-momentum tensor : $M_{KJ} = W \delta_{KJ} - F_{iK} P_{iJ}$

Variational Formulation – Static

Material force on a defect

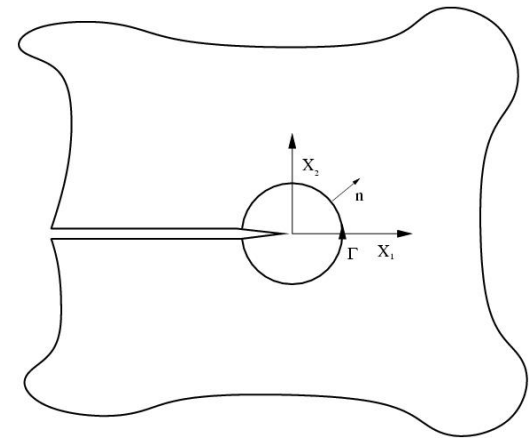
Defect (imperfections):

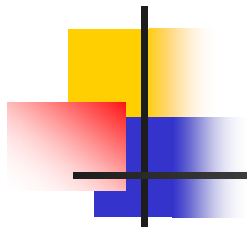
$$\mathbf{R} = \int_{S_0} \mathbf{M} \cdot \mathbf{N} \, dS_0$$

- J-integral : path independent

Tangential crack node material force

$$J = R_1 = \int_{\Gamma} m_{1j} n_j \, d\Gamma$$





Material forces

Continuous case :

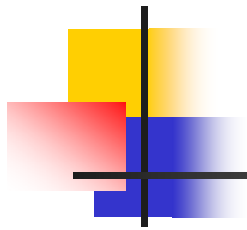
Homogeneous case : $I = \int_{\Omega} W(\mathbf{F}) \, dV_0$

Invariant under translation in reference configuration

Euler-Lagrange Equations : $\nabla_0 \cdot \mathbf{P} = 0 \Rightarrow$ translation invariance

Inhomogeneous case : $I = \int_{\Omega} W(\mathbf{F}, \mathbf{X}) \, dV_0$

Euler-Lagrange Equations : $\nabla_0 \cdot \mathbf{P} = 0 \not\Rightarrow$ translational invariance



Material forces

Discrete case :

Homogeneous case :

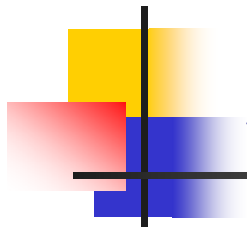
$$I_h[\mathbf{x}_h, \mathbf{X}_h] = \sum_{e=1}^E \int_{\Omega_0^e(\mathbf{X}_h)} W(\nabla_0 \mathbf{x}_h) dV_0$$

No translational symmetry :

$$\frac{\partial I_h}{\partial x_h} = 0 \not\Rightarrow \frac{\partial I_h}{\partial X_h} = 0$$

