Workshop on Verification and Validation in Solid Mechanics and Life Prediction Software

On the role of hierarchic spaces and models in verification & validation

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Outline

- Simulation & Simulation Governance
  - What is simulation
  - What is simulation governance
    - The process of numerical simulation
- Aspects of implementation
  - The finite element method
  - Computation of fracture mechanics parameters
    - Computation of SIFs by the contour integral method
    - Computation of ERRs by the separated J-integral
- Concluding remarks

Simulation & **Simulation Governance**

- What is simulation?
  - Simulation is a transformation of data **D** to the results of interest **R**.

$$\boxed{\mathbf{D} \rightarrow \mathbf{R}}$$

- What is simulation governance (SimGov)?
  - Simulation governance is the exercise of **command and control** over all aspects of **D** → **R**.
    - The procedures that must be established for the purposes of ensuring and enhancing the reliability of predictions based on numerical simulation.

Simulation & **Simulation Governance**

D → R

- How does SimGov exercise command & control?
  - Establishes and enforces rules by which **D** is collected, verified, recorded and archived.
  - Ensures that the transformation **D → R** is based on established principles and procedures of computational science.
  - Ensures that the analysts are properly qualified.
  - Establishes protocols for the incorporation of new information to continuously improve the simulation process.
  - Utilizes standard analysis processes whenever possible.

Simulation & **Simulation Governance**

- Why is SimGov important?
  - Properly exercised, SimGov will provide
    - Reduction of reliance on physical testing
    - Improved reliability of predictive performance of simulation tools
    - Improved design and decision-making
  - Properly exercised, SimGov will provide substantial economic benefits
    - Prevent expensive retrofits
    - Improve product life cycle management

Simulation & Simulation Governance

D → R

- <u>Key technical requirements of Sim Gov</u>: VVUQ
  - **Verification:** Control of the errors of approximation.
    - This includes Code Verification, Solution Verification and Verification of Input Data.
  - **Validation:** Quantitative assessment of the predictive accuracy of a model.
    - Objective means for assessing the predictive accuracy of mathematical models by comparison of simulation results with experimental data.
  - **Uncertainty Quantification:** Evaluation of the effects that uncertainties in **D** have on the results of interest **R**.
    - Random (aleatoric) & Cognitive (epistemic) uncertainties.

Numerical simulation
Validation

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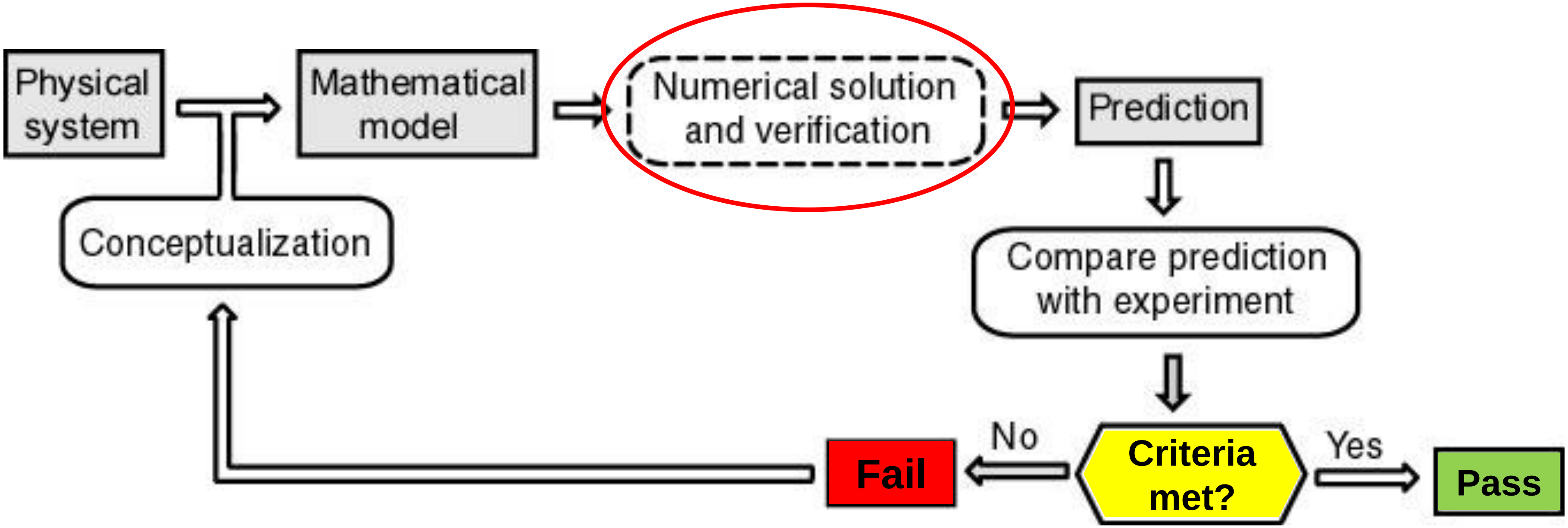
- Numerical simulation involves the formulation of a mathematical model and its numerical solution.

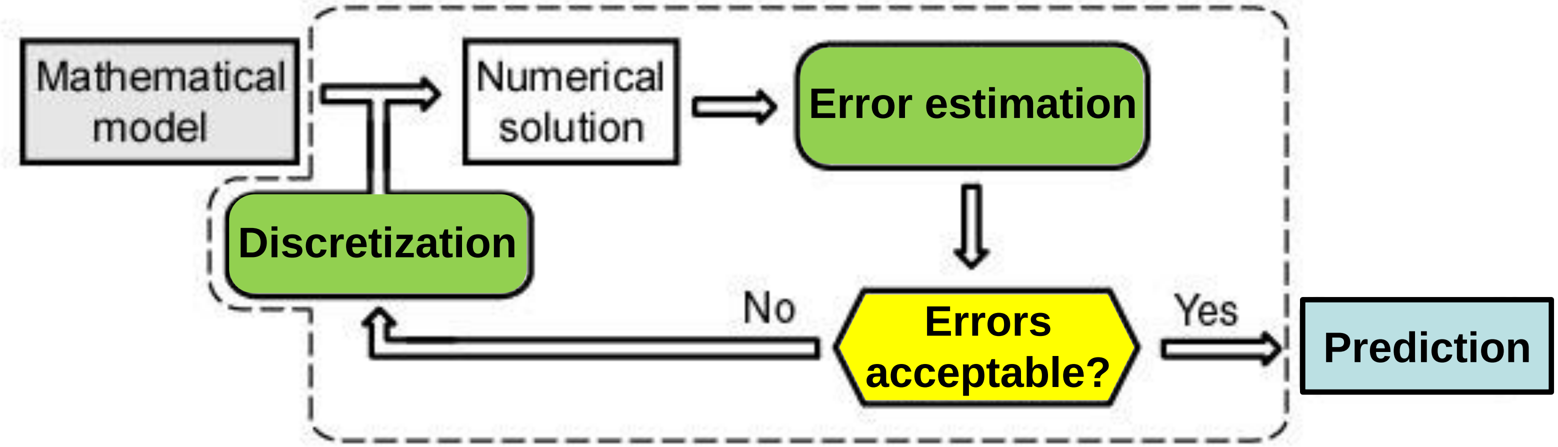


- A Validation assessment is well defined only in terms of the <u>results of interest</u> **R** and the accuracy needed for the use of the model.

