MDStressLab
Computing Stress in Atomistic Simulations

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Motivation

nature physics
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Breakdown of continuum mechanics for nanometre-wavelength rippling of graphene

Levente Tapasztó[1]*, Traian Dumitrică[2], Sung Jin Kim[3], Péter Nemes-Incze[1], Chanyong Hwang[3] and László P. Biró[1]

Understanding how the mechanical behaviour of materials deviates at the nanoscale from the macroscopically established concepts is a key challenge of particular importance for graphene, given the complex interplay between its nanoscale morphology and electronic properties[1–5]. In this work, the (sub)nanometre-wavelength periodic rippling of suspended graphene nanomembranes has been realized by thermal strain engineering and investigated using scanning tunnelling microscopy. This allows us to explore the rippling of a crystalline membrane with wavelengths comparable to its lattice constant. The observed nanorippling mode violates the predictions of the continuum model[6], and evidences the breakdown of the plate idealization[7] of the graphene monolayer. Nevertheless, microscopic simulations based on a quantum mechanical description of the chemical binding accurately describe the observed rippling mode and elucidate the origin of the continuum model breakdown. Spatially resolved tunnelling spectroscopy measurements indicate a substantial influence of the nanoripples on the local electronic structure of graphene and reveal the formation of one-dimensional electronic superlattices.

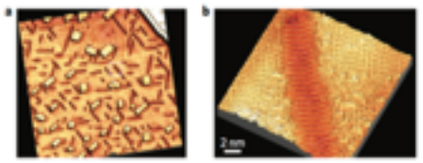

Figure 1 | Three-dimensional STM images of nanotrenches and graphene nanoripples. a, STM image (300 × 300 nm) of a reconstructed Cu(111) surface continuously covered by graphene. The rectangular protrusions are single-atom-height Cu adatom-clusters, whereas the trench-like features correspond to vacancy islands with well-defined widths of 5 nm and oriented along three particular directions. **b**, High-resolution STM image of a nanotrench revealing the nanoscale periodic rippling of the graphene membrane suspended over the trench.

To exploit the nanomechanical characteristics of graphene, it is of particular interest to explore down to which length scale

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Molecular modeling of mechanical stresses on proteins in glassy matrices: Formalism

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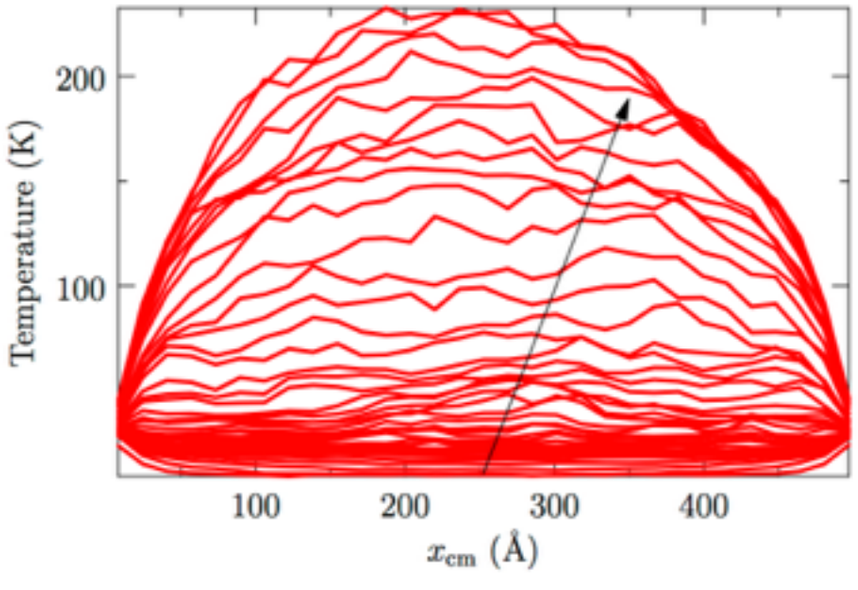
(Received 10 January 2012; accepted 22 June 2012; published online 18 July 2012)

We present an expression for the calculation of microscopic stresses in molecular simulation, which is compatible with the use of electrostatic lattice sums such as the Ewald sum, with the presence of many-body interactions, and which allows local stresses to be calculated on surfaces of arbitrarily complex shape. The ultimate goal of this work is to investigate microscopic stresses on proteins in glassy matrices, which are used in the pharmaceutical industry for the long-term storage and stabilization of labile biomolecules. We demonstrate the formalism's usefulness through selected results on ubiquitin and an α-keratin fragment, in liquid and glassy states. We find that atomic-level normal stresses on hydrophilic side-chains exhibit a similar fingerprint in both proteins, and protein-level normal stresses increase upon vitrification. Both proteins experience compressive stresses of the order of 10^2 bar in the glassy state. © *2012 American Institute of Physics*.
[http://dx.doi.org/10.1063/1.4734007]

