SAND2013-1340C

MultiScale Modeling Methods for Solid Mechanics

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

Major discussion points…

- Why even consider Multiscale ?
- What do we mean by consistent deformation ?
- Solver design for Multiscale modeling
- Can explict-to-implicit scale coupling be considered ?

Ref: Heinstein M.W. ,“A Finite Element Multiscale Capability for Nonlinear Quasistatic stress Analysis,” Finite Elements in anlysis and Design, Vol 4. April 2005, pp. 800-817

Fish, J., Chen, W. 2001, “Higher-order homogenization of Initial/Boundary value problem,” Journal of Engineering Mechanics, Vol 127, No. 12, pp. 1223-1230

Motivation for Multiscale Modeling

Computational Simulation & Parallel Computing:

- Routine models are now (O 10^6-10^7),

  and are run on many processors (O 10^2-10^3)

Observation: as problem sizes ⇧, # processors ⇧

- QS: solvers loose scalability (complexity increases greater than compute cycles)

- ETD: Courant limited time integrators stagnate (cost increases extra (h) with refinement)

Acknowledgements

Computational Contact Algorithms/ Multi-Length Scale Algorithms

- parallel, scalable proximity search algorithm
  Stephen Attaway, Kevin Brown, Bruce Hendrickson,
  Steve Plimpton (SNL)

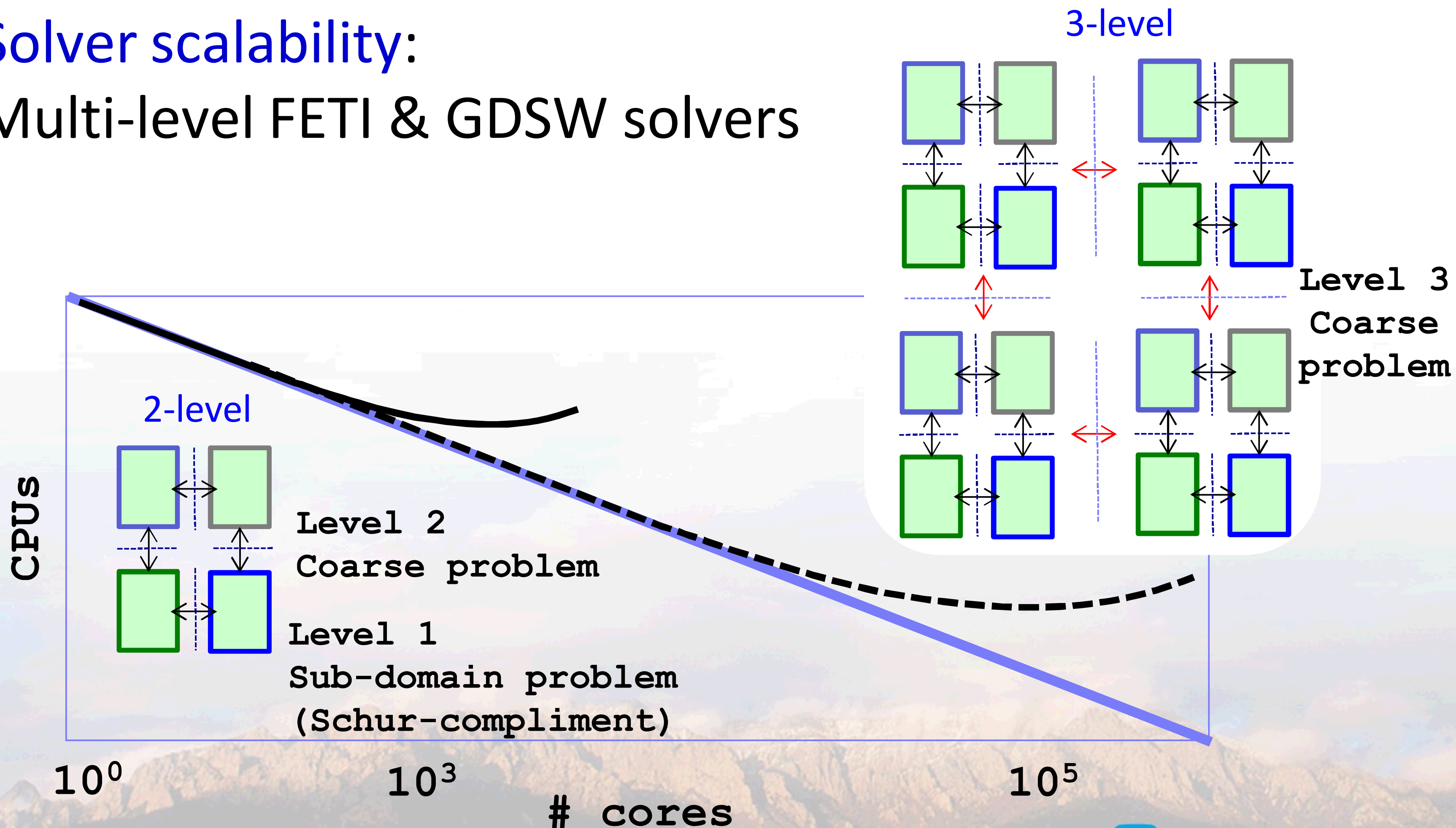
- iterative constraint enforcement methods for Explicit Transient Dynamics
  Kevin Brown, Tom Voth (SNL)

- Nested iterative constraint enforcement for Quasistatics
  Tod Laursen (Duke U.)

- Consistent interface algorithms for Quasistatic / Implicit Dynamics
  Clark Dohrmann, Sam Key (SNL), Tod Laursen (Duke U.)

Performance: Solver scalability

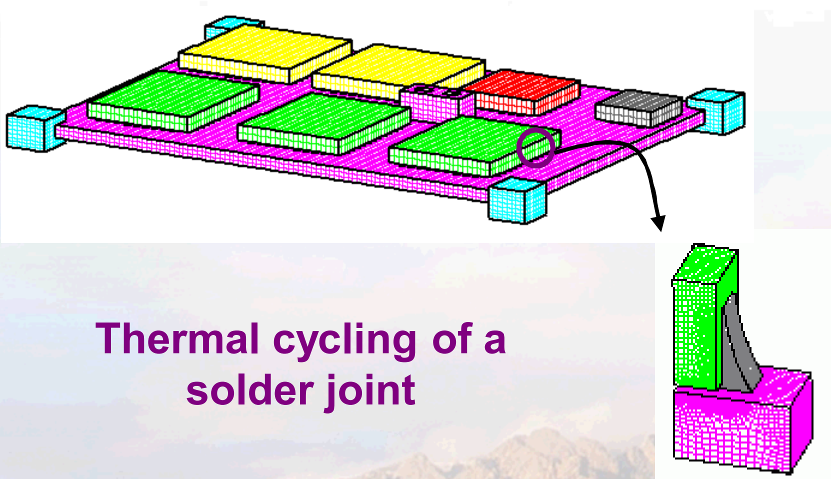
Emerging strategy for
Solver scalability:
Multi-level FETI & GDSW solvers



Physics Modeling: Failure

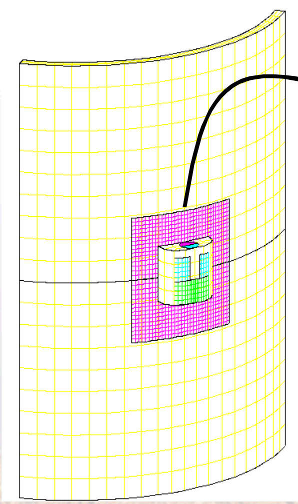
Failure modeling is inherently a multilength scale phenomenon that requires a failure model and a computational method that solves for solution gradients at interesting locations.

Although, adaptive mesh refinement (h-adaptivity) allows us to capture solution gradients for a class of problems, there is another class of problems where structural idealizations made in the reference calculation require a fine length scale with a different mesh topology, e.g.:

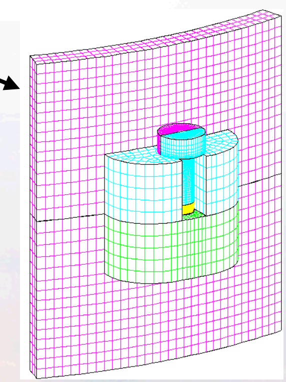


Thermal cycling of a solder joint

Failure of a bolted joint



Reference Length Scale Model with solid connection



Fine Length Scale Model with bolted connection

Multiscale FE Modeling

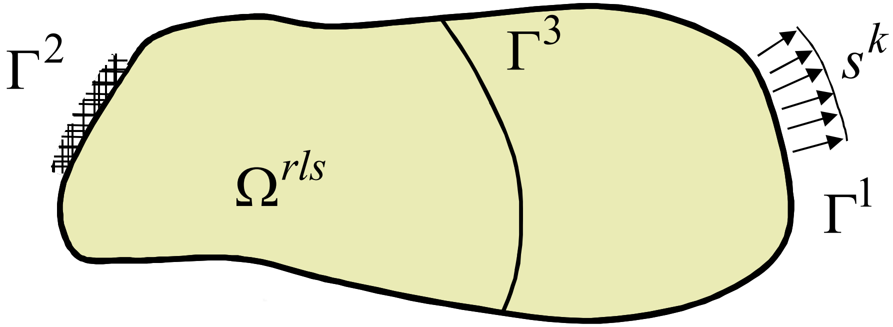
Multilength scale modeling is a computational technique aimed to provide detailed strain and stress results where failure prediction is critical.

The ability to "freely insert" a fine length scale mesh requires a solution of a coupled boundary value problem.

We anticipate that for many applications, multiscale modeling & mutiscale material modeling (e.g. RVEs) determines ultimately how well failure can be predicted.

Multilength-Scale Modeling

Reference length scale (*rls*) body, Ω^{rls}, with surfaces Γ^1, Γ^2 and Γ^3

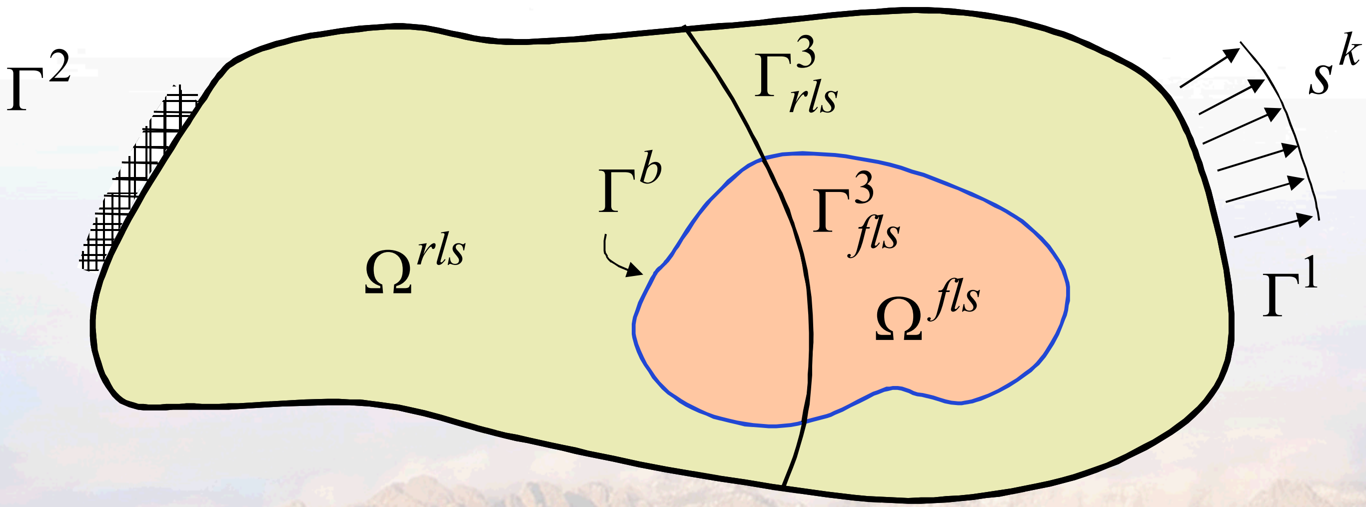


where, the following variational principle applies

$$\delta\Pi = \int_{\Omega^{rls}} \mathrm{T}^{ij}\,\delta u_{i,j}\,dv + \int_{\Omega^{rls}} \rho\,\ddot{x}^k \delta u_k\,dv - \int_{\Omega^{rls}} \rho\, b^k \delta u_k\,dv - \int_{\Gamma^1} s^k \delta u_k\,da + \int_{\Gamma^3} (-t_N \delta g_N)\,da \qquad \text{eqn. (1)}$$

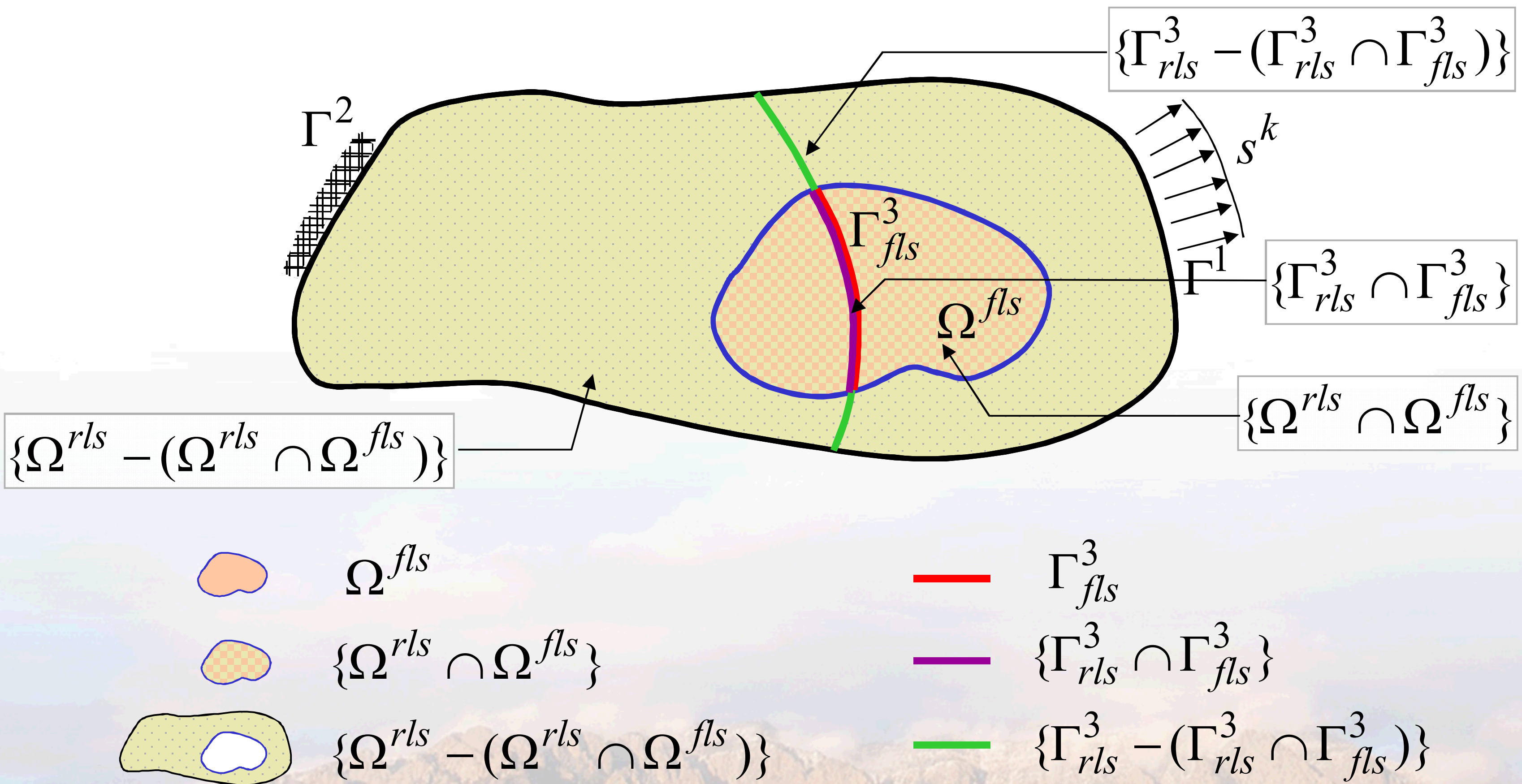
Introducing a second length scale

Lets introduce a second length scale, called the fine length scale (*fls*) body, Ω^{fls} with surface Γ^3_{fls} and Γ^b. Note that the *fls* body with exterior (boundary) surface Γ^b is fully inside the *rls* body and consequently overlaps it.



Domains and Surfaces

If the following sub-domains and sub-surfaces are defined…



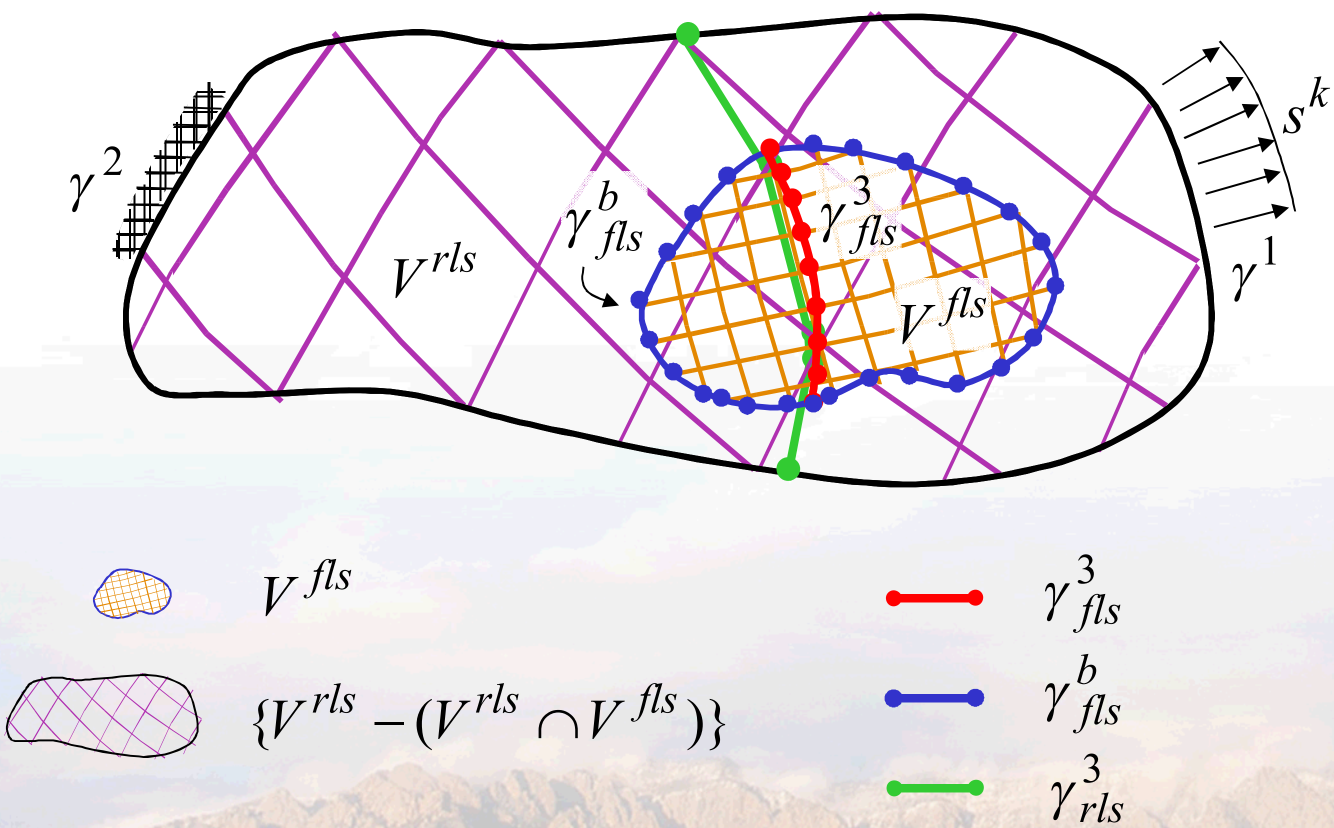
Variational statement

…then we argue that the following variational statement holds:

$$
\begin{aligned}
\delta\Pi = & \int_{\Omega^{rls}-(\Omega^{rls}\cap\Omega^{fls})} \mathrm{T}^{ij}\,\delta u_{i,j}\,dv + \int_{\Omega^{fls}} \mathrm{T}^{ij}\,\delta u_{i,j}\,dv \\
& + \int_{\Omega^{rls}-(\Omega^{rls}\cap\Omega^{fls})} \rho\,\ddot{x}^k\,\delta u_k\,dv + \int_{\Omega^{fls}} \rho\,\ddot{x}^k\,\delta u_k\,dv \\
& - \int_{\Omega^{rls}-(\Omega^{rls}\cap\Omega^{fls})} \rho\,b^k\,\delta u_k\,dv - \int_{\Omega^{fls}} \rho\,b^k\,\delta u_k\,dv \\
& - \int_{\Gamma^1_{rls}-\Gamma^1_{rls}\cap\Gamma^1_{fls}} s^k\,\delta u_k\,da - \int_{\Gamma^1_{fls}} s^k\,\delta u_k\,da \\
& + \int_{\Gamma^3_{rls}-\Gamma^3_{rls}\cap\Gamma^3_{fls}} (-t_N\,\delta g_N)\,da + \int_{\Gamma^3_{fls}} (-t_N\,\delta g_N)\,da
\end{aligned}
\qquad \text{eqn. (2)}
$$

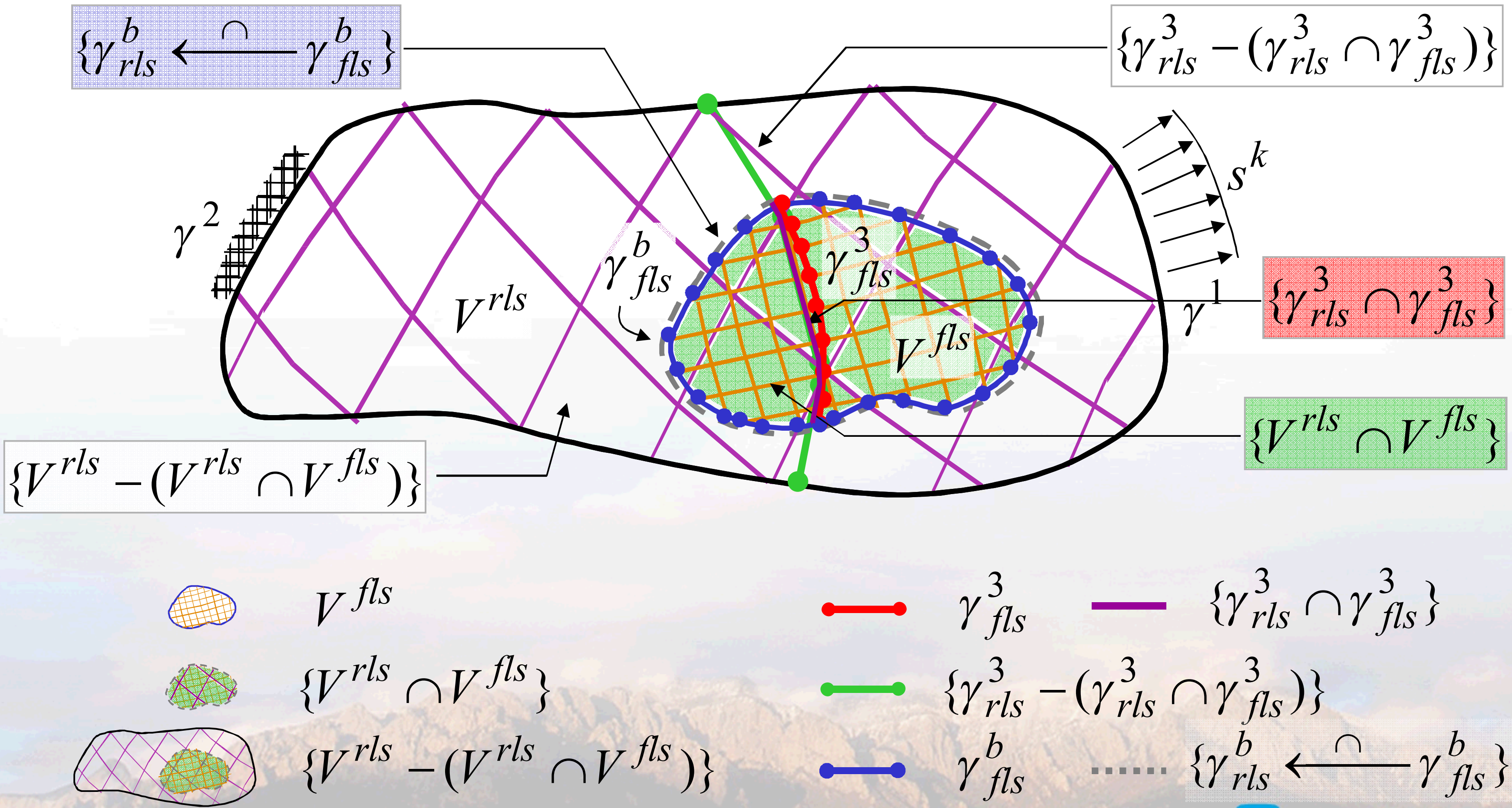
rls terms *fls* terms

FE Discretization of the Multi-length Scale problem



Imprinting the FE Discretizations

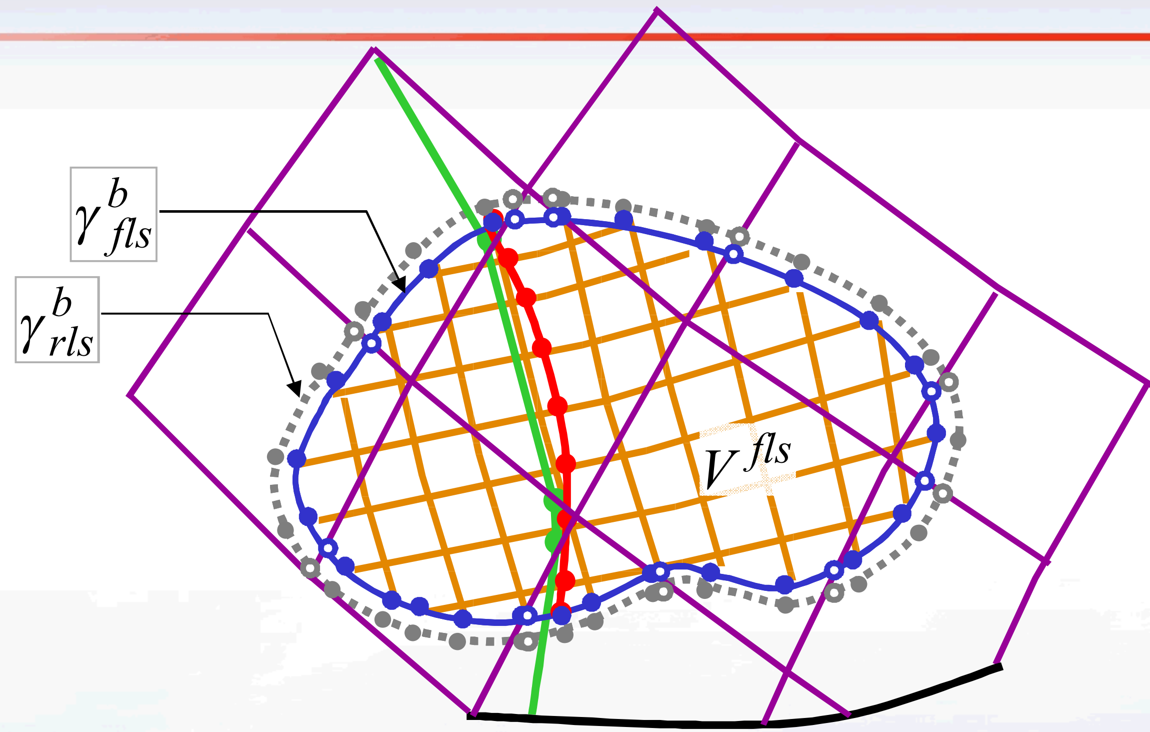
In order to perform the integrals in eqn. (2), we need to define the following sub-volumes and sub-surfaces via intersection (an algorithm which we call imprinting):



Imprinting: $\{\gamma^b_{rls} \xleftarrow{\cap} \gamma^b_{fls}\}$

Imprint of V^{rls} onto γ^b_{fls} yields nodes ○ and ○

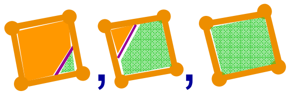
Imprint of γ^b_{fls} onto $V^{rls} : \{e^{rls}_k, k = 1,2,...\}$ yields facets γ^b_{rls} and γ^b_{fls}



The discretization of the *fls* boundary is imprinted onto the *rls* volume within *rls* elements $\{e^{rls}_k, k = 1,2,...\}$. Additionally, the *rls* element edges are imprinted onto γ^b_{fls} - thereby completing the intersection $\{\gamma^b_{rls} \xleftarrow{\cap} \gamma^b_{fls}\}$