Numerical simulation **Verification**

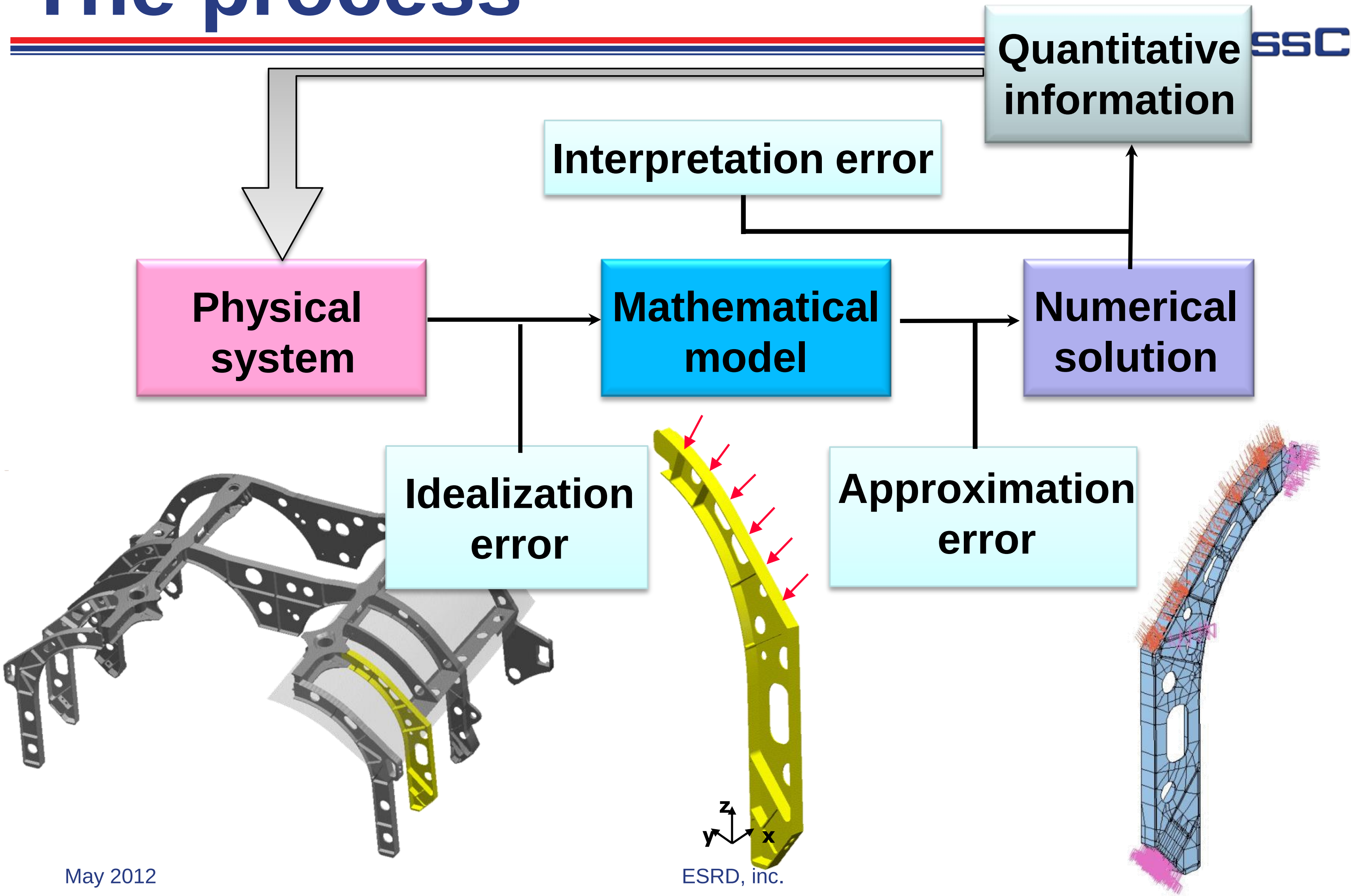
D → R

- Solution Verification is a process by which it is ascertained that the <u>results of interest</u> **R** satisfy necessary conditions for acceptance.



- In practice this means to verify that the results of interest are not sensitive to the mesh or the polynomial degree of elements.
- **Verification is a prerequisite to validation.**

Numerical simulation
The process



Quantitative information

Interpretation error

Physical system

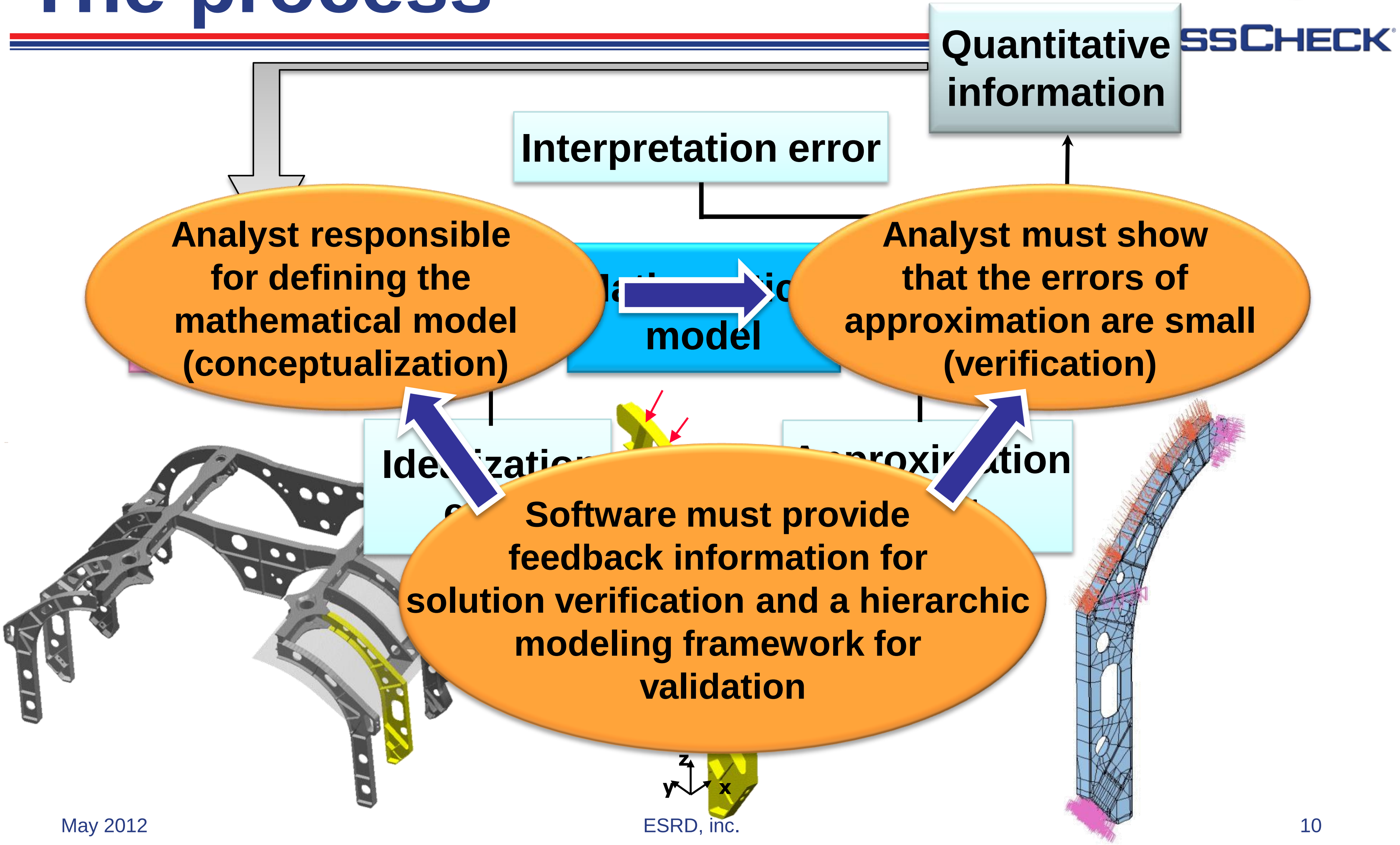
Mathematical model

Numerical solution

Idealization error

Approximation error

Numerical simulation
The process



Quantitative information

Interpretation error

model

Analyst responsible for defining the mathematical model (conceptualization)

Analyst must show that the errors of approximation are small (verification)

Software must provide feedback information for solution verification and a hierarchic modeling framework for validation

Aspects of implementation
Technical requirements

- What is available and what is needed?