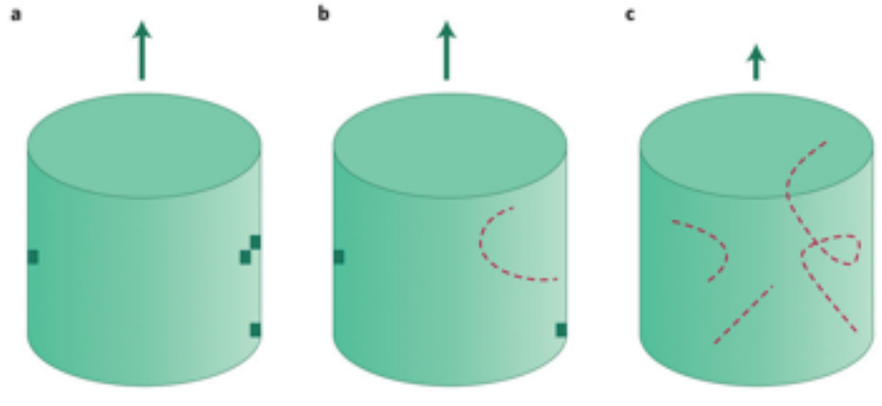
Connection with continuum models



Visualization

Amit Singh, *PhD thesis, University of Minnesota*

Stability of protein molecules under stress



Nucleation of defects

Ju Li, *Nature Materials* 14, 656–657 (2015)

Current implementation of atomistic stress

- LAMMPS: Stress/atom

Not a field

$$
\begin{aligned}
S_{ab} = -\Bigg[& m v_a v_b + \frac{1}{2}\sum_{n=1}^{N_p}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) + \frac{1}{2}\sum_{n=1}^{N_b}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b}) + \\
& \frac{1}{3}\sum_{n=1}^{N_a}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b}) + \frac{1}{4}\sum_{n=1}^{N_d}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) + \\
& \frac{1}{4}\sum_{n=1}^{N_i}(r_{1_a}F_{1_b} + r_{2_a}F_{2_b} + r_{3_a}F_{3_b} + r_{4_a}F_{4_b}) + \mathrm{Kspace}(r_{i_a}, F_{i_b}) + \sum_{n=1}^{N_f} r_{i_a}F_{i_b} \Bigg]
\end{aligned}
$$

Thompson, Plimpton, Mattson, J Chem Phys, 131, 154107 (2009).

- Goal: Implement a atomistic stress calculator that identically satisfies the balance law (in the absence of body forces):

Div (Stress) = 0

Outline

- The notion of stress in atomistic systems
- MDStressLab
- Example
- Conclusions

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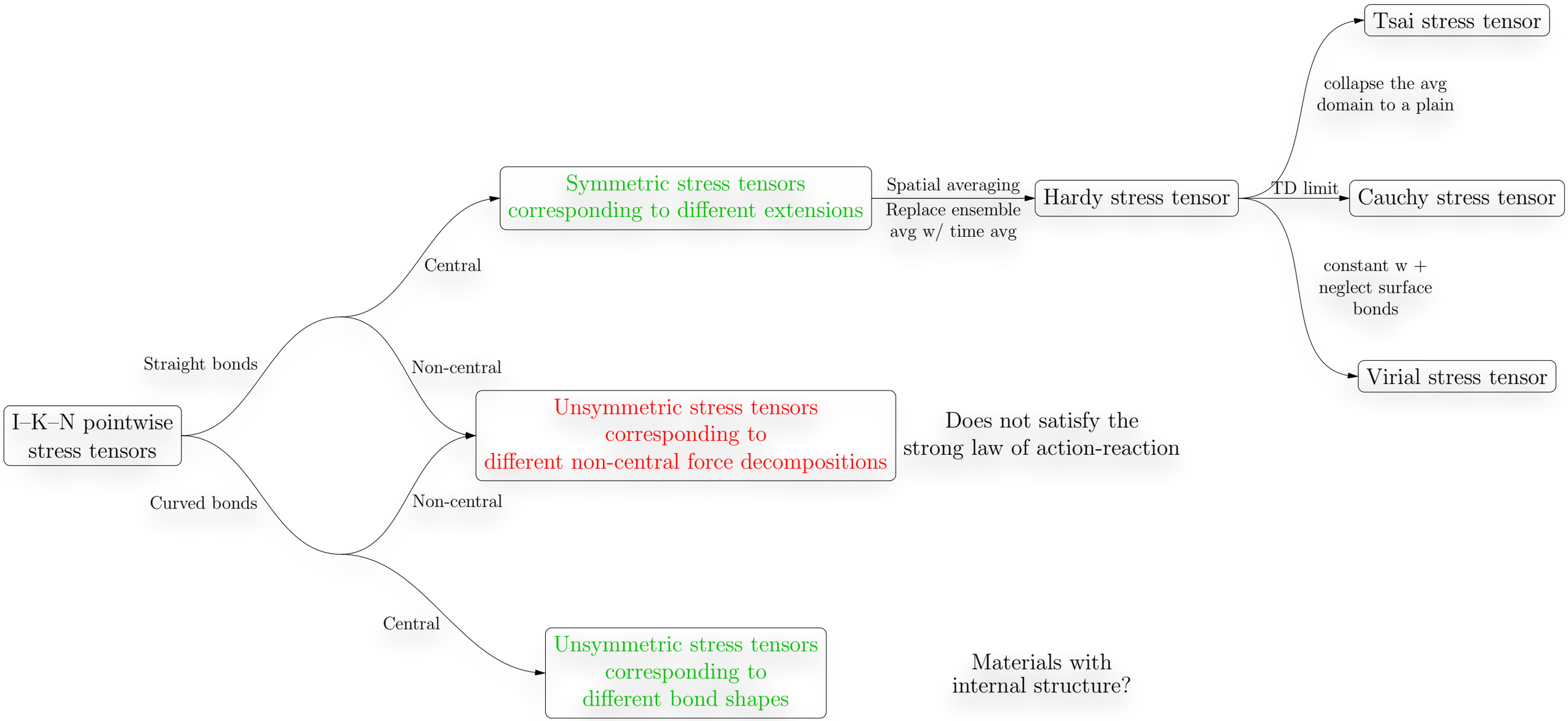
Atomistic stress



Admal, Nikhil Chandra, and Ellad B. Tadmor. "A unified interpretation of stress in molecular systems." *Journal of elasticity* 100.1 (2010): 63-143.