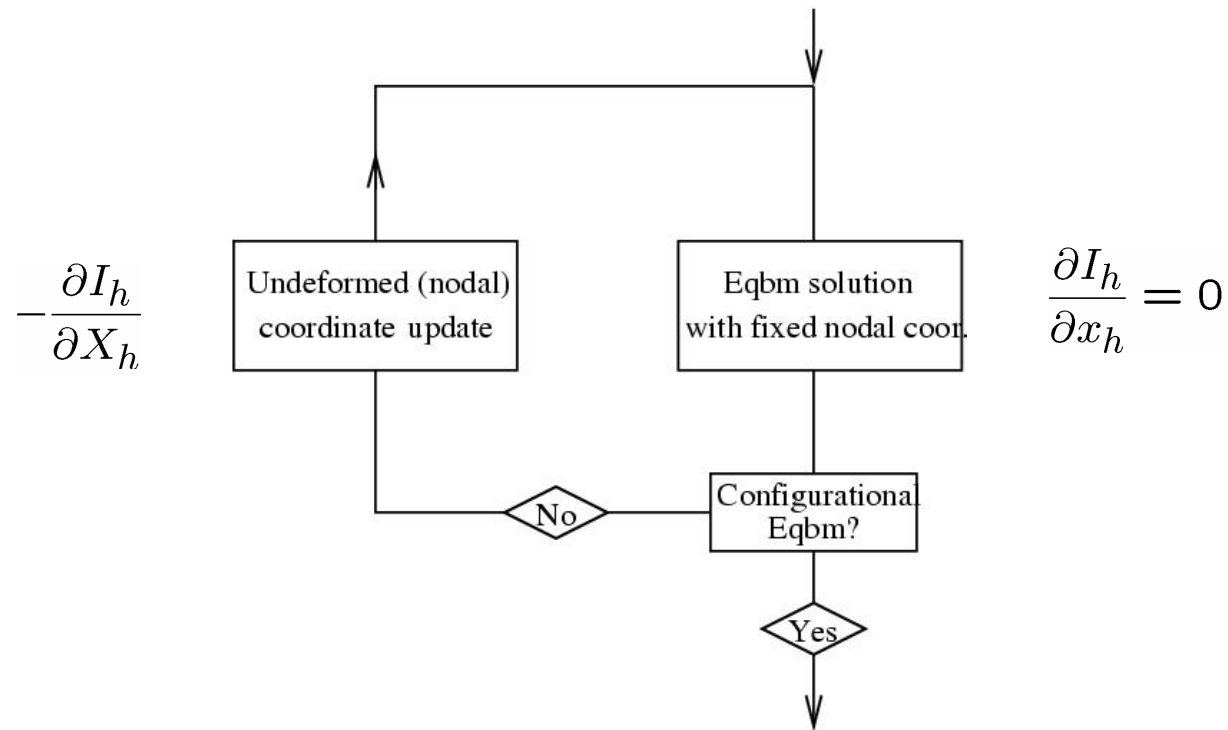
Nodes : Distribution of defects

Optimal mesh : no material forces on nodes



Solution Method

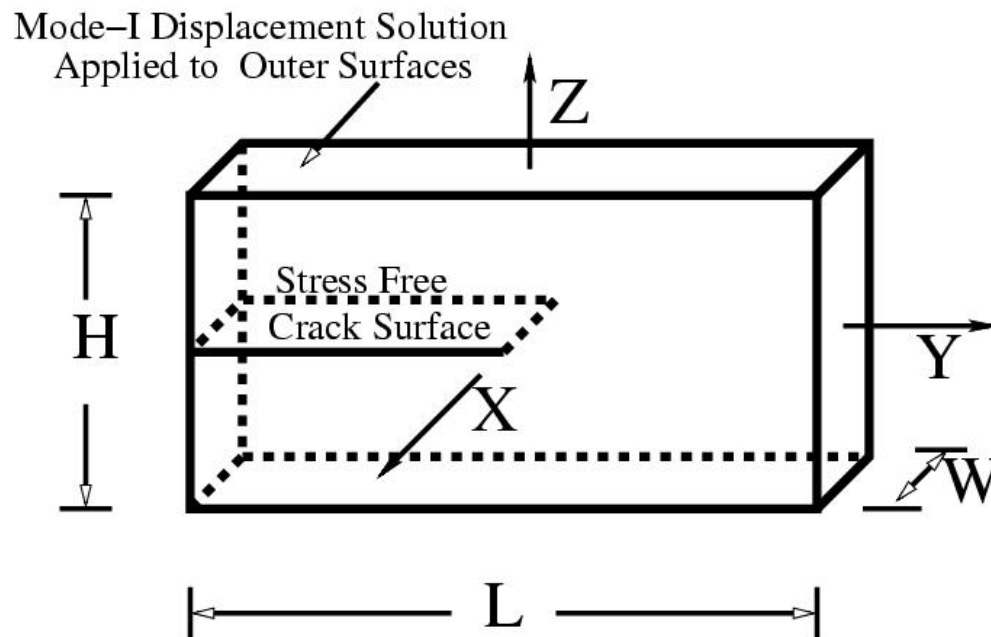
- Conjugate Gradient Method (Polak-Ribiere)



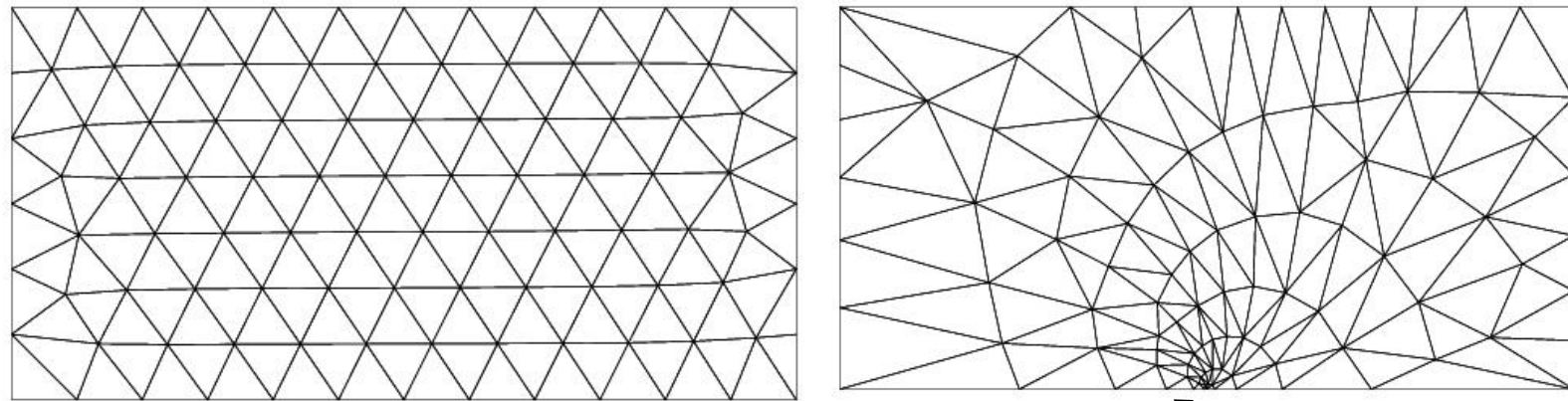
Mesh Optimization

Plane strain crack geometry with applied K_I -field

- Known analytic solution - singular



Mesh Optimization-2d



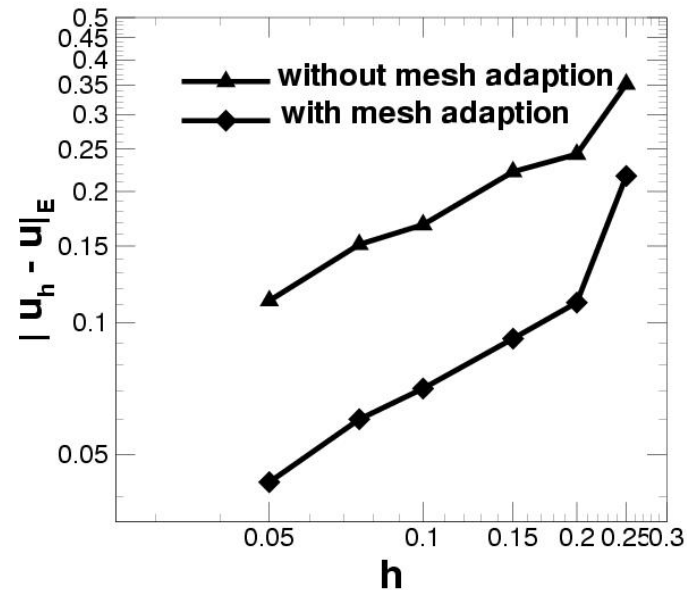
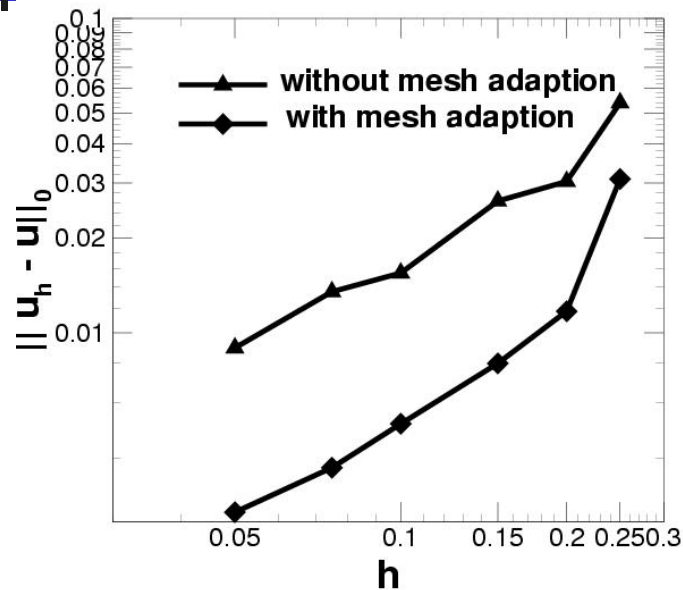
symmetry