Numerical Simulation	Traditional FEA	SimGov-Ready FEA
Focus	Element-Centric	Model-Centric
Implementation	**FE Model** Mixes model definition with the approximation	**FE Method** Model definition separate from the approximation
Quality Assessment	Subjective	Objective
FEA Results	Analyst-dependent	Analyst-independent
Standardization	Not supported	Supported

Aspects of implementation
The finite element method

Fundamental theorem in FEA (displacement formulation):

$$\|u_{EX} - u_{FE}\|_{E(\Omega)} = \min_{u \in S} \|u_{EX} - u\|_{E(\Omega)}$$

where $S = S(\Omega, \Delta, p, Q) \subset E(\Omega)$.

h-version: $h_{max} \to 0$, p-version: $p_{min} \to \infty$.

Convergence guaranteed by increasing the size of S

- In practice h_{max} cannot be close to zero and p_{min} cannot be close to infinity.
  - Therefore it is necessary to design reasonable meshes and assign reasonable values for p.
- <u>The distinction between *h*- and *p*-versions is related to implementation rather than to the conceptual basis of FEA</u>.

Aspects of implementation
The finite element method

- Mixing the “What?” (model definition) with the “How?” (approximation)
  - Definition of strain {ε} adopted by traditional FEA implementations

$$\boxed{\{\epsilon\} = [D]\{u\} = [D][N]\{a\} \equiv [B]\{a\}}$$

[*D*] = Differential operator → model definition

[*N*] = Element shape functions → Approximation

  - Stiffness matrix (element-level)

$$\boxed{[K_e] = \int_{\Omega_e} [B]^T [E][B]\, dV.}$$

[*B*] matrix → Mixes model definition with approximation

  - This led to the development of large element libraries (element-centric implementation).

Aspects of implementation
The finite element method

> “C3D20RHT: 20-node triquadratic displacement, trilinear temperature, hybrid, linear pressure, <u>reduced integration</u>.”

Aspects of implementation
The finite element method

- Reduced integration: What's the problem?
  - Reduced integration was introduced because low-order elements were found to be "too stiff" and locking occurred.
  - It was found that when the number of quadrature points is reduced, then the elements become more "compliant".
    - Unrealistic expectation: The error of approximation caused by low p-values is always canceled by the error in integration.
    - Reduced integration elements are prone to instability ("hour-glassing")
    - Users cannot control the errors caused by hour-glassing.
- This type of elements makes solution verification very difficult.
  - Solution may not converge when $h_{\max} \to 0$.

Aspects of implementation
The finite element method

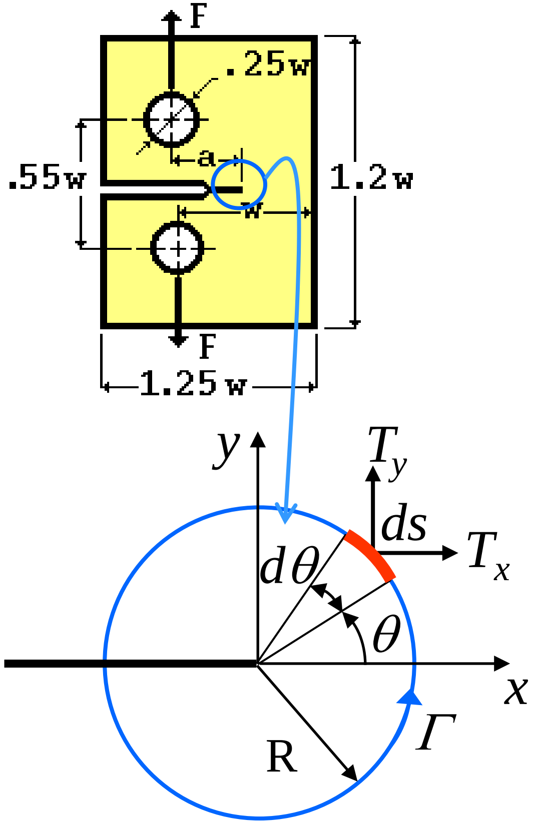
- The software infrastructure required to support V&V must provide for
  - Hierarchic FE Spaces to control errors of approximation.
  - Hierarchic Modeling to assess errors of idealization.
- Extraction procedures must be based on algorithms that exist independently from the mesh.
  - The data of interest (such as stress intensity factors, energy release rates, etc.) must converge to their exact values as the number of degrees of freedom is increased.

Aspects of implementation
Computation of SIFs

- Reliable prediction of crack growth and residual strength in metallic structures require accurate computation of SIFs.
  - Since analytical solutions for complex configurations are not available, estimates of SIFs have to be obtained by numerical methods.
- There are many procedures for extracting SIFs from finite element solutions.
  - However, most implementations in commercial FEA software tools do not provide feedback information to assess the error of approximation.
- The <u>Contour Integral Method</u> (CIM) provides for accurate extraction of SIFs for any crack configuration
  - Combined with hierarchic FE spaces provides convergence information in support of <u>solution verification</u>.

Computation of SIFs
The contour integral method

- The Stress Intensity Factor K_1 is computed using a path-independent Integral(*):



$$K_1 = \sqrt{2\pi}\oint_\Gamma \left(\vec{W}_1 \vec{T}_{EX} - \vec{u}_{EX}\vec{T}^{W_1}\right) R\,d\theta$$

$\vec{u}_{EX}$ is the displacement vector and $\vec{T}_{EX}$ is the traction vector from the exact solution of the actual crack configuration and loading.

$$\vec{W}_1 = \frac{1}{2G} R^{-1/2}\vec{\phi}_1, \qquad \vec{T}^{W_1} = -G R^{-3/2}\vec{\psi}_1$$

$\vec{W}_1$ and $\vec{T}^{W_1}$ are known extraction functions obtained from the asymptotic expansion in the vicinity of the crack tip.

* Szabó, B. A. and Babuska, I. *Finite Element Analysis,* John Wiley and Sons, Inc. New York, 1991.

Computation of SIFs
The contour integral method

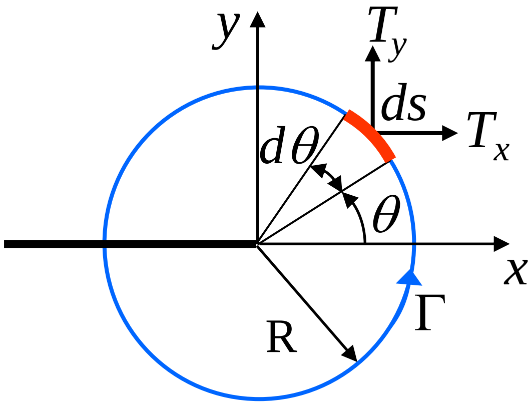
Exact value of SIF

$$K_{1EX} = \sqrt{2\pi}\oint_{\Gamma}\left(\vec{W}_1\vec{T}_{EX} - \vec{u}_{EX}\vec{T}^{W_1}\right)R\,d\theta$$

$\vec{u}_{EX}$ and $\vec{T}_{EX}$ are replaced by the finite element solution.