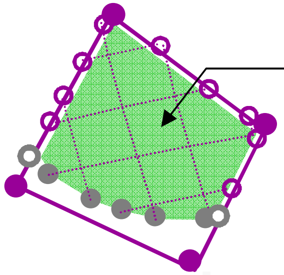
Imprinting: $\{V^{rls} \cap V^{fls}\}$

Elements of V^{fls} that intersect e^{rls}



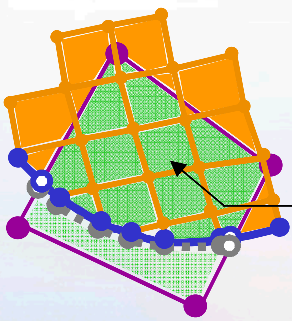
$V^{fls} : \{e_k^{fls}, k = 1,2,\ldots\}$

defining the imprint



$\{e^{rls} \cap V^{fls}\}$

and

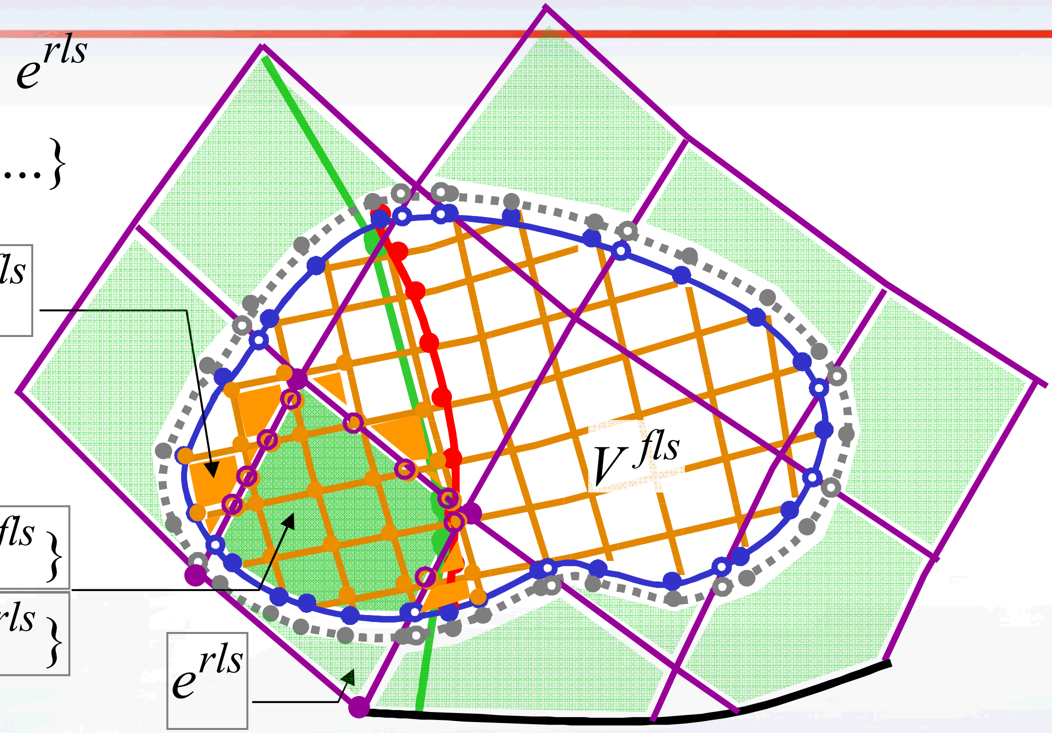


$V^{fls} : \{e_k^{fls}, k = 1,2,\ldots\} \cap e^{rls}$

$\{e^{rls} \cap V^{fls}\}$

$\{V^{fls} \cap e^{rls}\}$

e_k^{fls}



e^{rls}

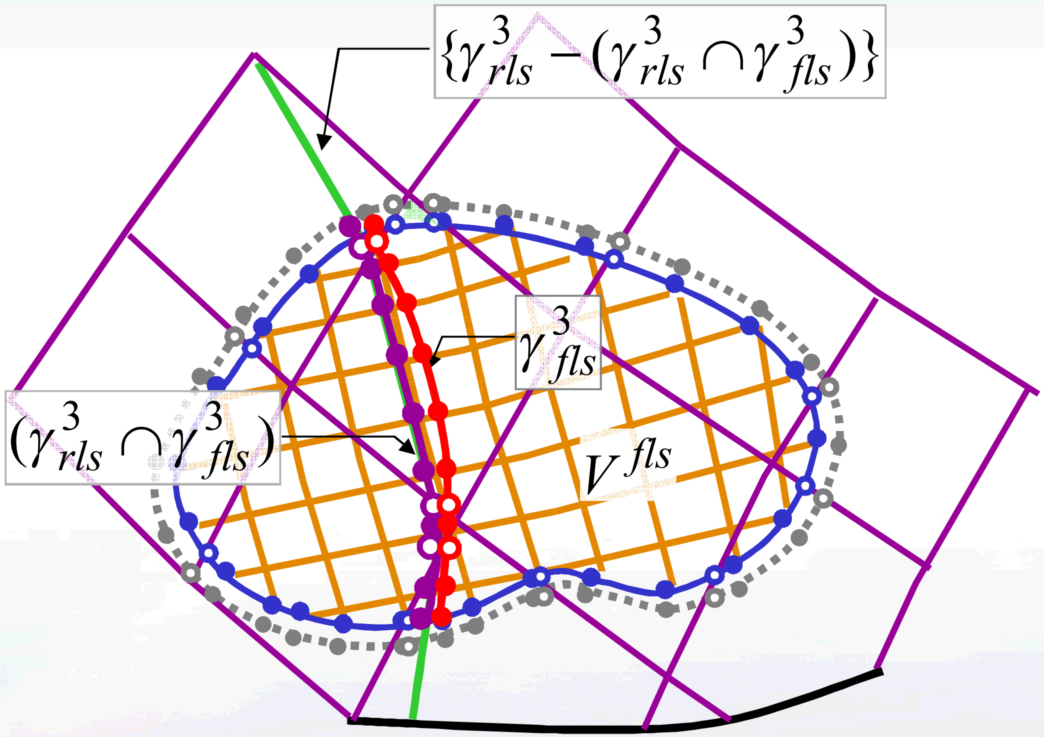
A reference length scale element e^{rls} is intersected with a collection of fine length scale elements $\{e_k^{fls}, k = 1,2,\ldots\}$, defining the intersection $\{e^{rls} \cap V^{fls}\}$ and $\{V^{fls} \cap e^{rls}\}$

Imprinting: $\{\gamma^3_{rls} \cap \gamma^3_{fls}\}$

Imprint of γ^3_{rls} onto γ^3_{fls} yields nodes ○ and ○

Imprint of γ^3_{fls} onto γ^3_{rls}

yields facets γ^3_{rls} and γ^3_{fls}



The discretization of the *fls* interface surface γ^3_{fls} is imprinted onto the *rls* interface surface γ^3_{rls}

Constraints between Multiscales

With these definitions in hand, there are two computational mechanics arguments that need to be addressed:

A Boundary Constraint s.t the boundary between the length scales described by the 2 discretizations γ^{b}_{fls} and γ^{b}_{rls} deform consistently

An Interior Constraint s.t the material described by both length scales $V^{fls} : \{e^{fls}_{k}, k = 1,2,...\}$ and $\{e^{rls} \cap V^{fls}\}$ deform consistently

Multiscale Boundary Constraint

A Boundary Constraint s.t the boundary between the length scales described by the 2 discretizations γ^{b}_{fls} and γ^{b}_{rls} deform consistently

- what are the deformations described by the 2 surface discretizations γ^{b}_{fls} and γ^{b}_{rls} ?
- what methods are there to enforce the boundary constraint?
- what does it mean to deform consistently?

Boundary deformation

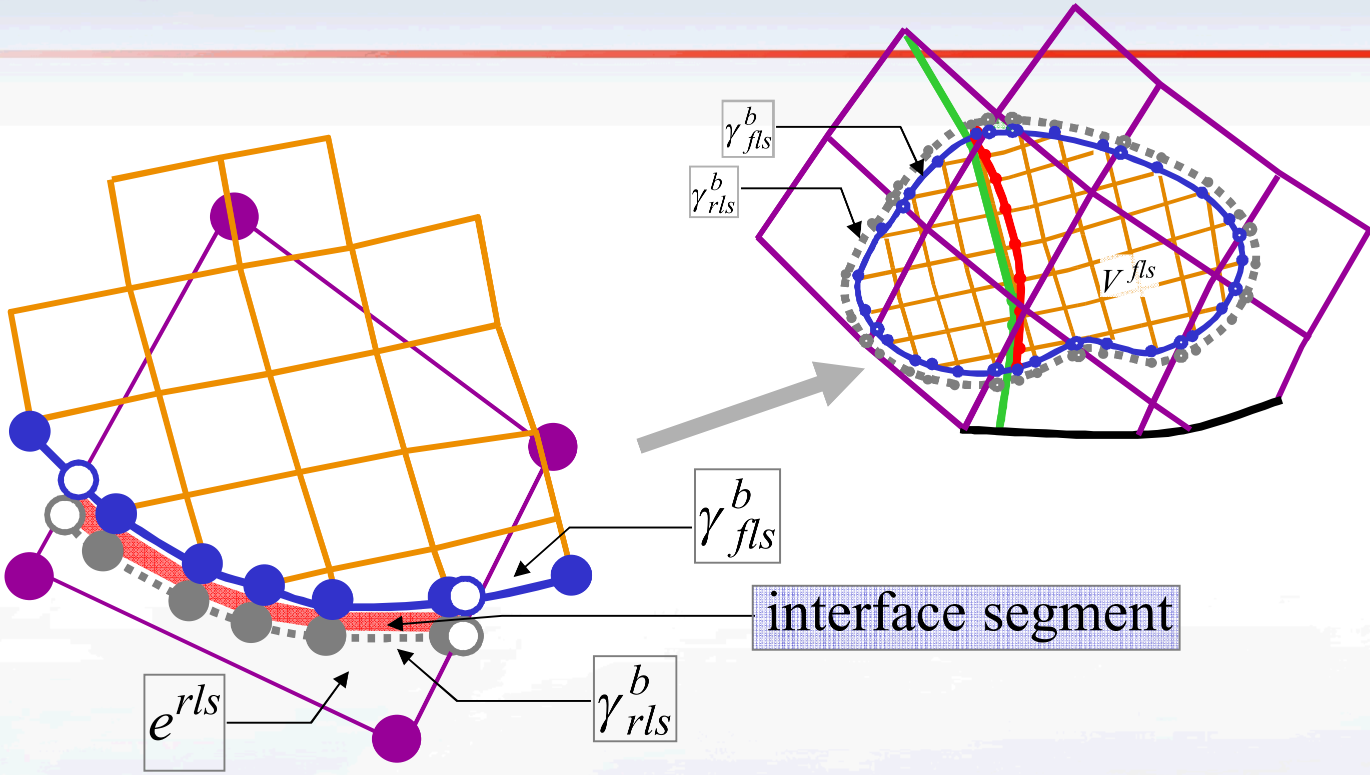
$\varphi_{\gamma^{b}_{rls}}, \varphi_{\gamma^{b}_{fls}}$

Constraints:

$d^{b\,●}_{rls} = \mathrm{N}_I \, d^{I\,●}_{rls}$

$d^{b\,○}_{rls} = \mathrm{N}_I \, d^{I\,●}_{rls}$

$d^{b\,○}_{rls} = \mathrm{N}_I \, d^{I\,●}_{rls}$



The deformation of the discretized *fls* boundary is dictated by the motion of nodes ●, and the deformation of the *rls* imprinted boundary is dictated by the motion of nodes ● of element e^{rls}, allowing the interface segment to deform differently on the *fls* and *rls*

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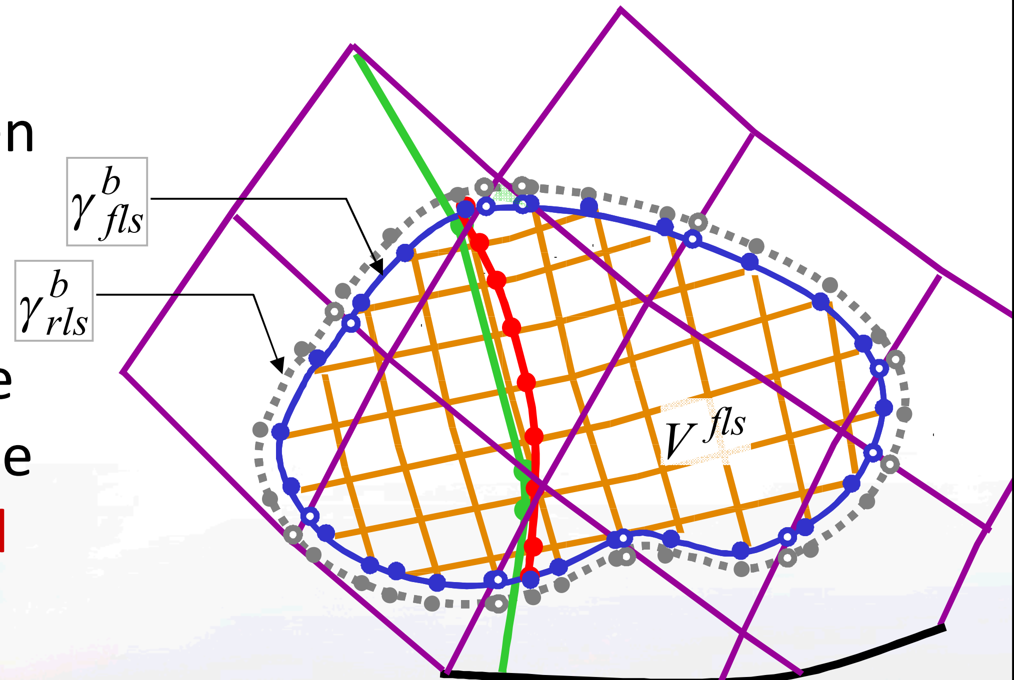
Multiscale Interface BCs: Comparison of known methods

A node-colocation algorithm for the boundary constraint between the length scales is an MPC

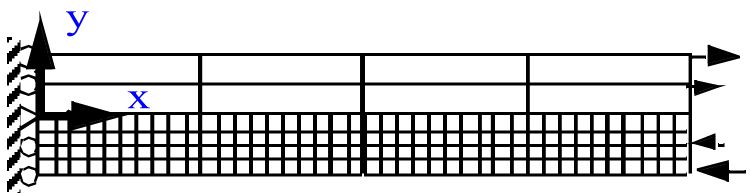
A least-squares algorithm for the boundary constraint between the length scales is a mortar method

A linearly-consistent algorithm for the boundary constraint between the length scales admits the solution to a first order patch test for general curved surfaces



Multiscale Interface BCs: issues

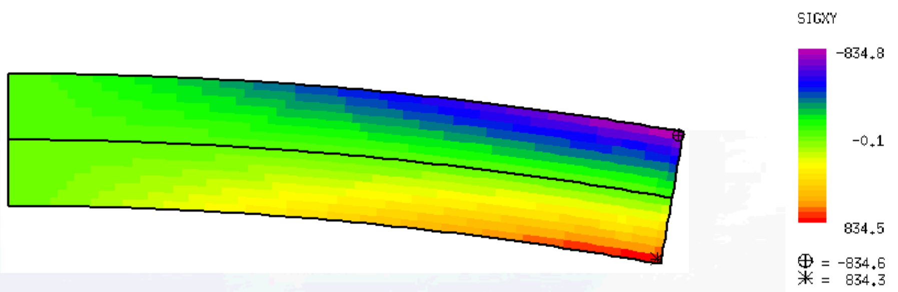
The issues involved in the Boundary Constraint are similar, we realized, to properly tying meshes together, e.g.



Prescribed moment

8x80 mesh

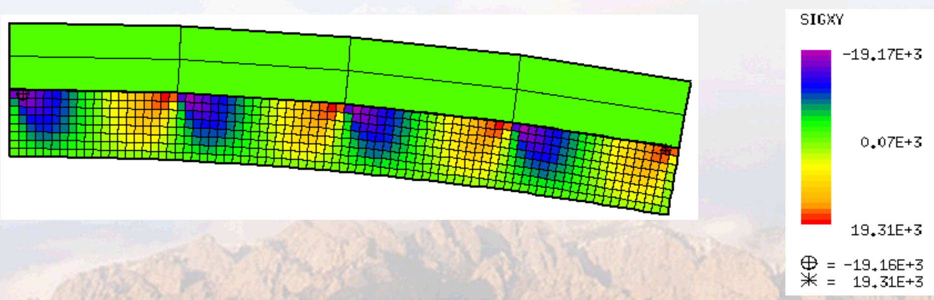
8x80 mesh



Analytic solution is "pure bending"

2x4 mesh

8x80 mesh

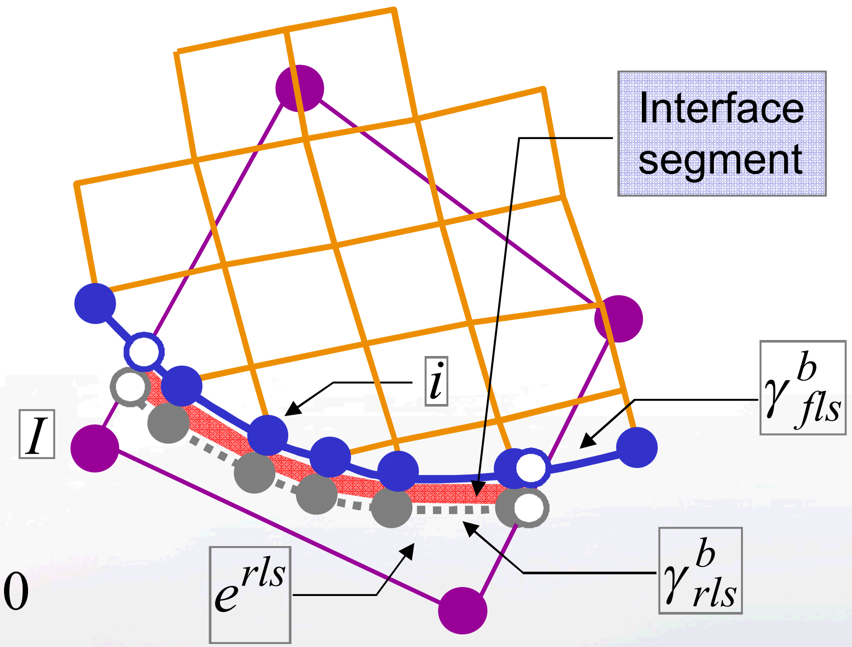


Node colocation or mesh tying can produce enormous errors in some cases (this being a good example)

Multi-pont Constraint Interface BC

An MPC for the boundary constraint between the length scales enforces pointwise compatibility

In order to admit such a solution, the deformations of nodes on γ^{b}_{fls} must be equivalent to mapped nodal deformations on γ^{b}_{rls}



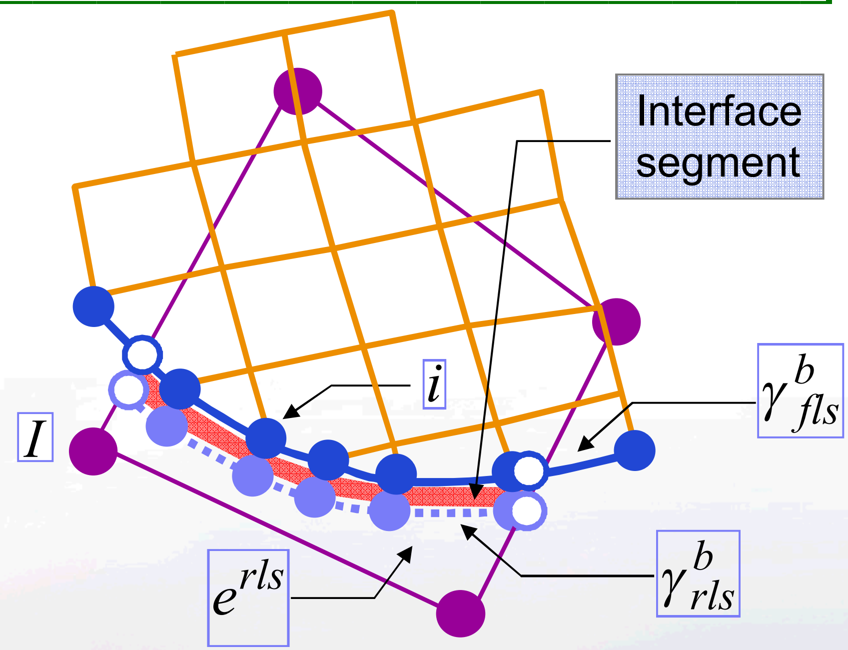
$$d^{i}_{fls} - d^{@i}_{rls} = d^{i}_{fls} - \mathrm{N}_I(\xi^{i})\, d^{I}_{rls} = 0$$

pointwise values (nodal degrees of freedom)

Mortar method as Interface BC

A mortar method for the boundary constraint between the length scales is a weak enforcement of compatibility

In order to admit such a solution, the deformations of γ^b_{rls} and γ^b_{fls} must be equivalent in a least squares integral sense across the interface in every *rls* element e^{rls}, i.e.



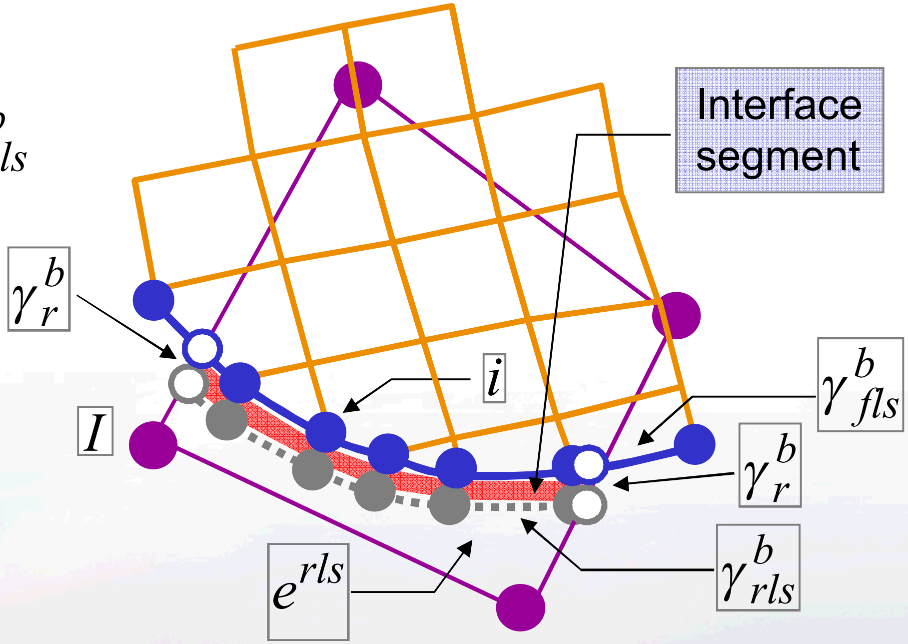
$$W_b = \int_{\gamma^b_{rls}} \lambda (d_{fls} - d_{rls}) d\gamma = \int_{\gamma^b_{e^{rls}}} N_J \lambda^J (N_i d^i_{fls} - N_I d^I_{rls}) d\gamma = 0$$

functional representation (interpolation of nodal degrees of freedom)

linearly-consistent Interface BC

A linearly-consistent algorithm for the boundary constraint between the length scales admits the solution to a first order patch test

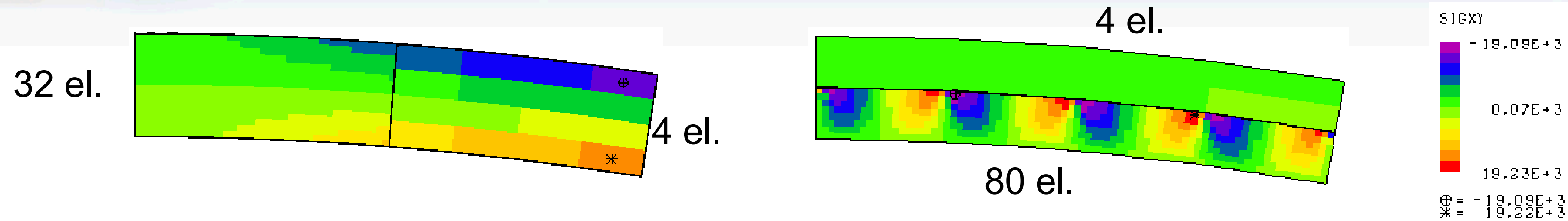
In order to admit such a solution, the deformations of γ^b_{rls}, γ^b_{fls}, and γ^b_r must produce a constant stress acting in the interface segment within every *rls* element e^{rls}.



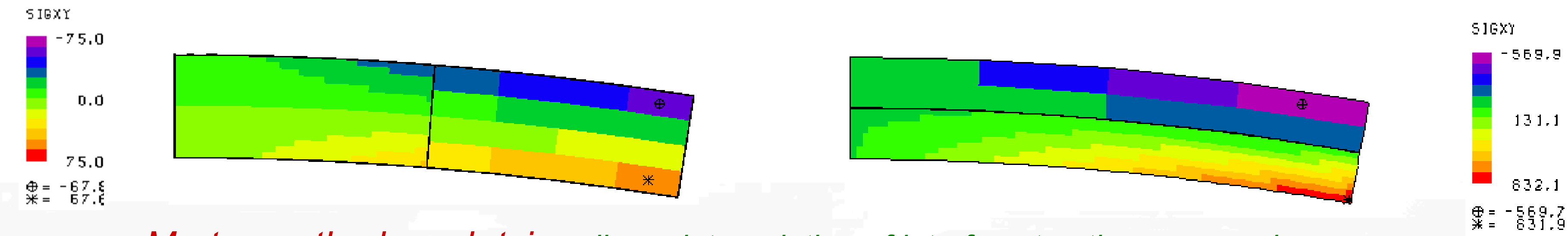
Since γ^b_{rls} is an imprint of γ^b_{fls} the work must balance, i.e.:

$$\delta W_b = \sigma^{(0)}_{ij} \left(\int_{\gamma^b_{rls}} n_j \delta(d_i)_{rls} \, d\gamma - \int_{\gamma^b_{fls}} n_j \delta(d_i)_{fls} \, d\gamma + \int_{\gamma^b_{rls}} n_j \delta(d_i)_r \, d\gamma \right) = 0$$

Multiscale Interface BC: beam example



MPC mesh tying: no modes are unresisted can produce unrealistic results (overconstrained)



Mortar method mesh tying: linear interpolation of interface tractions, no modes are unresisted but cannot pass patch test for general curved interfaces

Consistent mesh tying: A constant stress field is accurately transmitted across the interface, but higher order modes are left stress-free (analogy: mean strain modes , hourglass modes)

Multiscale Interface BCs: summary

Linearly consistent approach

+ properly treats non-zero interface volume

- currently only allows for a constant interface stress

mortar method

+ allows for a linear variation of the interface traction (converges at the same rate as the displacements)

- the unknown Lagrange multiplier is a traction and not a stress (cannot pass the patch test for general curved surfaces)

Bottom line: the appropriate interface BC depends on the problem

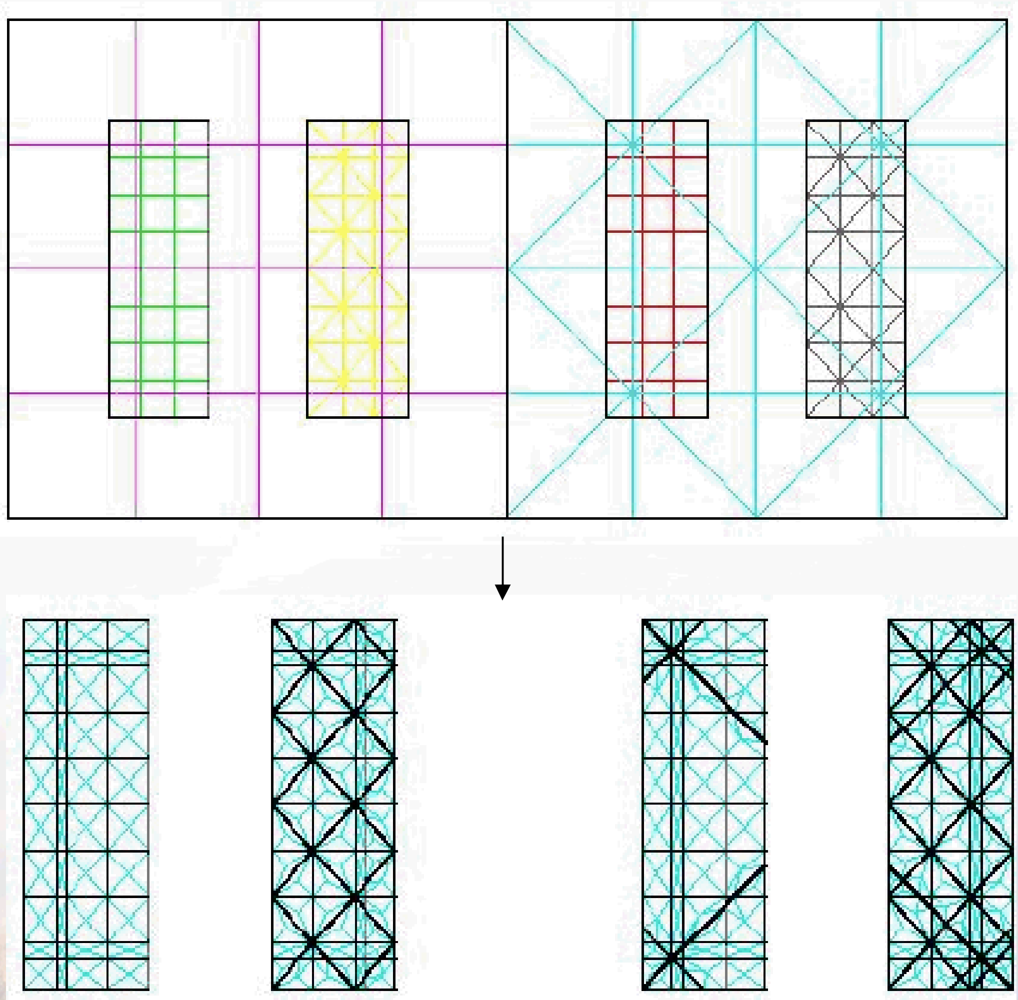
When there is initially gaps or overclosures on the interface, a consistent tying approach is the only known method to properly handle the work done by the non-zero interface volume

When the interface has zero initial “volume” a mortar method is preferred because of its linear variation (and hence higher order rate of convergence)

Interface BCs: "imprinting" algorithm

A linearly-consistent algorithm or a mortar method for the boundary constraint requires an imprinting of one discretization on the other.