Crack tip

Mesh before and after mesh optimization

$$E = 217.5 \text{ MPa} \quad \nu = 0.3 \quad K_I = 1.0 \text{ MPa}\sqrt{m}$$

Convergence Rate – 2d

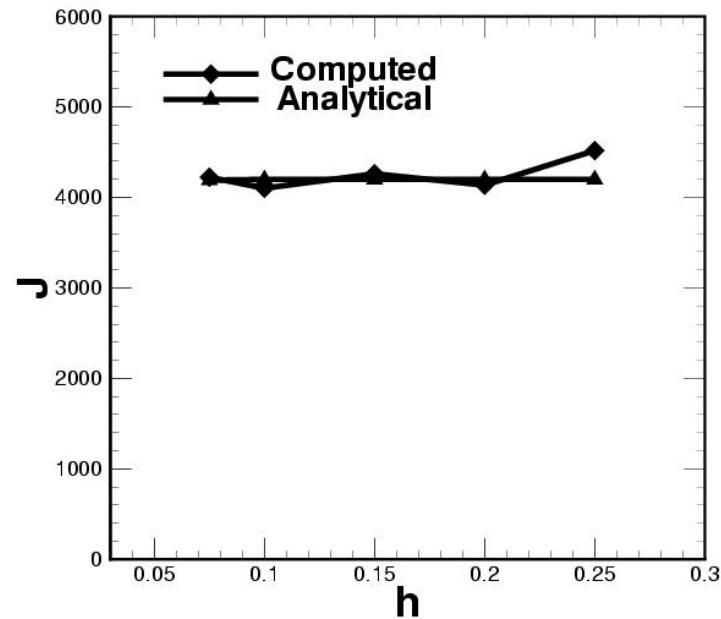


	$\ \mathbf{u}_h - \mathbf{u} \ _0$	$ \mathbf{u}_h - \mathbf{u} _E$
without adaption	0.8794	0.5172
with adaption	1.1369	0.6662

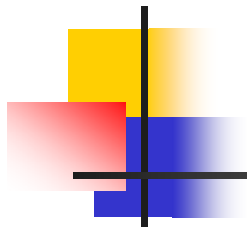
$$\|\mathbf{u}\|_0 = \left\{ \int_{\Omega} |\mathbf{u}|^2 d\Omega \right\}^{1/2}, \quad |\mathbf{u}|_E = \left\{ \int_{\Omega} \sigma_{ij} u_{i,j} d\Omega \right\}^{1/2}$$

J-integral

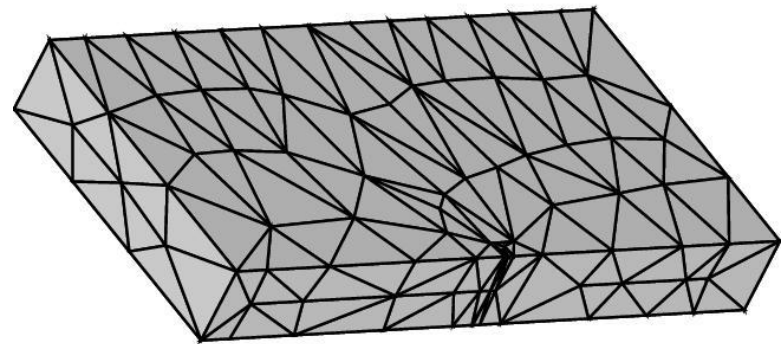
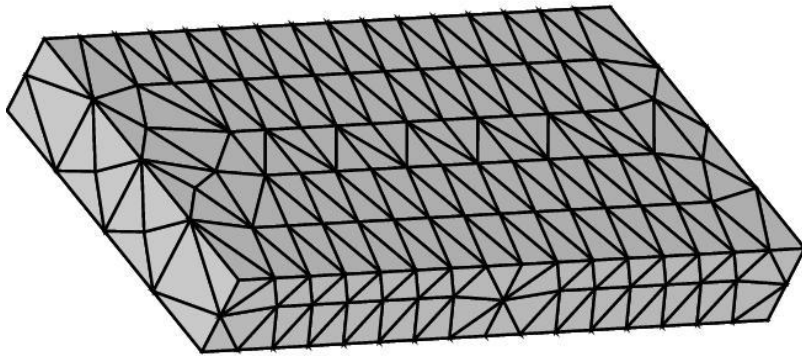
J-integral : Pointwise calculation, $J_h = -\frac{\partial I_h}{\partial X_{01}}$