Spatial averaging

- IKN pointwise Cauchy stress

$$\boldsymbol{\sigma}_v(\boldsymbol{x},t) = \sum_{\substack{\alpha,\beta \\ \alpha<\beta}} -\boldsymbol{f}_{\alpha\beta} \otimes (\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta) \int_{s=0}^{1} \delta((1-s)\boldsymbol{x}_\alpha + s\boldsymbol{x}_\beta - \boldsymbol{x})\, ds$$

Not a continuum stress field

- A true macroscopic quantity is by necessity an average over some spatial region surrounding the continuum point where it is nominally defined

- The Hardy Cauchy stress is obtained by spatially averaging the IKN point wise stress.

Atomistic stress tensor fields

- Hardy Cauchy stress

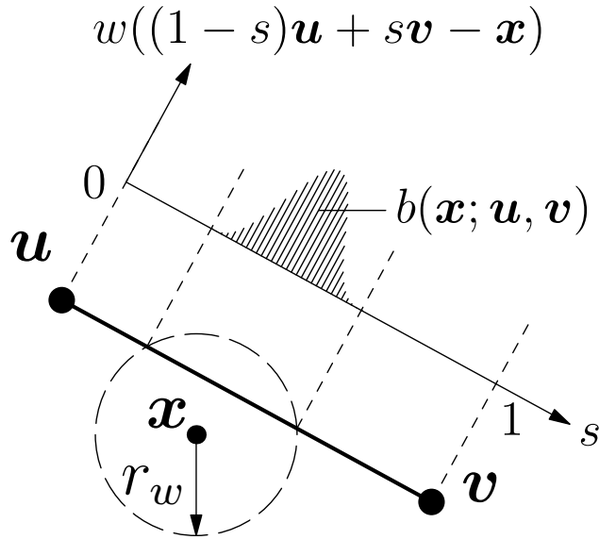
$$\boldsymbol{\sigma}_w = \boldsymbol{\sigma}_{w,v} + \boldsymbol{\sigma}_{w,\mathrm{k}},$$

$$\boldsymbol{\sigma}_{w,v}(\boldsymbol{x},t) = \sum_{\substack{\alpha,\beta \\ \alpha<\beta}} -\boldsymbol{f}_{\alpha\beta} \otimes (\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta) b(\boldsymbol{x}, \boldsymbol{x}_\alpha, \boldsymbol{x}_\beta),$$

$$\boldsymbol{\sigma}_{w,\mathrm{k}}(\boldsymbol{x},t) = -\sum_\alpha m_\alpha (\boldsymbol{v}_\alpha^{\mathrm{rel}} \otimes \boldsymbol{v}_\alpha^{\mathrm{rel}}) w(\boldsymbol{x}_\alpha - \boldsymbol{x})$$

$$b(\boldsymbol{x}, \boldsymbol{x}_\alpha, \boldsymbol{x}_\beta) := \int_{s=0}^{1} w((1-s)\boldsymbol{x}_\alpha + s\boldsymbol{x}_\beta - \boldsymbol{x})\, ds$$

$$\boldsymbol{f}_{\alpha\beta} = -\frac{\partial \mathcal{V}}{\partial r_{\alpha\beta}} \frac{\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta}{r_{\alpha\beta}}$$



- Tsai Cauchy stress

$$\boldsymbol{t}(\boldsymbol{x},\boldsymbol{n}) = \lim_{T\to\infty} \frac{1}{AT} \left[\int_0^T \sum_{\alpha\beta\cap\mathfrak{l}} \boldsymbol{f}_{\alpha\beta} \frac{(\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta)\cdot\boldsymbol{n}}{|(\boldsymbol{x}_\alpha - \boldsymbol{x}_\beta)\cdot\boldsymbol{n}|}\, dt - \sum_{\alpha\leftrightarrow\mathfrak{l}}^{T} \frac{m_\alpha \boldsymbol{v}_\alpha(t_\leftrightarrow)(\boldsymbol{v}_\alpha(t_\leftrightarrow)\cdot\boldsymbol{n})}{|\boldsymbol{v}_\alpha(t_\leftrightarrow)\cdot\boldsymbol{n}|} \right],$$

- Virial stress

Outline

- The notion of stress in atomistic systems
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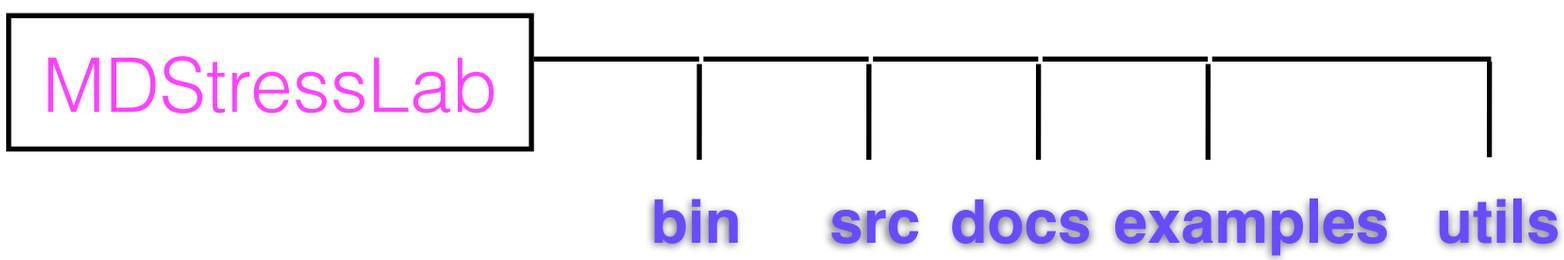
MDStressLab

