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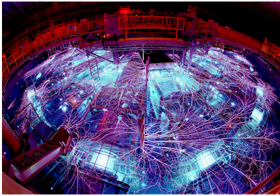

Round Robin: PROMs Using Hyper-Dual Numbers

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Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

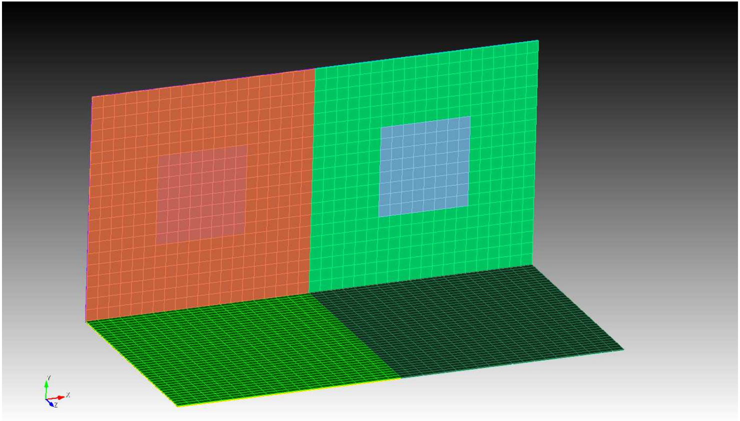
Test Case Summay

Comparison Between Codes

- Mesh Convergence Study
- Mode Shapes

PROM Comparison

Test Case Geometry



- Plates are nominally 0.4 mm thick
- Square patch in center of vertical plates increased by up to 6 mm

Parameterized Reduced-Order Models (PROMs)

Create parameterized models using a Taylor series expansion about the nominal design:

$$\tilde{f}(x + \Delta x) = f(x) + (\Delta x) f'(x) + \frac{(\Delta x)^2}{2} f''(x) + \frac{(\Delta x)^3}{6} f'''(x) + \ldots .$$

Quantity of interest $f(x)$:

- Mass and stiffness matrices from Finite-Element Analysis (FEA)
- Outputs of FEA, such as displacements or natural frequencies

Perturbations Δx: variations in geometry or material properties

Terminology:

- Parameterized Full-Order Model if applied to FEA quantities
- Parameterized Reduced-Order Model (PROM) if applied to a Reduced-Order Model (ROM)
  - Craig-Bampton (C-B) Component Mode Synthesis (CMS) approach [Craig and Bampton 1968]

Derivative Calculations Using Hyper-Dual Numbers

The derivative calculations are performed using Hyper-Dual Numbers [Fike and Alonso 2011]:

- Derivative calculations are exact to machine precision
- Perturbations applied to non-real part of the number
  - Real part contains nominal design and is unperturbed
  - Requires only one mesh for the nominal design, and information on how mesh would change with geometric variations
  - Derivatives produced using information at a single point, may only be valid for small perturbations from nominal
- Modified version of Salinas produces up to exact third derivatives with respect to input parameters

Hyper-Dual Numbers

Complex Numbers:

$$a + bi$$

$$i^2 = -1$$

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Dual Numbers: [Study 1903]

$$a + b\epsilon$$

$$\epsilon^2 = 0,\ \epsilon \neq 0$$

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Dual Numbers: [Study 1903]

$$a + b\epsilon$$

$$\epsilon^2 = 0, \ \epsilon \neq 0$$

Quaternions: [Hamilton 1843]

$$a + bi + cj + dk$$

$$i^2 = j^2 = k^2 = -1$$

$$ij = -ji = k$$

Hyper-Dual Numbers

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Complex Numbers:

$$a + bi$$

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Quaternions: [Hamilton 1843]

$$a + bi + cj + dk$$

$$i^2 = j^2 = k^2 = -1$$

$$ij = -ji = k$$

Hyper-Dual Numbers: [Fike and Alonso 2011]

$$a + b\epsilon_1 + c\epsilon_2 + d\epsilon_1\epsilon_2$$

$$\epsilon_1^2 = \epsilon_2^2 = (\epsilon_1\epsilon_2)^2 = 0$$

$$\epsilon_1 \neq \epsilon_2 \neq \epsilon_1\epsilon_2 \neq 0$$

$$\epsilon_1\epsilon_2 = \epsilon_2\epsilon_1$$

Derivative Calculations using Complex Numbers

Taylor series for a real valued function subject to a perturbation in the imaginary direction:

$$f(x+hi) = f(x) + hf'(x)i - \frac{1}{2!}h^2 f''(x) - \frac{h^3 f'''(x)}{3!}i + \ldots$$

Derivative Calculations using Complex Numbers

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$$f(x+hi) = \underbrace{\left(f(x) - \frac{1}{2!}h^2 f''(x) + \ldots\right)}_{\text{real}} + \underbrace{h\left(f'(x) - \frac{1}{3!}h^2 f'''(x) + \ldots\right)i}_{\text{imaginary}}$$

Derivative Calculations using Complex Numbers

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First-Derivative Complex-Step Approximation: [Martins, Kroo, and Alonso 2000 and Martins, Sturdza, and Alonso 2003]

$$f'(x) = \frac{\text{Im}\left[f(x+hi)\right]}{h} + \mathcal{O}(h^2)$$

Derivative Calculations using Hyper-Dual Numbers

Taylor series with a dual number perturbation:

$$f(x+h\epsilon) = \underbrace{f(x)}_{\text{real}} + \underbrace{hf'(x)\epsilon}_{\text{non-real}}$$

Derivative Calculations using Hyper-Dual Numbers

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Taylor series with a dual number perturbation:

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Taylor series with a hyper-dual perturbation:

$$f(x+h_1\epsilon_1+h_2\epsilon_2+0\epsilon_1\epsilon_2) = f(x)+h_1f'(x)\epsilon_1+h_2f'(x)\epsilon_2+h_1h_2f''(x)\epsilon_1\epsilon_2$$

Derivative Calculations using Hyper-Dual Numbers

Taylor series with a dual number perturbation:

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Taylor series when including an ϵ_3 perturbation:

$$\begin{aligned} f(x + h_1\epsilon_1 + h_2\epsilon_2 + h_3\epsilon_3 + 0\epsilon_1\epsilon_2 + 0\epsilon_1\epsilon_3 + 0\epsilon_2\epsilon_3 + 0\epsilon_1\epsilon_2\epsilon_3) \\ = f(x) + h_1f'(x)\epsilon_1 + h_2f'(x)\epsilon_2 + h_3f'(x)\epsilon_3 + h_1h_2f''(x)\epsilon_1\epsilon_2 \\ + h_1h_3f''(x)\epsilon_1\epsilon_3 + h_2h_3f''(x)\epsilon_2\epsilon_3 + h_1h_2h_3f'''(x)\epsilon_1\epsilon_2\epsilon_3 \end{aligned}$$