Must be parallel, scalable



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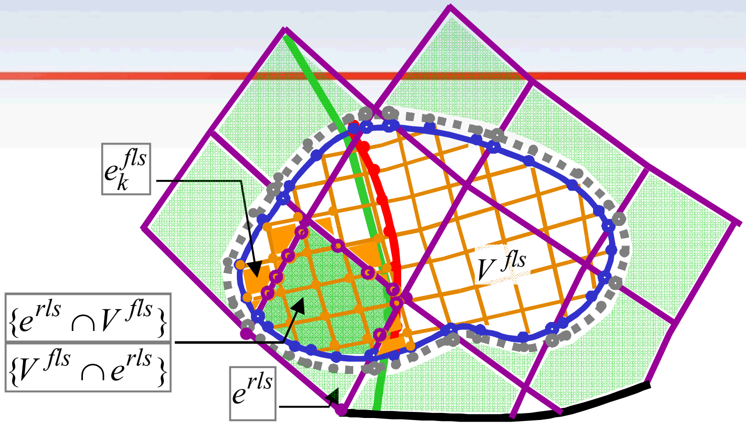
Mutliscale Interior Constraint

An Interior Constraint s.t the material described by both length scales $V^{fls} : \{e_k^{fls}, k = 1,2,...\}$ and $\{e^{rls} \cap V^{fls}\}$ deform consistently

- what are the deformations described by the 2 volume discretizations?
- what does it mean to deform consistently?
- why do we want consistent deformations?
- what methods are there to enforce the interior constraint?

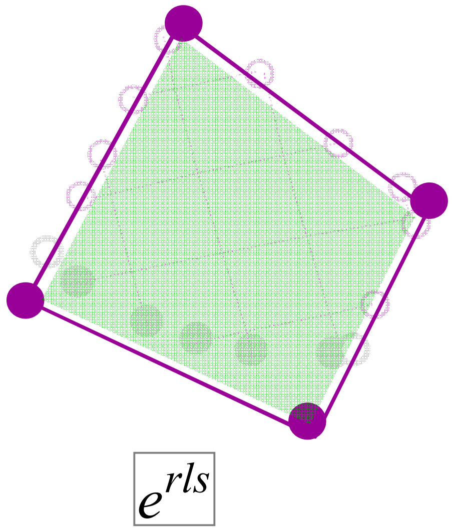
Element Deformations

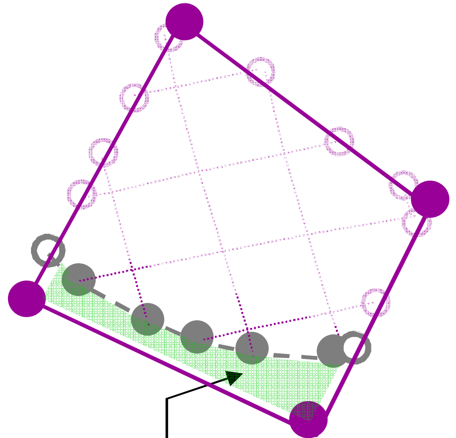
$\varphi_{e^{rls}_{MLS}}, \varphi_{e^{fls}_k}, k=1,2,...$

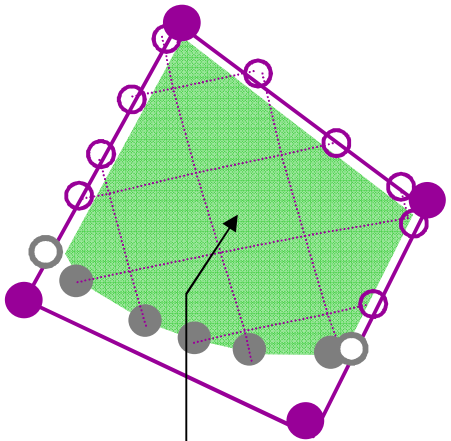


Deformation of a reference length scale element is decomposed into two parts:

$\varphi_{e^{rls}}$ = $\varphi_{e^{rls}-(e^{rls} \cap V^{fls})}$ + $\varphi_{e^{rls} \cap V^{fls}}$

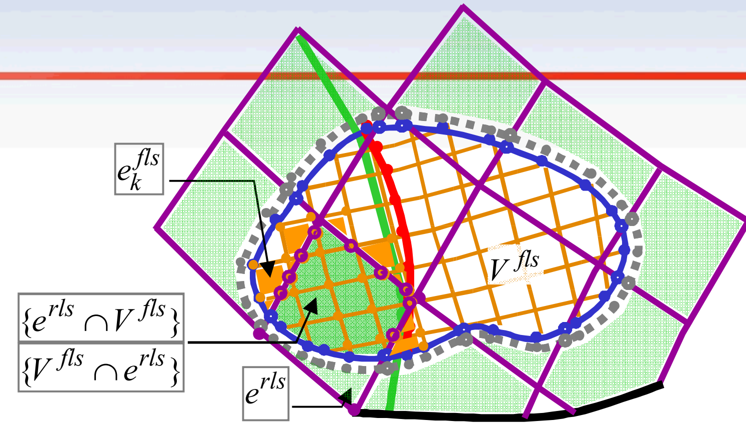






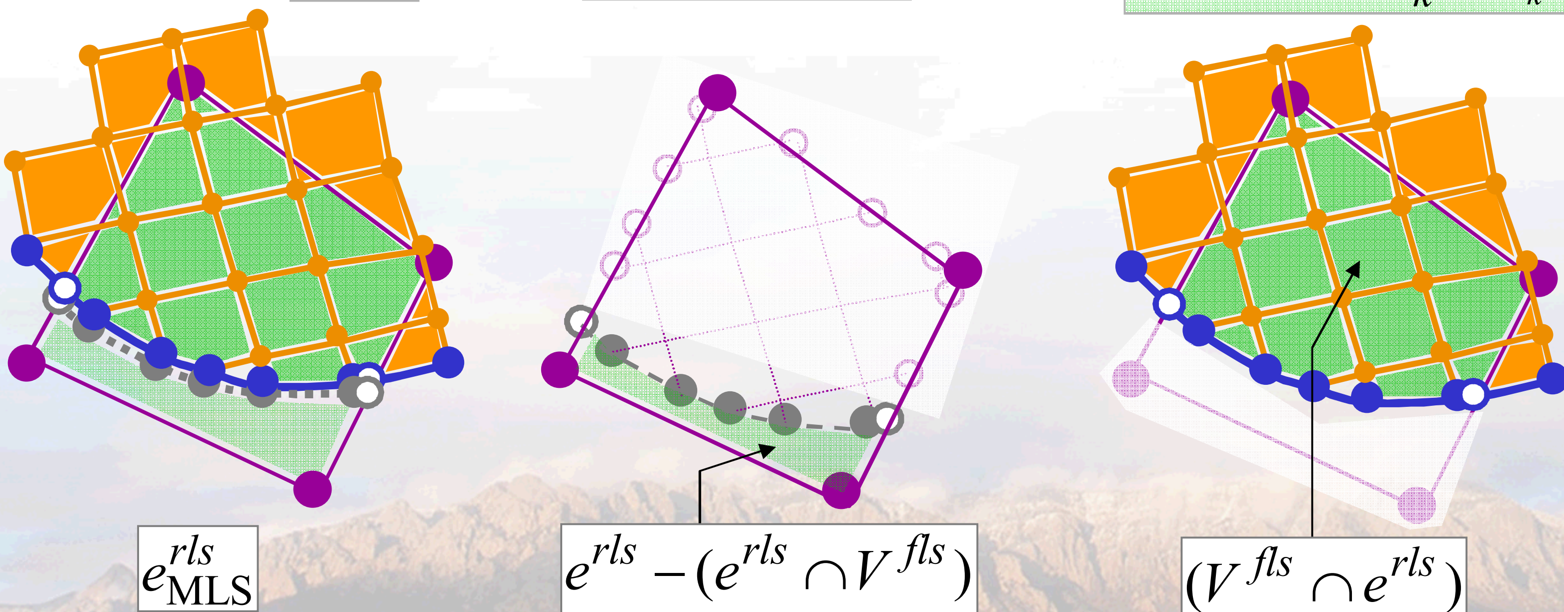
Element Deformations

$\varphi_{e^{rls}_{\mathrm{MLS}}}, \varphi_{e^{fls}_k}, k=1,2,\ldots$



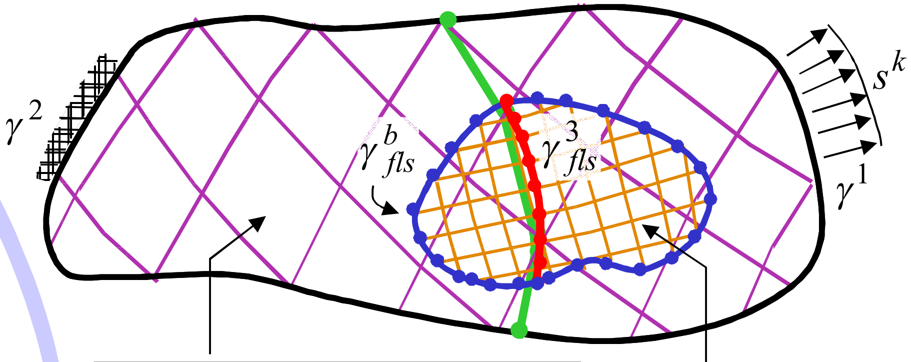
Deformation of a MLS reference length scale element is re-composed of two parts:

$$\varphi_{e^{rls}_{\mathrm{MLS}}} = \varphi_{e^{rls} - (e^{rls} \cap V^{fls})} + \varphi_{V^{fls} \cap e^{rls}} = \underset{k}{\mathrm{A}}(\varphi_{e^{fls}_k})$$



Multiscale Internal Energy

$$\delta\Pi = \int_{\Omega^{rls}-(\Omega^{rls}\cap\Omega^{fls})} \mathrm{T}^{ij}\,\delta u_{i,j}dv + \int_{\Omega^{fls}} \mathrm{T}^{ij}\,\delta u_{i,j}dv$$
$$+ \int_{\Omega^{rls}-(\Omega^{rls}\cap\Omega^{fls})} \rho\,\ddot{x}^k\delta u_k dv + \int_{\Omega^{fls}} \rho\,\ddot{x}^k\delta u_k dv$$
$$- \int_{\Omega^{rls}-(\Omega^{rls}\cap\Omega^{fls})} \rho\,b^k\delta u_k dv - \int_{\Omega^{fls}} \rho\,b^k\delta u_k dv$$
$$- \int_{\Gamma^1_{rls}-\Gamma^1_{rls}\cap\Gamma^1_{fls}} s^k\delta u_k da - \int_{\Gamma^1_{fls}} s^k\delta u_k da$$
$$+ \int_{\Gamma^3_{rls}-\Gamma^3_{rls}\cap\Gamma^3_{fls}} (-t_N\delta g_N)da + \int_{\Gamma^3_{fls}} (-t_N\delta g_N)da$$



$$\{e_L^{rls}, L=1,2,\ldots\}$$
$$\{e_k^{fls}, k=1,2,\ldots\}$$

$$\sum_L\Big[\int_{V^{e_L^{rls}}-(V^{e_L^{rls}}\cap V^{fls})} \mathbf{B}^T_{e_L^{rls}}\mathbf{T}_{e_L^{rls}}dv + \sum_k\Big(\int_{V^{e_k^{fls}}\cap e_L^{rls}} \mathbf{B}^T_{e_k^{fls}}\mathbf{T}_{e_k^{fls}}dv\Big)\Big]$$

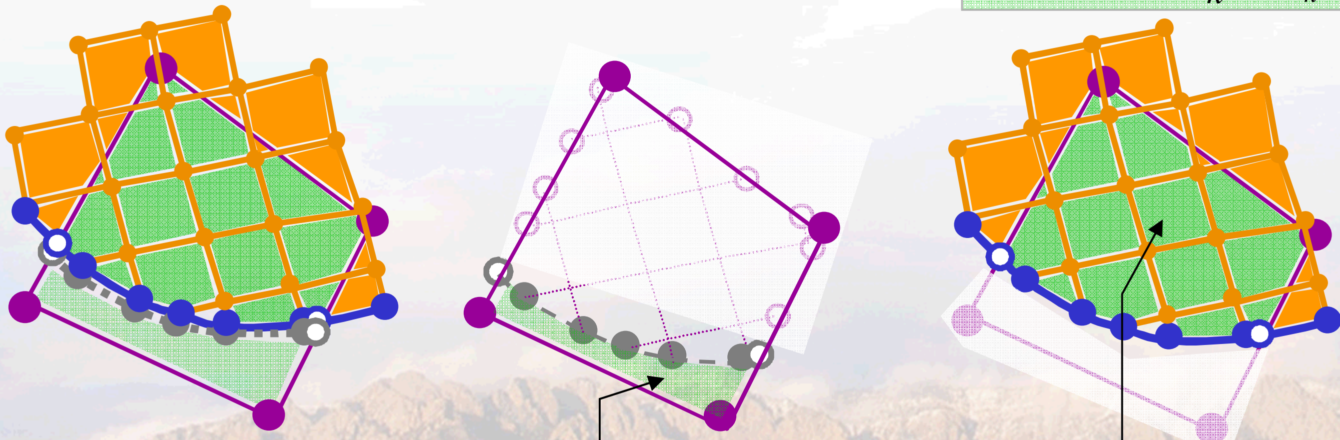
Specific *rls* element contribution

Contribution of a MLS reference length scale element is composed of two parts

$$\int_{V^{e^{rls}_{\mathrm{MLS}}}} \mathrm{T}^{ij}\,\delta u_{i,j}\,dv = \int_{V^{e^{rls}_L} - (V^{e^{rls}_L} \cap V^{fls})} \mathbf{B}^T_{e^{rls}}\,\mathbf{T}_{e^{rls}}\,dv + \sum_k \Big(\int_{V^{e^{fls}_k} \cap e^{rls}_L} \mathbf{B}^T_{e^{fls}_k}\,\mathbf{T}_{e^{fls}_k}\,dv \Big)$$

which is coincident w/ the deformations:

$\varphi_{e^{rls}_{\mathrm{MLS}}}$ = $\varphi_{e^{rls} - (e^{rls} \cap V^{fls})}$ + $\varphi_{V^{fls} \cap e^{rls}} = \mathop{\mathrm{A}}_{k}(\varphi_{e^{fls}_k})$



e^{rls}_{MLS} $\quad$ $e^{rls} - (e^{rls} \cap V^{fls})$ $\quad$ $(V^{fls} \cap e^{rls})$

Solution strategy: separate scales

To allow a more efficient solution of the Multi-length scale problem, it is desirable to separate the length scales, i.e. in any *rls* element , L:

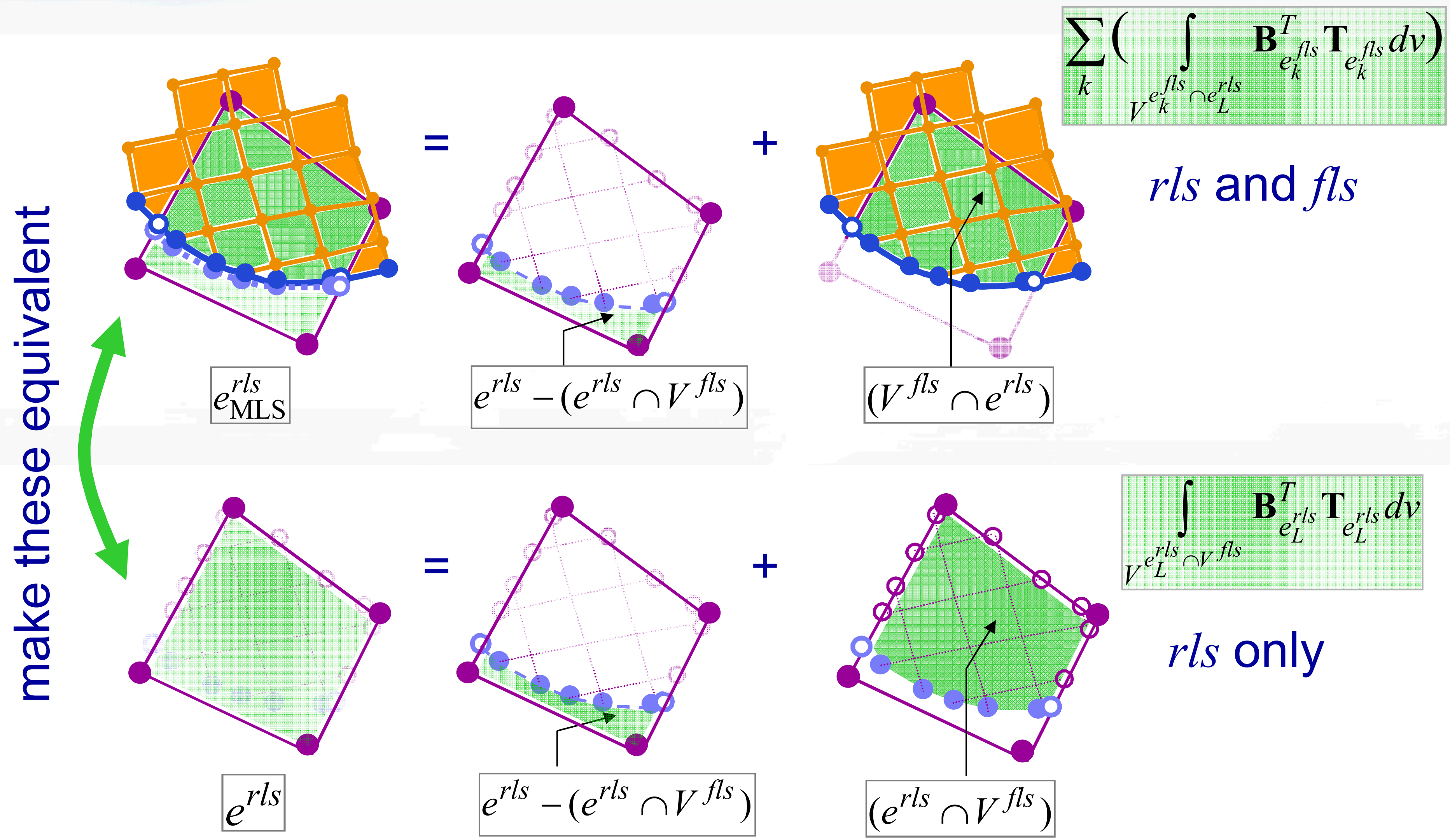
$$\int_{V^{(e_L^{rls})_{MLS}}} \mathrm{T}^{ij}\,\delta u_{i,j}dv = \int_{V^{e_L^{rls}} - (V^{e_L^{rls}} \cap V^{fls})} \mathbf{B}^T_{e_L^{rls}} \mathbf{T}_{e_L^{rls}} dv + \int_{V^{e_L^{rls}} \cap V^{fls}} \mathbf{B}^T_{e_L^{rls}} \mathbf{T}_{e_L^{rls}} dv$$

which is a proper statement iff,

$$\int_{V^{e_L^{rls}} \cap V^{fls}} \mathbf{B}^T_{e_L^{rls}} \mathbf{T}_{e_L^{rls}} dv = \sum_k \Big(\int_{V^{e_k^{fls}} \cap e_L^{rls}} \mathbf{B}^T_{e_k^{fls}} \mathbf{T}_{e_k^{fls}} dv \Big)$$

rls element where it intersects *fls* elements

Separating length scales within a specific *rls* element



Approximation within a specific *rls* element

Contribution of a MLS reference length scale element is approximated by considering the mean contribution:

$$\int_{V^{e_L^{rls}} \cap V^{fls}} \mathbf{B}^T_{e_L^{rls}} \mathbf{T}_{e_L^{rls}} dv = \sum_k \Big(\int_{V^{e_k^{fls}} \cap e_L^{rls}} \mathbf{B}^T_{e_k^{fls}} \mathbf{T}_{e_k^{fls}} dv \Big)$$

$$= \overline{\mathbf{T}}_{e^{fls}} \sum_k \int_{V^{e_k^{fls}} \cap e_L^{rls}} \mathbf{B}^T_{e_k^{fls}} dv$$

$$+ \sum_k \Big(\int_{V^{e_k^{fls}} \cap e_L^{rls}} \xi^m (\mathbf{B}^m)^T_{e_k^{fls}} (\mathbf{T}^m)_{e_k^{fls}} dv \Big) = 0$$

higher order terms

Enforcing the Interior constraint within a specific *rls* element

The mean stress is computed as:

$$\overline{\mathbf{T}}_{e^{fls}} = \frac{\sum_k \left(\int_{V^{e_k^{fls}} \cap e_L^{rls}} V^{e_k^{fls}} \mathbf{T}_{e_k^{fls}} \, dv \right)}{\sum_k \left(\int_{V^{e_k^{fls}} \cap e_L^{rls}} V^{e_k^{fls}} \, dv \right)}$$

One method to enforce that the mean strain energy is equivalent is to construct an equivalent hypo-elastic material :

$$\overline{T}_{rls}^{ij} = 2\tilde{G}_{e_L^{rls}} \varepsilon_{rls}^{ij} + \left(\tilde{K}_{e_L^{rls}} - \frac{2\tilde{G}_{e_L^{rls}}}{3}\right) \varepsilon_{rls}^{kk} \delta_{ij}$$

where:

$$\tilde{K}_{e_L^{rls}} = \frac{tr(\mathbf{T}_{e^{fls}})}{tr(\varepsilon_{e^{fls}})} \qquad 2\tilde{G}_{e_L^{rls}} = \frac{\left\| dev(\mathbf{T}_{e^{fls}}) \right\|_2}{\left\| dev(\varepsilon_{e^{fls}}) \right\|_2}$$

Enforcing the Interior constraint within a specific *rls* element

Another method to enforce that the mean strain energy is equivalent is to construct an equivalent hypo-elastic material :

$$\overline{T}_{rls}^{ij} = 2\widetilde{G}_{e_L^{rls}} \varepsilon_{rls}^{ij} + (\widetilde{K}_{e_L^{rls}} - \frac{2\widetilde{G}_{e_L^{rls}}}{3}) \varepsilon_{rls}^{kk} \delta_{ij}$$

where:

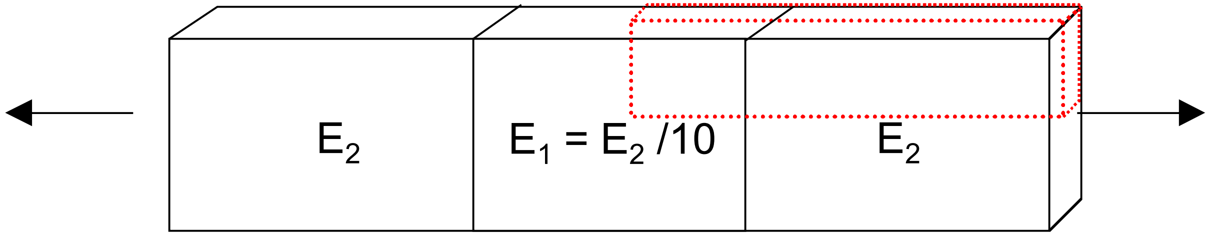
$$\widetilde{K}_{e_L^{rls}} = \frac{tr(\mathbf{T}_{e^{fls}})}{tr(\varepsilon_{e^{fls}})} \qquad 2\widetilde{G}_{e_L^{rls}} = \frac{\left\| dev(\mathbf{T}_{e^{fls}}) \right\|_2}{\left\| dev(\varepsilon_{e^{fls}}) \right\|_2}$$

And to enforce the constraint that:

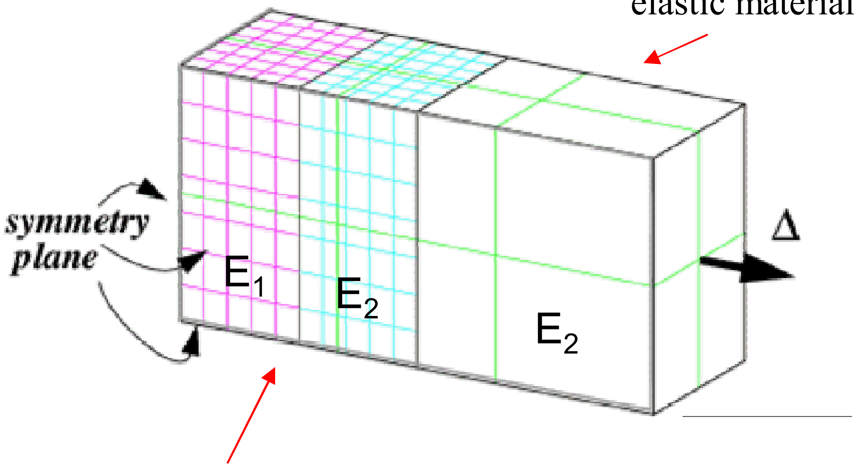
$$H_{ij}(u) = \left[B_j^{rls} \right] u_i^{rls} - \left[\mathop{\mathrm{A}}_{k} (B_j^{e_k^{fls}}) \right] u_i^{fls}$$

Multiscale Solver

The solver is explored by way of the following example:

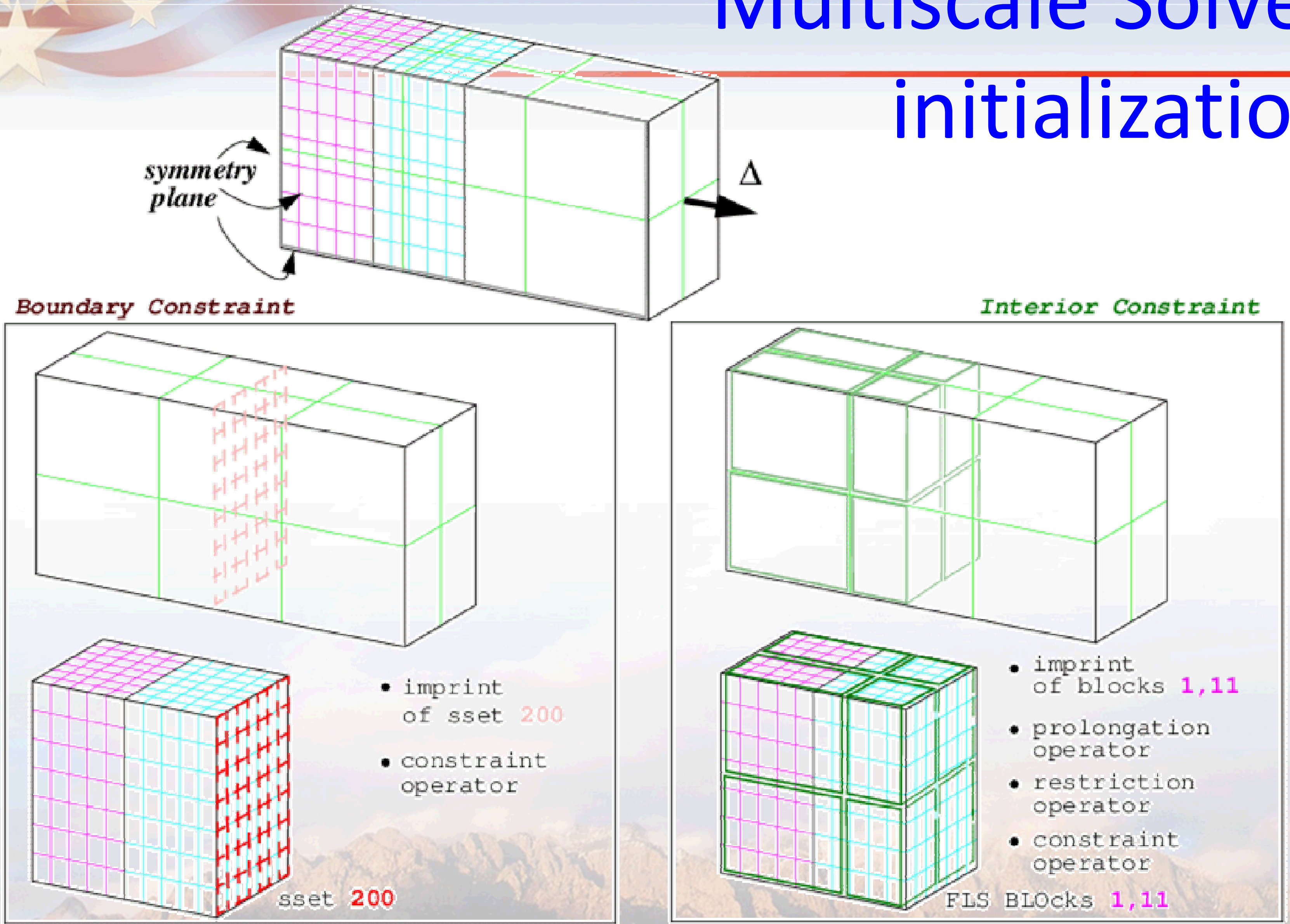


reference length scale model is an isotropic elastic material which has modus E_2