$$J = \frac{(1 - \nu^2) K_I^2}{E}$$

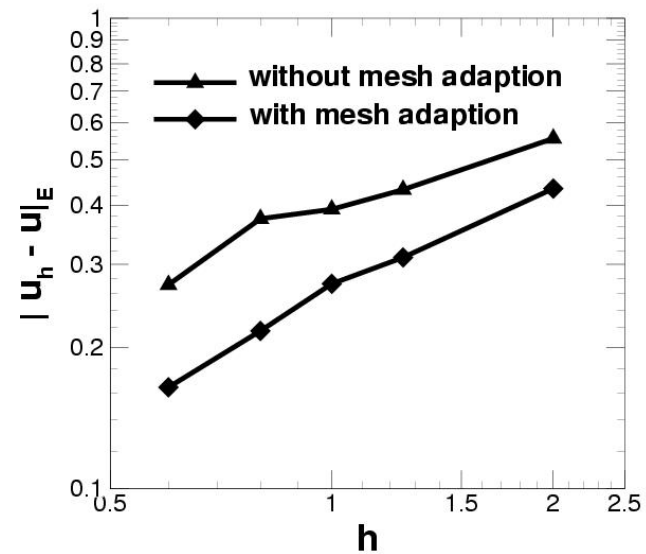
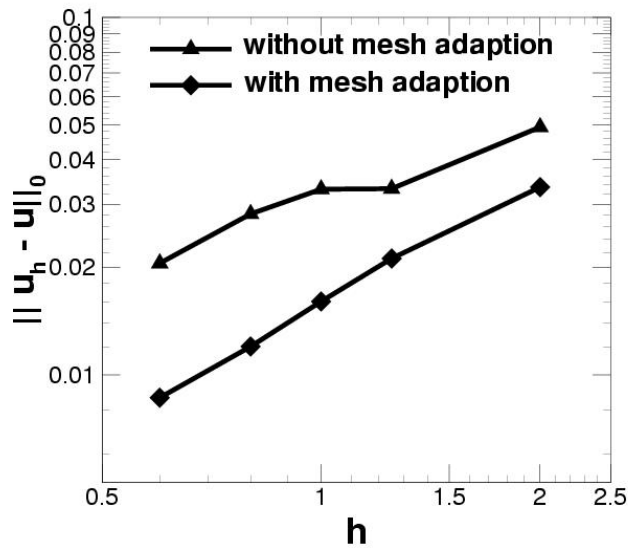


Mesh Optimization-3d

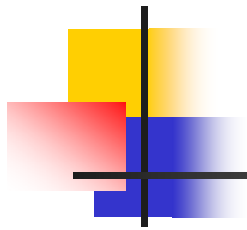


Mesh before and after mesh optimization

Convergence Rate – 3d



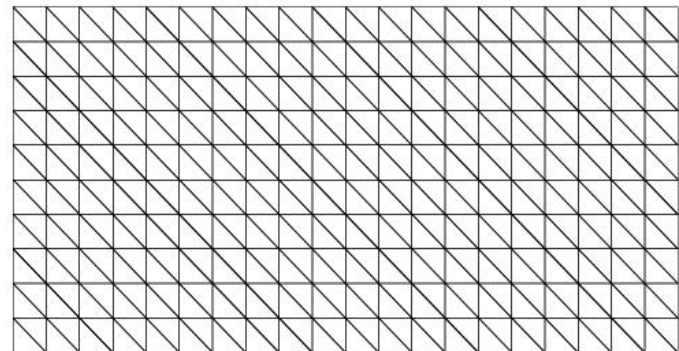
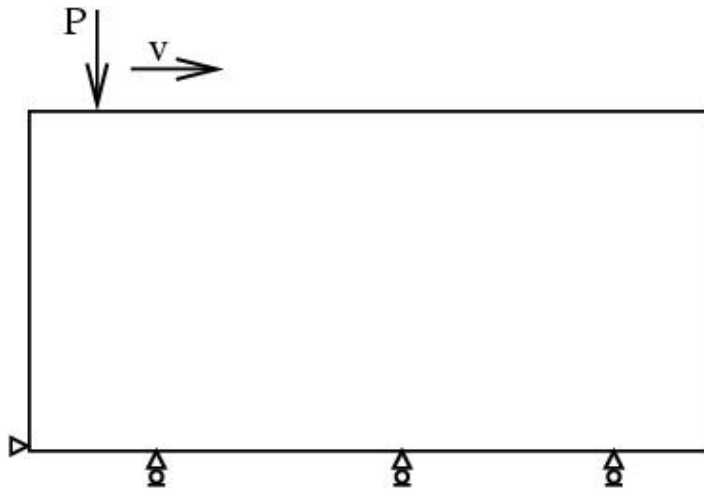
	$\ \mathbf{u}_h - \mathbf{u} \ _0$	$ \mathbf{u}_h - \mathbf{u} _E$
without adaption	0.728	0.5849
with adaption	1.1265	0.8079