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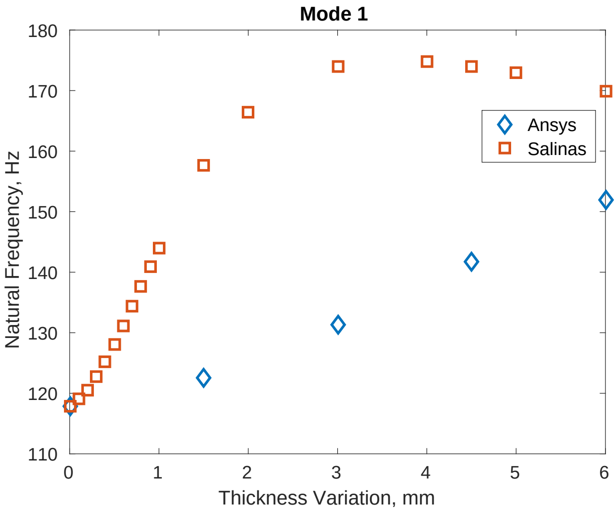
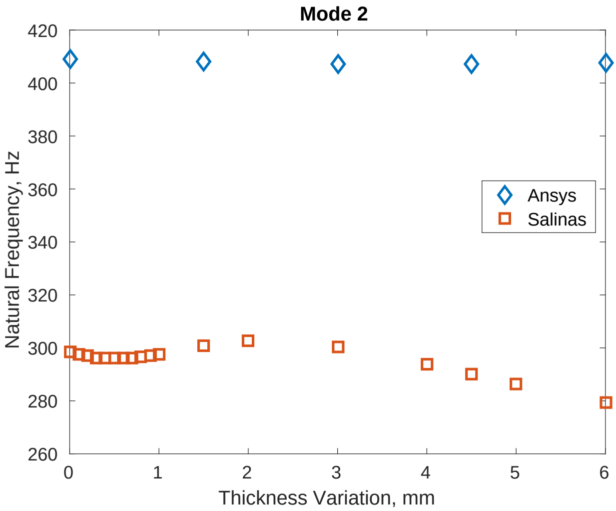
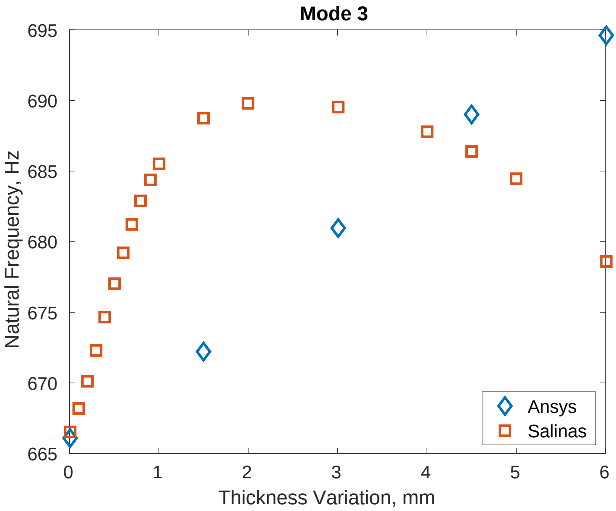
Natural Frequency as Thickness is Varied, Mode 1



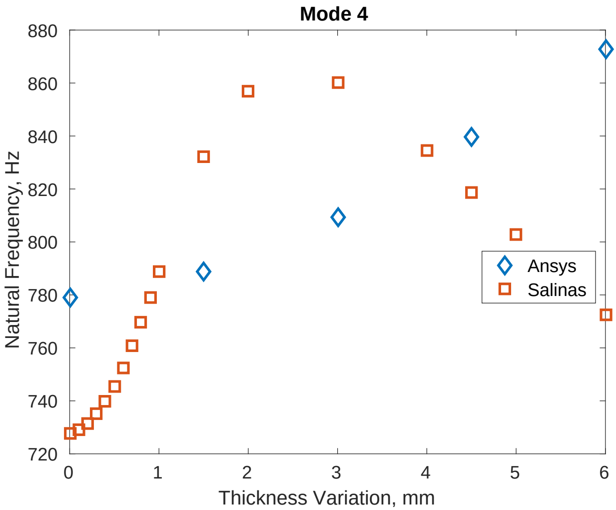
Natural Frequency as Thickness is Varied, Mode 2



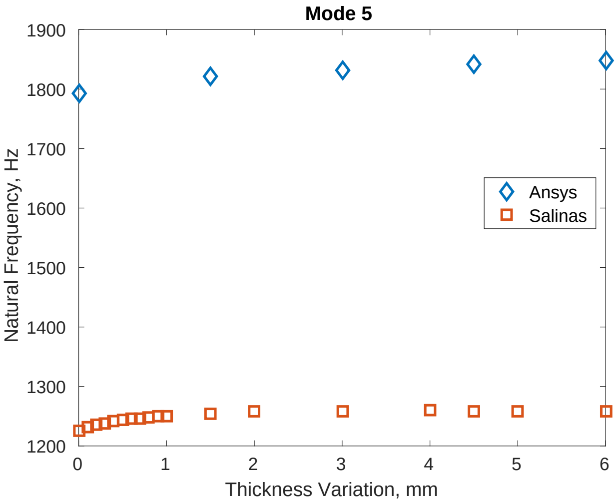
Natural Frequency as Thickness is Varied, Mode 3



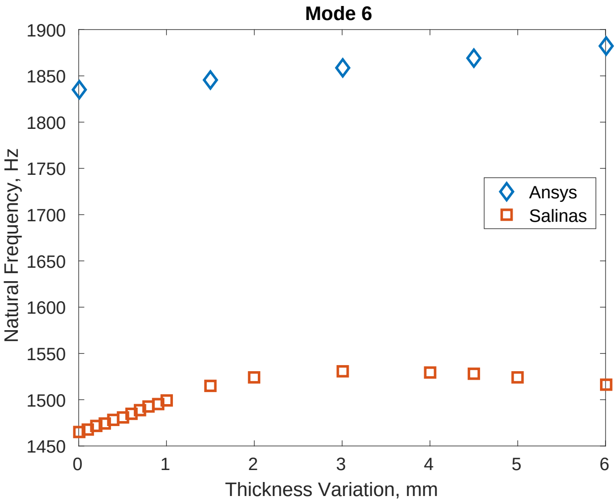
Natural Frequency as Thickness is Varied, Mode 4