- Available at www.mdstresslab.org



- What is MDStressLab, and what can it do?
  - A tool to post-process MS or MD simulation results to obtain various notions of stress fields
  - A KIM-compliant test simulator that can couple with any interatomic potential in the Open KIM repository
  - Cauchy and Piola—Kirchhoff versions of the Hardy, Tsai and viral stresses
  - Helmholtz-Hodge-Beltrami type decomposition of the atomistic stress

Input file

```
% Read in atomic configuration and species information
read
    spec,species
    conf,config
end

% Set up the grid for computing the stress field
grid
    gfit,300,300,0
end

% Define the KIM model used to compute the atomic interactions
potential
    modl,Pair_LJ_Smooth_Bernardes_Ar__MO_764178710049_000
end

% Specify whether to decompose stress into unique and non-unique parts
uniqueness
    project,T
end

% Setup and begin stress calculation
stress
    pkstr,F
    avgsize,10.0
    virial,F
    tsai,F
    hardy,T
end

stop
```

Input file

```
% Read in atomic configuration and species information
read
    spec,species
    conf,config
end
```

species.data

```
Al      0.0027964393
Ar      0.0041406102
Si      0.0029111119
```

config.data

```
3   58260
1000.00   1000.00   26.46   1000.00   1000.00   26.46
F   F   T
    Al      -129.658  -148.180  2.6460  0.00  0.00  0.00
    Al      -129.658  -148.180  13.230  0.00  0.00  0.00
    Al      -129.658  -148.180  7.9382  0.00  0.00  0.00
    ..
```

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stress
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    virial,F
    tsai,F
    hardy,T
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stop
```

OpenKIM

Jump to: Tests | Visualizers | Files

Pair_LJ_Smooth_Bernardes_Ar__MO_764178710049_000

Title	A smoothed Lennard-Jones pair potential for Argon
Short KIM ID	MO_764178710049_000
Extended KIM ID	Pair_LJ_Smooth_Bernardes_Ar__MO_764178710049_000
KIM Item Type	Parameterized Model using Model Driver Pair_LJ_Smooth__MD_716364606252_000
Contributor	Admal
Maintainer	Admal
Author	Nikhil Chandra Admal
Publication Year	2015
Species	Ar
Description	A smoothed Lennard-Jones pair potential for Argon with parameter from Bernardes.
Disclaimer	
Source Citations	Bernardes, N., 1958. Theory of solid Ne, Ar, Kr, and Xe at 0K. Phys. Rev. 112 (5), 1534–1539.
Programming Language(s)	N/A
Item Citation	Pair LJ Smooth Bernardes Ar MO_764178710049_000 Click here to download a citation in BibTeX format.

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stop
```

Spherical averaging domain of radius 10 Angstrom

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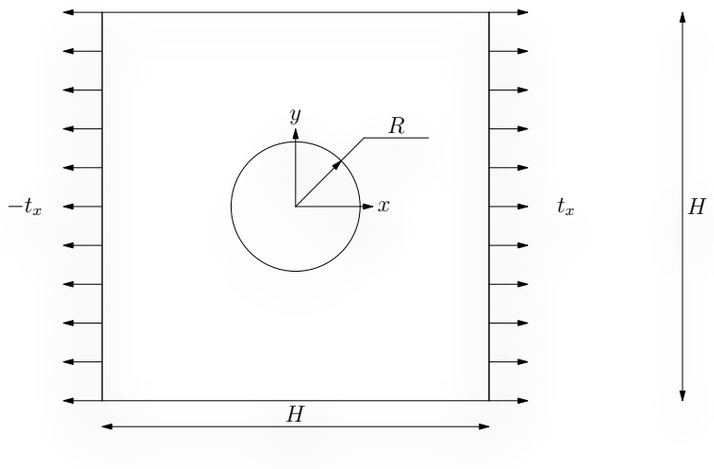
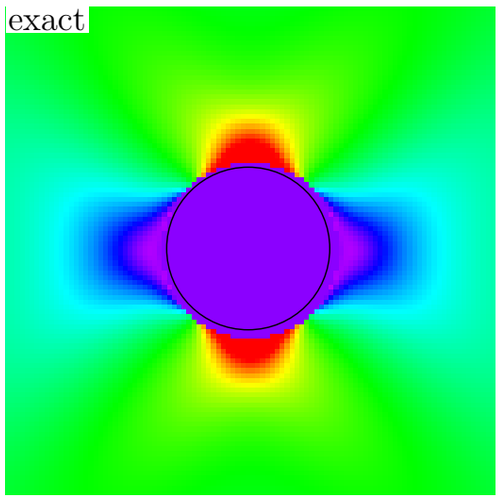
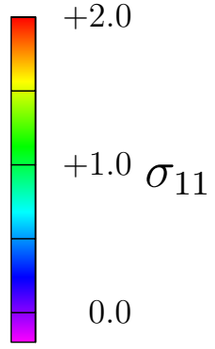
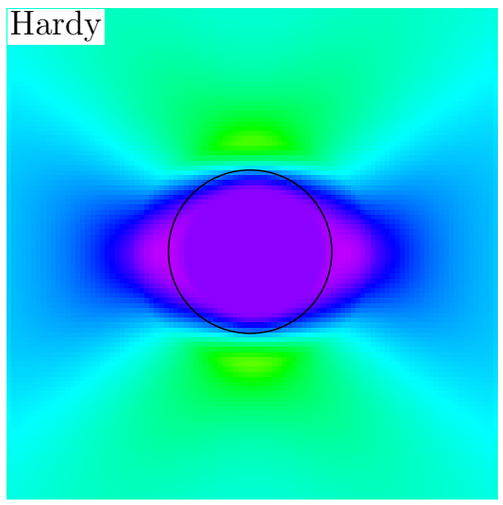
Example