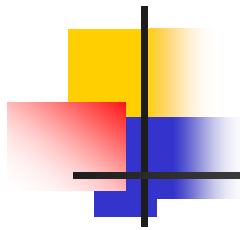


Neoohookean solid

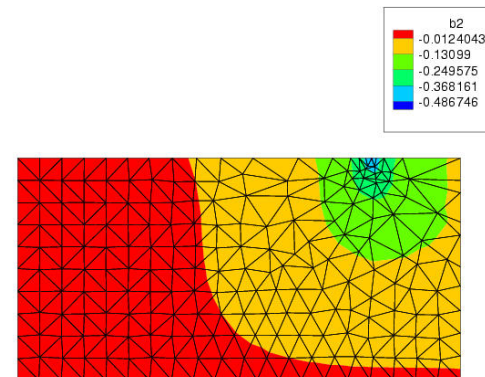
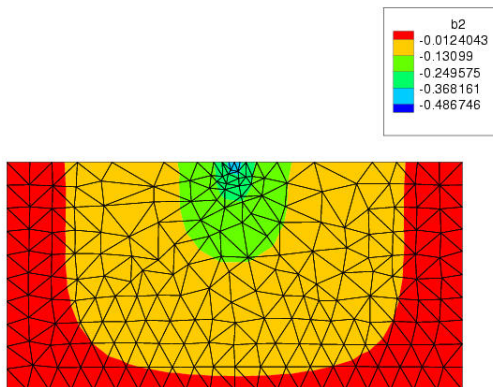
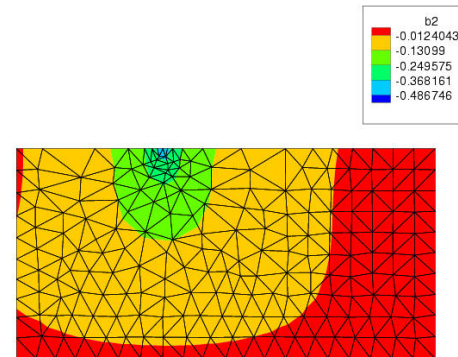
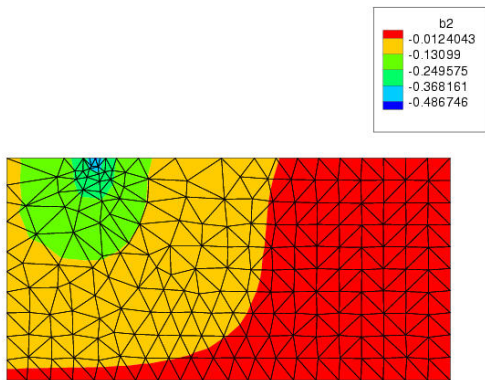
- Finite deformation – quasi-static :

$$W(F) = \frac{1}{2}\lambda_0(\log J)^2 - \mu_0 \log J + \frac{\mu_0}{2}\text{tr}(F^T F)$$



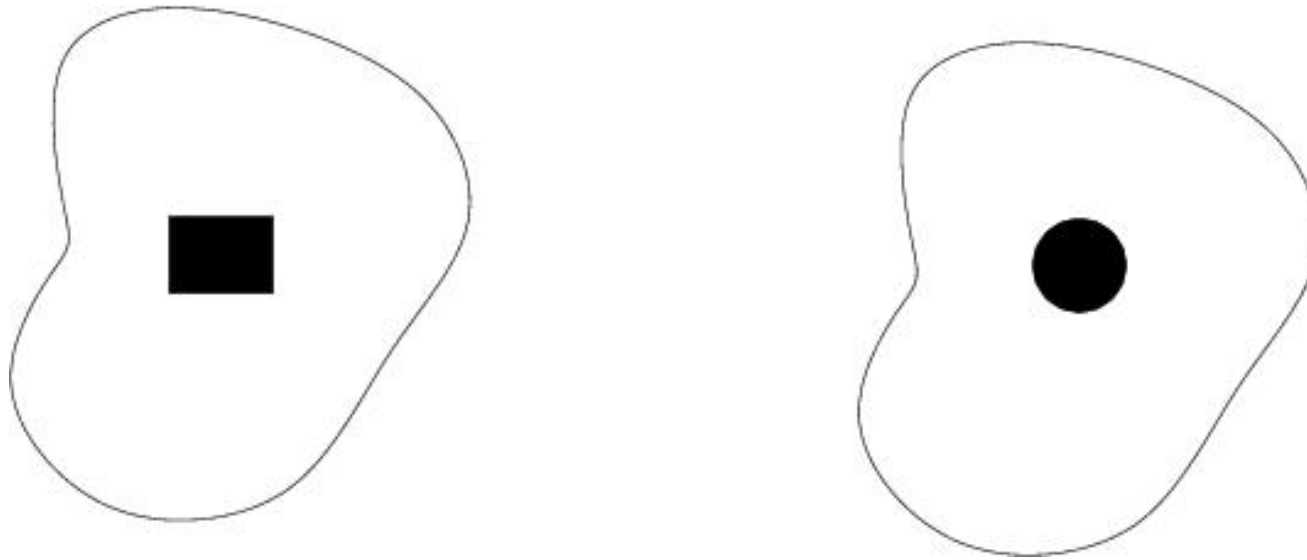


Neohookean solid





Shape Optimization

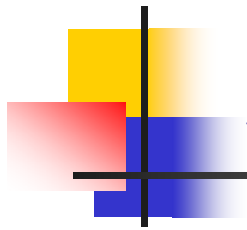


Precipitates of two different shapes of same size

What is the Optimal shape ?

$$I_h = \int_{B_0} W(\nabla_0 \varphi_h) dV_0 + \int_{\partial B_{02}} \gamma dS_0 + \frac{1}{2} \alpha (A_0 - \int_{B_2} dV_0)^2$$

$$B_0 = B_{01} \cup B_{02}$$



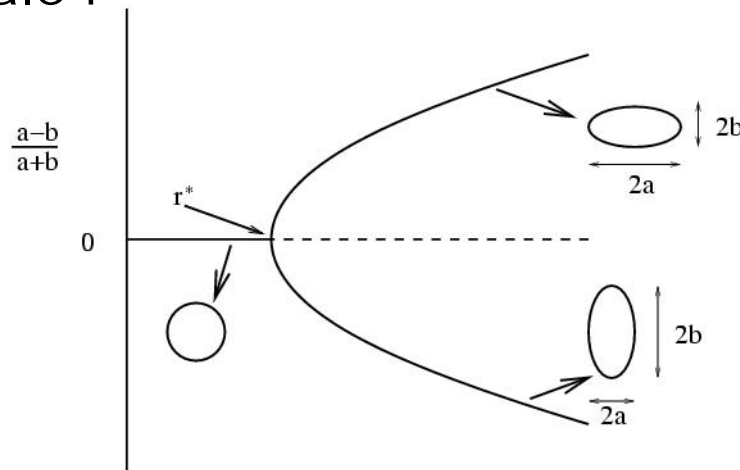
Shape Optimization

Numerical Example – dilatational misfit :