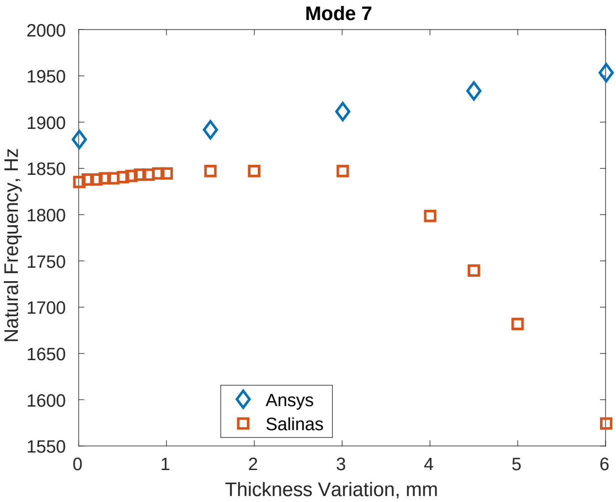
Natural Frequency as Thickness is Varied, Mode 5



Natural Frequency as Thickness is Varied, Mode 6



Natural Frequency as Thickness is Varied, Mode 7



Natural Frequency as Thickness is Varied, Mode 8

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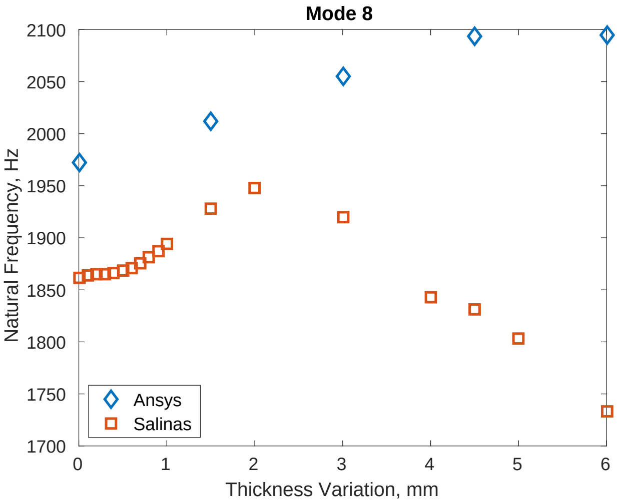
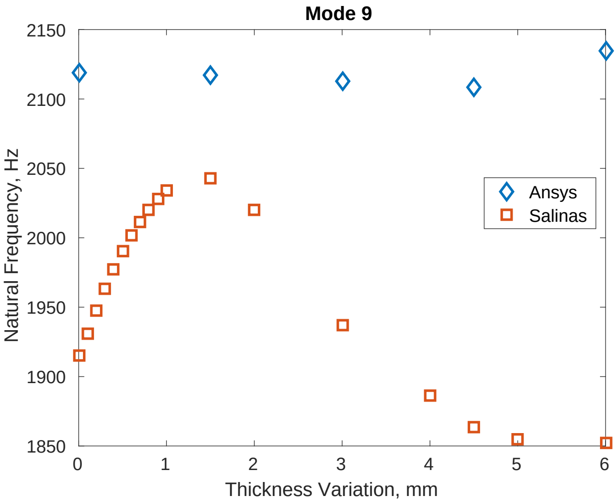
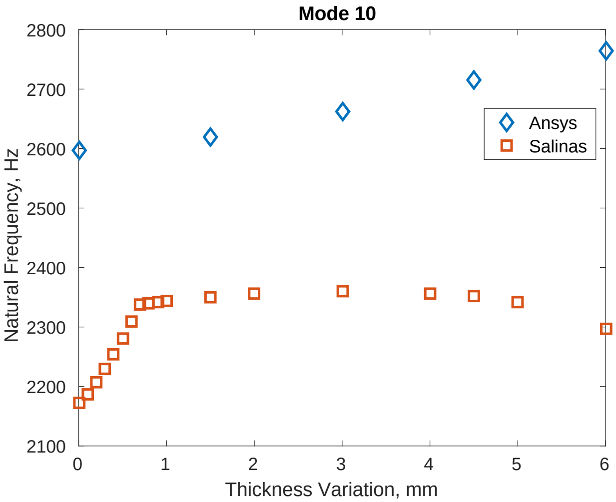


Natural Frequency as Thickness is Varied, Mode 9



Natural Frequency as Thickness is Varied, Mode 10

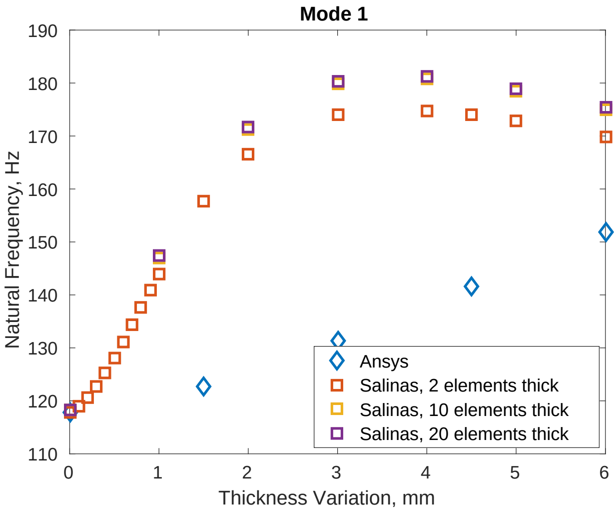


Discussion

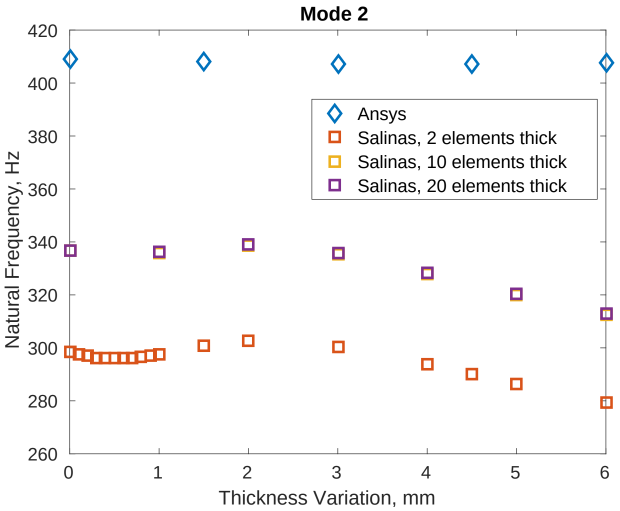
There are significant differences in the results