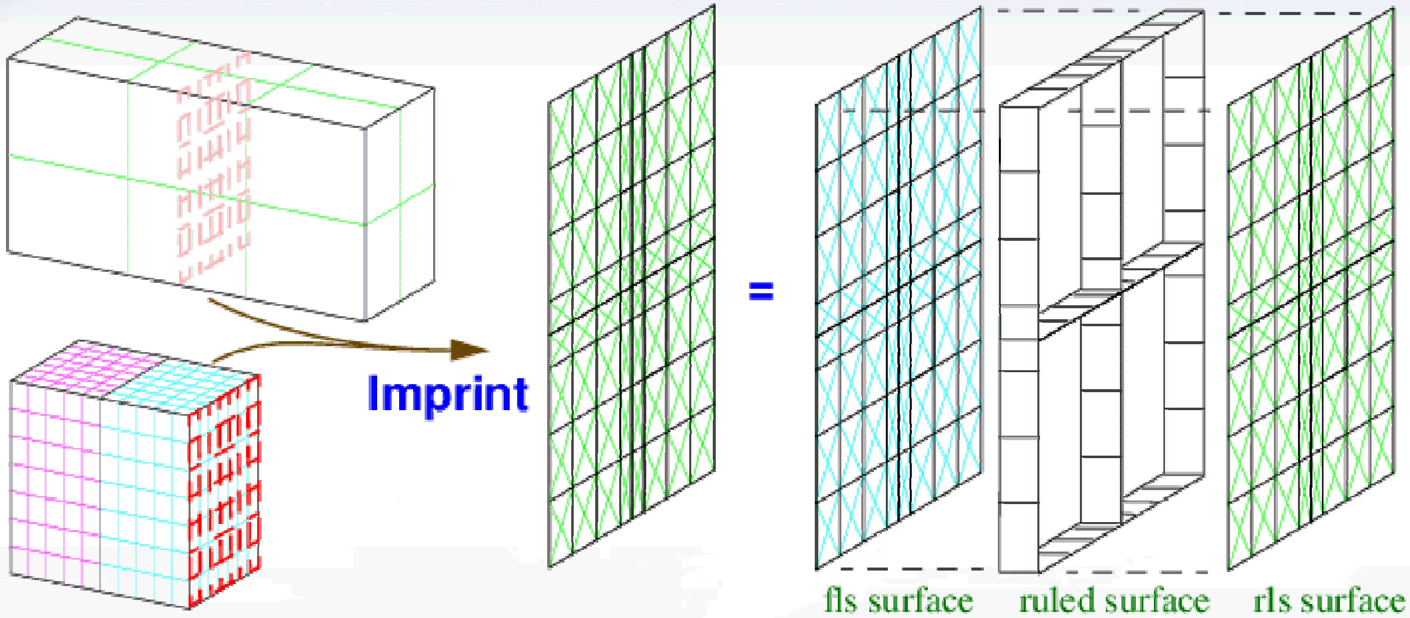


fine length scale model has two element blocks composed of isotropic elastic material with modulii E_2 ,and $E_1 = E_2/10$ respectively

Multiscale Solver initialization



MLS surface -in- volume imprinting

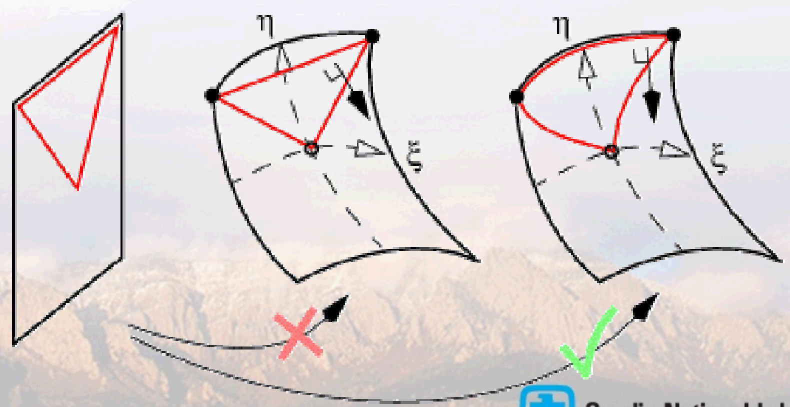


The purpose of the imprint is to define ***regions*** over which the integrand of the boundary constraint equation is ***piecewise continuous***

The triangular facets describing the regions are actually scribed on the faces and interior of the parent element. (The ruled surface is a connection of the fls&rls edge of the region)

*position & normals are **defined by** interpolation within **the parent element** and NOT on the triangle itself*

on the face of a parent element, e.g.



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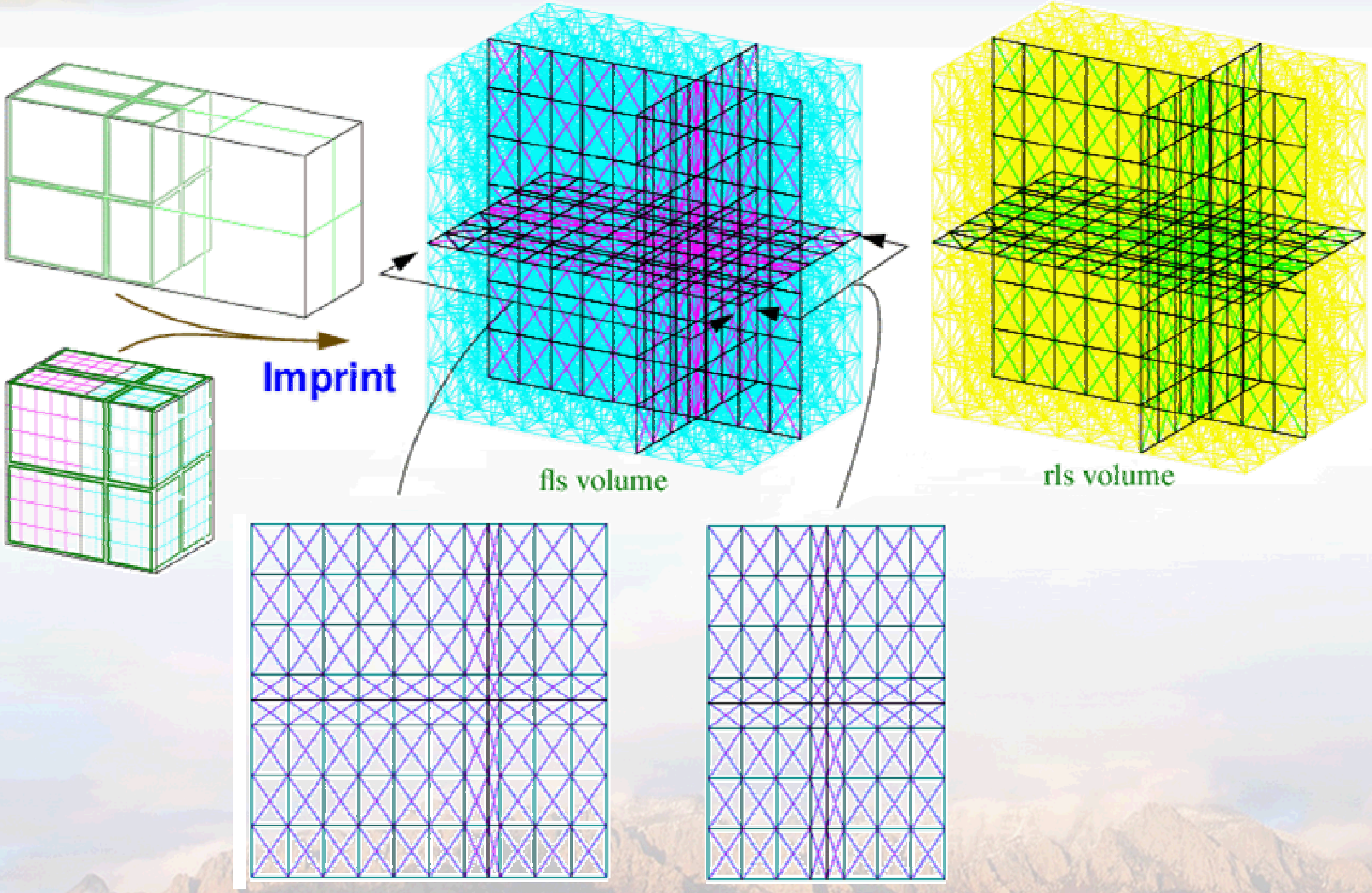
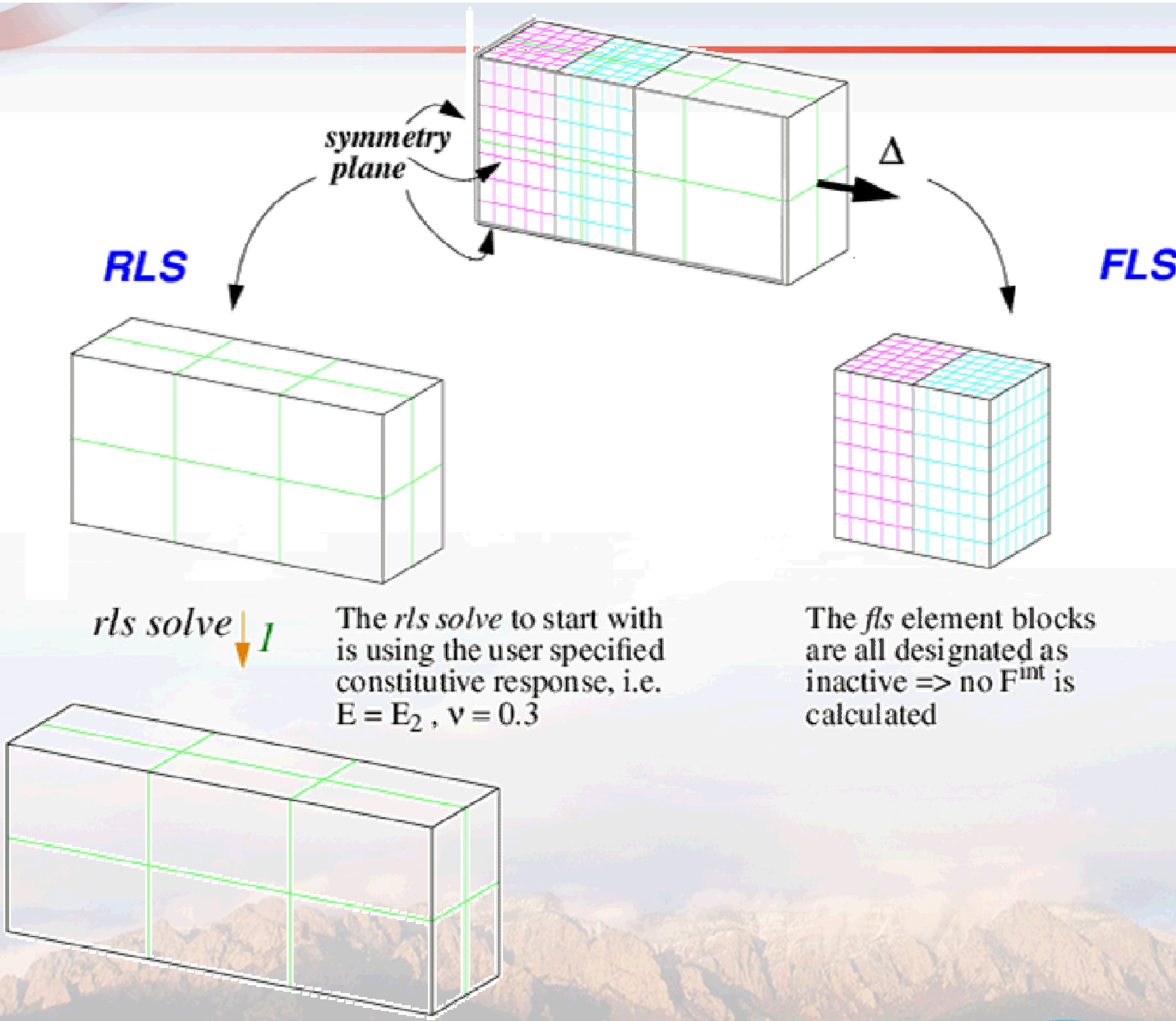
MLS volume -in- volume imprinting



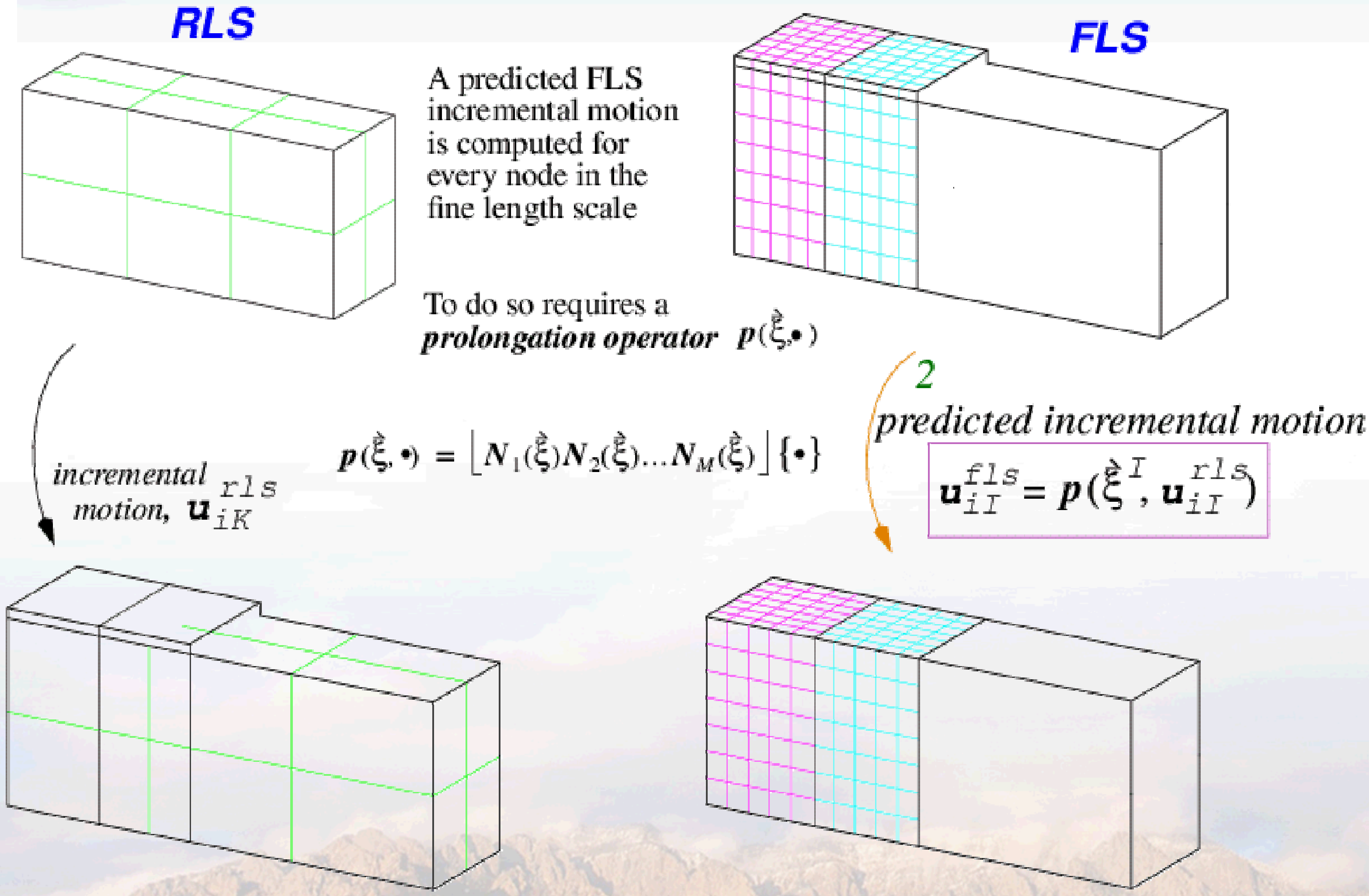
Multiscale solver: *RLS* solve



The *rls solve* to start with is using the user specified constitutive response, i.e. $E = E_2$, $\nu = 0.3$

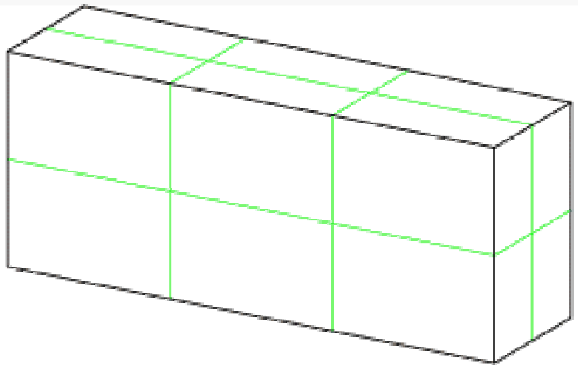
The *fls* element blocks are all designated as inactive => no F^{int} is calculated

Multiscale solver: *FLS* predictor



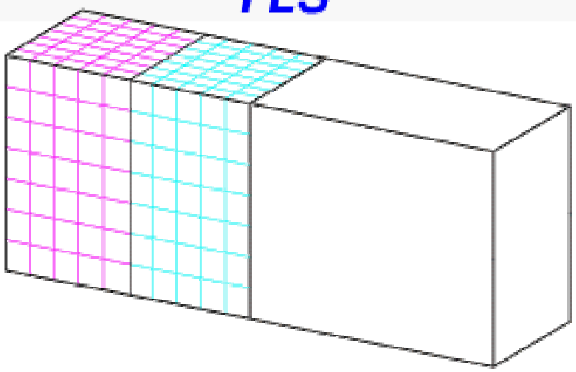
Multiscale solver: *FLS* solve

RLS



The *rls* element blocks are all designated as inactive => no F^{int} is calculated

FLS



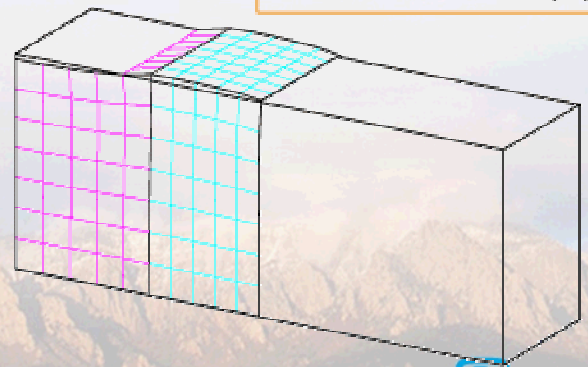
fls solve ↓ *3*

The *fls solve* is subjected to the Boundary Constraint:

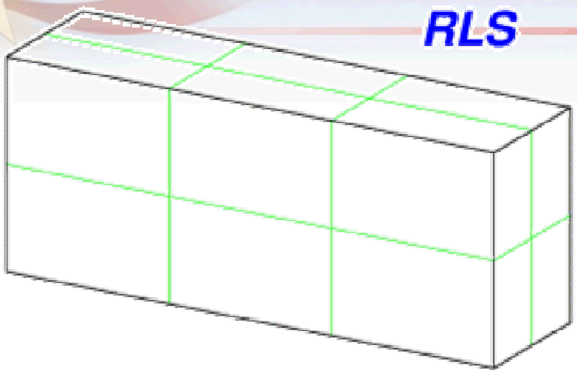
$$H^{mpc}(u) = 0$$

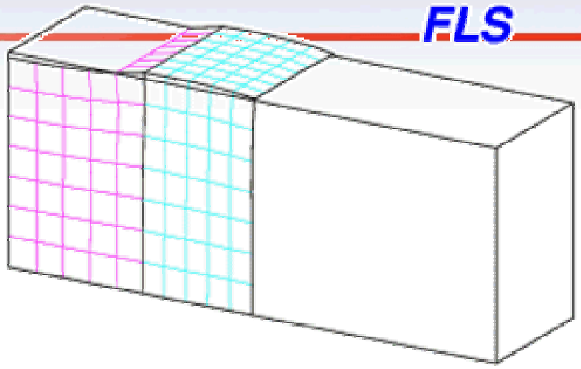
or

find λ^b s.t. $H^b(u) = 0$



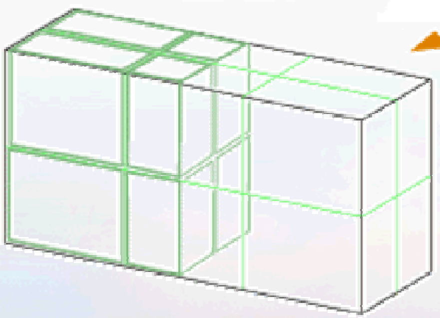
Multiscale solver: homogenization



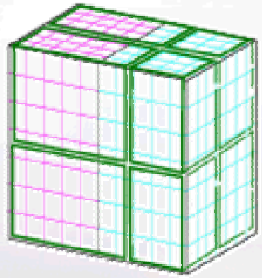


Equivalent hypo-elastic material properties are computed for every *rls* element which has fls material in it. To do so requires a ***volume operator*** $vratio$ and a ***restriction operator*** $m(\xi,\bullet)$

4 *homogenization*



$$\tilde{C}^{e^{rls}} = (1 - v_r) \cdot C^{e^{rls}} + v_r \cdot \overline{C}^{e^{rls}}(2\overline{G}, \overline{K})$$



where:

$$v_r = \frac{V^{f \cap e^{rls}}}{V^{e^{rls}}} \qquad 2\overline{G} = \frac{\left\| dev\left(m\left(\bar{\sigma}_{ij}^{f}\right)\right)\right\|_2}{\left\| dev\left(m\left(\bar{\varepsilon}_{ij}^{f}\right)\right)\right\|_2} \qquad \overline{K} = \frac{tr\left(m\left(\bar{\sigma}_{ij}^{f}\right)\right)}{tr\left(m\left(\bar{\varepsilon}_{ij}^{f}\right)\right)}$$

mean stress in a RLS element

$$\bar{\sigma}_{ij}^{f} = \frac{1}{V^c} \int_{V^c} \sigma_{ij} dv = \frac{1}{V^c} \sum_f \int_{V^f} \sigma_{ij} dv = \frac{1}{V^c} \sum_f V^{f \cap e^{rls}} \sigma_{ij}^{f} = m\left(\sigma_{ij}^{f}\right)$$

mean strain in a RLS element

$$\bar{\varepsilon}_{ij}^{f} = \frac{1}{V^c} \sum_f V^{f \cap e^{rls}} \varepsilon_{ij}^{f}$$

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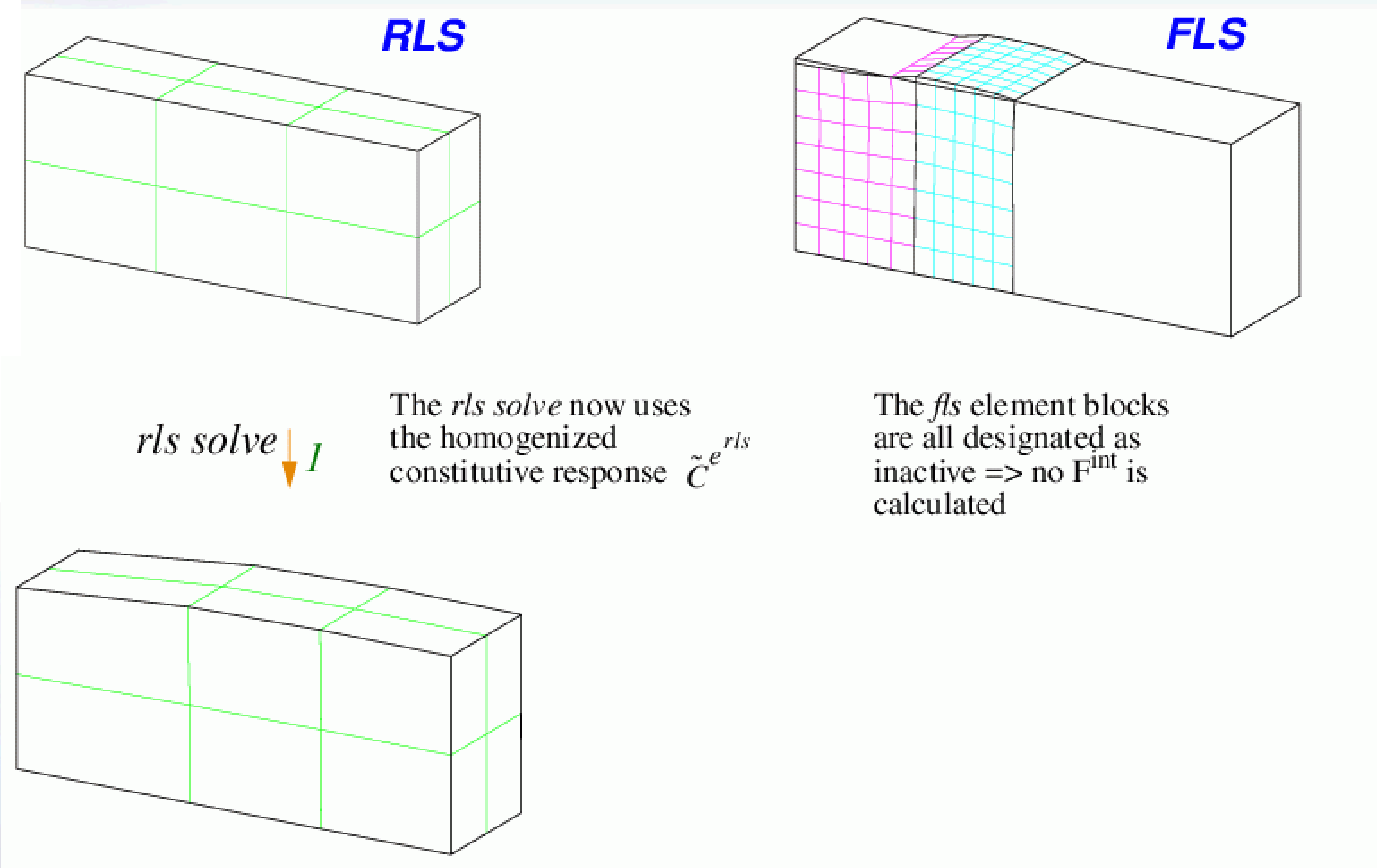
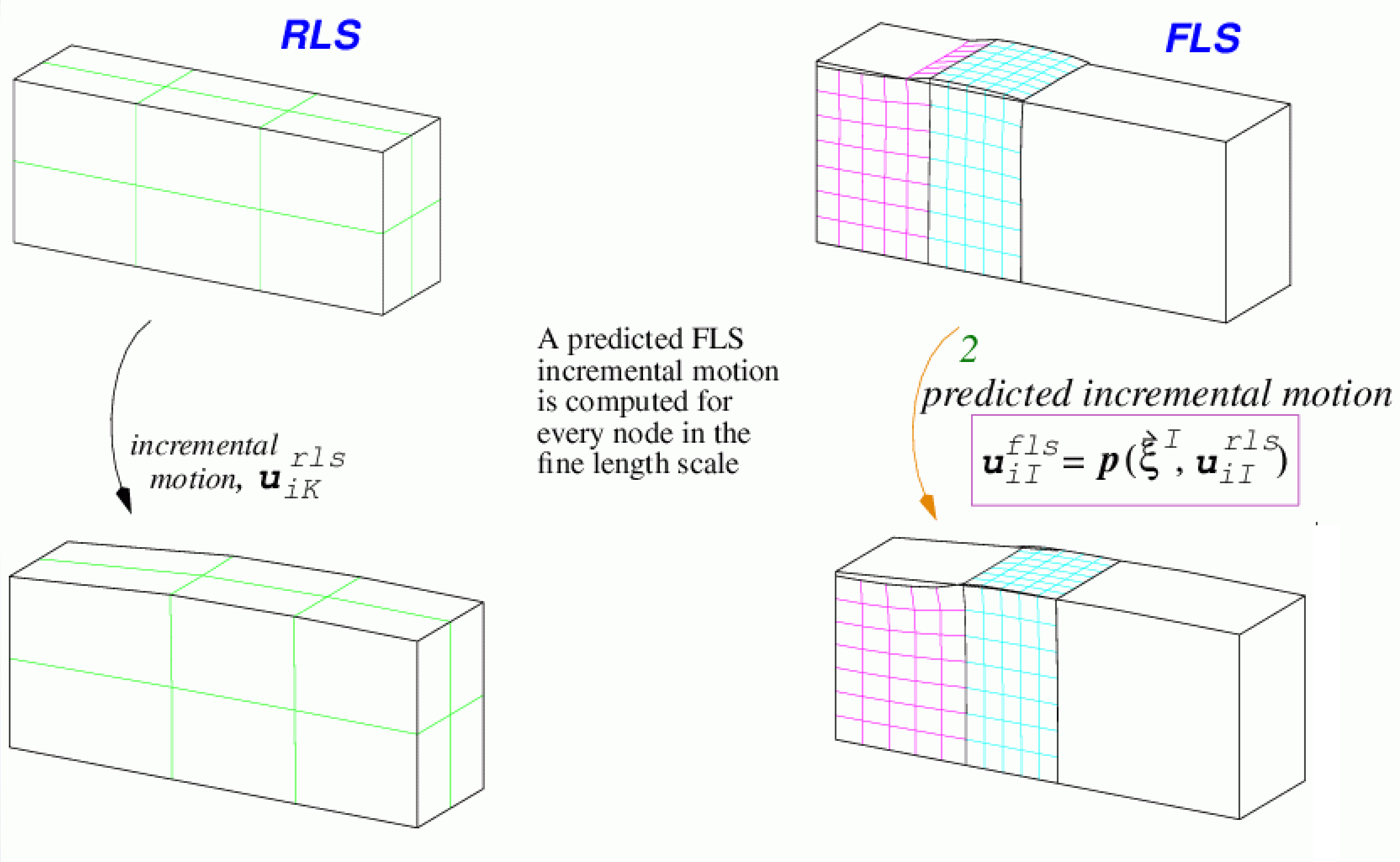
Multiscale solver: repeat *RLS* solve