Approximate value of SIF

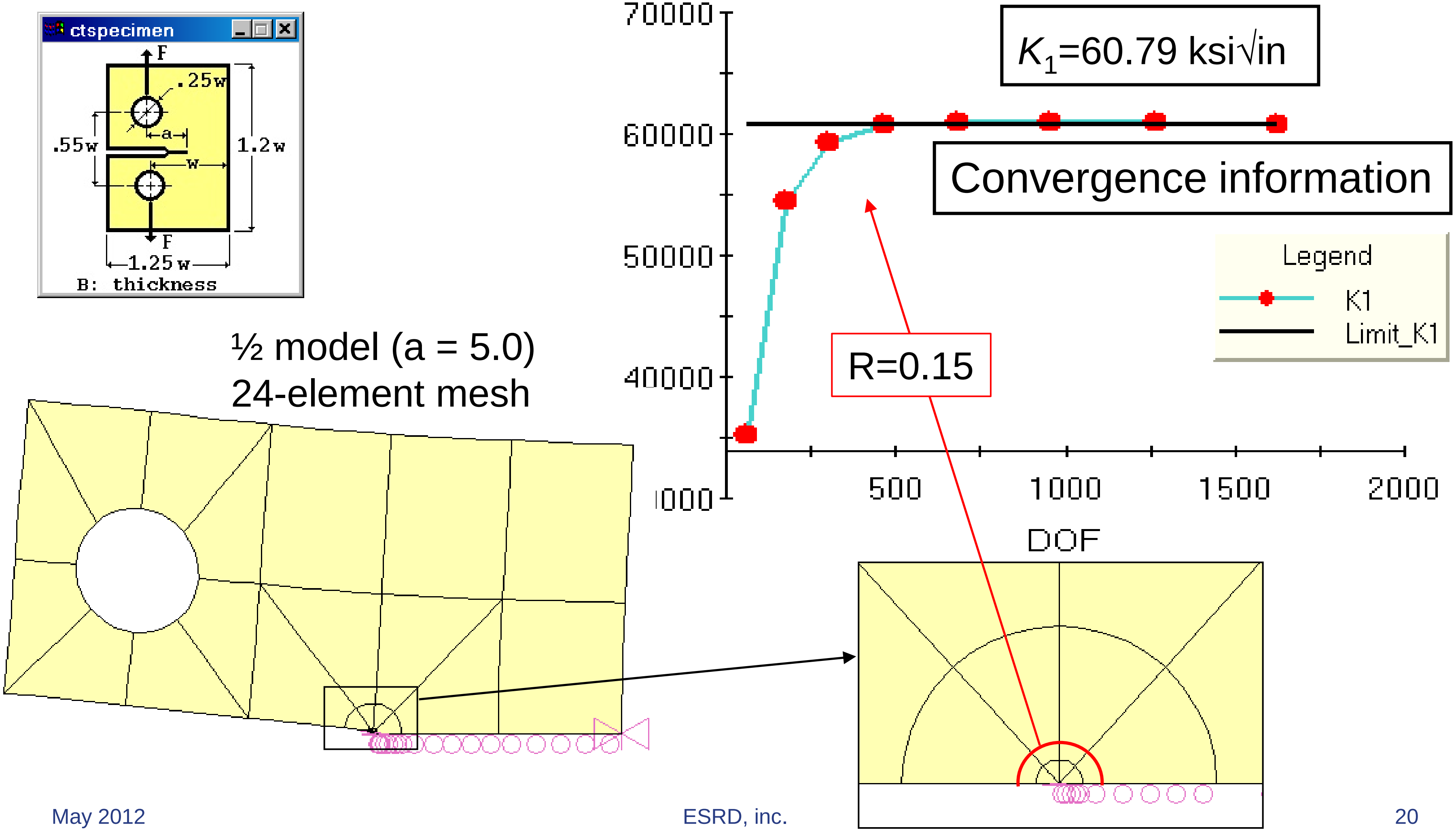
$$K_{1FE} \approx \sqrt{2\pi}\oint_{\Gamma}\left(\vec{W}_1\vec{T}_{FE} - \vec{u}_{FE}\vec{T}^{W_1}\right)R\,d\theta$$



K_1 converges to the exact value as the number of DOF increases (essential for solution verification).

As $\|u_{FE}\| \rightarrow \|u_{EX}\|$, $K_{1FE} \rightarrow K_{1EX}$

Example of Solution Verification
2D-SIFs for a CTS



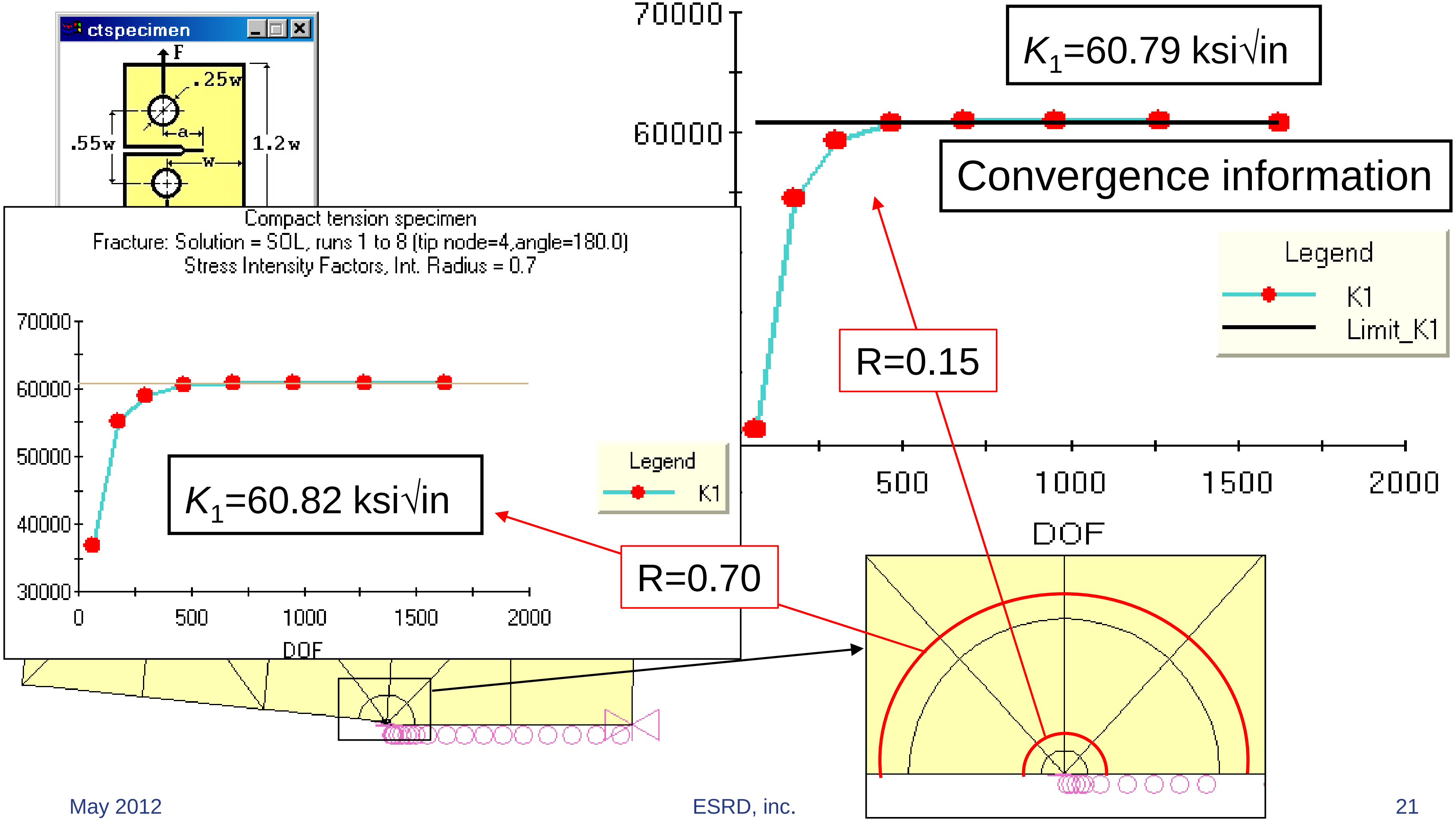
K_1=60.79 ksi√in

Convergence information

½ model (a = 5.0)
24-element mesh

R=0.15

Example of Solution Verification
2D-SIFs for a CTS



Compact tension specimen
Fracture: Solution = SOL, runs 1 to 8 (tip node=4,angle=180.0)
Stress Intensity Factors, Int. Radius = 0.7