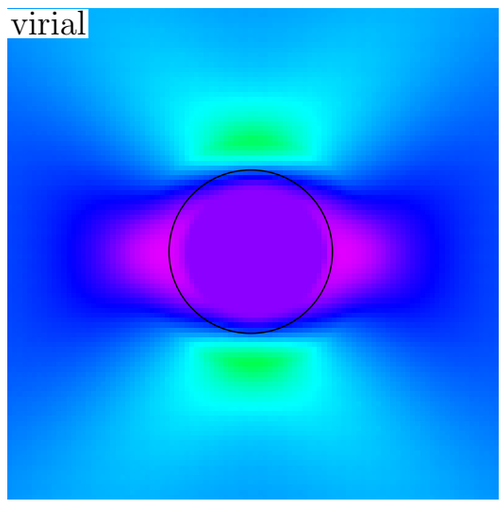




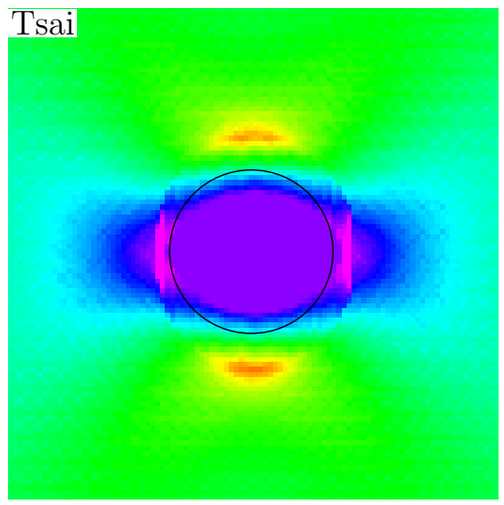
Exact



Hardy

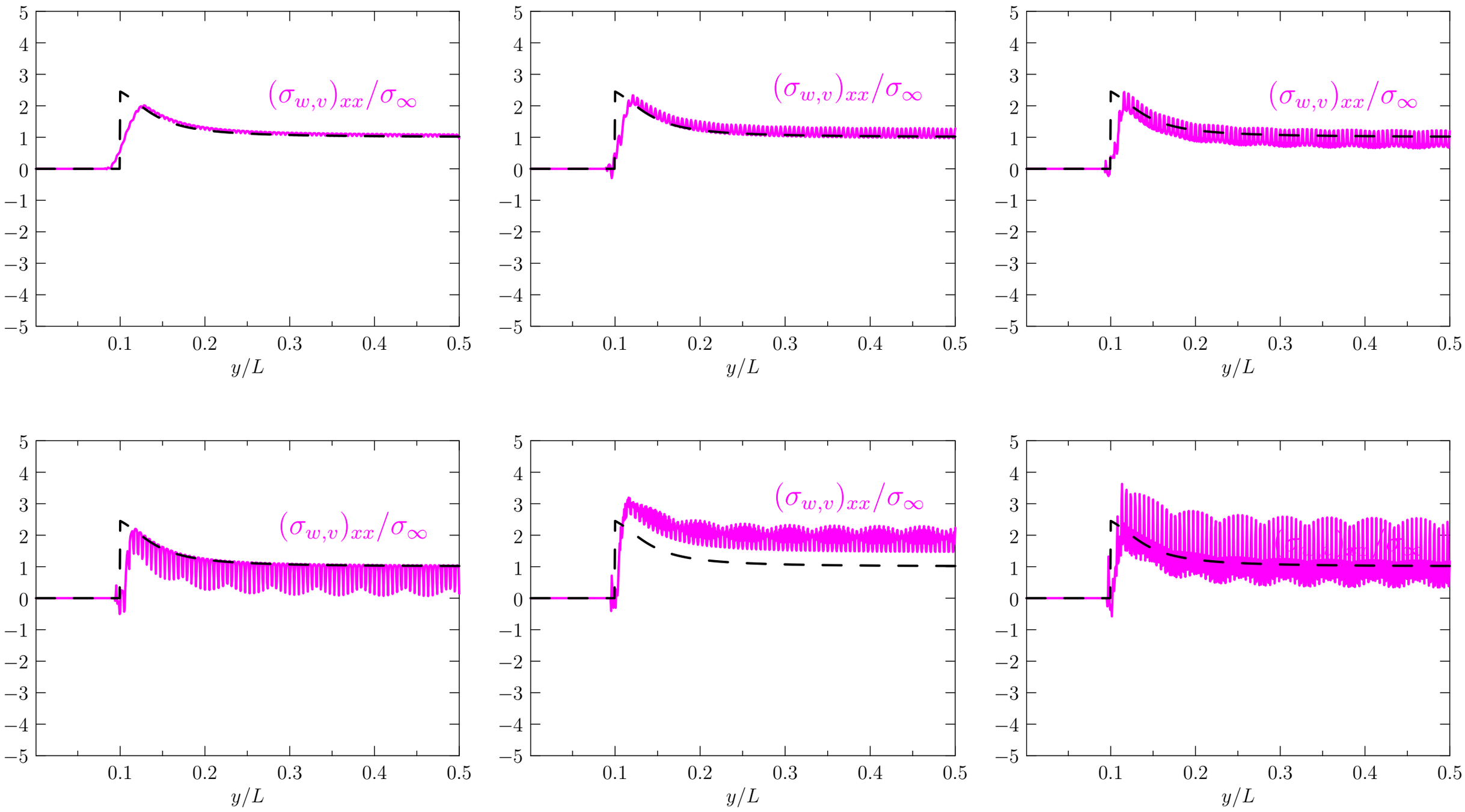


Virial

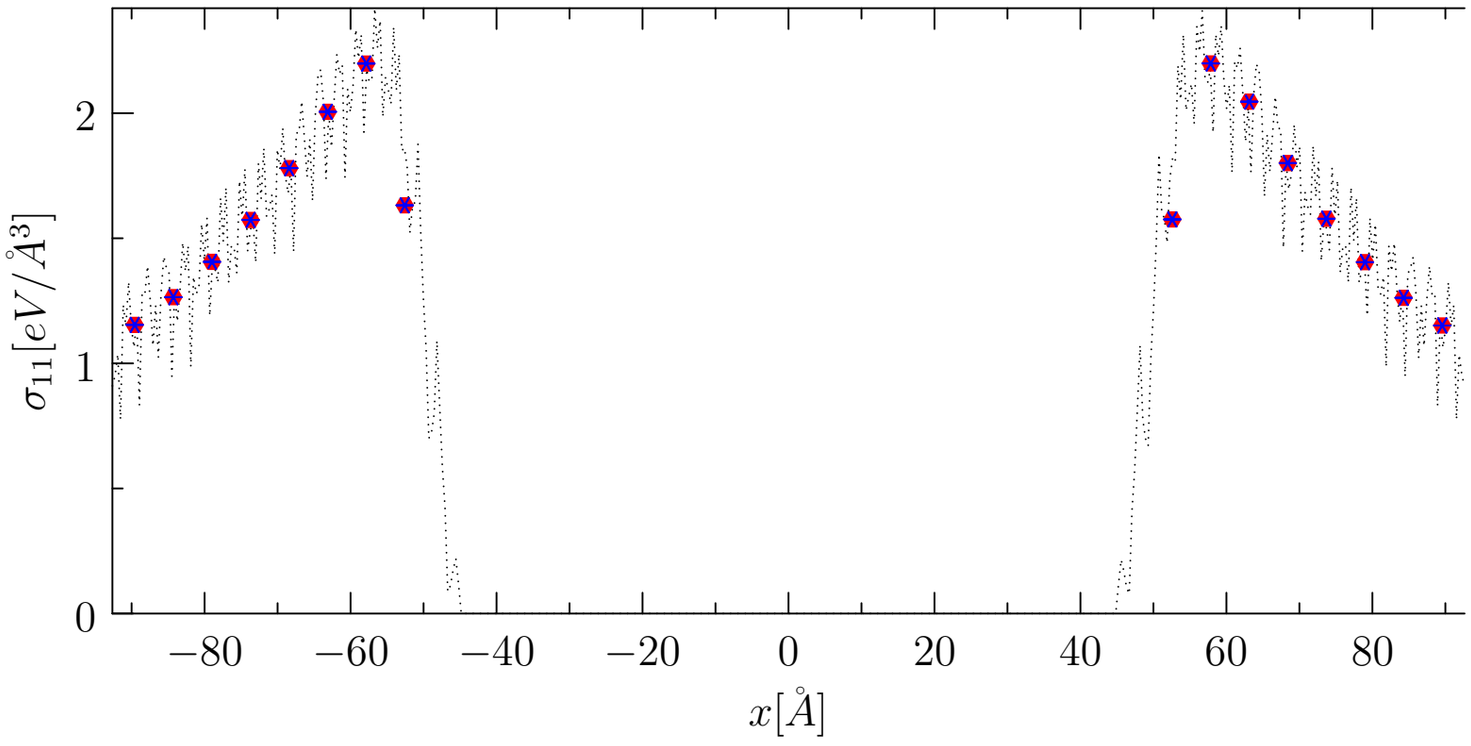


Tsai

Role of the averaging domain



Comparison with LAMMPS



Helmholtz-Hodge-Beltrami decomposition

- Non-uniqueness due to force decomposition

$$\boldsymbol{f}_\alpha = \sum_{\substack{\alpha,\beta \\ \alpha \neq \beta}} \boldsymbol{f}_{\alpha\beta}$$

