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

![Graphs comparing Atomistic and Cauchy-Born Method strains](image-url)
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