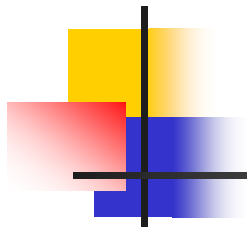
- Transformational strains ϵ^T differ by dilatation component

$$\sigma = \mathbf{C} : (\epsilon - \epsilon^T)$$

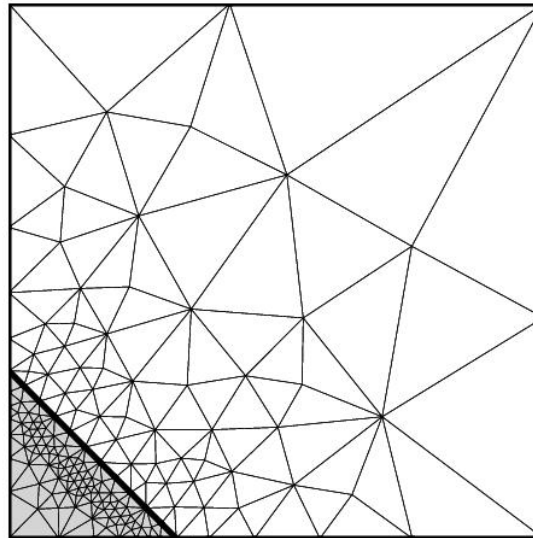
- Misfit strain energy scales with volume
- Interface energy scales with interface area
- Due to the competition between the two, there is a critical length scale r^*



Symmetry Bifurcation

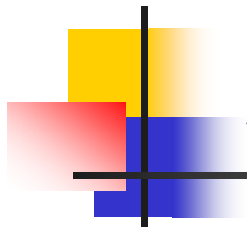


Initial Mesh



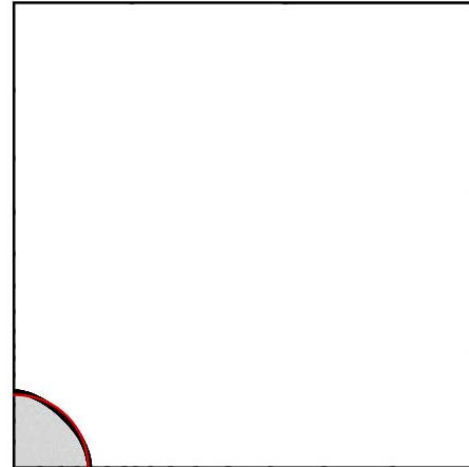
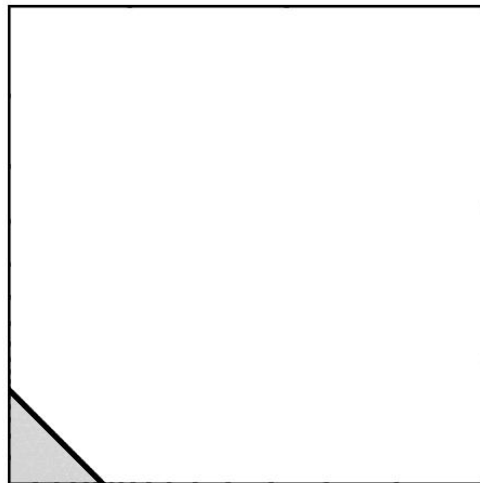
Initial mesh for shape optimization

- Element faces coincide with interface
- Elements retain material identification



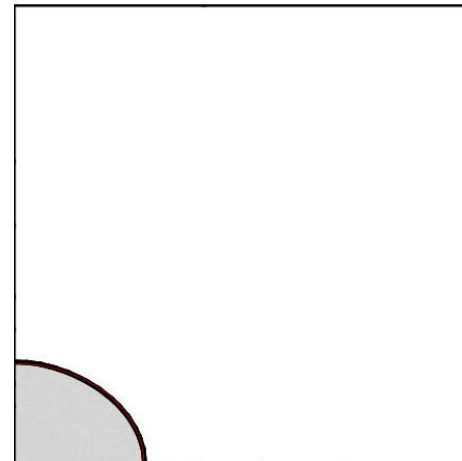
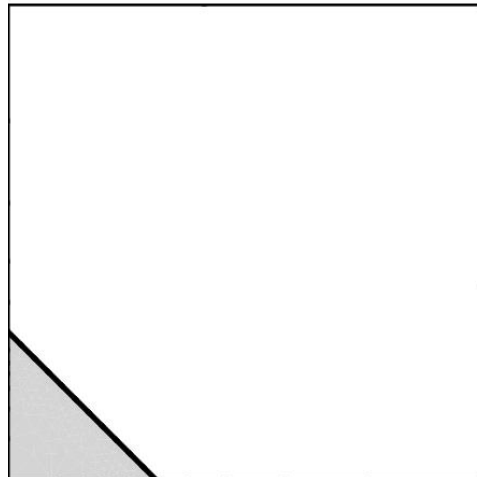
Symmetry Bifurcation

$r(=31.8\text{nm}) < r^*$



$r^* = 35.62\text{nm}$

$r(=50\text{nm}) > r^*$



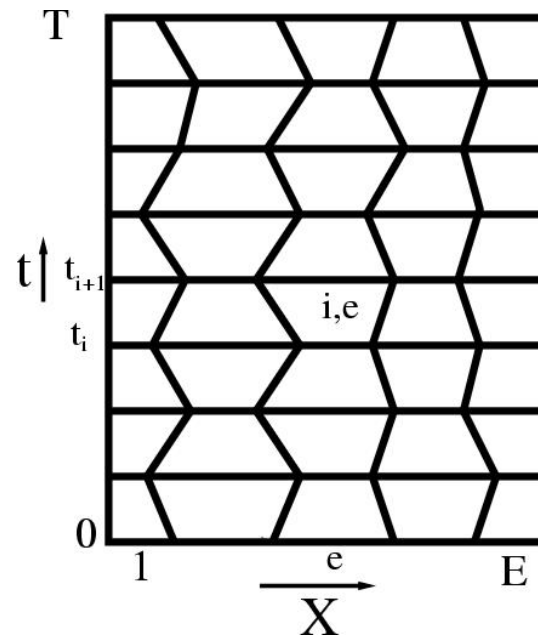
Precipitate shape before and after shape optimization