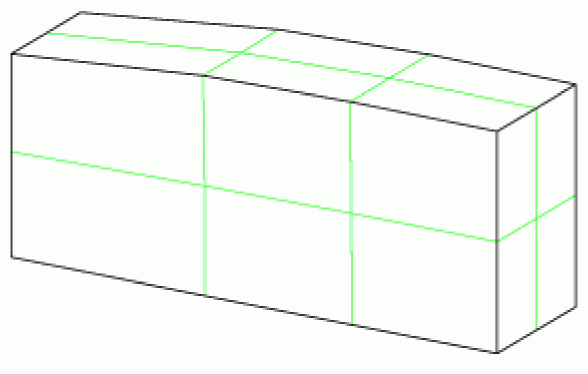


Multiscale solver: *FLS* predictor



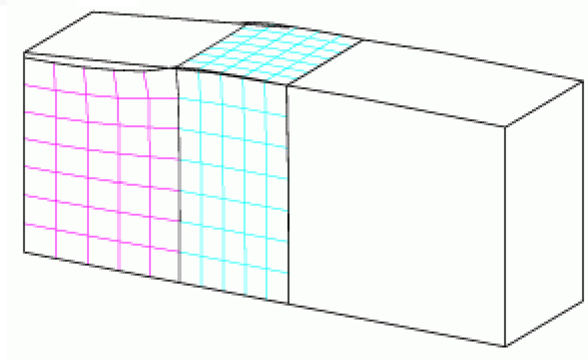
Multiscale solver: *FLS* solve

RLS



The *rls* element blocks are all designated as inactive => no F^{int} is calculated

FLS



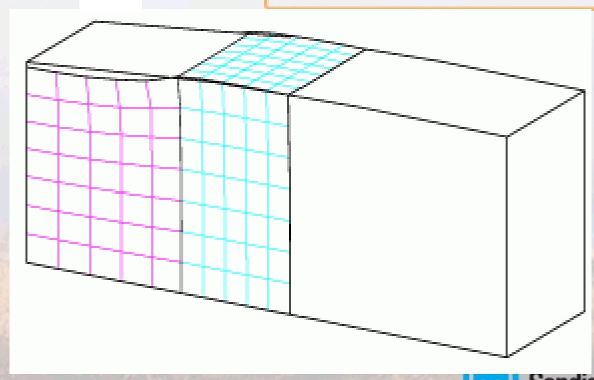
fls solve ↓ *3*

The *fls solve* is subjected to the Boundary Constraint:

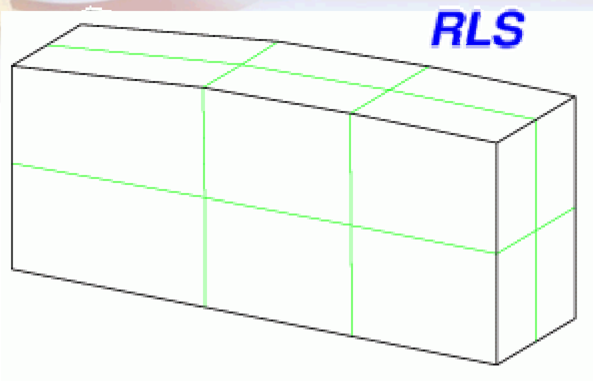
$$H^{mpc}(u) = 0$$

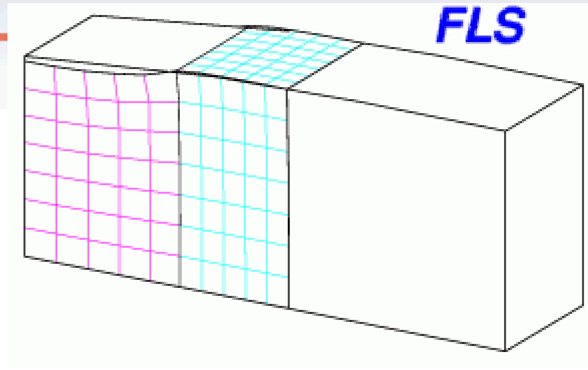
or

find λ^b s.t. $H^b(u) = 0$



Multiscale solver: homogenization





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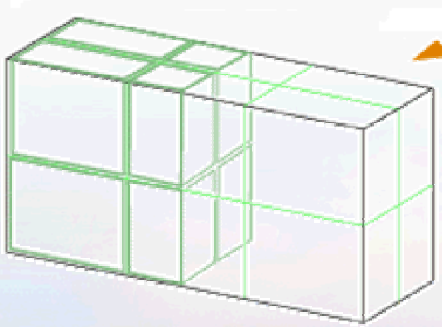
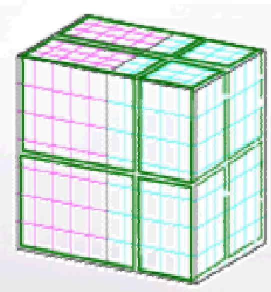
4 homogenization



$$\tilde{C}^{e^{rls}} = (1 - v_r) \cdot C^{e^{rls}} + v_r \cdot \bar{C}^{e^{rls}}(2\bar{G}, \bar{K})$$



where:

$$v_r = \frac{V^{f \cap e^{rls}}}{V^{e^{rls}}} \qquad 2\bar{G} = \frac{\left\| dev\left(m\left(\bar{\sigma}_{ij}^{f}\right)\right)\right\|_2}{\left\| dev\left(m\left(\bar{\varepsilon}_{ij}^{f}\right)\right)\right\|_2} \qquad \bar{K} = \frac{tr\left(m\left(\bar{\sigma}_{ij}^{f}\right)\right)}{tr\left(m\left(\bar{\varepsilon}_{ij}^{f}\right)\right)}$$

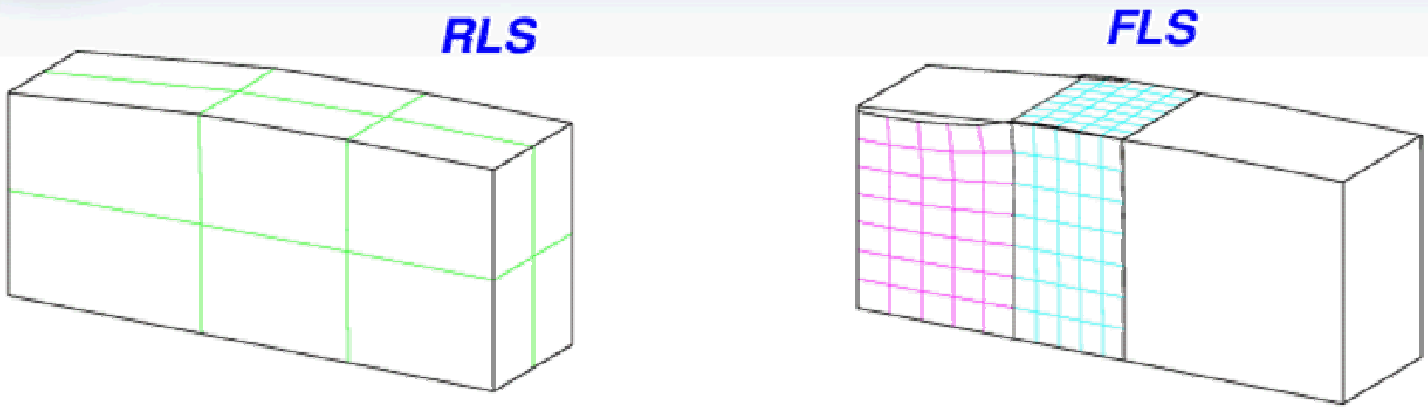
mean stress in a RLS element

$$\bar{\sigma}_{ij}^{f} = \frac{1}{V^c}\int_{V^c} \sigma_{ij}\,dv = \frac{1}{V^c}\sum_f \int_{V^f} \sigma_{ij}\,dv = \frac{1}{V^c}\sum_f V^{f \cap e^{rls}} \sigma_{ij}^{f} = m\left(\sigma_{ij}^{f}\right)$$

mean strain in a RLS element

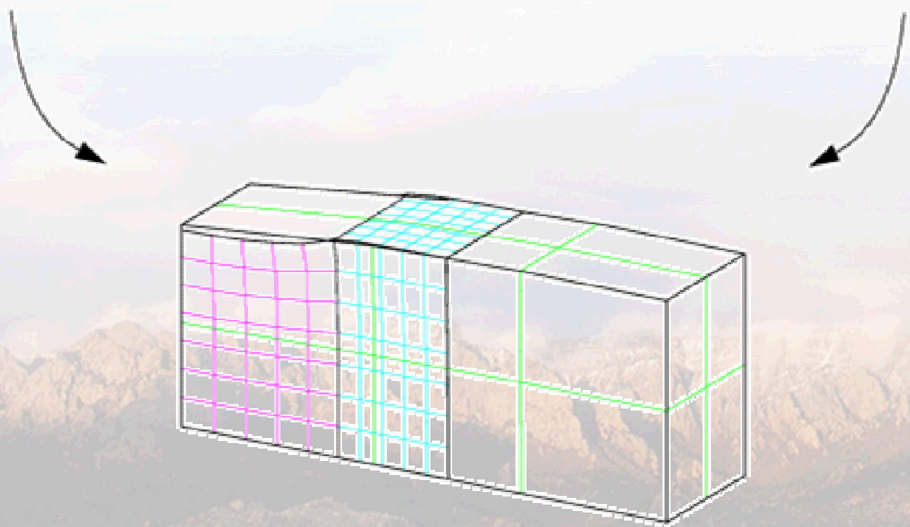
$$\bar{\varepsilon}_{ij}^{f} = \frac{1}{V^c}\sum_f V^{f \cap e^{rls}} \varepsilon_{ij}^{f}$$

Multiscale solver: converged load step

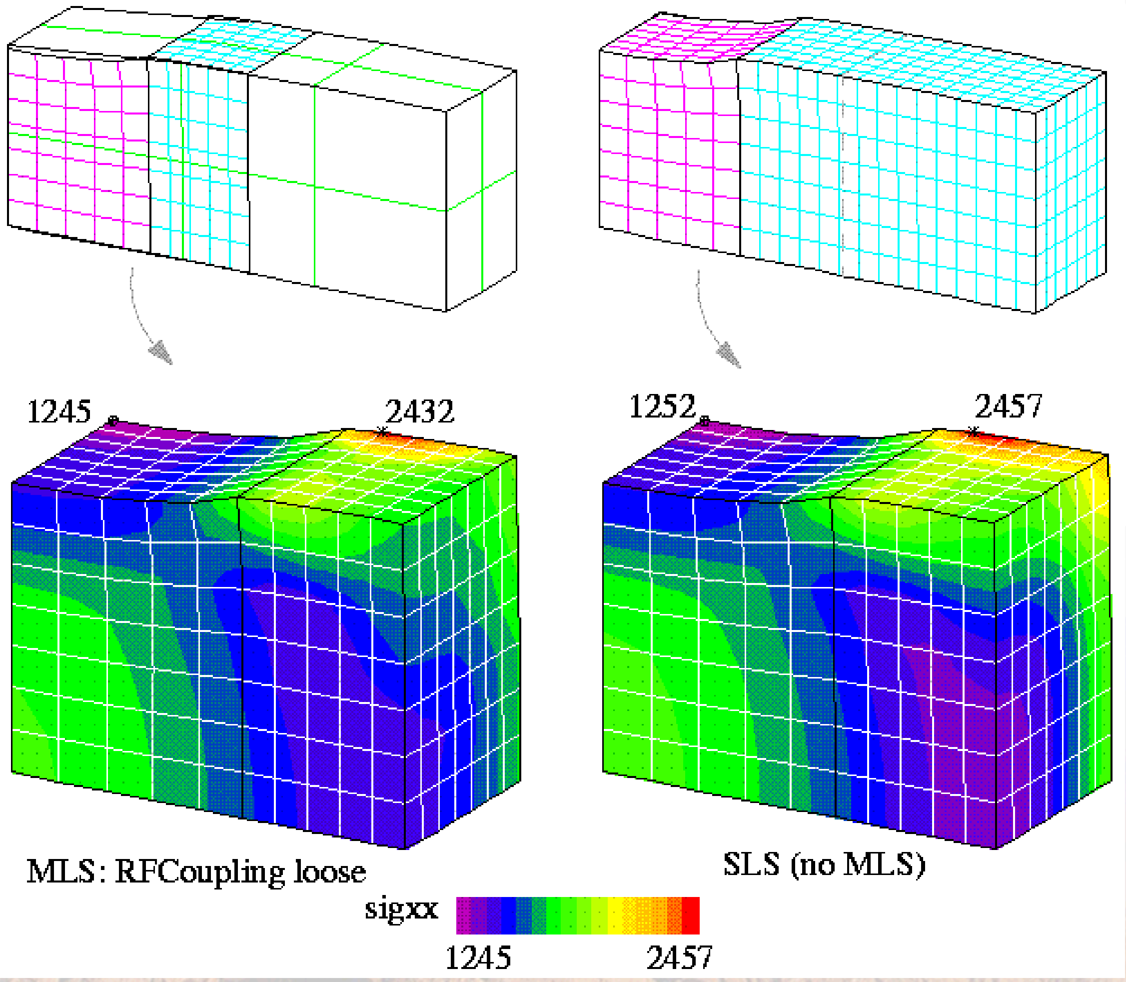


equilibrium iff: If after homogenization the residual on the rls dofs are acceptable small

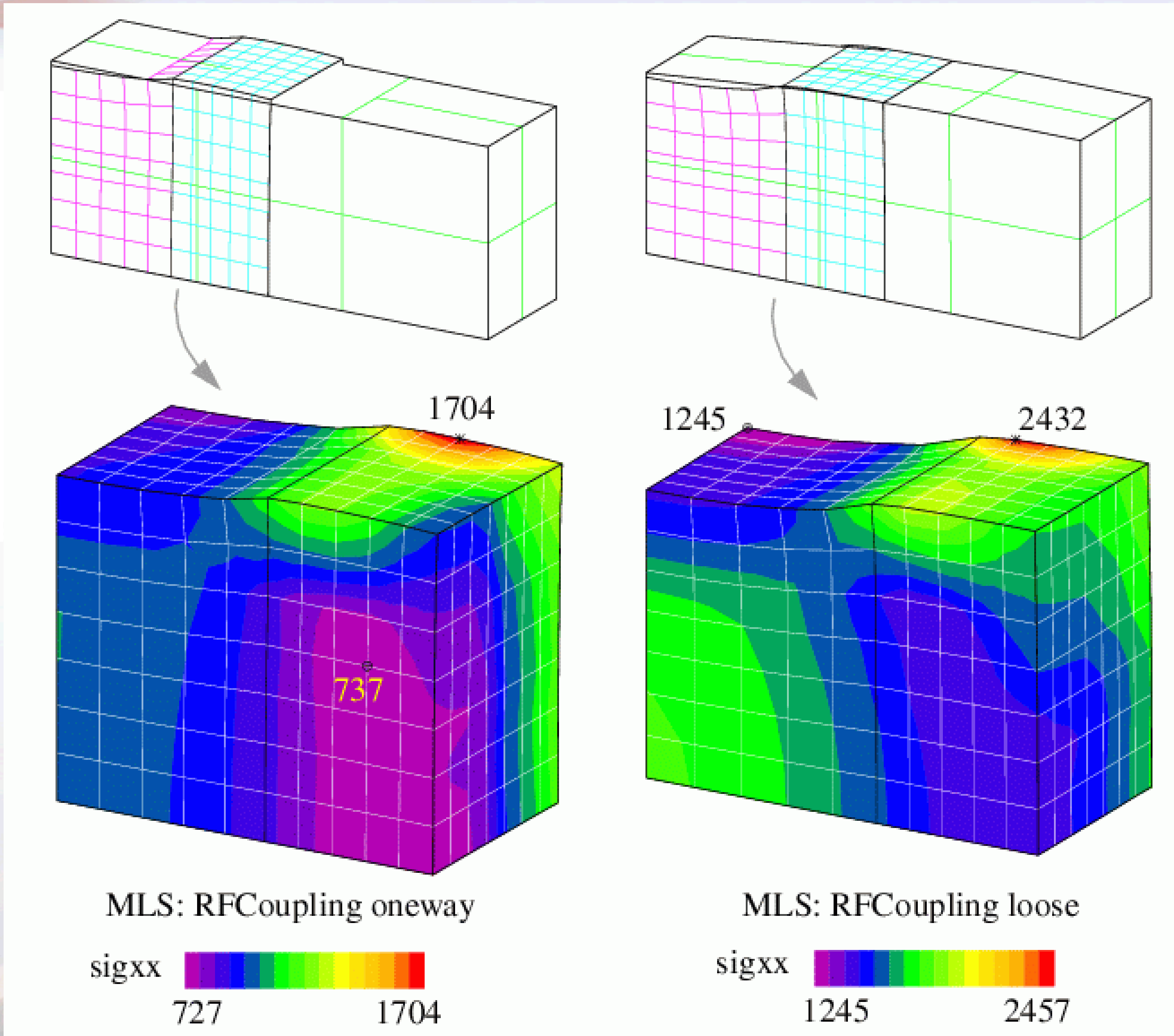
If so then update state on both length scales



MLS example: Bar with a soft inclusion

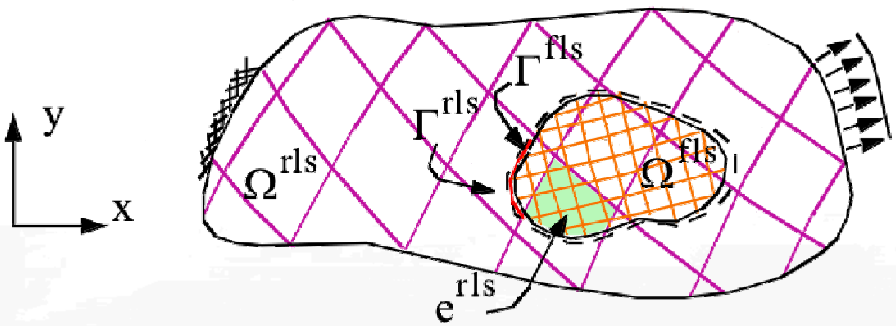


Submodeling vs. Multiscale modeling



Interactions between Global system model and a local detailed model

- Boundary constraint
  - Ensures that deformation of boundary of the fine length scale (*fls*) mesh is consistent with the imprint of that boundary in the reference length scale (*rls*) mesh.
  - Methods for enforcement:
    - » Multi-Point Constraint (MPC)
    - » Mortar Methods
    - » Consistent mesh tying

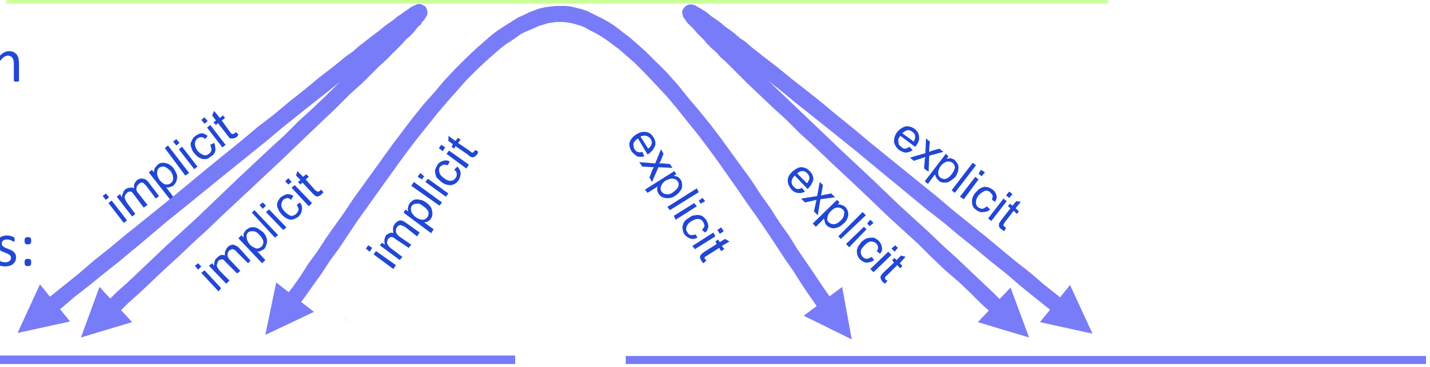


- Interior constraint
  - Ensures that deformation of material in *fls* and *rls* domains is consistent.
  - Methods for enforcement
    - » Homogenization: Effective moduli for *rls* material are computed based on *fls* behavior.
    - » Tight coupling: *rls* response computed from volume-weighted *fls* stress divergence

MLS Implementation in Sierra

Tempo : data manager for handoff and coupled problems

- Flexibility in *rls* and *fls* modeling approaches:



QS: solves the class of nonlinear large deformation quasi-static and implicit dynamics problems using advanced (Newton-like) solvers

ETD: solves the class of nonlinear large deformation dynamic problems using explicit central difference time integrator

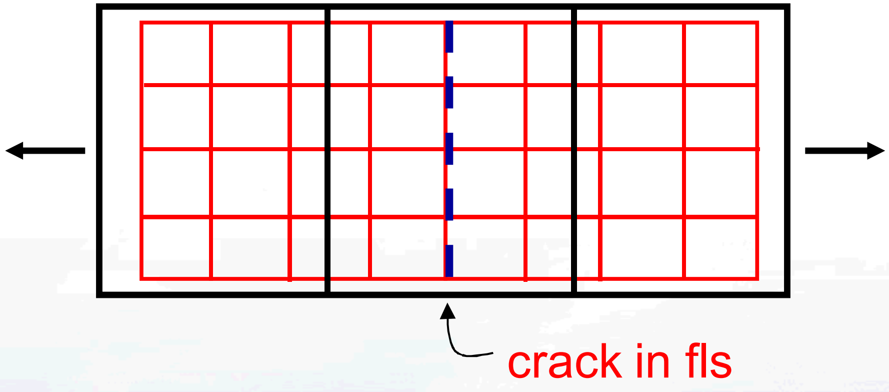
MLS coupling approach via homogenization has limitations

- In what is commonly referred to as a ***loose-coupling approach***, homogenization of the fine length scale response (for each reference length scale element) is used to give the reference length scale an approximate incremental material response.

  In the implicit-implicit case, any approximations in this homogenization are sorted-out via successive solves on the *rls* & *fls* within the same load step.

Homogenization techniques is a simplifying approach for MLS… but has limitations

- **Limiting assumption:**
  - **material model in *rls* elements must be capable of representing *fls* domain.**



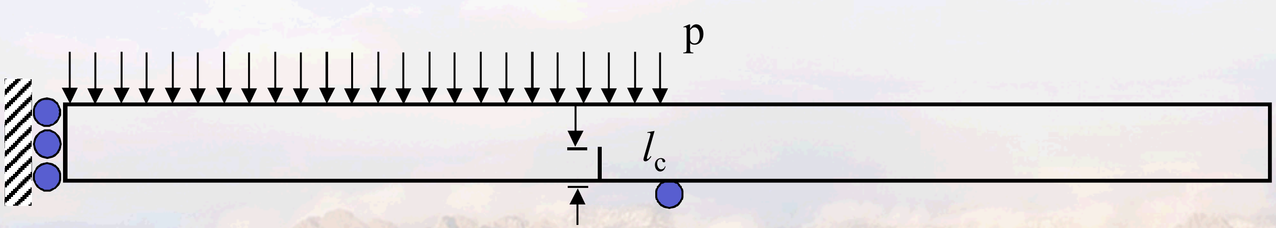
for intact material (no crack), modulus must be: $$E_{rls} = \frac{\Delta\sigma_{rls}}{\Delta\varepsilon_{fls}}$$

for failed material (thru-thickness crack), modulus must be: $$E_{rls} = \frac{\Delta\sigma_{fls}}{\Delta\varepsilon_{fls}}$$

MLS coupling approach via tight coupling

Consider the following class of problems…

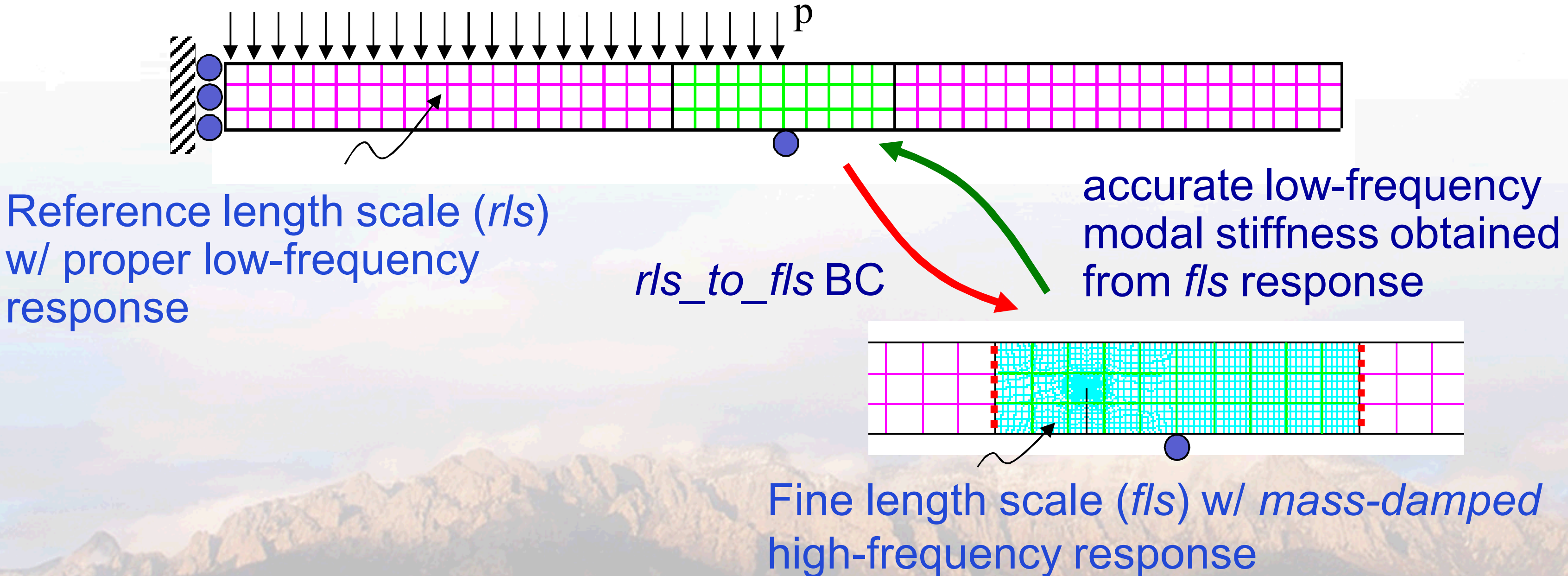
- Structural response of this thin flexible continuum is predominately low-mode response
- Yet, the stress concentrations & stiffness variability in the structure (around the support, and due to the crack tip) can only be obtained via a detailed model
- This is an ideal case for explicit-explicit MLS.
  → consider a ***tight-coupling approach***



Explicit-explicit MLS

concept…

- Solve two nonlinear problems… one for the reference length scale (*rls*) and one for the fine length scale (*fls*) in a ***tight-coupling approach***
- where explicit control modes is used as a modal filter to decompose response into low-frequency (*rls*) + high-frequency (*fls*) modes