Not unique

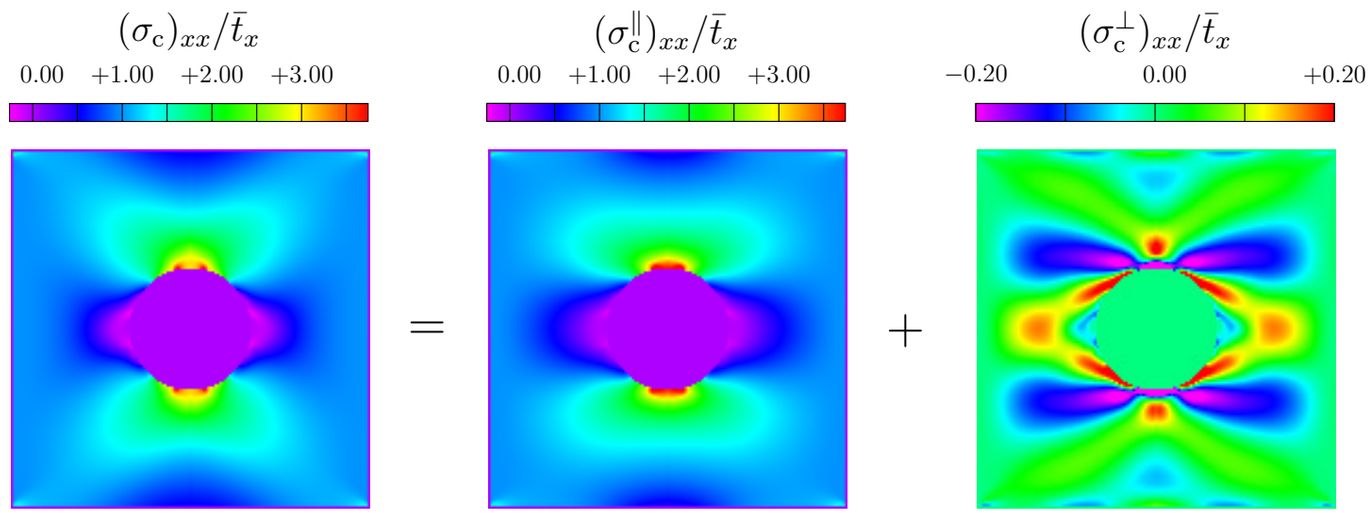
Results from a QM calculation

- Decomposition of interatomic forces using rigidity theory

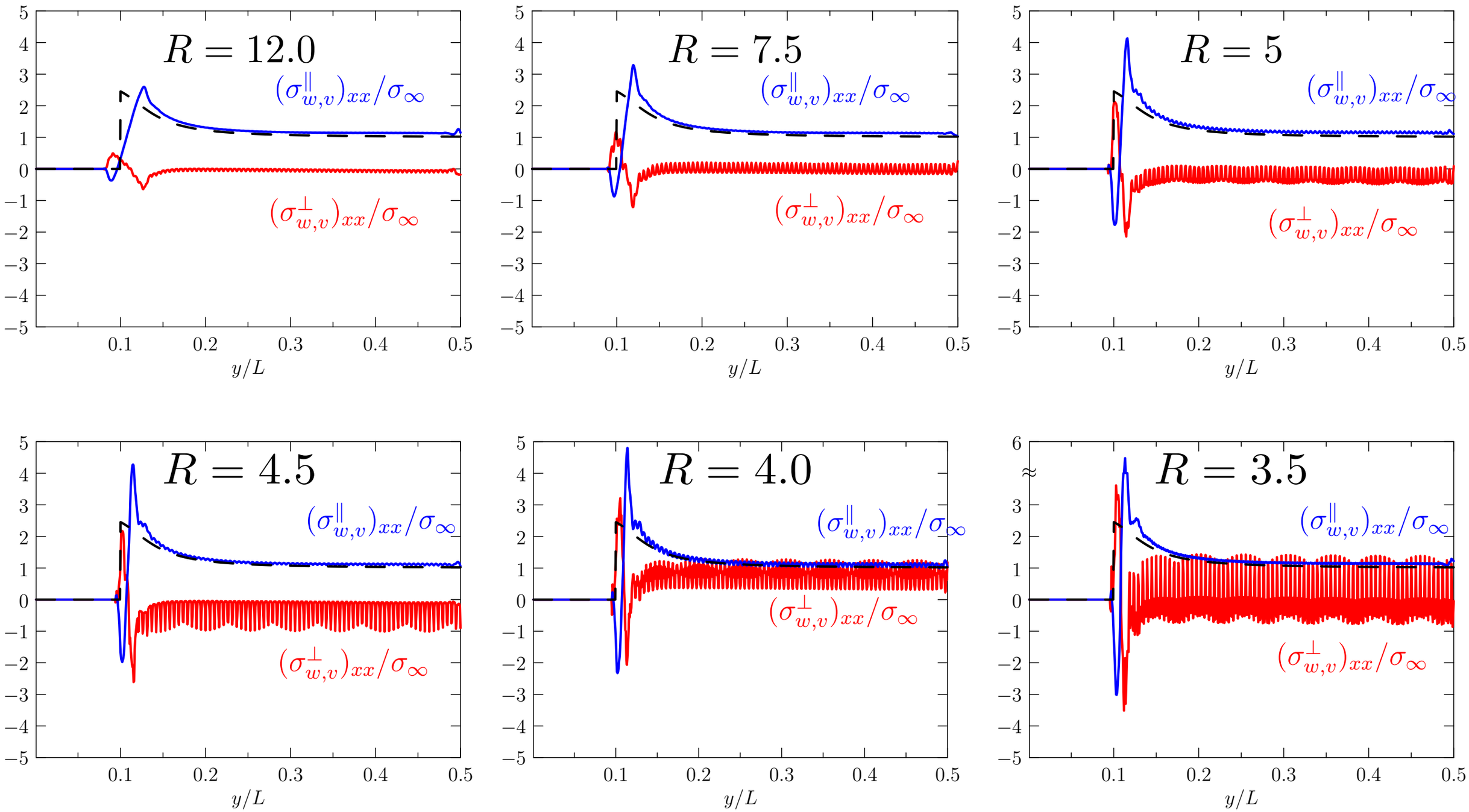
$$(f_{\alpha\beta}) = (f^{\parallel}_{\alpha\beta}) + (f^{\perp}_{\alpha\beta})$$