VALE – dynamic

Hamilton's principle : stationarity solution for

$$S = \int_0^T \int_{B_0} \left(\frac{1}{2} \rho_0 |\dot{\varphi}|^2 - W(\nabla_0 \varphi) \right) dV_0 dt$$

Spacetime Formalism :



VALE – dynamic

Introducing spacetime discretization

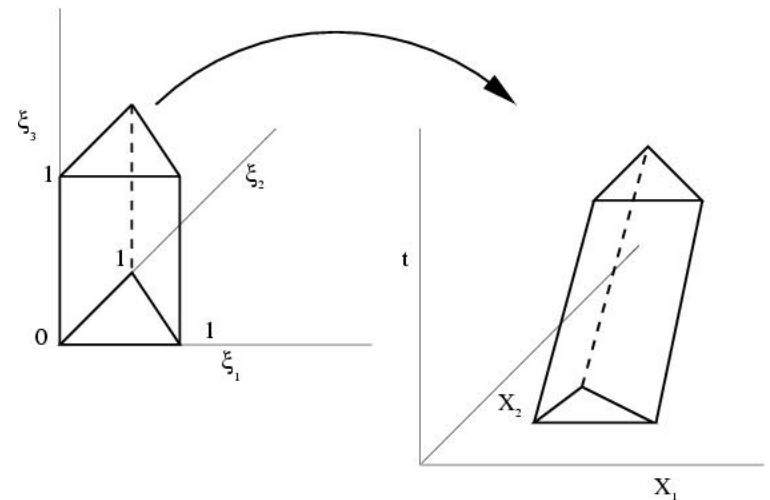
$$\varphi_h(\mathbf{X}, t) = \sum_{a=1}^N \mathbf{x}_a \mathbf{N}_a(\mathbf{X}, t) = \sum_{e=1}^{m \times E} \sum_{a=1}^n \mathbf{x}_a^e \mathbf{N}_a^e(\mathbf{X}, t)$$

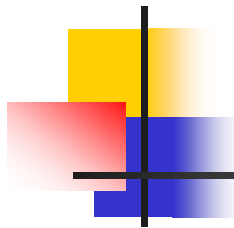
- Shape functions : space-time product

$$N(\xi_1, \xi_2, \xi_3) = N^s(\xi_1, \xi_2) N^t(\xi_3)$$

$$\frac{\partial N_a}{\partial \xi_\alpha} = \frac{\partial N_a}{\partial X_i} \frac{\partial X_i}{\partial \xi_\alpha}$$

$$\frac{\partial N_a}{\partial X_i} = \left(\frac{\partial X_i}{\partial \xi_\alpha} \right)^{-1} \frac{\partial N_a}{\partial \xi_\alpha}$$





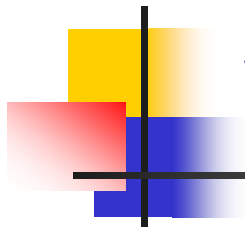
VALE – dynamic

Discrete action sum :

$$S_d = \sum_{i=1}^m \sum_{e=1}^E \int_{\Omega_e^i} \frac{1}{2} \rho_0 \left(\sum_{a=1}^n x_{ja} N_{a,t} \right)^2 - W \left(\sum_{a=1}^N x_{ja} N_{a,J} \right) d\Omega_e^i$$

Discrete Hamilton's principle :

$$\sum_{i=2}^m \langle DS_d, \delta \mathbf{x}_h^i \rangle \cdot \delta \mathbf{x}_h^i + \langle DS_d, \delta \mathbf{X}_h^i \rangle \cdot \delta \mathbf{X}_h^i = 0$$



Variational Integrator

Discrete Equations

for $\delta \mathbf{x}^i$ and $\delta \mathbf{X}^i$ are independent

$$\mathbf{r}^i = \langle DS_d, \delta \mathbf{x}_h^i \rangle = 0, \quad \mathbf{R}^i = \langle DS_d, \delta \mathbf{X}_h^i \rangle = 0, \quad i = 2 \dots m$$