Explicit-explicit MLS

conceptual implementation…

- **Boundary constraint**: use BC to tie *fls* boundary to *rls* mesh
- **Interior constraint**: distinguish between *rls* elements *rls_empty* & *rls_replaced* (*rls* inherits *fls* low-freq. modal response)

fls IBVP : *fls_response* obtained via *modal_decomposition*

use *fls* material model to compute F^{int}_{fls}

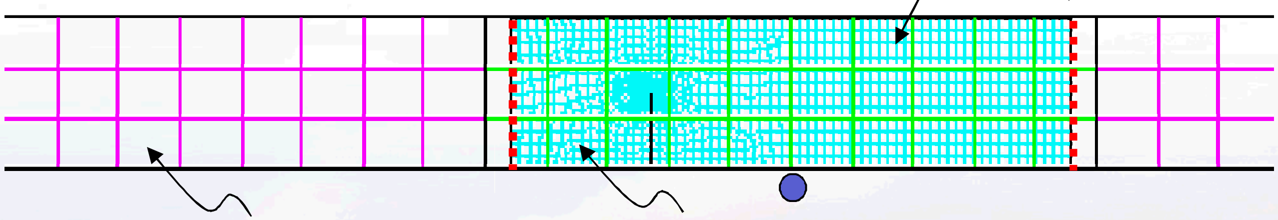
i.e. $F^{int}_{fls}\left(v + \Delta t^{rls}_{cr}\left(p(a^{lf}) + a^{hf}\right)\right)$

prolongation operator p( )

rls_with_boundary

enforce *fls* to *rls* BC

BC(fls_to_rls)



rls IBVP :

rls_empty

use *rls* material model to compute F^{int}_{rls}

i.e. $F^{int}_{rls} = div\,(\sigma_{rls})$

$\sigma_{rls} = C\varepsilon_{rls}$

rls_replaced

use *fls* material model to compute F^{int}_{rls}

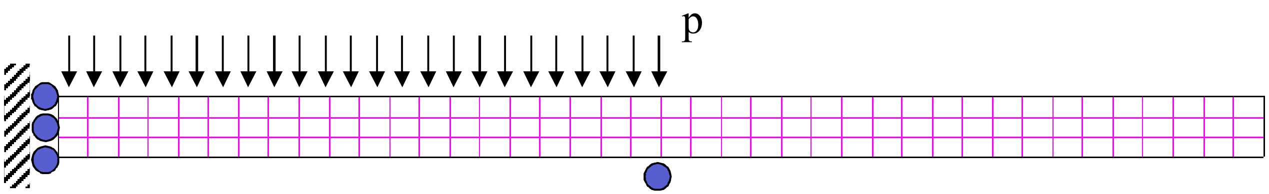
i.e. $F^{int}_{rls} = r(F^{int}_{fls})$

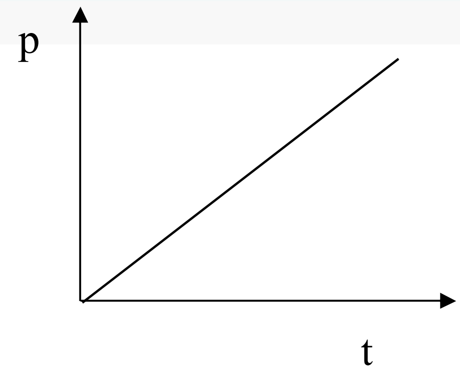
$F^{int}_{fls} = div\,(\sigma_{fls})$

restriction operator r( )

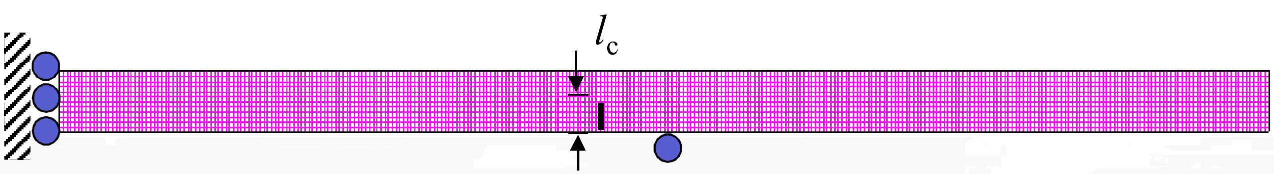
Explicit – explicit MLS

beambending_ecm_mls





Reference length-scale mesh (3 x 40 elements)



Fine length-scale mesh (w/ embedded crack)

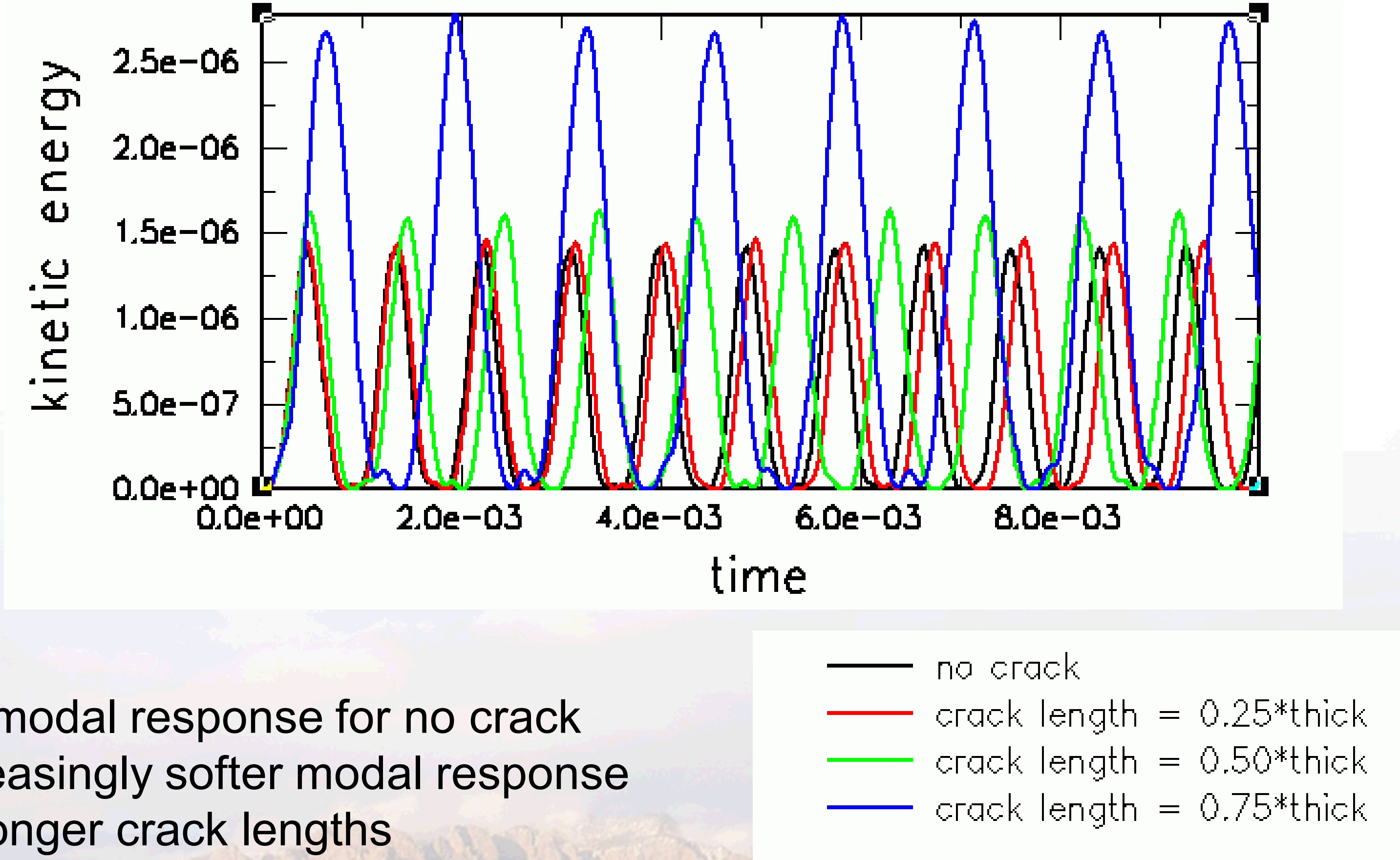
- **Critical time step is obtained from reference length scale**
- *fls* is the entire domain

Explicit – explicit MLS

beambending_ecm_mls

Stationary crack results

Kinetic energy vs time for various stationary crack lengths



Note:

- stiff modal response for no crack
- increasingly softer modal response for longer crack lengths

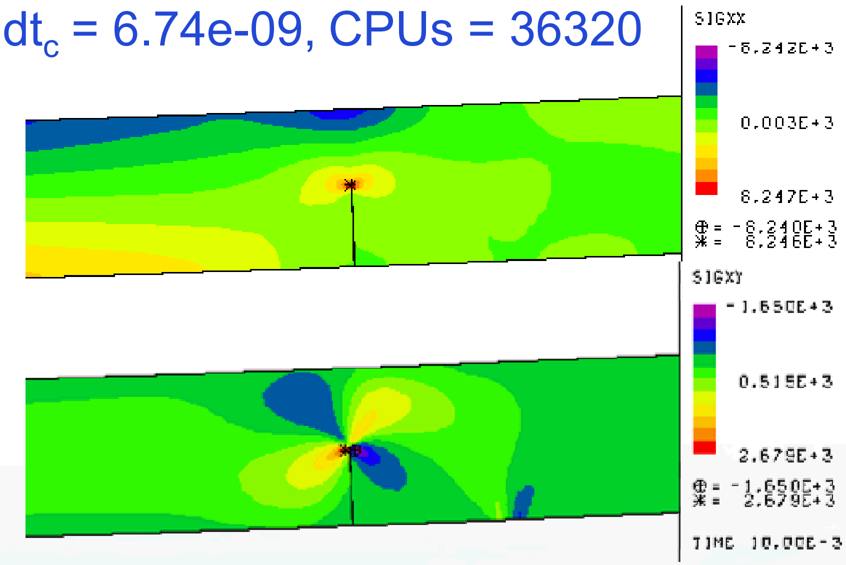
Explicit – explicit MLS

beambending_ecm_mls

Stationary crack results

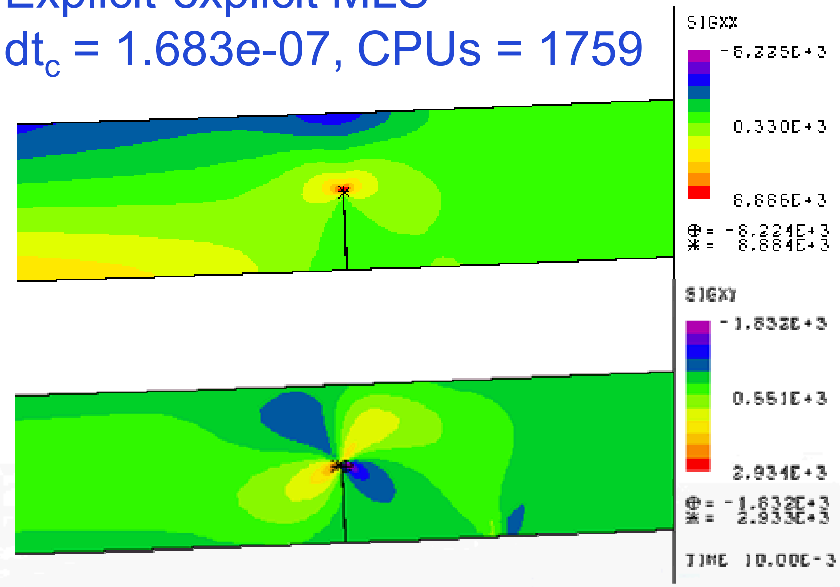
Explicit solution on *fls* only

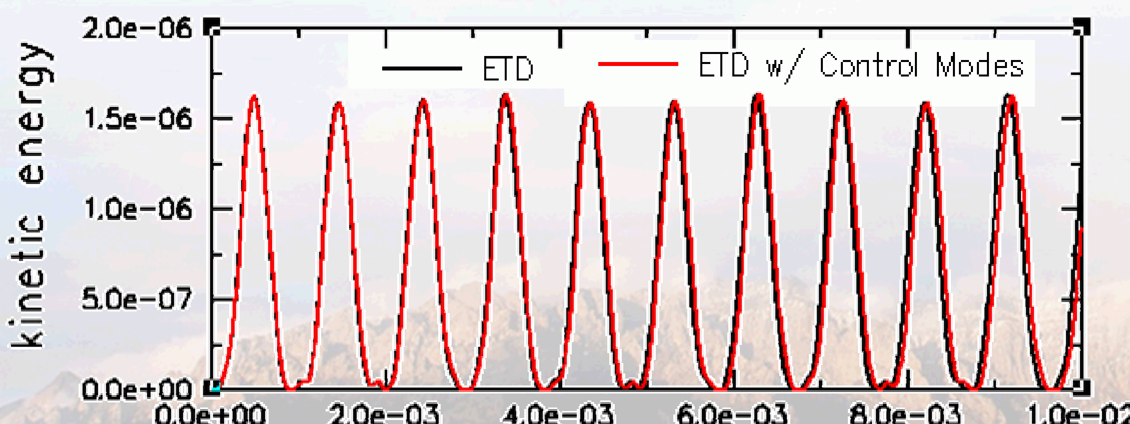
dt_c = 6.74e-09, CPUs = 36320



Explicit-explicit MLS

dt_c = 1.683e-07, CPUs = 1759





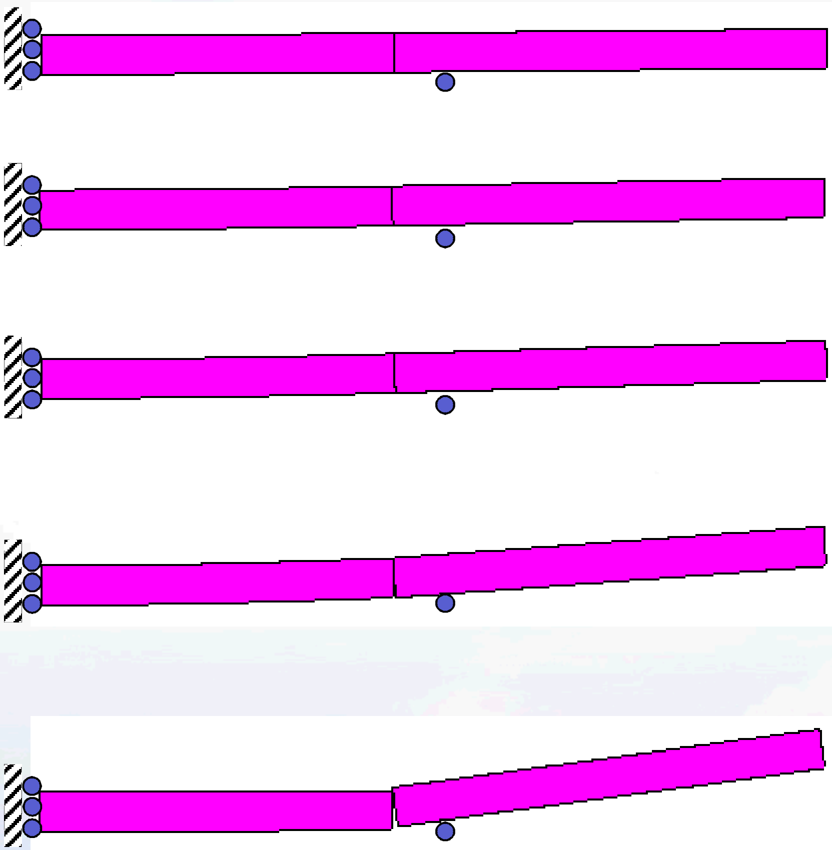
nearly identical dynamics for 1/20 of the cost:

CPUs_ratio = 1759/ 36320

Explicit – explicit MLS

beambending_ecm_mls

Running crack results



t = 0.0025

t = 0.005

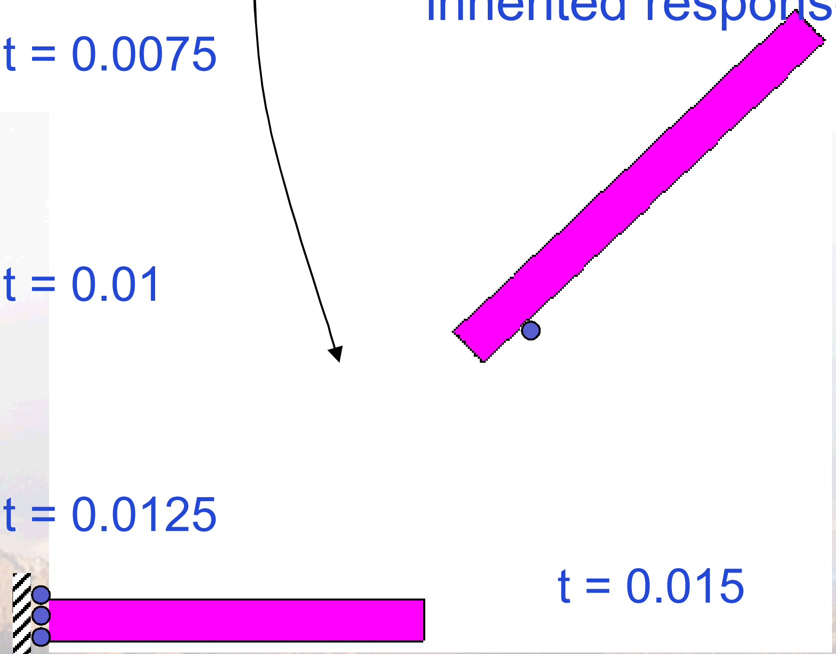
t = 0.0075

t = 0.01

t = 0.0125

fls: running crack solution transitions from “intact” to “failed”

rls: uniform mesh deforms with inherited response



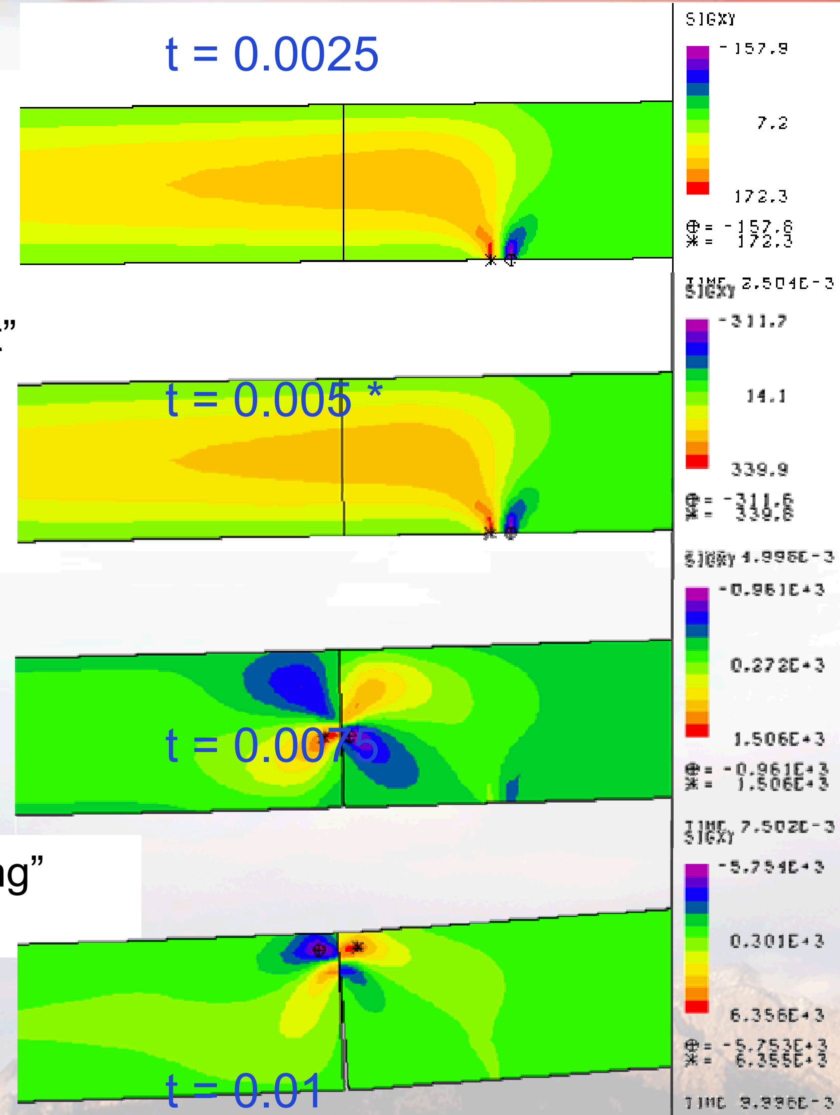
t = 0.015

Crack is *programmed* to run starting @ t=0.005

Explicit – explicit MLS

beambending_ecm_mls

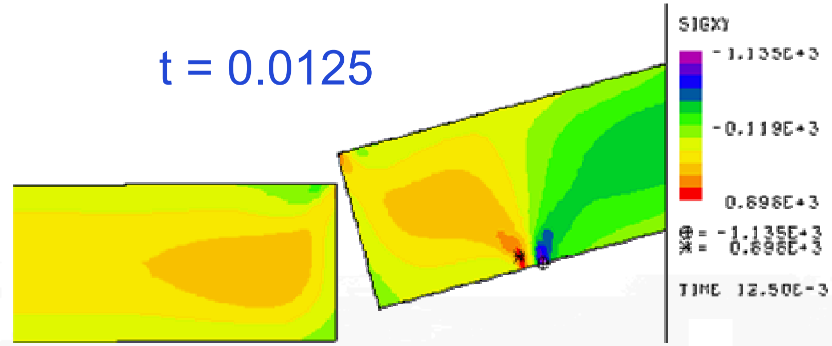
Running crack results
(crack begins to run @t=0.005)



fully "intact"

"running" crack

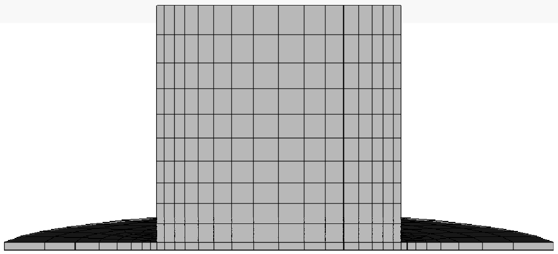
sigxy



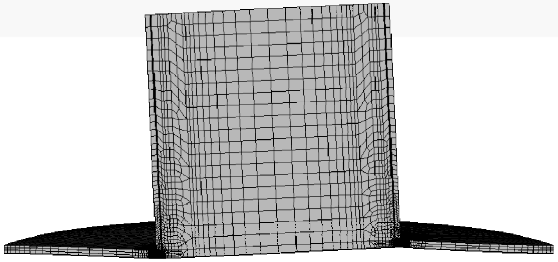
fully "failed"

Explicit Tight Coupling Application

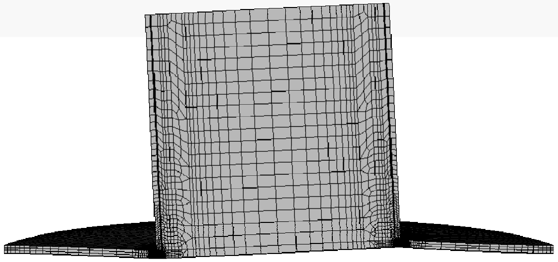
Surrogate test for laser welds connecting a component to a housing



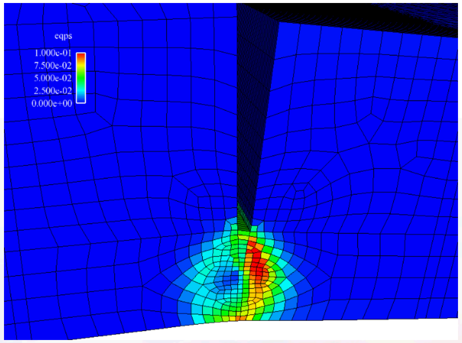
Constraint mesh
1732 elements



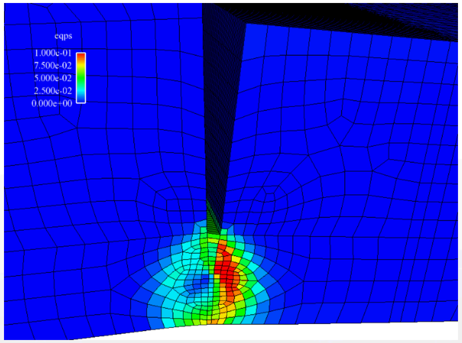
Deformed MLS fine mesh
2.23M elements



Deformed comparison
model



MLS solution
equivalent plastic strain



Comparison solution
equivalent plastic strain

Both cases run on 200 processors
MLS critical Δt = 5.3e-8
Comparison critical Δt = 2.2e-9
$\therefore$ Using MLS yields 24x increase in Δt, 16x speedup

Multiscale modeling: Example problems

1. EXAMPLE : Axial tension of a bar w/ an inclusion
2. EXAMPLE : Axial tension of fiber/matrix composite
3. EXAMPLE : Axial tension of a Toy-Bolt
4. EXAMPLE : Coesfeld tension test w/ edge crack
5. EXAMPLE : Contact patchtest
6. EXAMPLE : Axial tension of a Welded Plate
7. EXAMPLE : Axial tension of a Bolted Cylinder
8. EXAMPLE : Rolling tire w/ belt edge crack

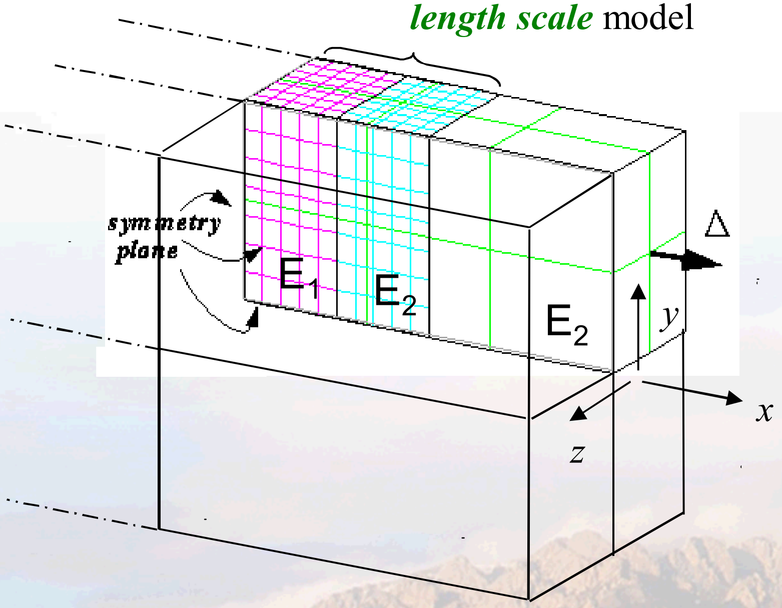
Multiscale Modeling Example

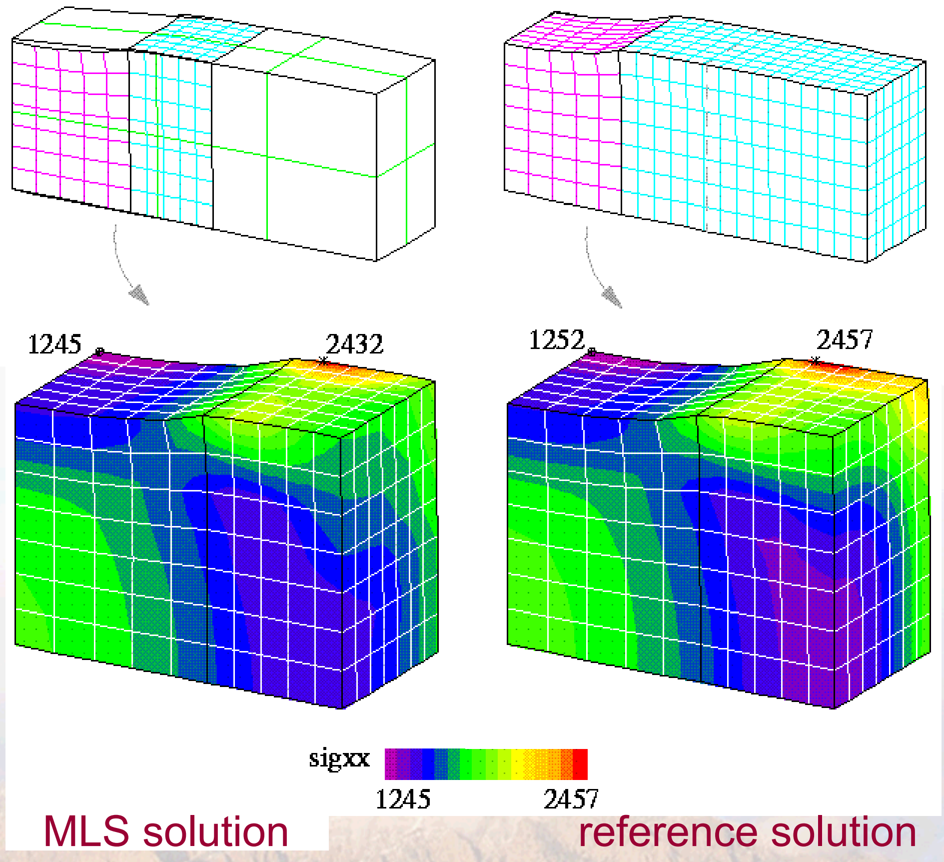
EXAMPLE : Axial tension of a bar w/ a soft inclusion

fine length scale model has modulii E_2 , $E_1 = E_2/10$

reference length scale model has initial modulus E_2

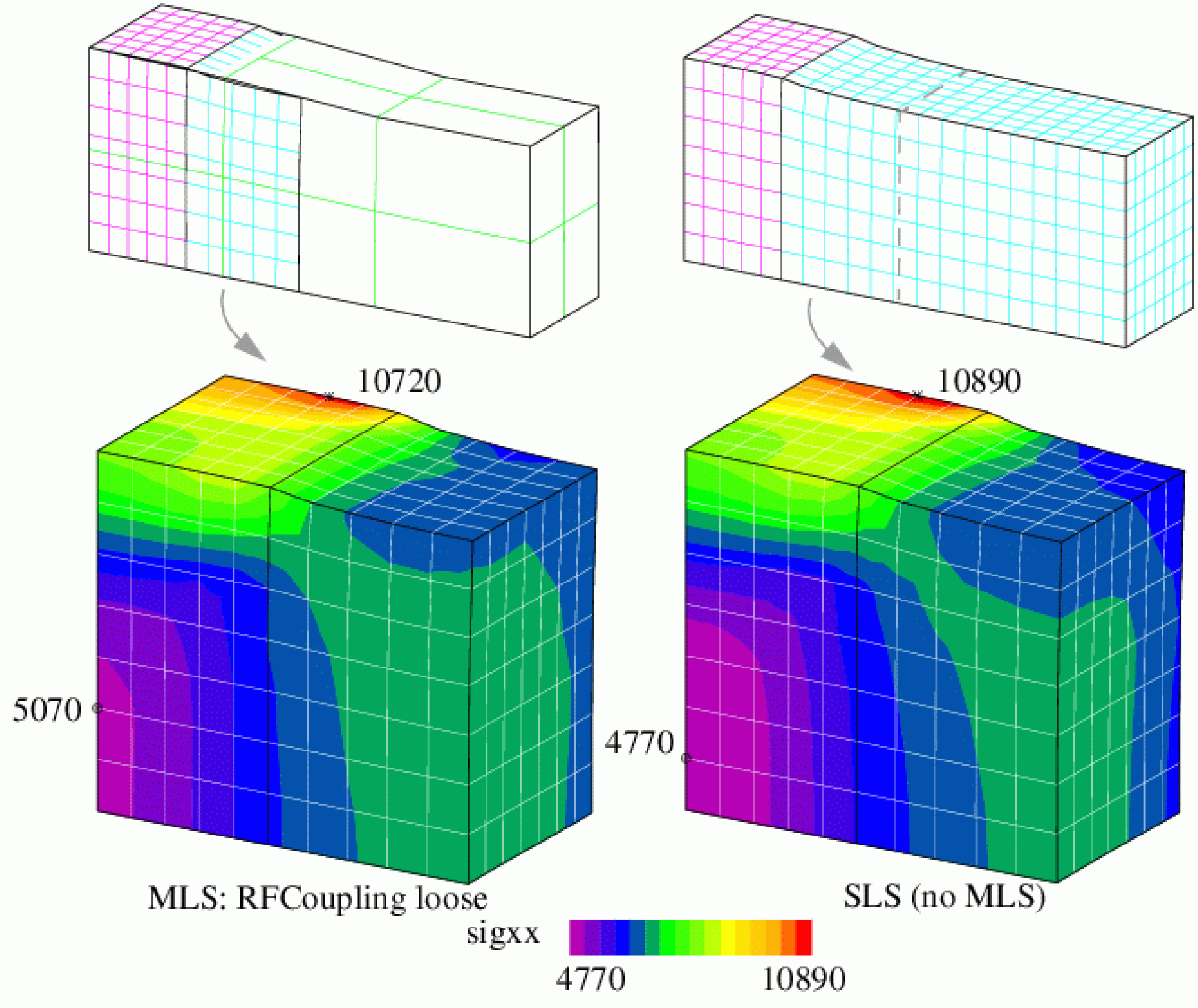
fine length scale model is embedded in the ***reference length scale*** model