K_1=60.79 ksi√in

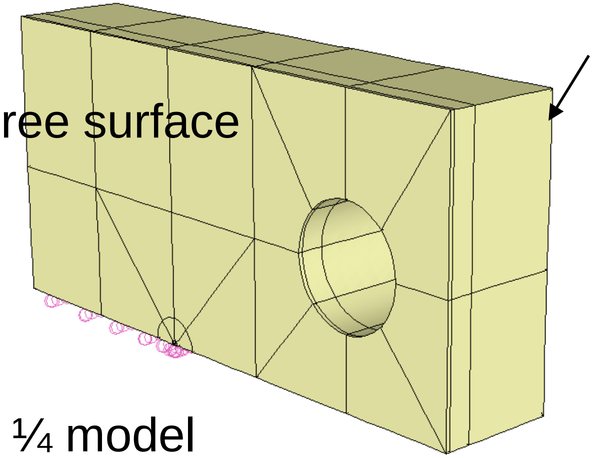
Convergence information

R=0.15

R=0.70

K_1=60.82 ksi√in

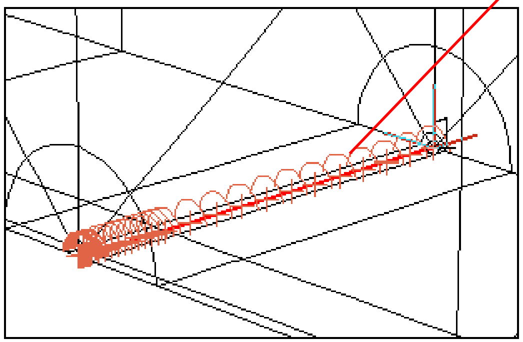
Example of Solution Verification
Thru-thickness crack



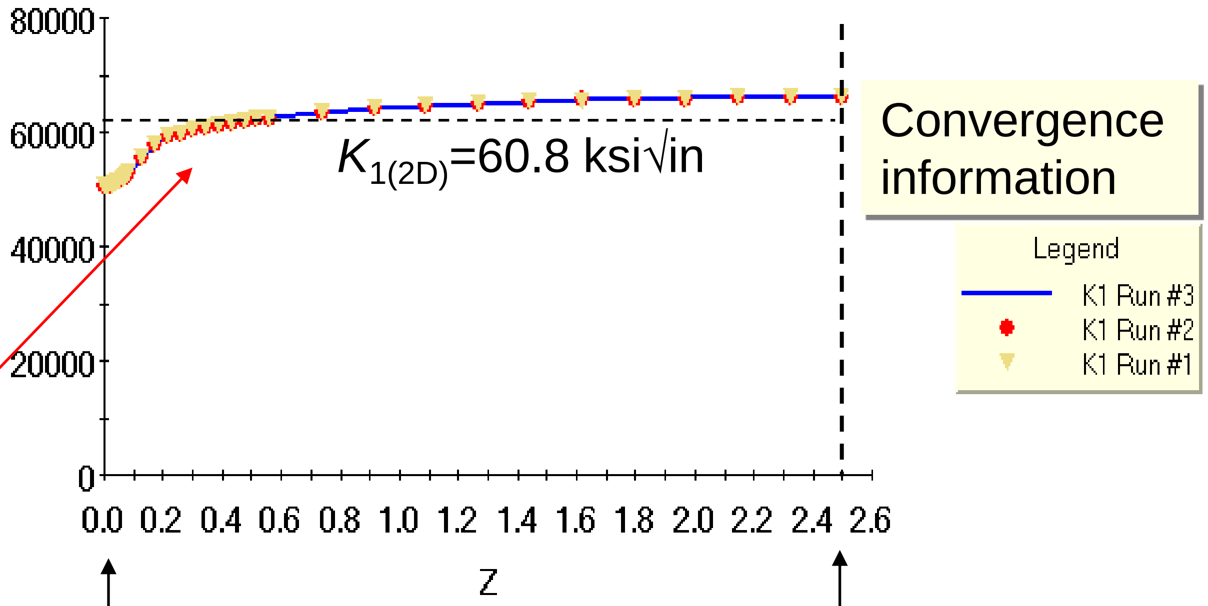
Free surface

Symmetry plane

¼ model
3 layers of elements
through the thickness



K1 along crack front



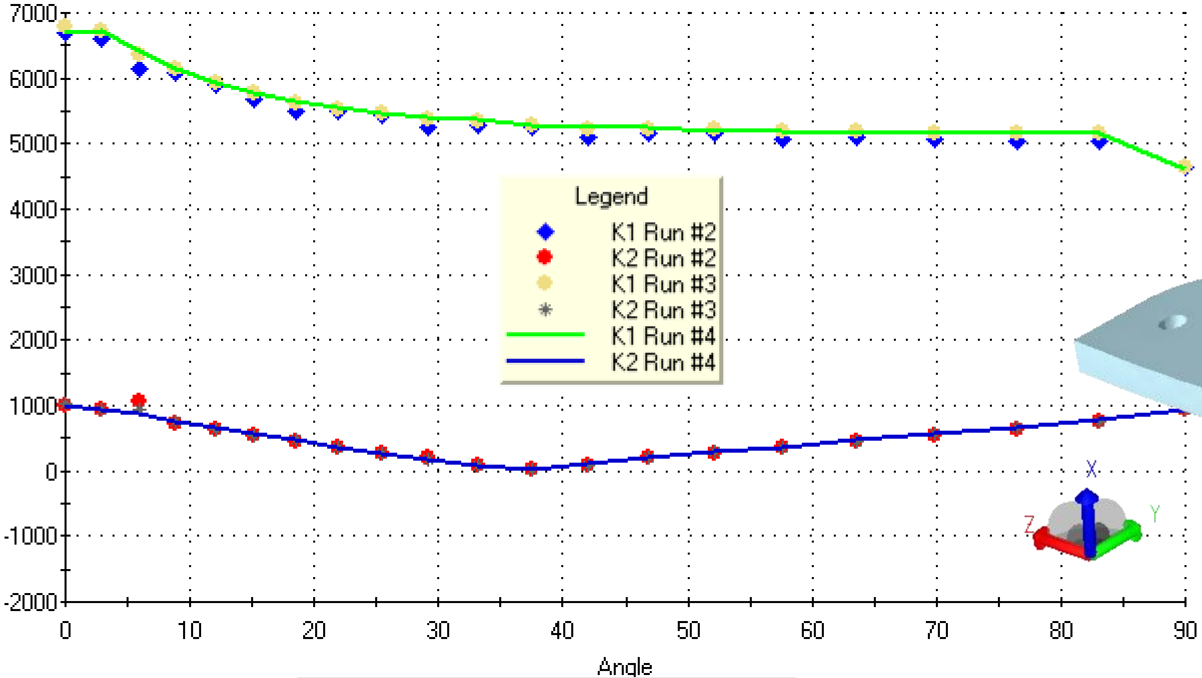
$K_{1(2D)}=60.8\ \text{ksi}\sqrt{\text{in}}$

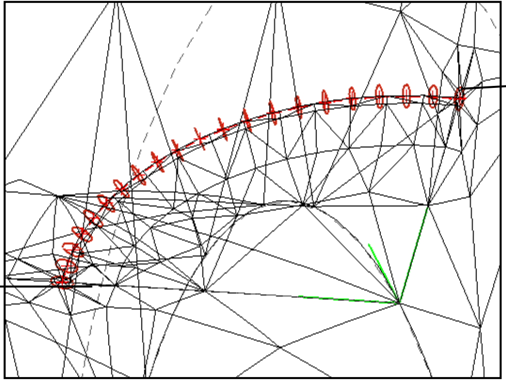
Convergence information

Free surface

Symmetry plane

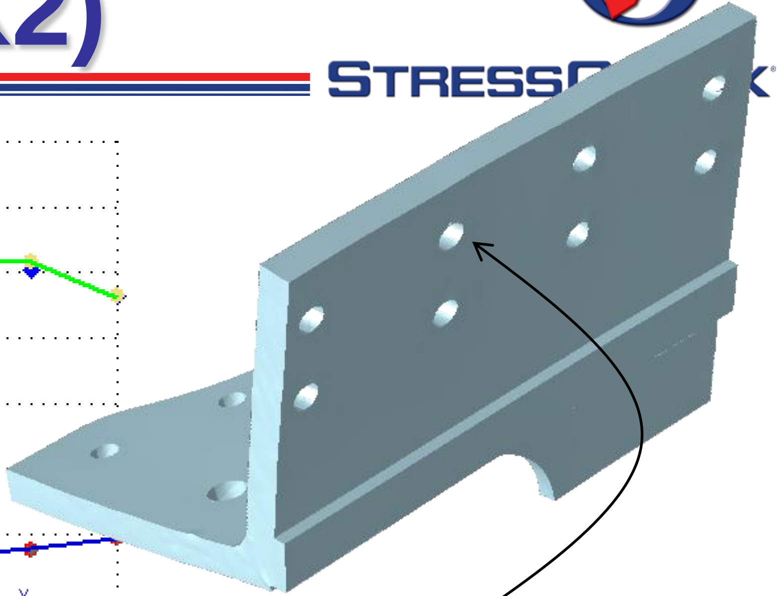
Example of Solution Verification
Corner crack (K1 & K2)