- Mode 1 and Mode 3 match well at 0 mm perturbation
  - Other modes do not match as well even for 0mm
- The behavior as the thickness is increased is different
  - Ansys seems to be almost linear in most cases
  - Salinas exhibits non-linear behavior
  - Are thicknesses for Ansys results correct?
- For these results, the plates are 2 elements thick
  - Refining the mesh shifts the behavior, but does not drive Salinas results towards Ansys results
- The element type choice in Salinas has a large impact
  - The chosen type is closer to a commercial code than the default (according to the Salinas documentation)
- Non-linear behavior suggests that HD PROMs constructed from 0mm case will not be very accurate for large perturbations

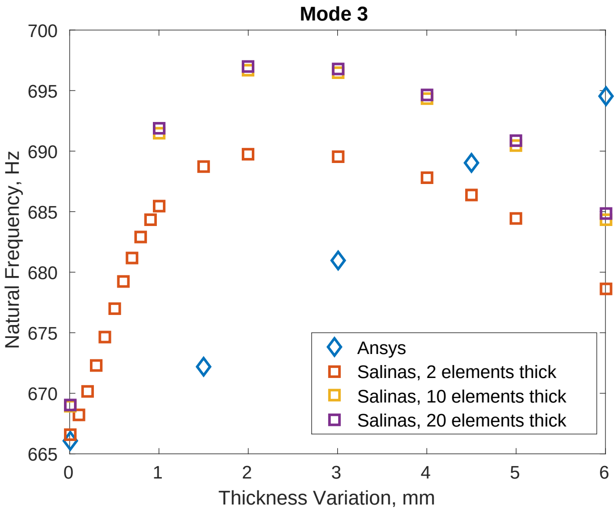