Multiscale Modeling Example

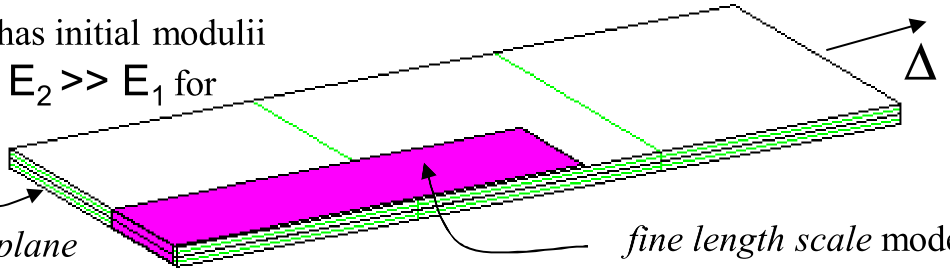
fine length scale model has modulii E_2 , $E_1 = 10E_2$



Multiscale Modeling Example

EXAMPLE : Axial tension of fiber/matrix composite

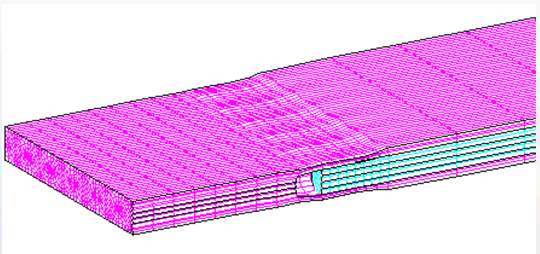
reference length scale model has initial modulii E_1 for matrix (hex elements), $E_2 >> E_1$ for fiber (membrane elements)



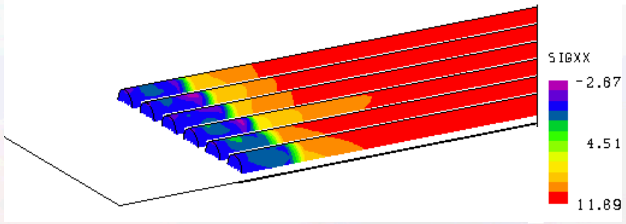
symmetry plane

fine length scale model has modulii E_1 for matrix (hex elements), $E_2 >> E_1$ for fiber (hex elements)

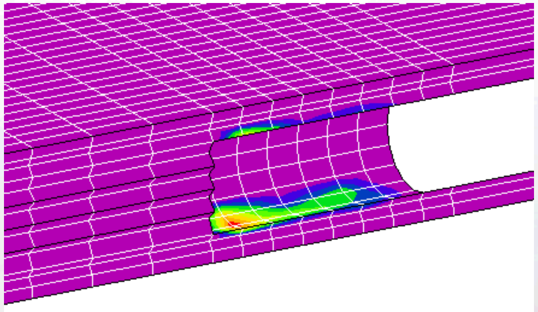
MLS solution:



Deformation of fine length scale model - displacements magnified x50



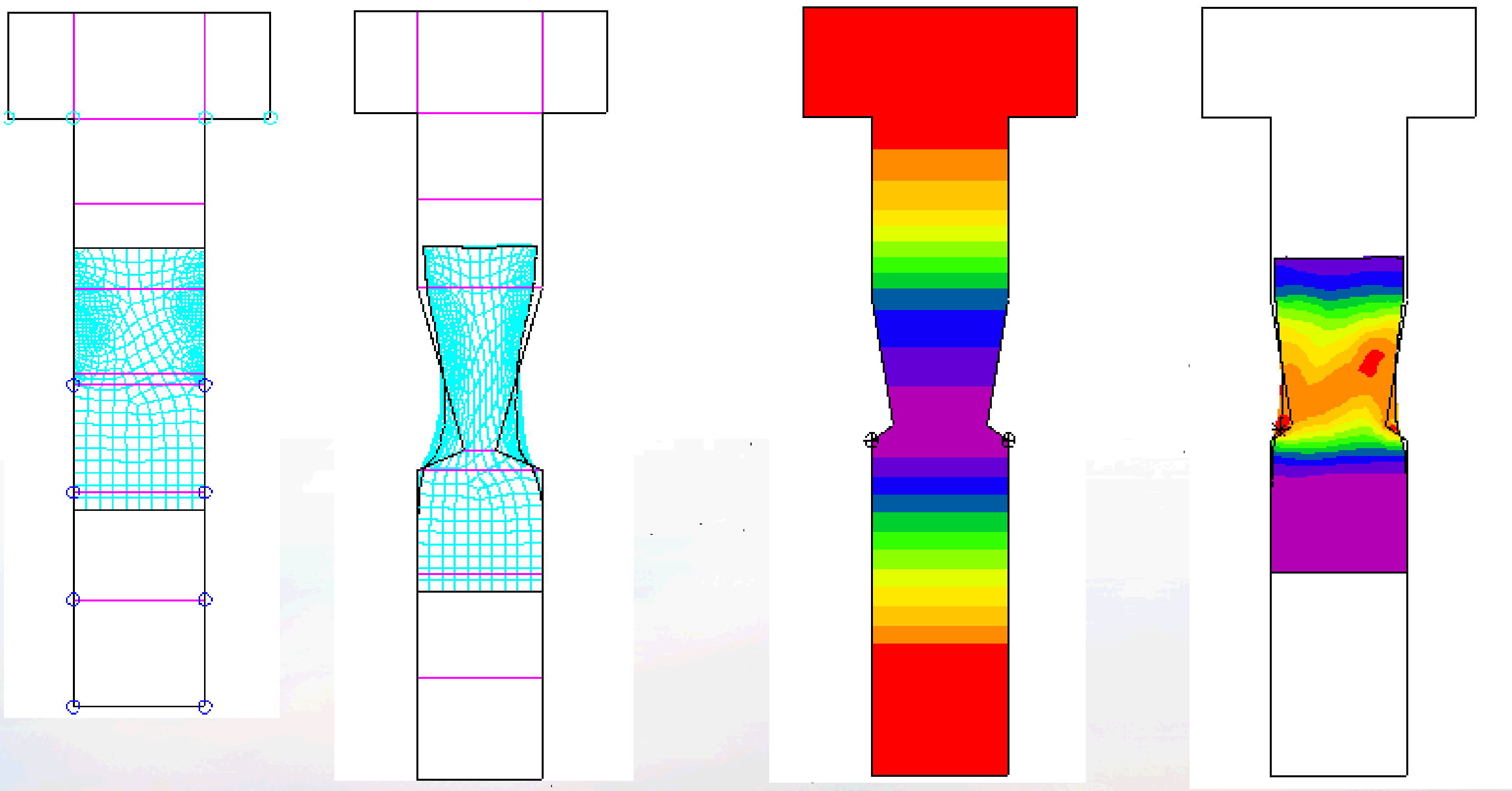
Axial stress in fiber



Frictional energy between fiber & rubber

Multiscale Modeling Example

EXAMPLE : Axial tension of a Toy-Bolt

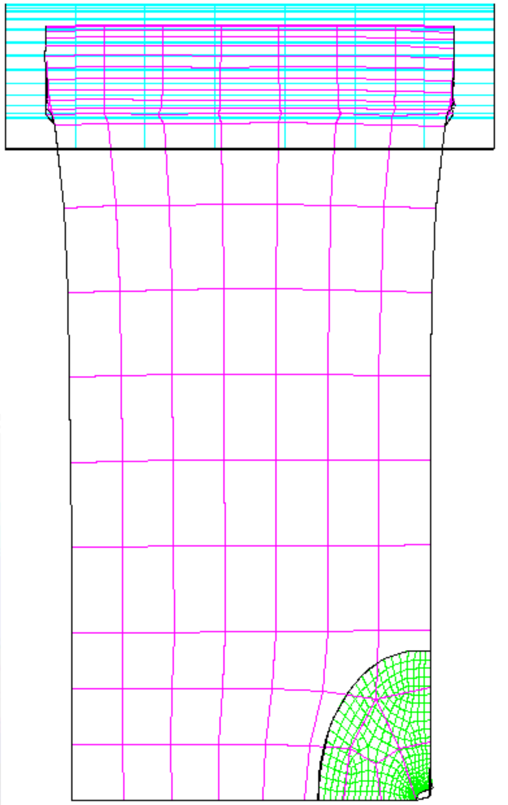


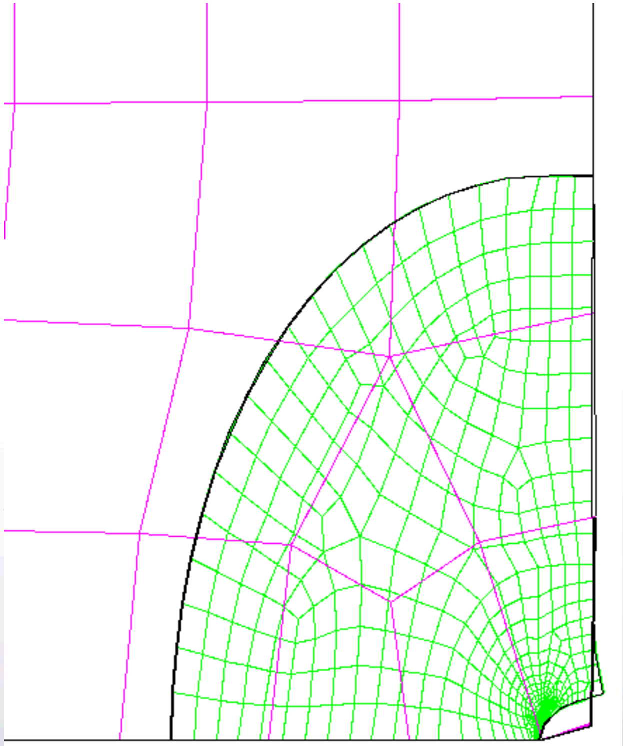
Deformations magnified x2 Effective modulus in RLS eqps

reference length scale model has initial modulii equal to fine length scale modulii, both described by the same material model (elastic plastic non-linear hardening)

Multiscale Modeling Example

EXAMPLE : Coesfeld tension test w/ edge crack





reference length scale model has initial modulii equal to fine length scale modulii, both described by the same material model (incompressible solid)

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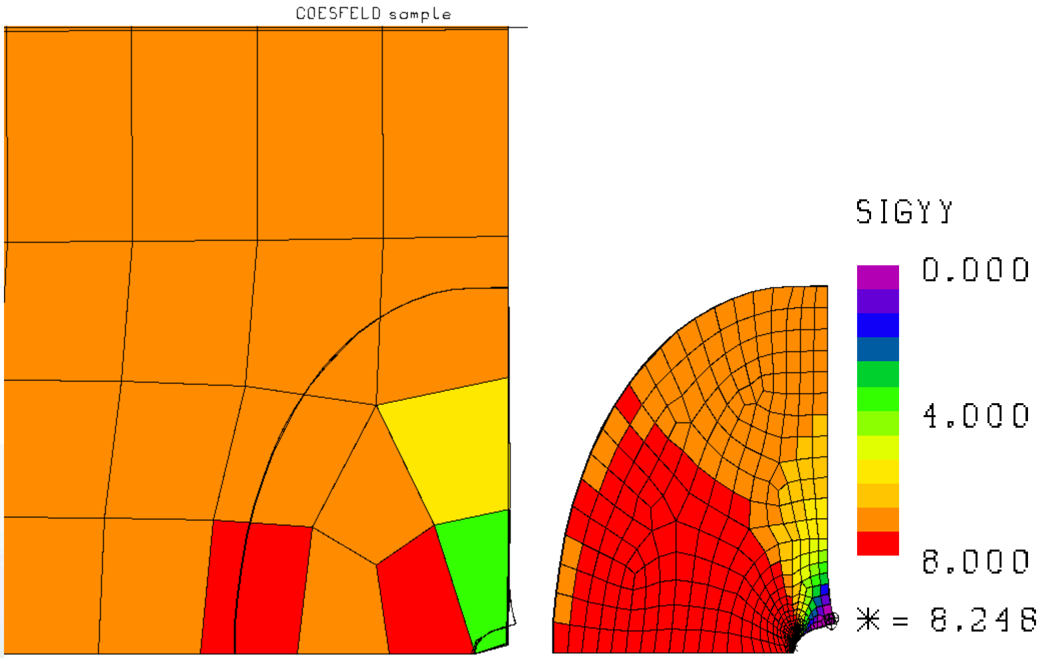
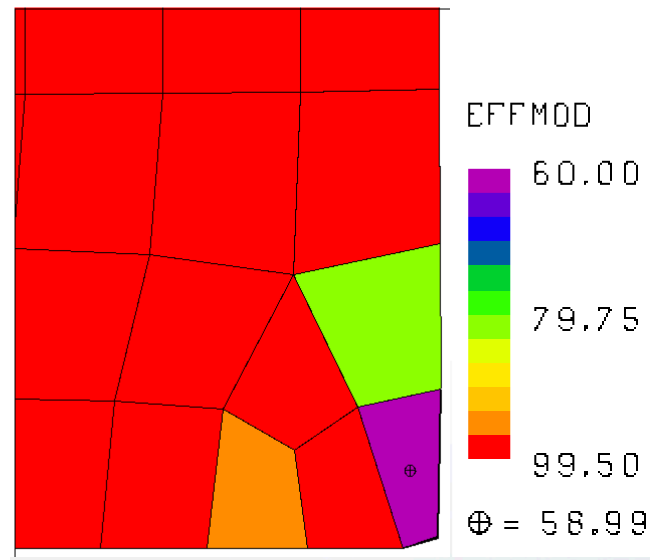
Multiscale Modeling Example

EXAMPLE : Coesfeld tension test w/ edge crack



Stress in pull direction

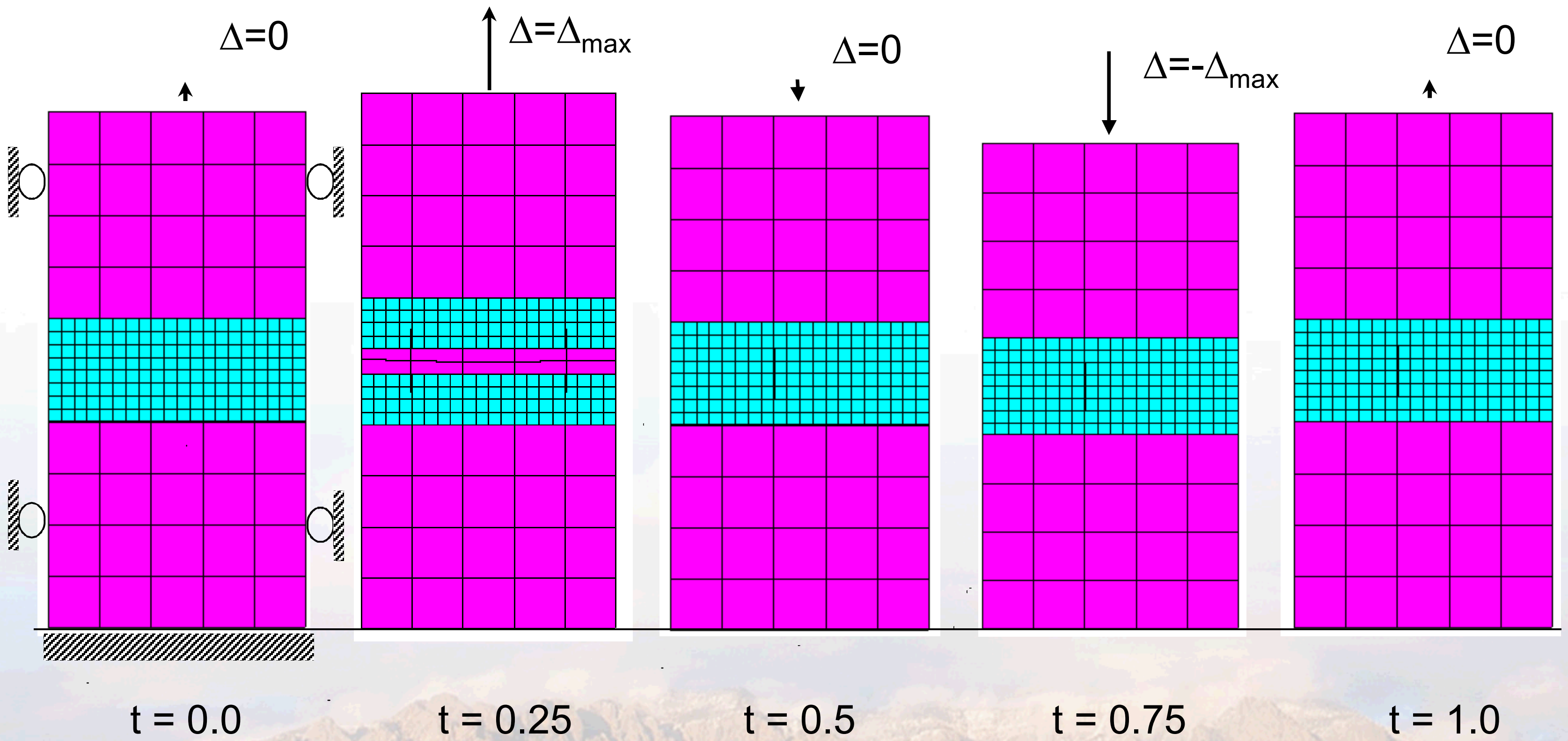


Effective modulus in RLS

Multiscale Modeling Example

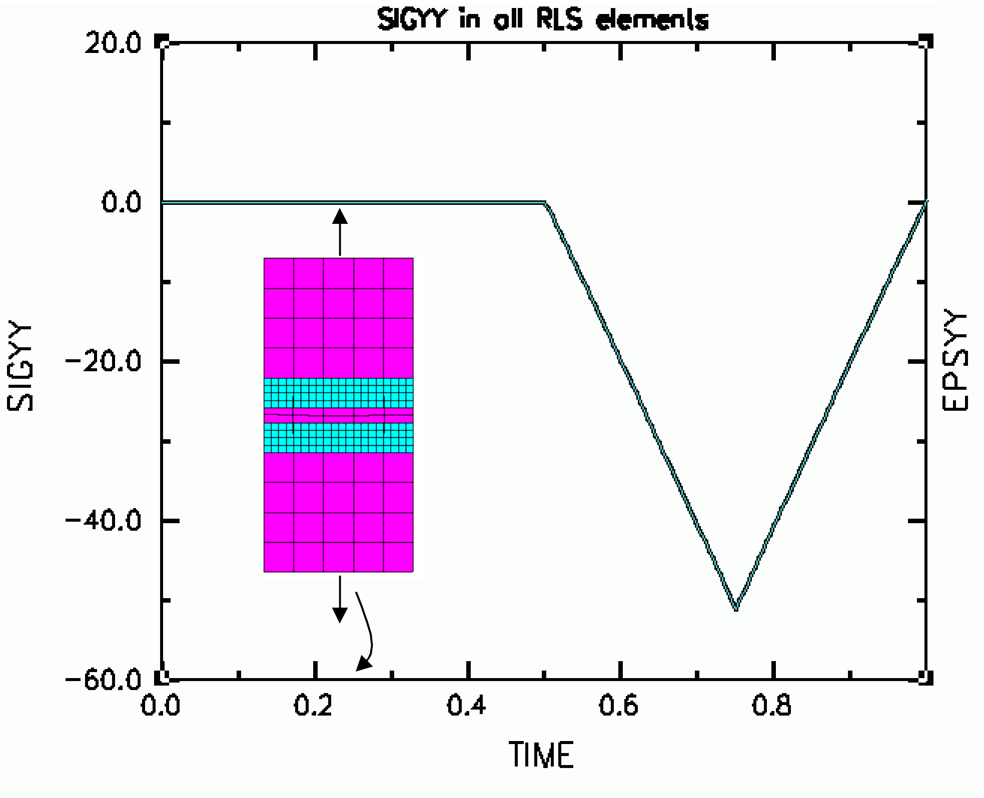
EXAMPLE : Contact patchtest

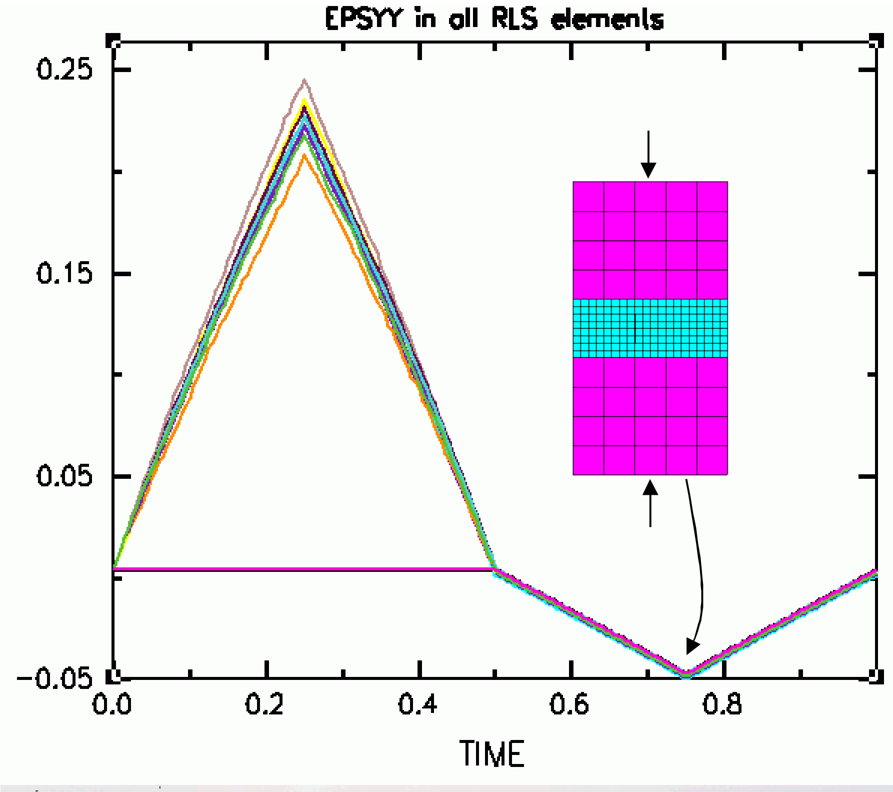
Reference length scale and fine length scale have identical, elastic properties



Multiscale Modeling Example

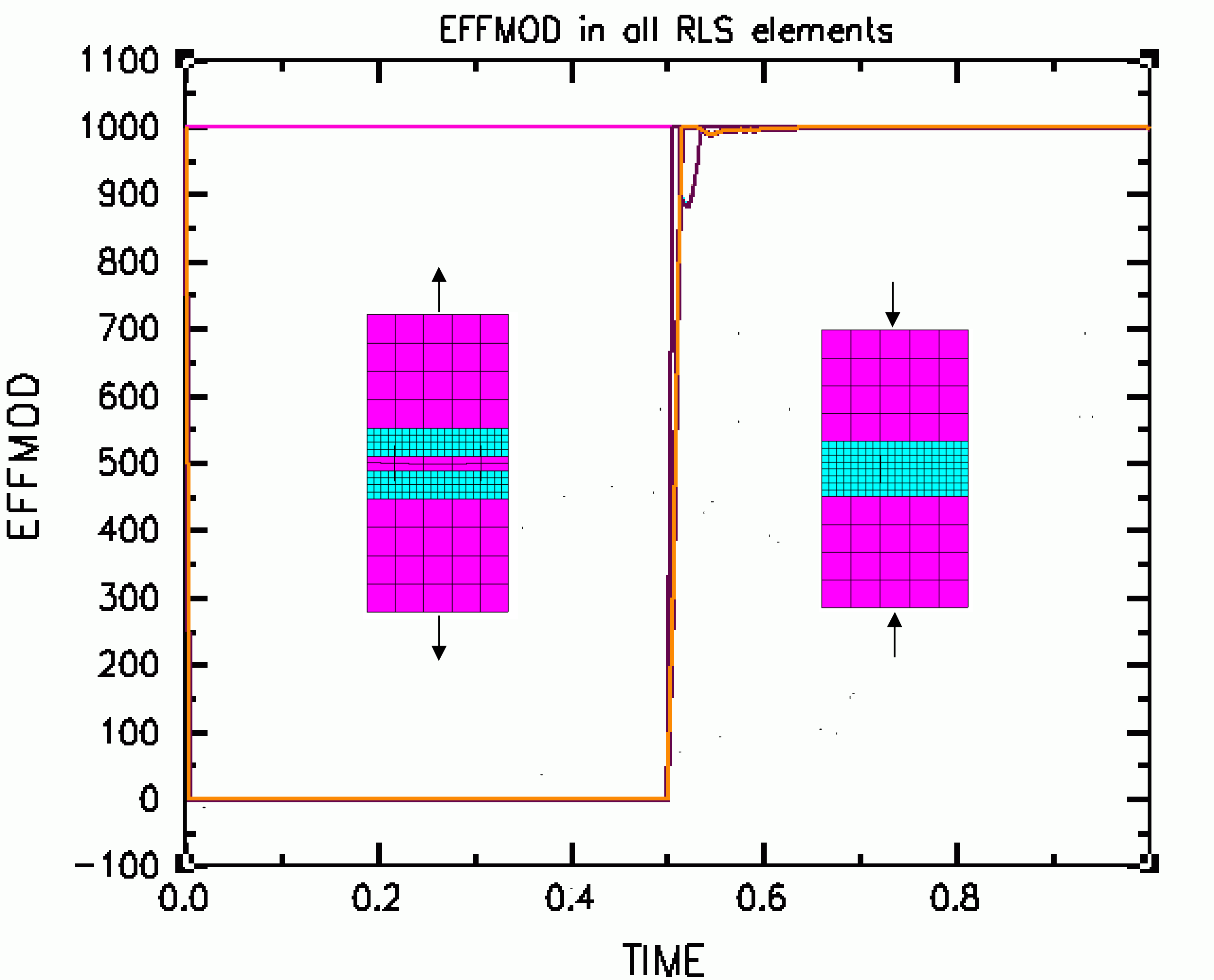
EXAMPLE : Contact patchtest





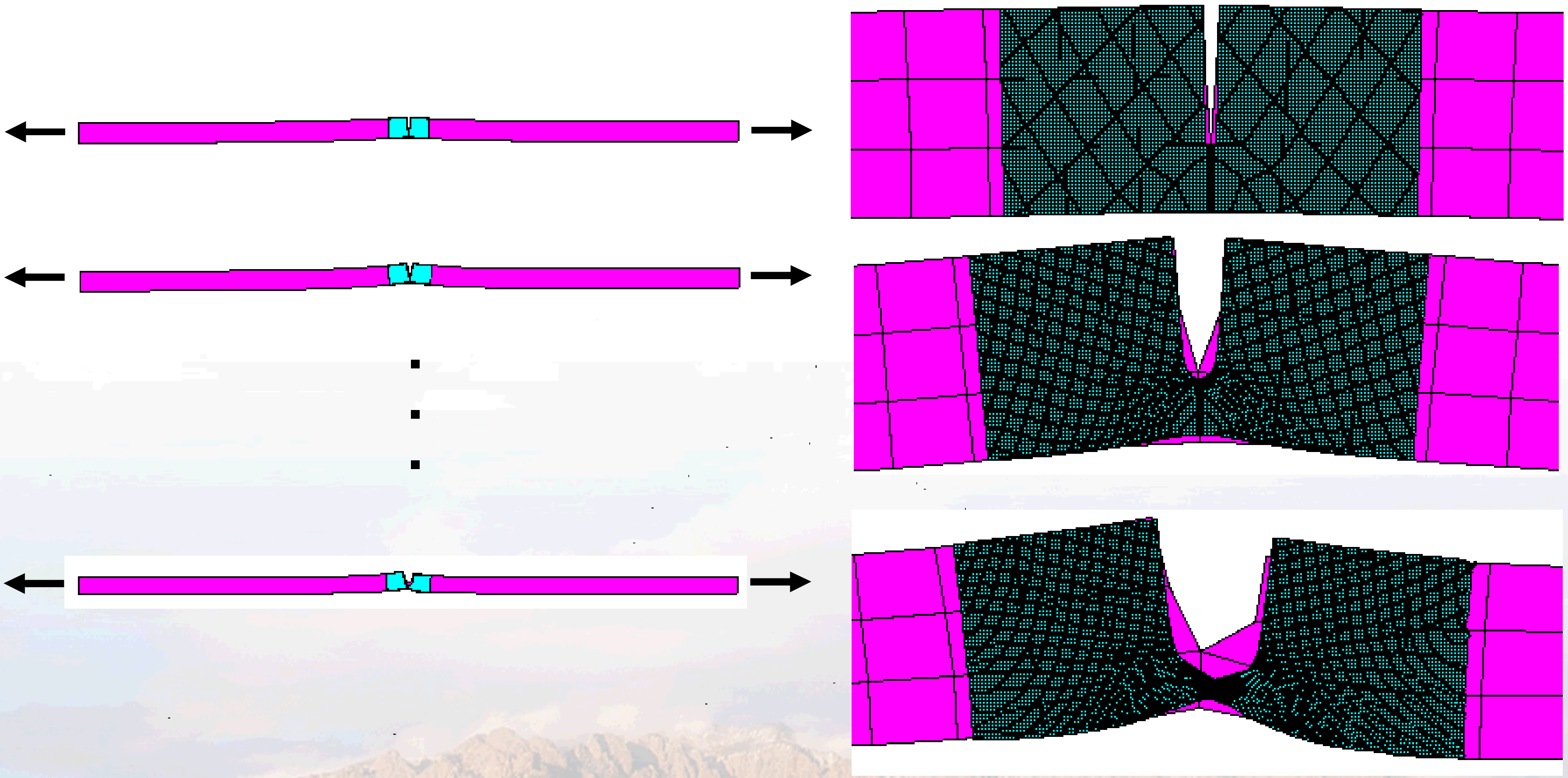
Multiscale Modeling Example

EXAMPLE : Contact patchtest



Multiscale Modeling Example

EXAMPLE : Axial tension of a Welded Plate



reference length scale model and ***fine length scale*** model have the same plasticity constitutive model