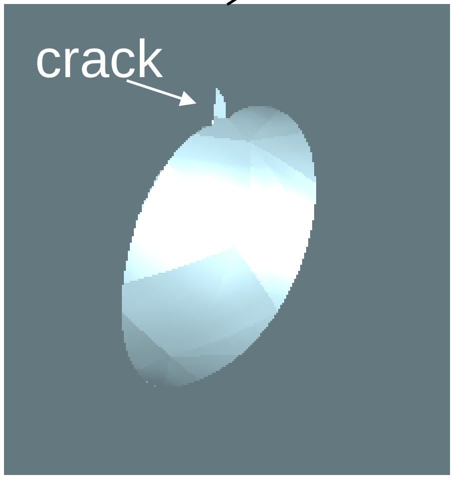




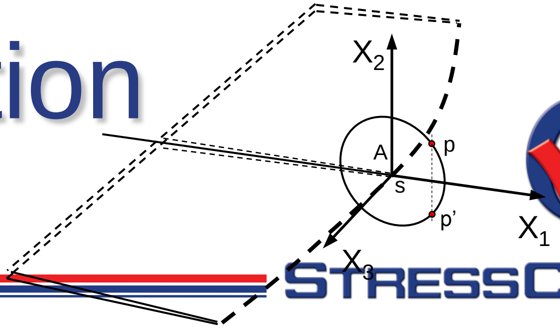
Angle = 90°

Angle = 0°





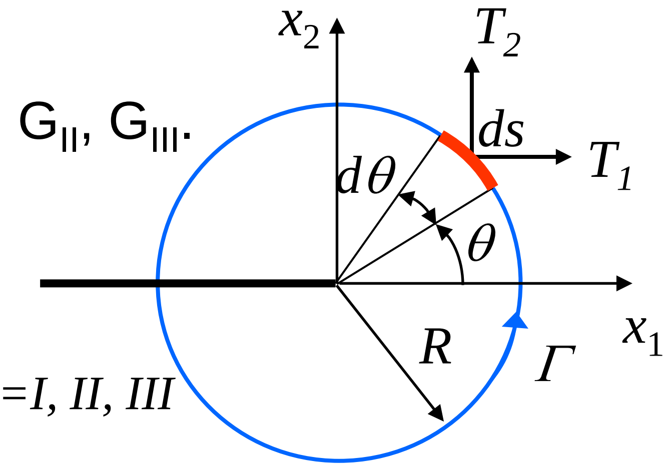
Aspects of implementation
Computation of ERRs



- The mode I (G_I), mode II (G_{II}) and mode III (G_{III}) components of the strain ERR must be determined to formulate and validate mixed-mode failure criteria for the determination of onset of instability of interlaminar flaws.
- The components of the energy release rate can be obtained using the separated J-integral:
  - Separated J-integrals$^{(*)}$ J_I, J_{II}, J_{III}
  - For linear elasticity are the same as G_I, G_{II}, G_{III}.

$$\boxed{J_M^{\Gamma} = \int_{-\pi}^{\pi} \left[\left(\int_0^{\varepsilon_{ij}} \sigma_{ij}^M \, d\varepsilon_{ij}^M \right) \cos\theta - t_i^M \frac{\partial u_i^M}{\partial x_1} \right] R \, d\theta}$$

$M = I, II, III$



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* **Rigby, R. H. and M. H. Aliabadi, 1998. "Decomposition of the mixed-mode J integral-revisited". *International Journal of Solids and Structures*, 35(17): 2073-2099.**

Aspects of implementation
The separated J-integral

- The implementation of the J-integral decomposition combined with hierarchic finite element spaces obtained by p-extension on a fixed mesh provides the framework for solution verification.

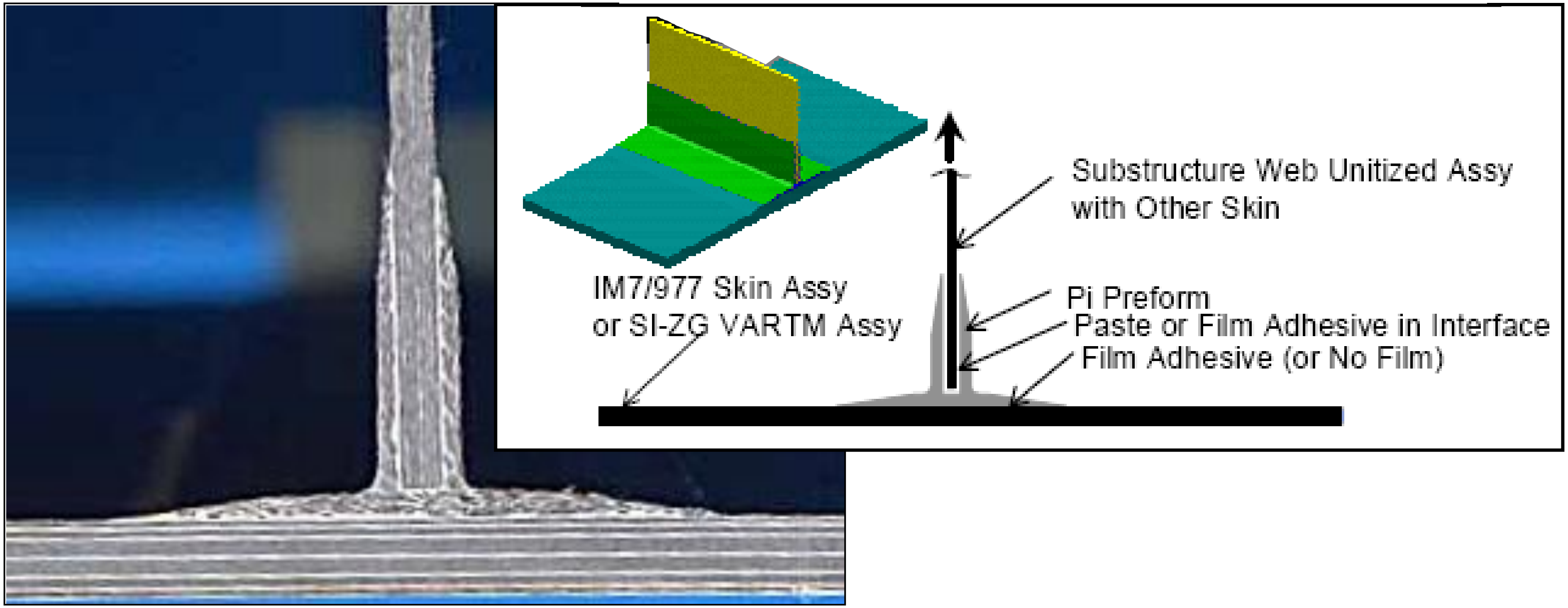
$$J_{EX} = J(\vec{u}_{EX}) \qquad J_{FE} = J(\vec{u}_{FE})$$

$$\boxed{\left\|\vec{u}_{FE}\right\| \to \left\|\vec{u}_{EX}\right\|, \quad J_{FE} \to J_{EX}}$$

- The implementation of the J-integral in a hierarchic modeling framework allows the assessment of modeling assumptions in the results.
- The next example demonstrates the use of hierarchic FE spaces and Hierarchic modeling in the assessment of delamination of a composite PI-joint.

Example
PI-joint delamination

- Computation of the ERR components along a delamination front of a Pi-joint specimen.