Mesh Convergence Study, Mode 1



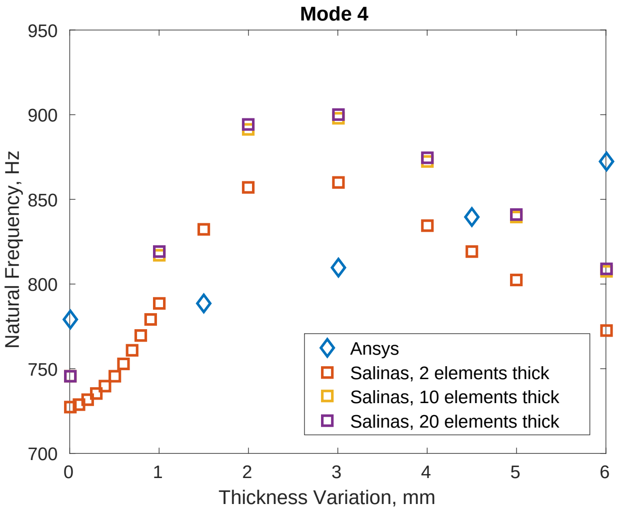
Mesh Convergence Study, Mode 2



Mesh Convergence Study, Mode 3

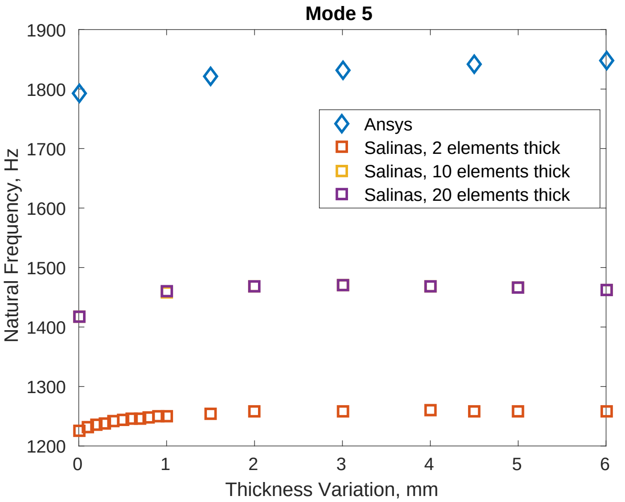


Mesh Convergence Study, Mode 4

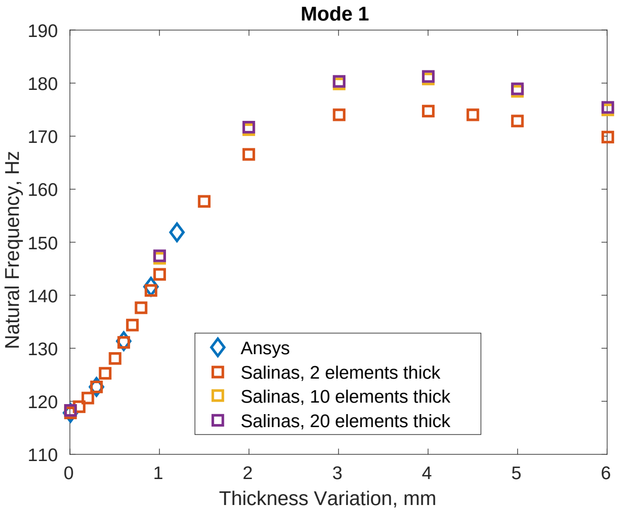


Unlimited Release

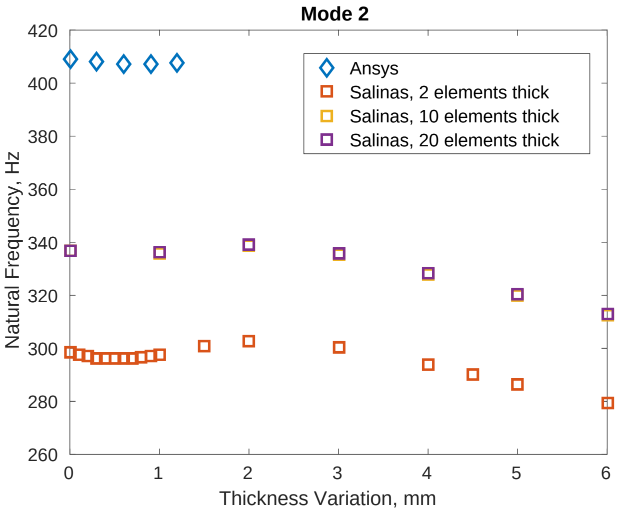
Mesh Convergence Study, Mode 5



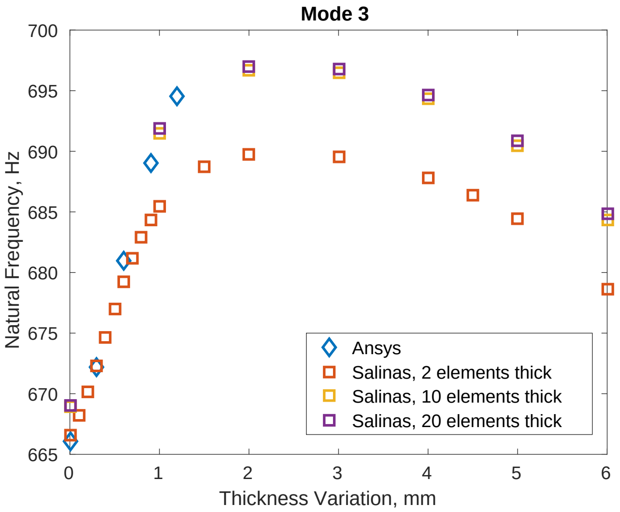
Change Thickness for Ansys Results, Mode 1



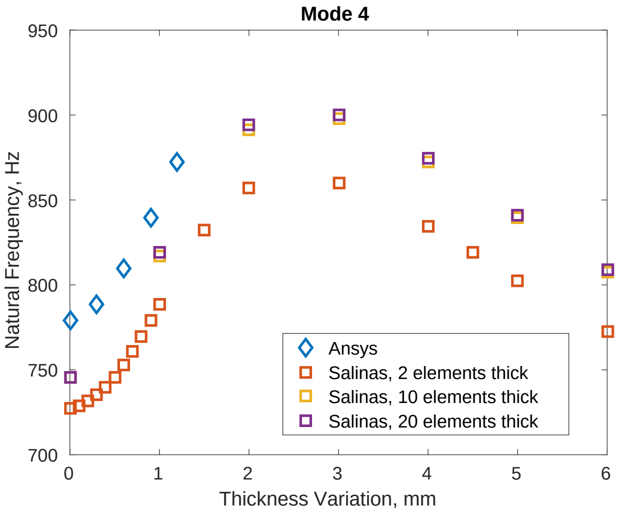
Change Thickness for Ansys Results, Mode 2



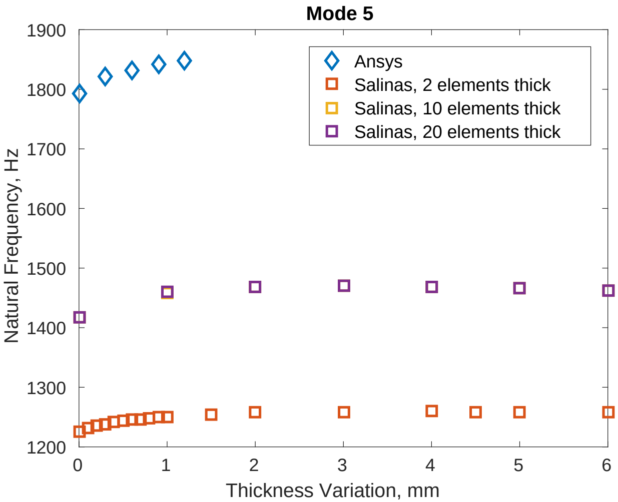
Change Thickness for Ansys Results, Mode 3



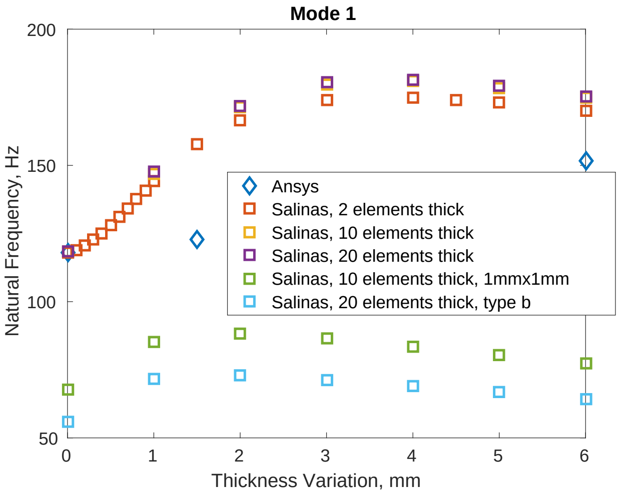
Change Thickness for Ansys Results, Mode 4



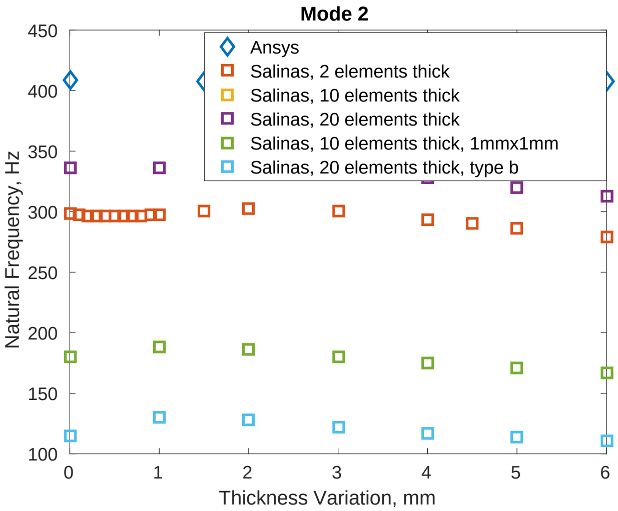
Change Thickness for Ansys Results, Mode 5