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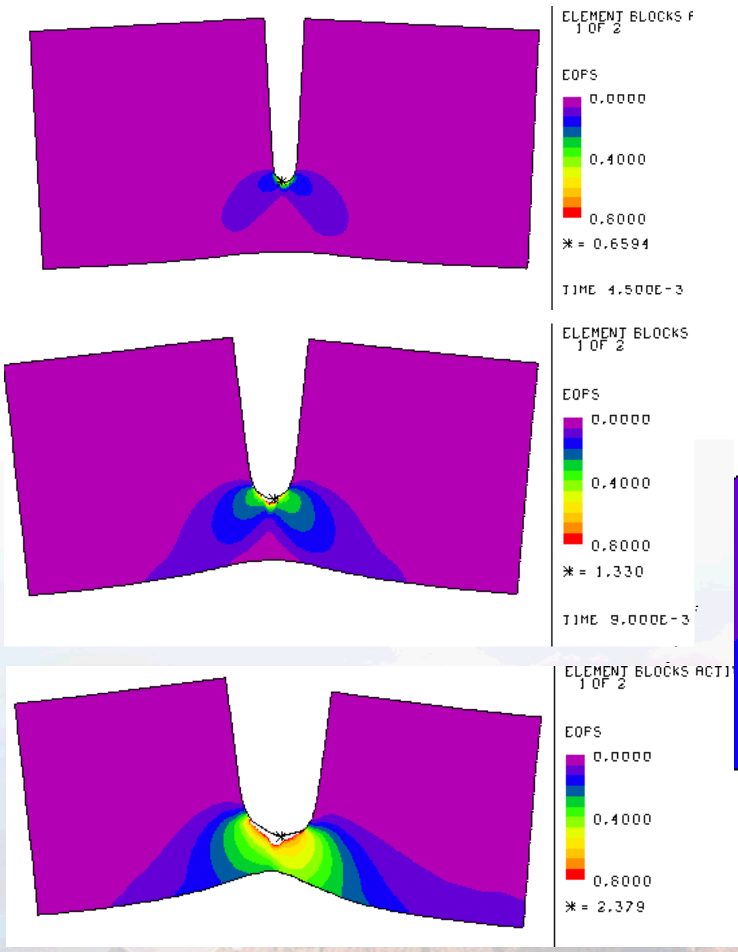
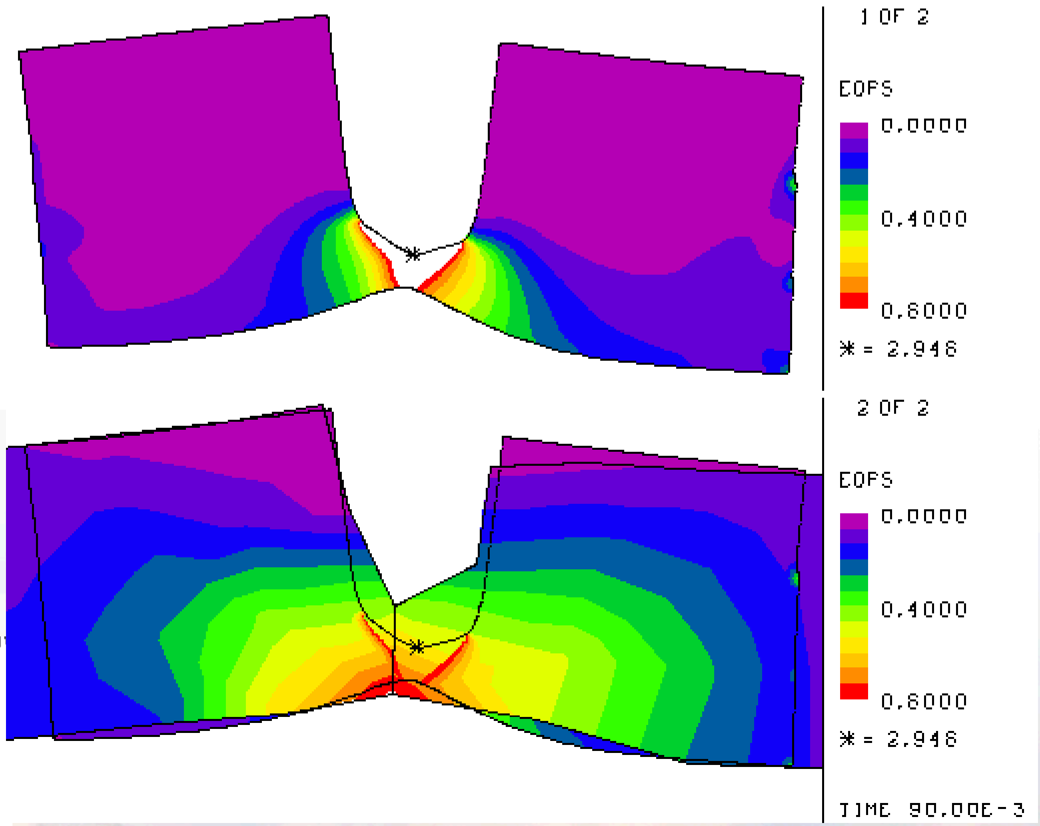
Multiscale Modeling Example

EXAMPLE : Axial tension of a Welded Plate

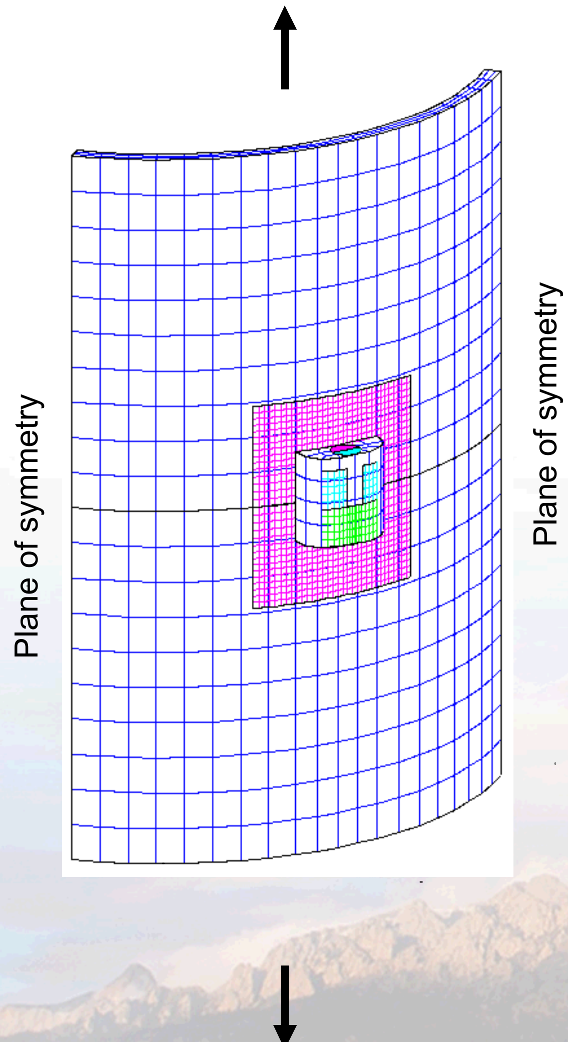




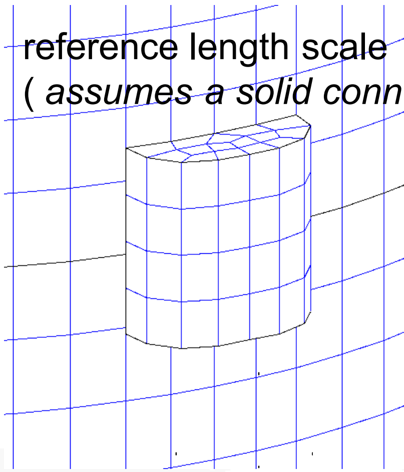
Equivalent plastic strain

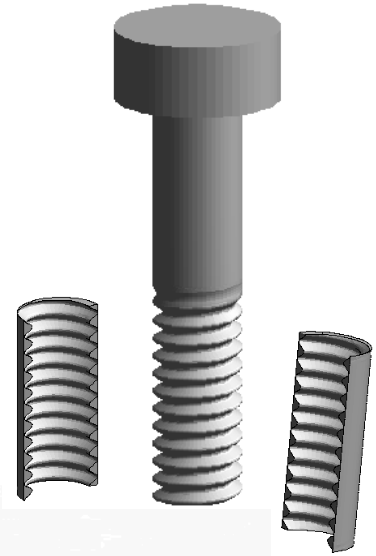
Multiscale Modeling Example

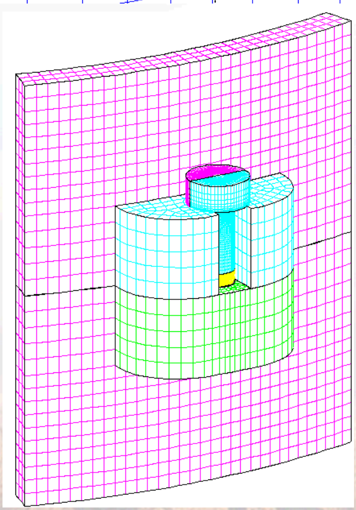
EXAMPLE : Axial tension of a Bolted Cylinder



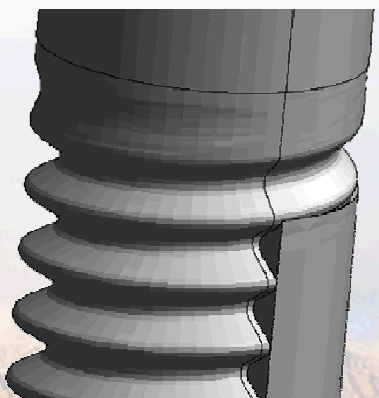
reference length scale
(*assumes a solid connection*)





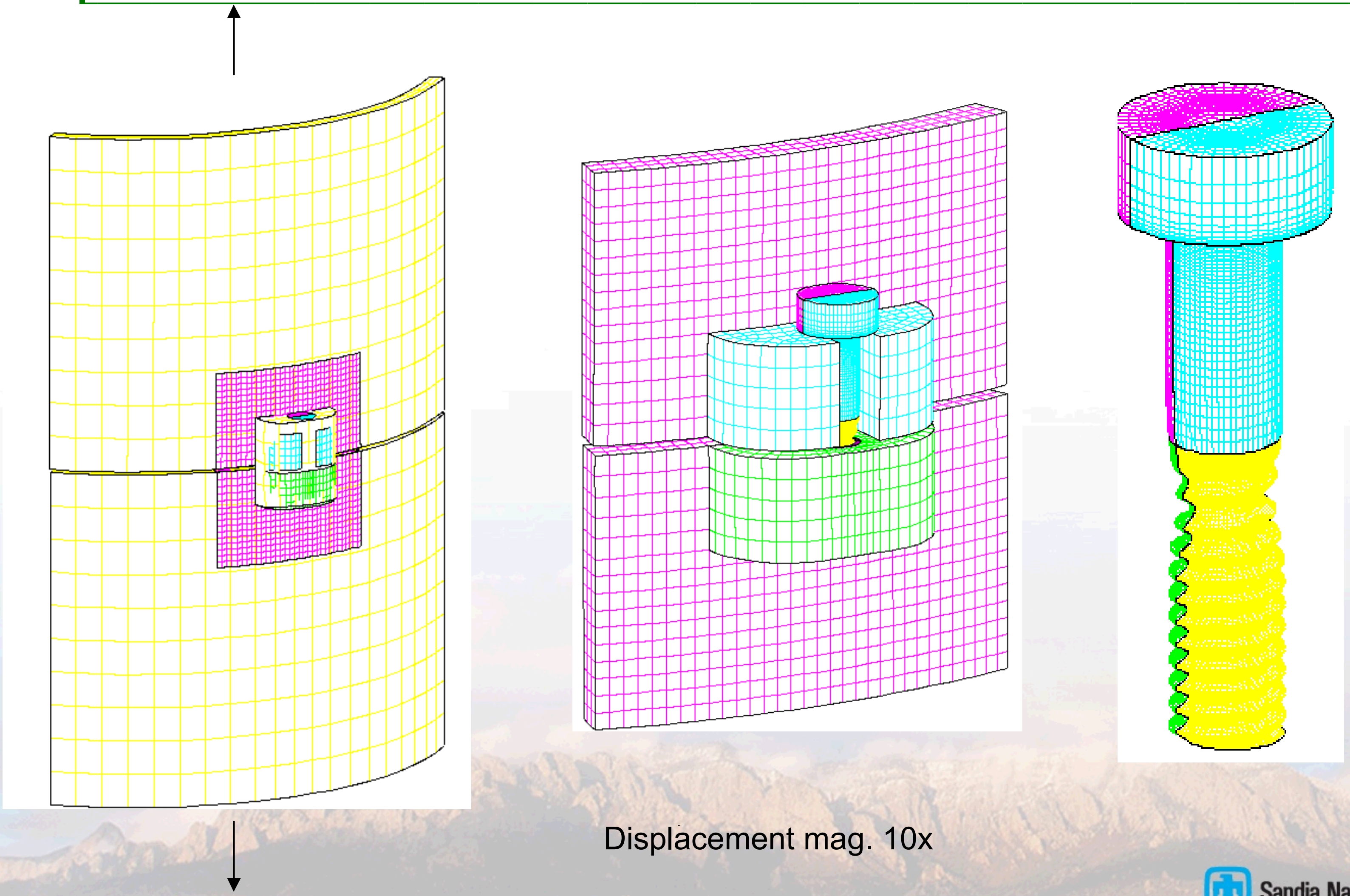


fine length scale
(*models a bolted joint*)



Multiscale Modeling Example

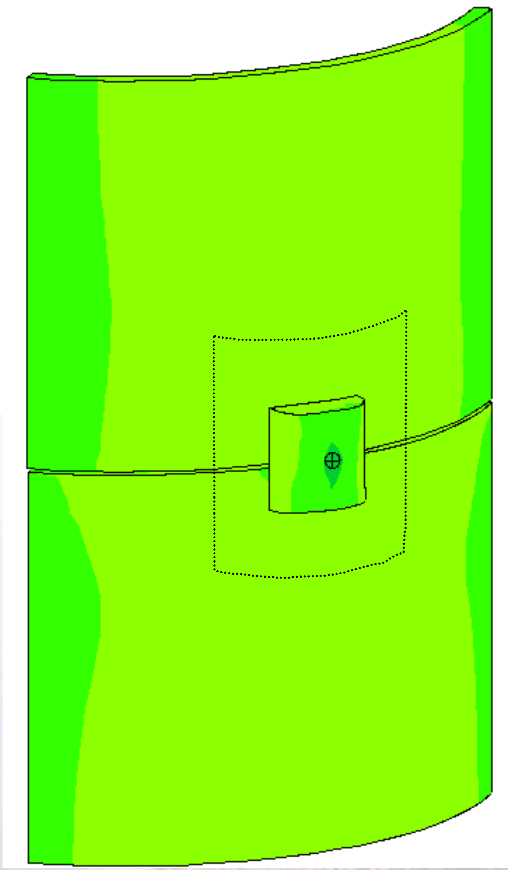
EXAMPLE : Axial tension of a Bolted Cylinder

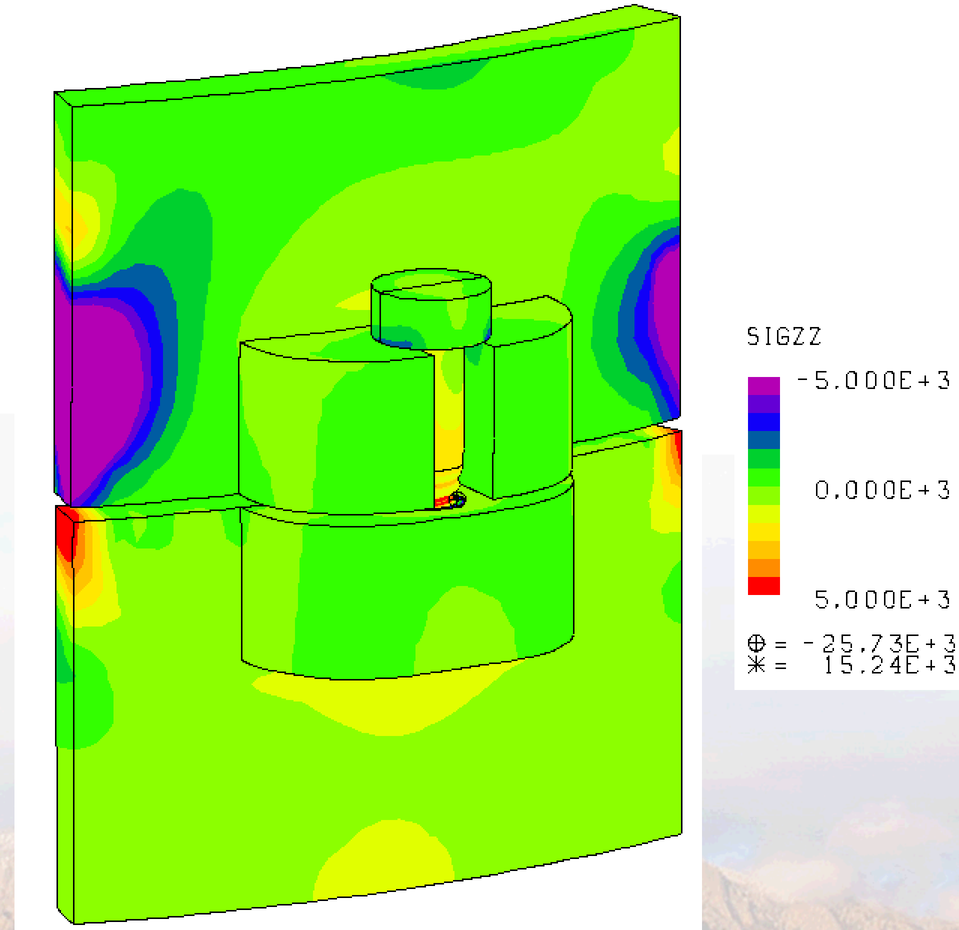


Displacement mag. 10x

Multiscale Modeling Example

EXAMPLE : Axial tension of a Bolted Cylinder

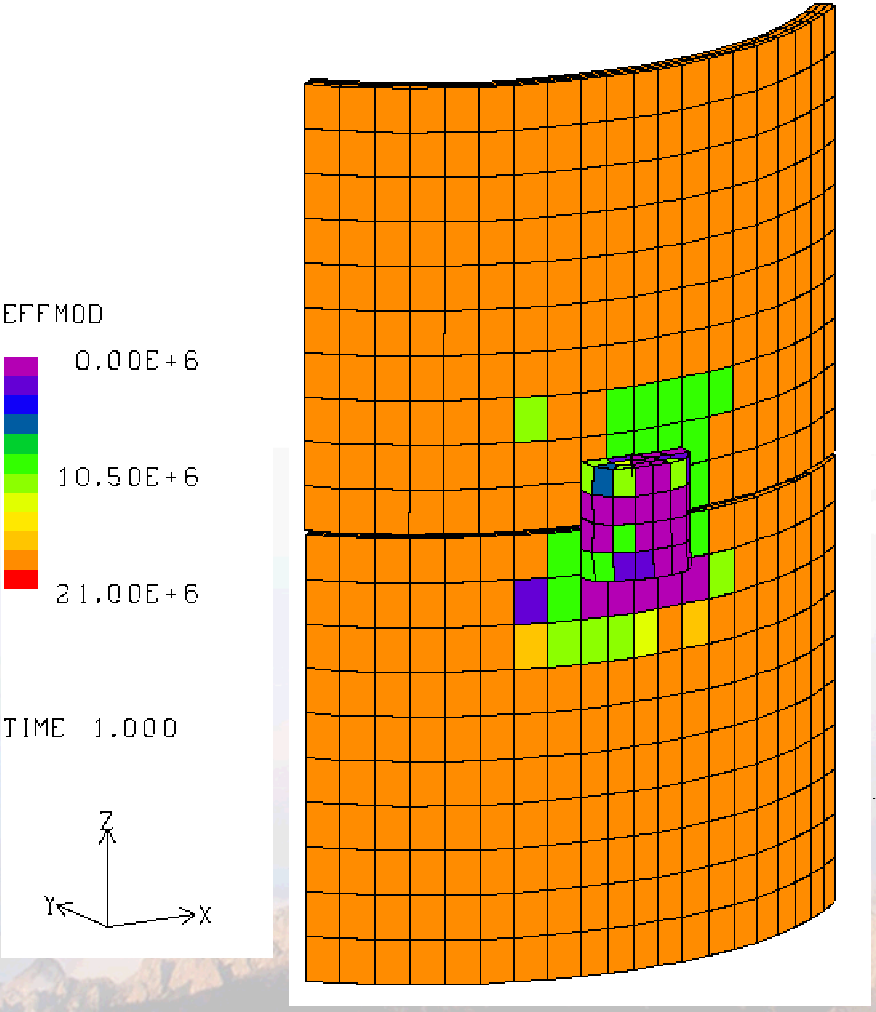


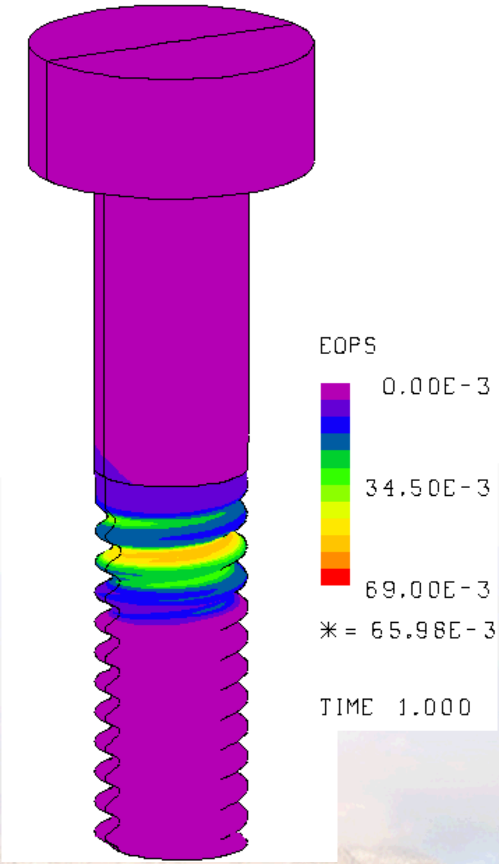


Displacement mag. 10x

Multiscale Modeling Example

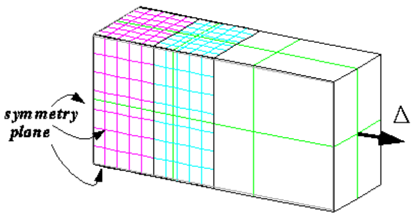
EXAMPLE : Axial tension of a Bolted Cylinder

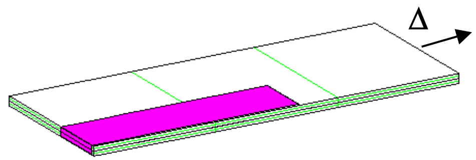


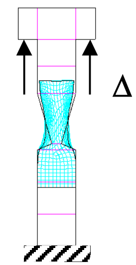


Multiscale modeling: Summary of Accomplishments to-date

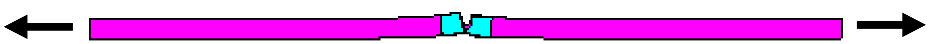
The current capability is implemented for Quasistatic problems and has been demonstrated on "proof-of-concept" examples



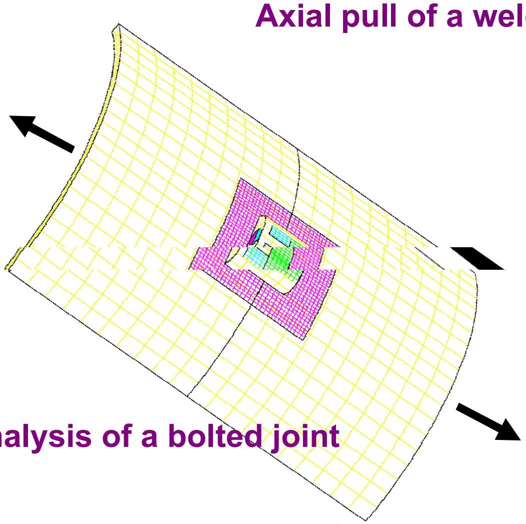


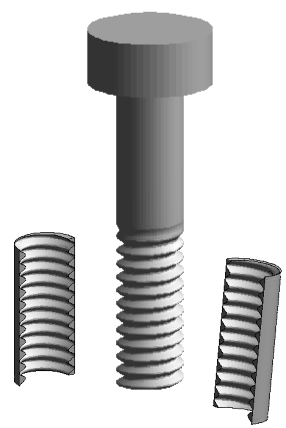


And some realistic Quasistatic applications, i.e.:

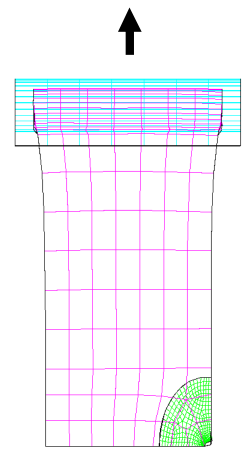


Axial pull of a welded joint





Analysis of a bolted joint



Coesfeld test

Multiscale modeling: To-Do List

We need to be able to say a lot more about

- Accuracy
- Convergence rates

Homogenization of non-isotropic response (contact, failure)

Hex *fls* embedded in Shell *rls* needs more demonstration

Combined explicit / implicit solver is functioning (but not yest w/ contact)