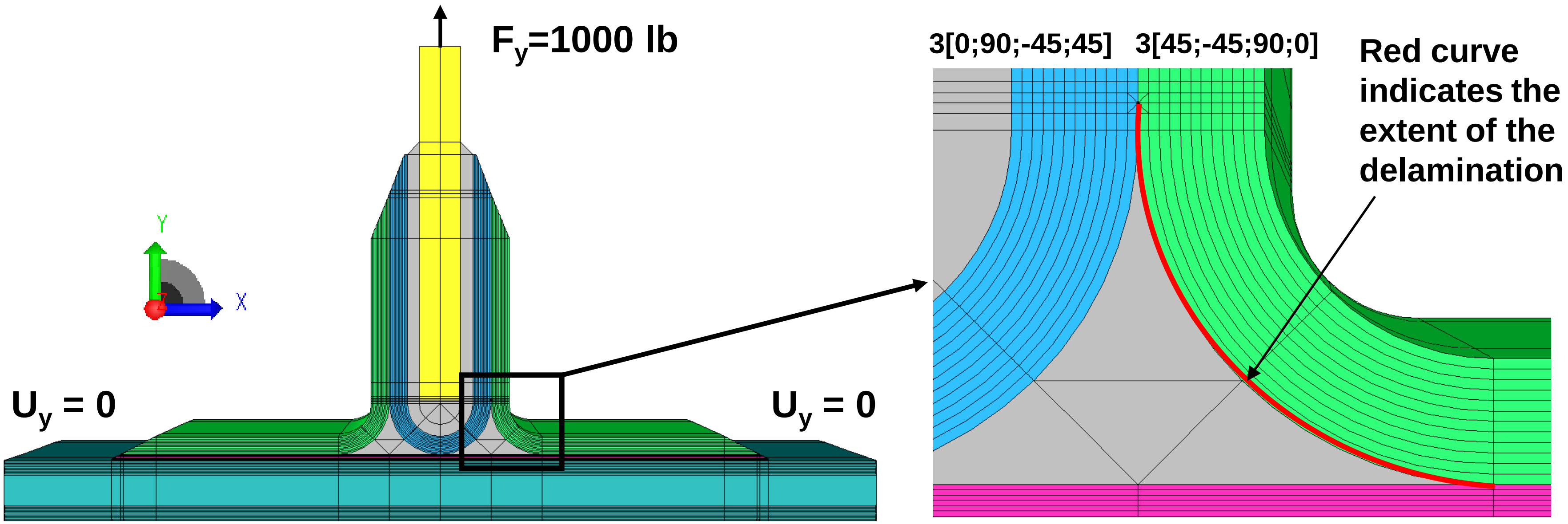


Pi-joint delamination
Problem description

- PI-joint specimen with an interlaminar thru-delamination between two 45 degree plies.
  - Loaded in three-point bending
  - Computation of G_I along delamination front

Problem Definition

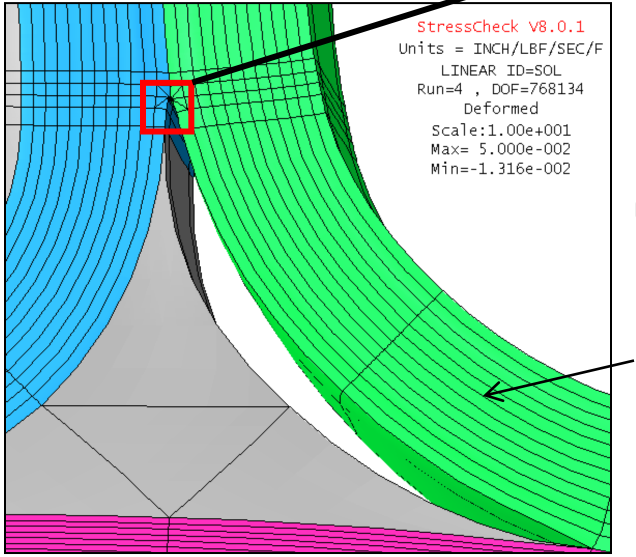
Local Ply Layup



Pi-joint delamination
ERR solution verification

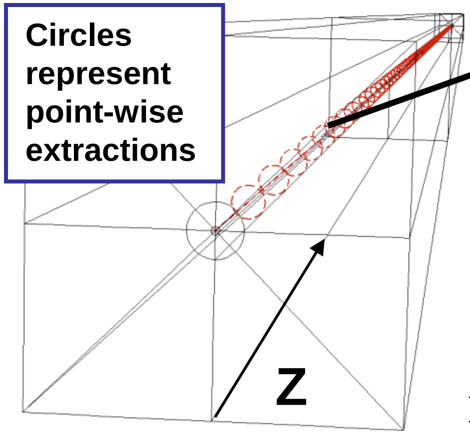
- Solution by p-extension (p=6 to 8) on a fixed mesh
  - Distribution of J1 along crack front (0<Z<1.0).
  - Convergence of J1 value at Z=0.5.

Deformed Shape of Delaminated Region (10:1)



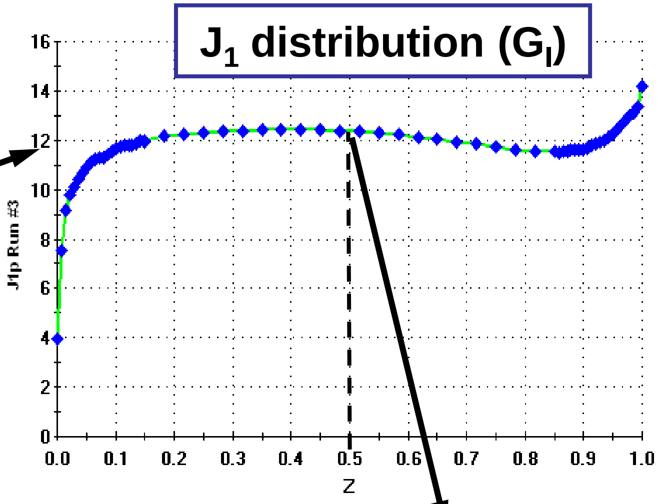
StressCheck V8.0.1
Units = INCH/LBF/SEC/F
LINEAR ID=SOL
Run=4 , DOF=768134
Deformed
Scale:1.00e+001
Max= 5.000e-002
Min=-1.316e-002

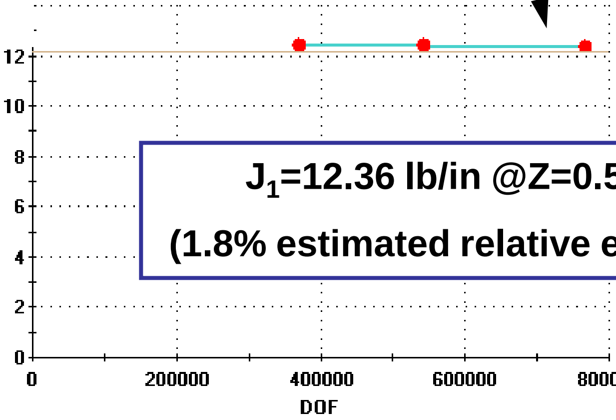
Circles represent point-wise extractions



Full ply-by-ply modeling

J_1 distribution (G_I)