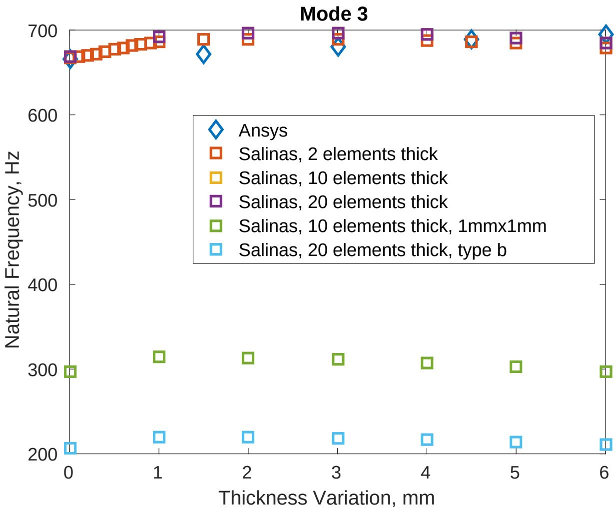
Additional Salinas Runs, Mode 1



Additional Salinas Runs, Mode 2



Additional Salinas Runs, Mode 3



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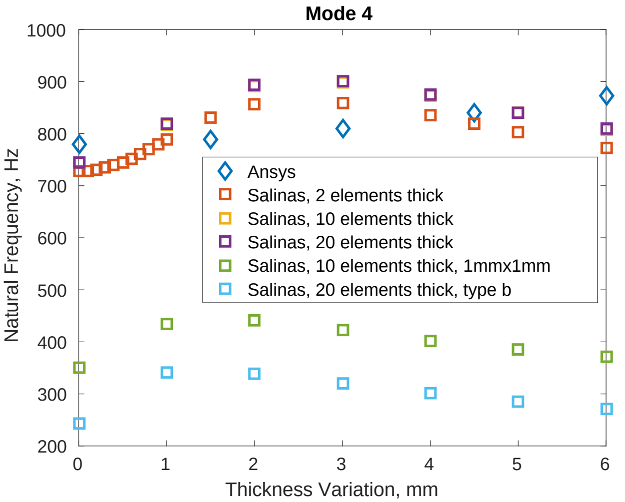

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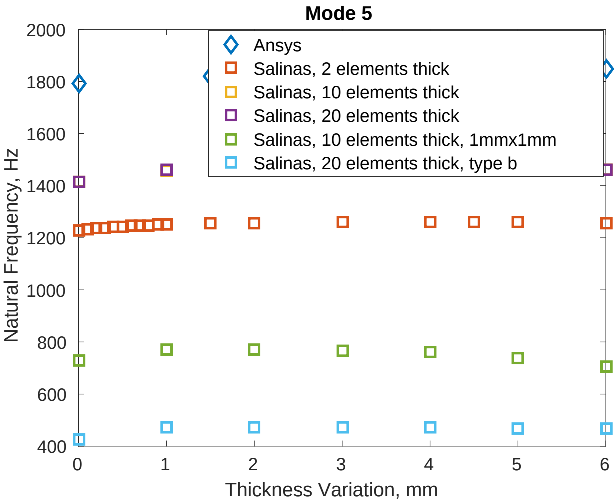
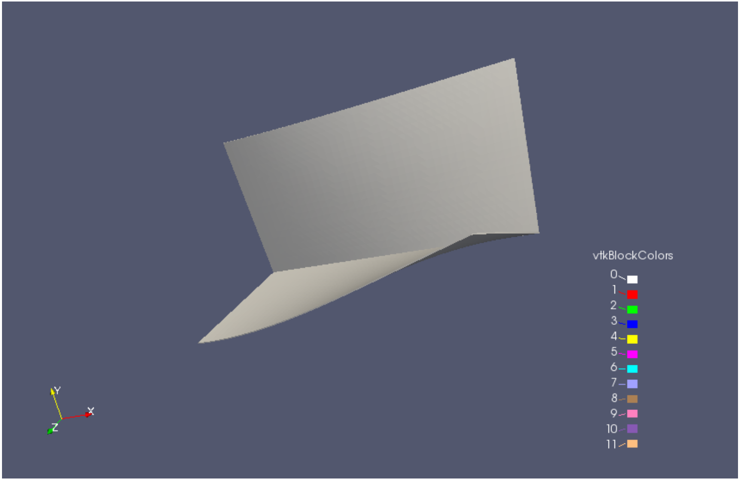
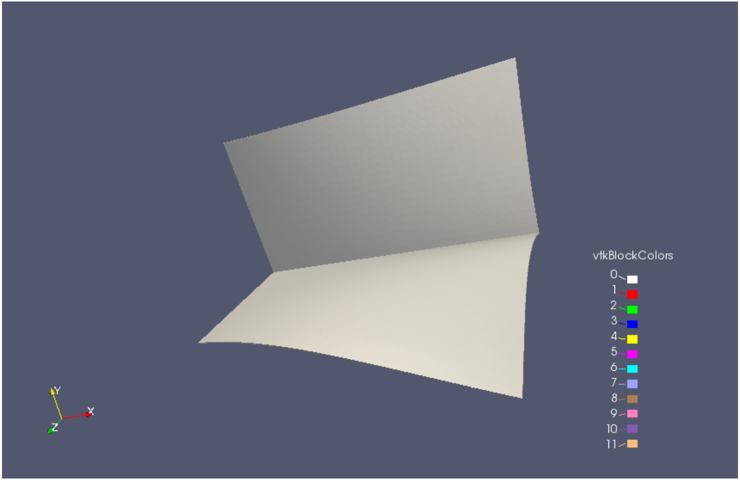