$(f^{\parallel}_{\alpha\beta})$: extension-independent

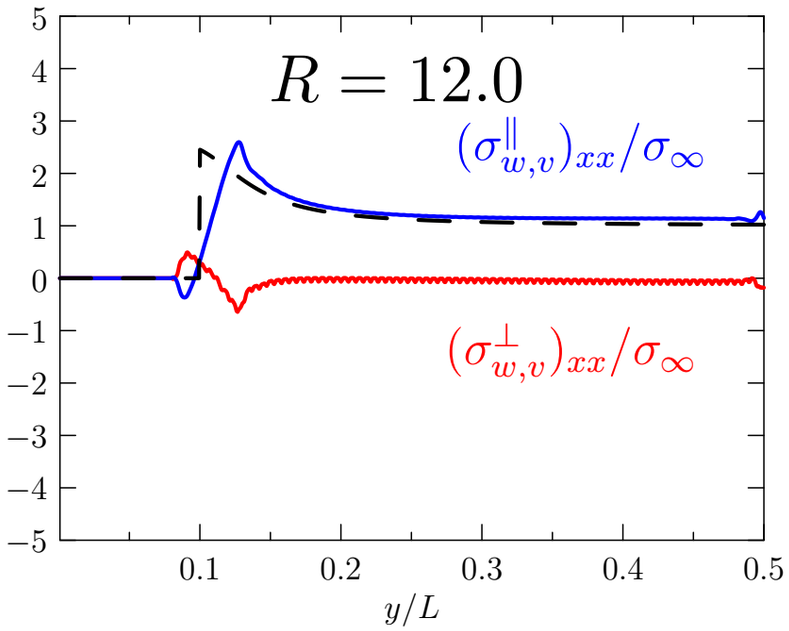
$(f^{\perp}_{\alpha\beta})$: extension-dependent

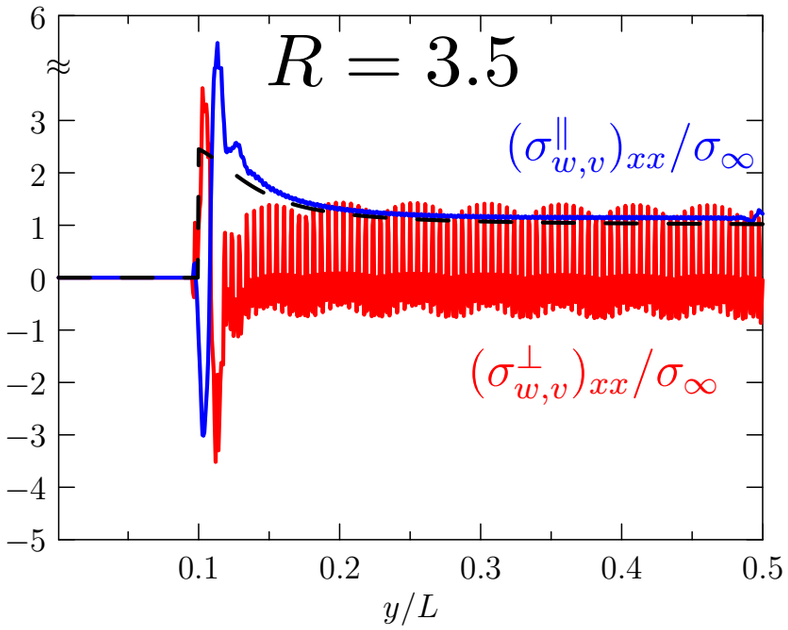


Helmholtz-Hodge-Beltrami decomposition



Helmholtz-Hodge-Beltrami decomposition





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Conclusions

- MDStressLab: A post-processing tool to compute stress fields that satisfy the exact balance laws of continuum mechanics. Available at

www.mdstresslab.org

A Unified Interpretation of Stress in Molecular Systems. Journal of Elasticity, 100(1–2), 63–143

The non-uniqueness of the atomistic stress tensor and its relationship to the generalized Beltrami representation. Journal of the Mechanics and Physics of Solids, 1–21.

Material fields in atomistics as pull-backs of spatial distributions. Journal of the Mechanics and Physics of Solids, 89, 59–76.

Stress and heat flux for arbitrary multibody potentials: A unified framework. Journal of Chemical Physics, 134(18)

- Currently MDStressLab computes the Cauchy and Piola—Kirchhoff stress corresponding to the Hardy, Virial and Tsai definition of atomistic stress

- In addition, a discrete Helmholtz—Hodge—Beltrami decomposition of the stress field can be computed. The demonstrated example highlights the use of this decomposition in the noise reduction of atomistic stress field.