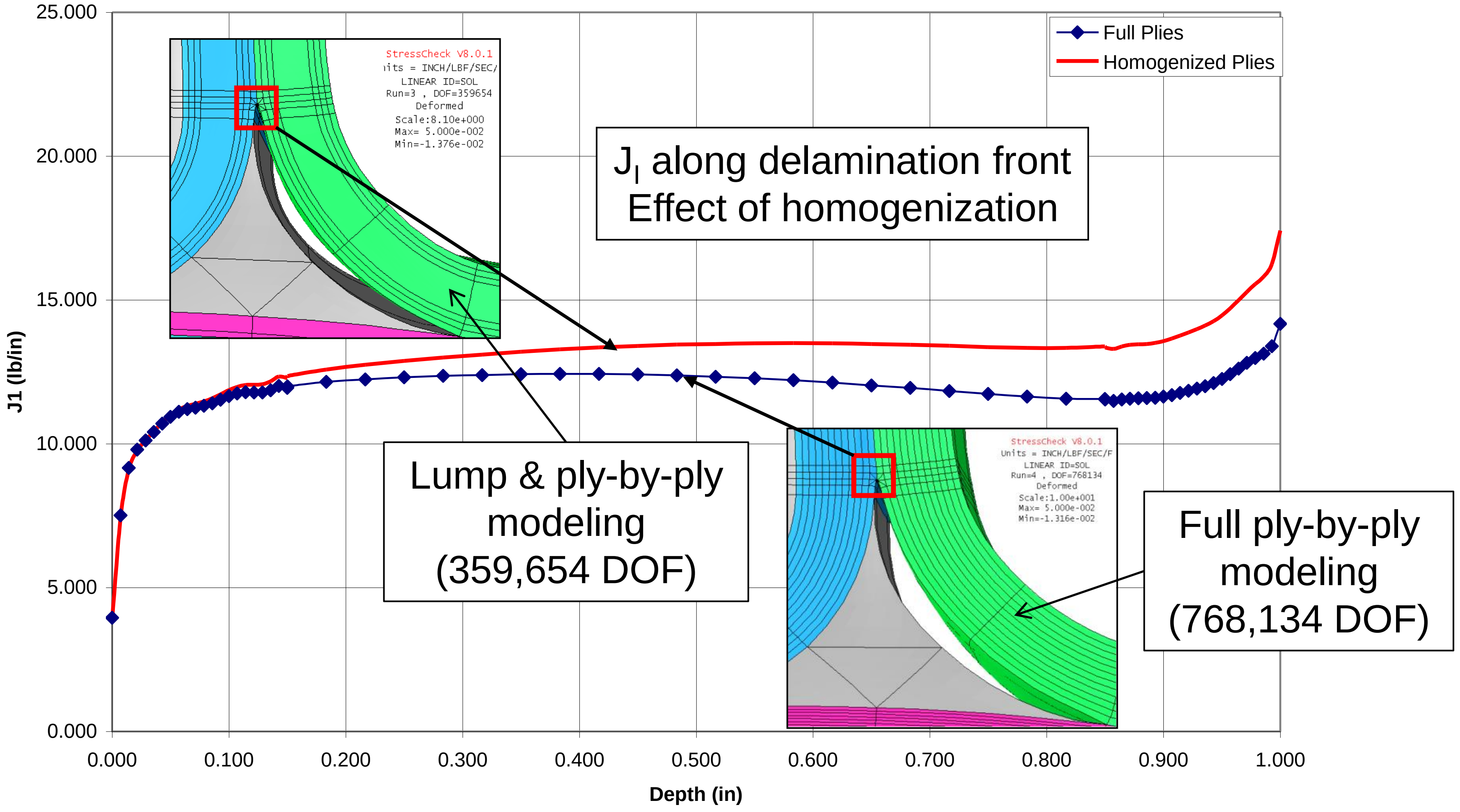




J_1=12.36 lb/in @Z=0.5

(1.8% estimated relative error)

Pi-joint delamination
Effects of modeling in ERR



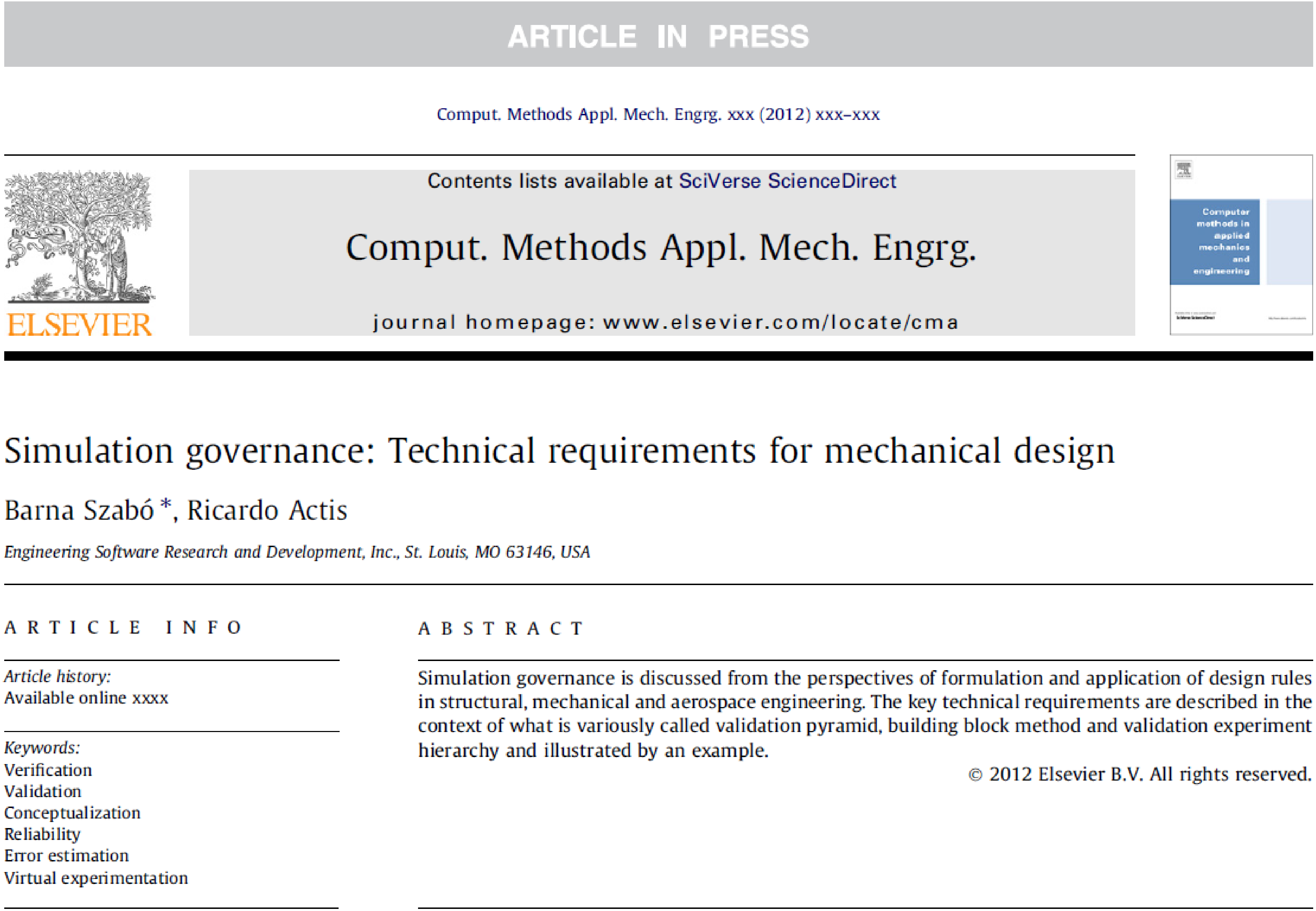
J_I along delamination front
Effect of homogenization

Lump & ply-by-ply
modeling
(359,654 DOF)

Full ply-by-ply
modeling
(768,134 DOF)

Concluding remarks

- There are strong economic incentives for decreasing reliance on physical experimentation and increasing reliance on computed information.
  - Simulation Governance provides a framework for systematic, consistent and progressive improvement of the predictive capabilities of mathematical models.
- Hierarchic spaces and models are essential for Verification and Validation
  - Verification refers to "Solving the equations right", which means the proper selection of the mesh, the mapping and p-level (discretization).
  - Validation refers to "Solving the right equations". Experiments should be used for assessing the predictive accuracy of mathematical models.
  - A hierarchic modeling framework in the software infrastructure provides for proper control of the errors of idealization and discretization.



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Simulation governance: Technical requirements for mechanical design

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A R T I C L E   I N F O

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Reliability
Error estimation
Virtual experimentation

A B S T R A C T

Simulation governance is discussed from the perspectives of formulation and application of design rules in structural, mechanical and aerospace engineering. The key technical requirements are described in the context of what is variously called validation pyramid, building block method and validation experiment hierarchy and illustrated by an example.

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