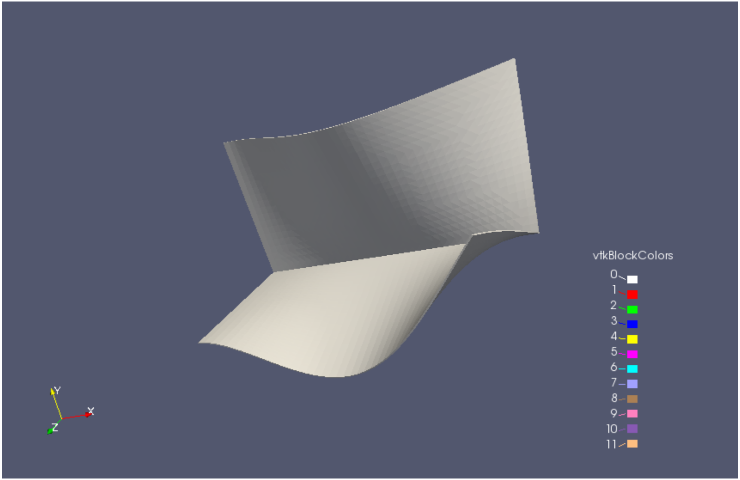
Mode Shapes: Mode 1



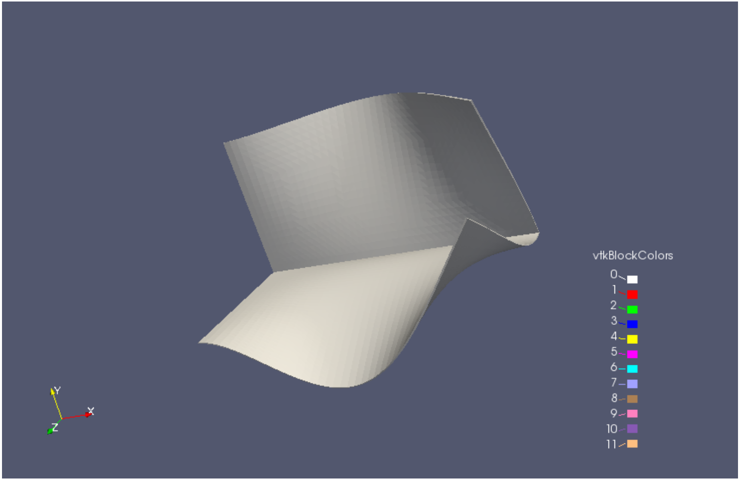
Mode Shapes: Mode 2



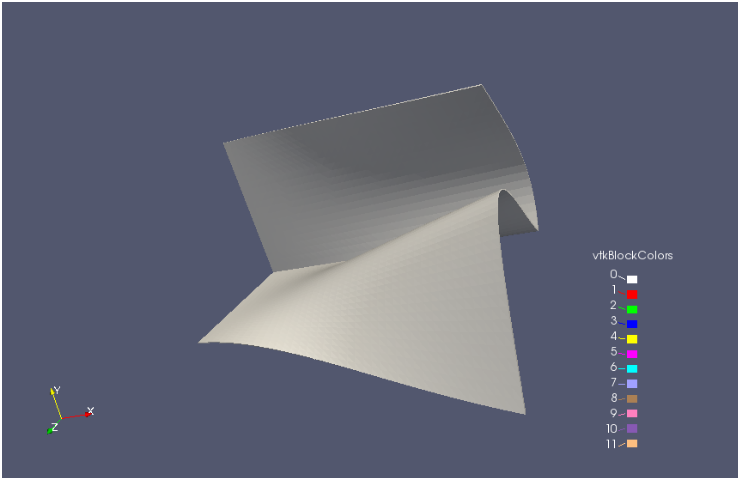
Mode Shapes: Mode 3



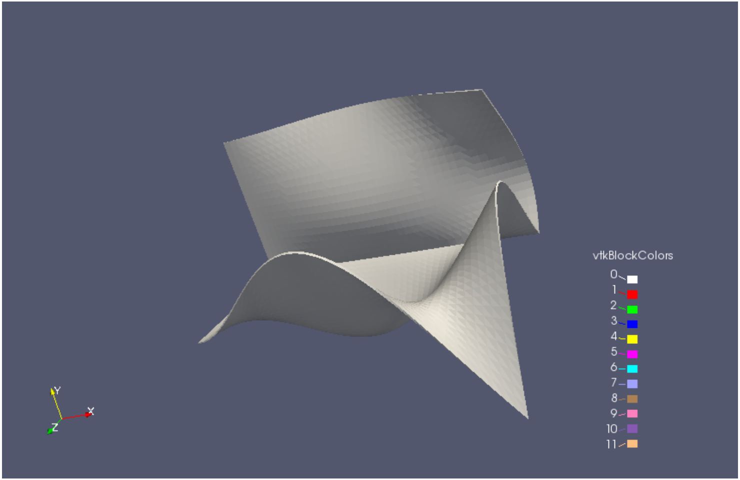
Mode Shapes: Mode 4



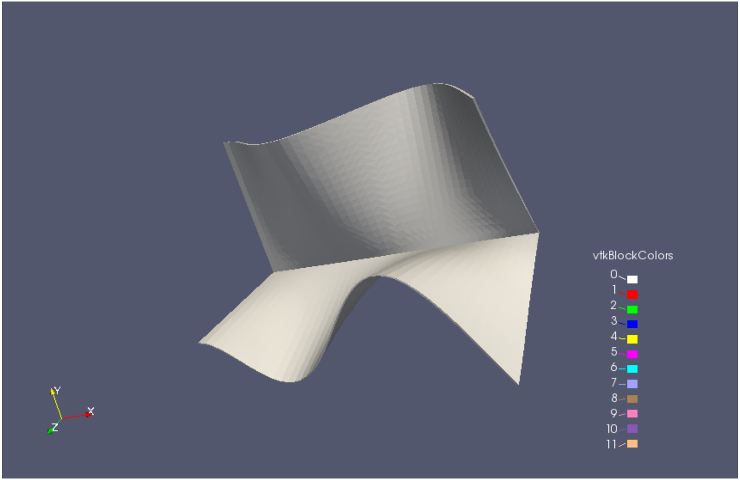
Mode Shapes: Mode 5



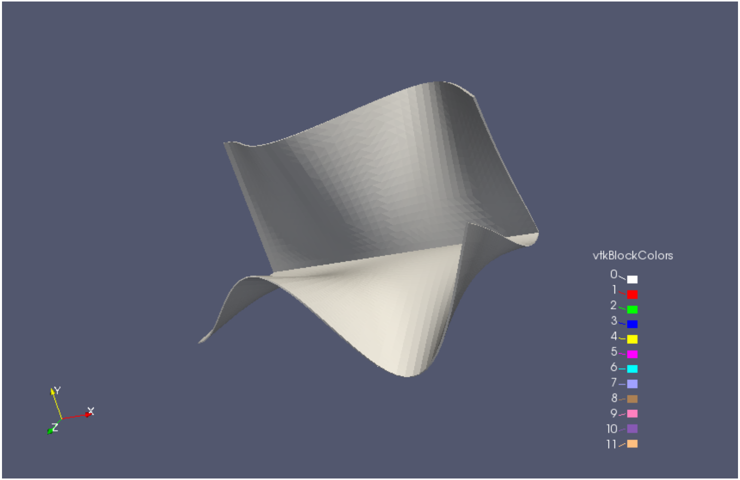
Mode Shapes: Mode 6



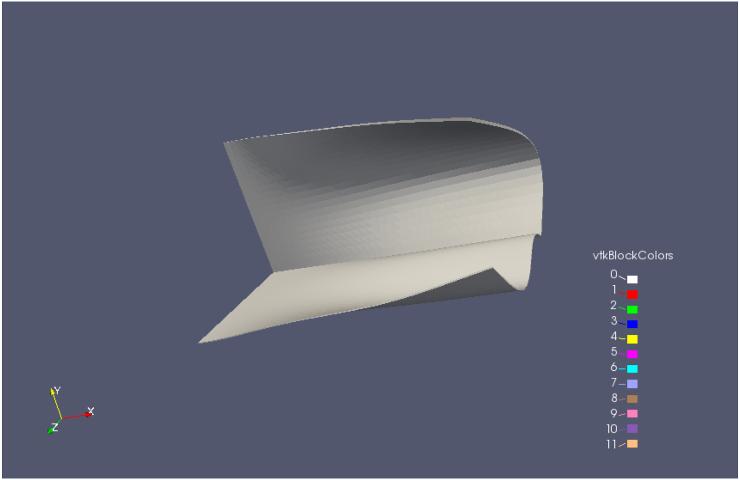
Mode Shapes: Mode 7



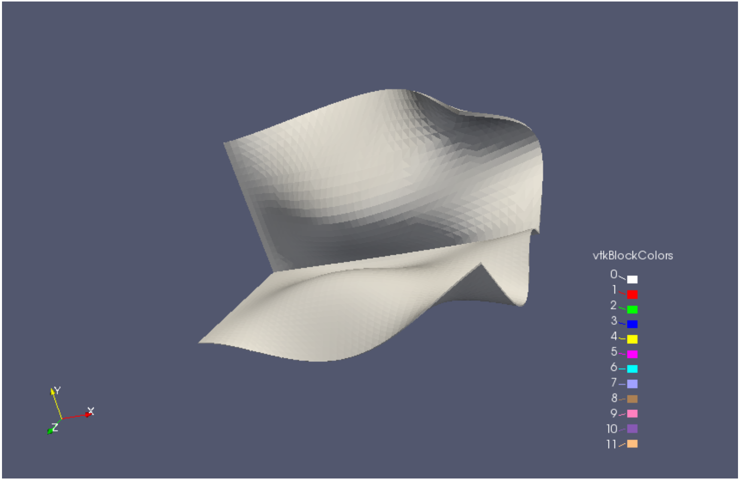
Mode Shapes: Mode 8



Mode Shapes: Mode 9



Mode Shapes: Mode 10



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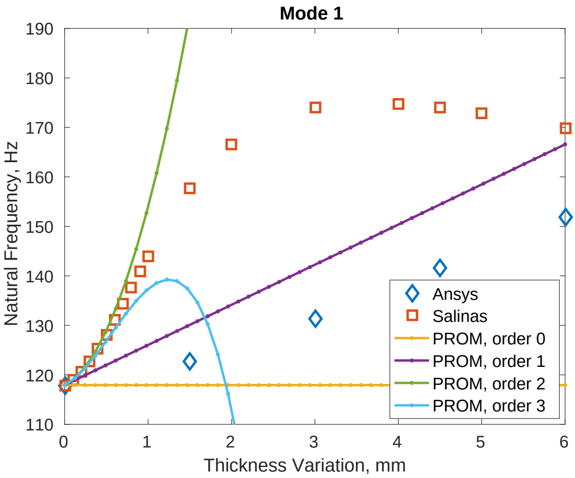
Two PROM Comparisons:

- PROM constructed using information from 0mm case
