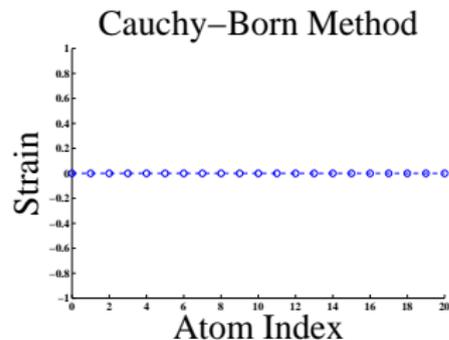
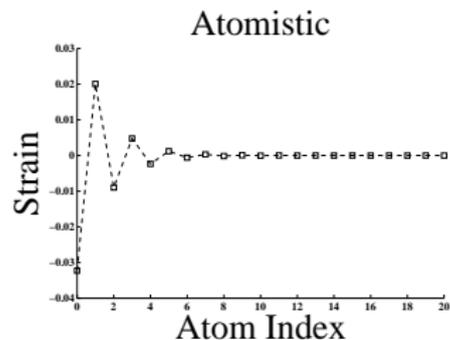


Analysis of a Predictor-Corrector Method for Computationally Efficient Modeling of Surface Effects in 1D

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Motivation:

- Regular Cauchy-Born method does not capture surface effects well
- Surface effects are important for nano-materials and for studying any behavior near a surface



Approach:

- Novel predictor-corrector method
- Regular Cauchy-Born method provides initial prediction of behavior
- Correct the solution at atomistic resolution over a boundary layer
- Introduces first-order surface term error

Features:

- Inherit efficiency of regular Cauchy-Born approach
- Systematic control over the error and ability to handle various surface geometries