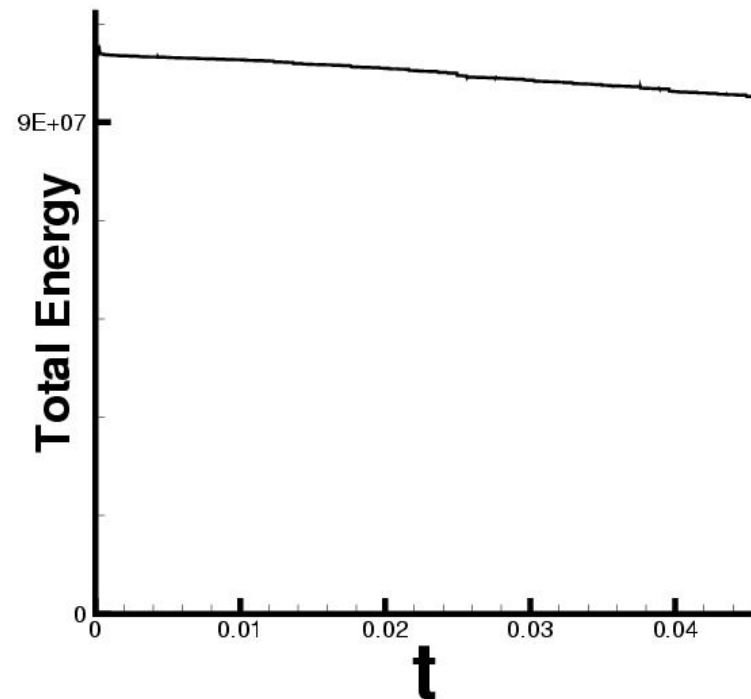
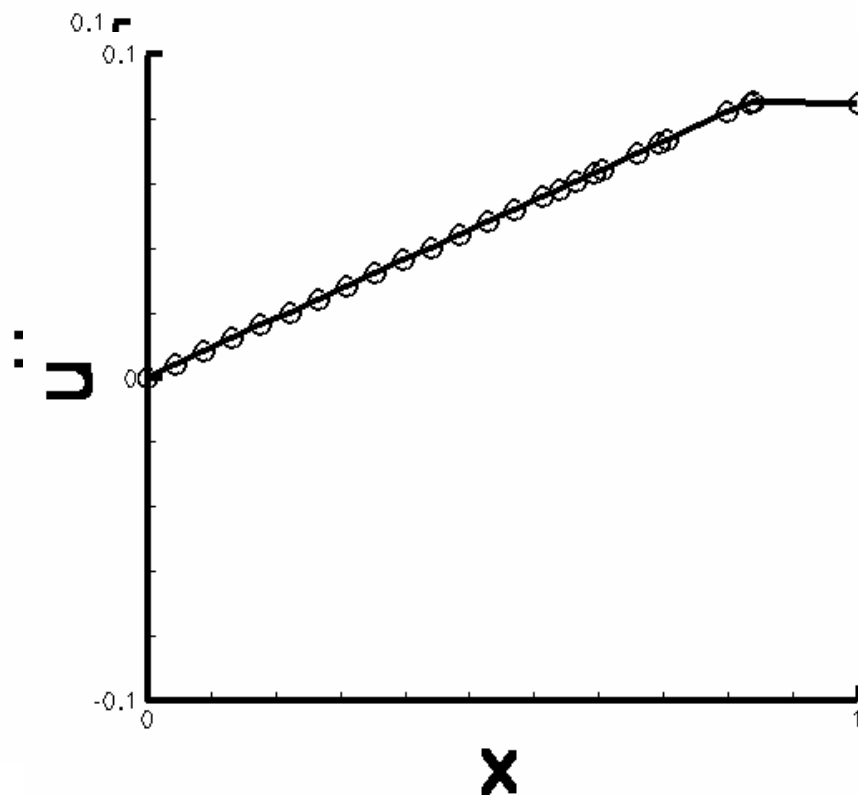
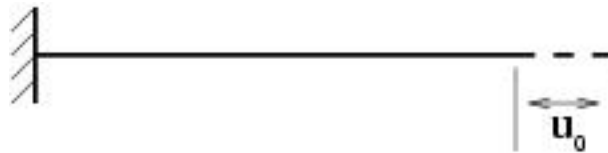
- These equations, corresponding to nodal and configurational force equilibrium, provide update for \mathbf{x}^{i+1} and \mathbf{X}^{i+1} and can be solved implicitly with Newton-Raphson method

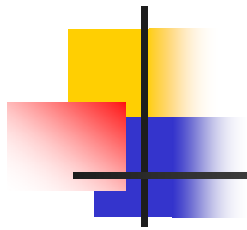
Element Equations :

$$r_{ck}^{i,e} = \frac{\partial S_d^{i,e}}{\partial x_{ck}} = \int_{\Omega_e^i} (\rho_0 x_{c,t} N_{k,t} - P_{cJ} N_{k,J}) d\Omega_e^i$$

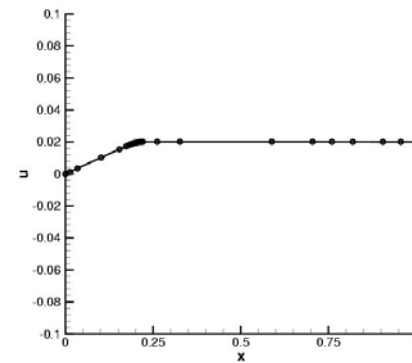
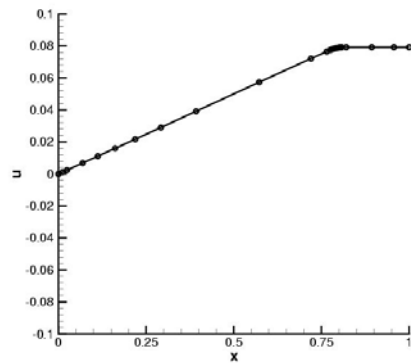
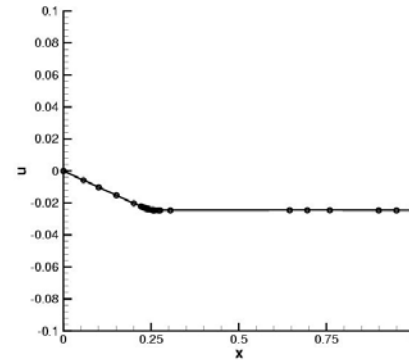
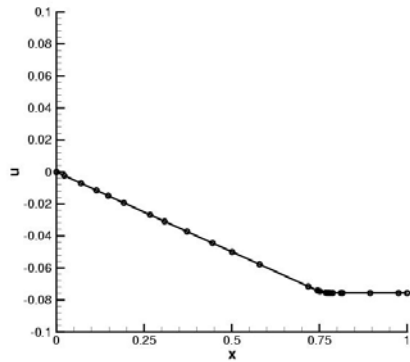
$$R_{Ck}^{i,e} = \frac{\partial S_d^{i,e}}{\partial X_{Ck}} = \int_{\Omega_e^i} \left(\frac{1}{2} \rho_0 x_{i,t} x_{i,t} N_{k,C} - \rho_0 x_{i,t} F_{iC} N_{k,t} - M_{CJ} N_{k,J} \right) d\Omega_e^i$$

Dynamic mesh optimization-1d





Dynamic mesh optimization-1d





Summary

☐ Mesh Optimization

- Precise criterion for mesh optimality
- Does not involve error estimation
- Devoid of mesh-to-mesh transfer and hence interpolation errors
- Accurate solution for a given number of nodes
- Ideal for parallel computation : no dynamic load balancing
- Symplectic-momentum preserving variational integrator with horizontal variations

☐ Ideally suited for solution of optimal reference configuration

- Shape/structural optimization

☐ Well suited for resolving steep gradients