  - Not expected to be accurate for entire range of variation due to non-linear behavior
  - Accurate only for small variations
- PROM constructed using information from 3mm case
  - Captures behavior better for larger variations

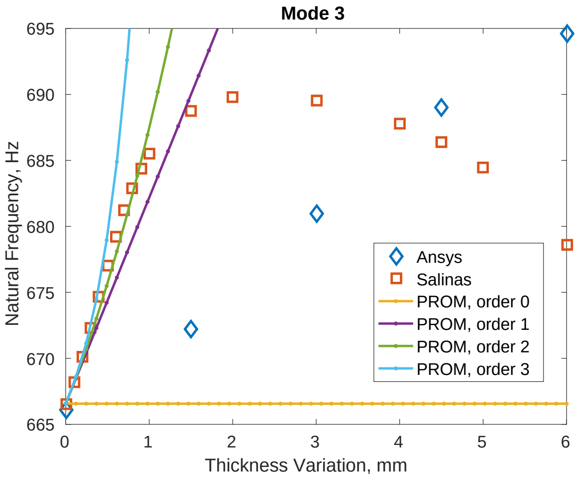
Vary order of parameterization from 0 (constant) to 3 (cubic)

Focus on Mode 1 and Mode 3, which matched better with Ansys results

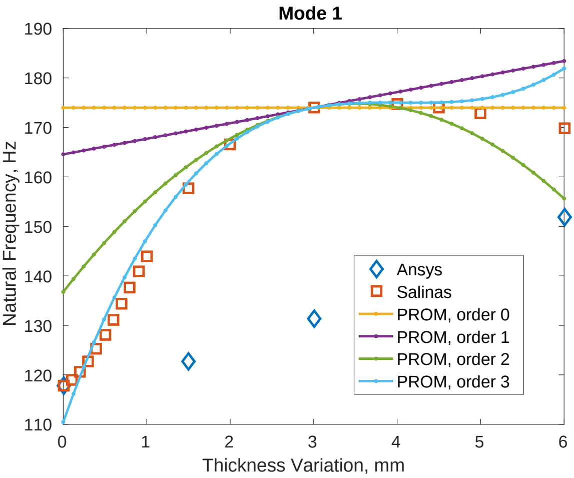
PROM Constructed from 0mm Case



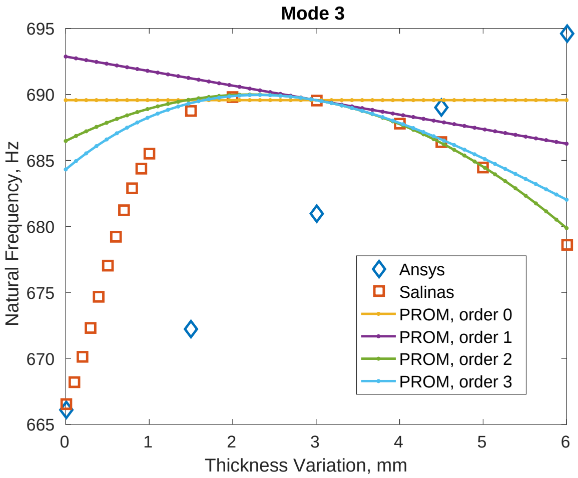
PROM Constructed from 0mm Case



PROM Constructed from 3mm Case



PROM Constructed from 3mm Case



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Questions?