MDStressLab
Computing Stress in Atomistic Simulations

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Motivation

Connection with continuum models

Stability of protein molecules under stress

Visualization

Amit Singh, PhD thesis, University of Minnesota

Nucleation of defects

Current implementation of atomistic stress

- **LAMMPS: Stress/atom**

\[
S_{ab} = - \left[ m v_a v_b + \frac{1}{2} \sum_{n=1}^{N_p} (r_1 a F_{1b} + r_2 a F_{2b}) + \frac{1}{2} \sum_{n=1}^{N_b} (r_1 a F_{1b} + r_2 a F_{2b}) + \frac{1}{3} \sum_{n=1}^{N_a} (r_1 a F_{1b} + r_2 a F_{2b} + r_3 a F_{3b}) + \frac{1}{4} \sum_{n=1}^{N_d} (r_1 a F_{1b} + r_2 a F_{2b} + r_3 a F_{3b} + r_4 a F_{4b}) + \frac{1}{4} \sum_{n=1}^{N_f} (r_1 a F_{1b} + r_2 a F_{2b} + r_3 a F_{3b} + r_4 a F_{4b}) + \text{Kspace}(r_i a, F_{ib}) + \sum_{n=1}^{N_f} r_i a F_{ib} \right]
\]


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

\[
\text{Div (Stress)} = 0
\]
Outline

• The notion of stress in atomistic systems

• MDStressLab

• Example

• Conclusions
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Symmetric stress tensors corresponding to different extensions

Unsymmetric stress tensors corresponding to different non-central force decompositions

Unsymmetric stress tensors corresponding to different bond shapes

I–K–N pointwise stress tensors

Hardy stress tensor

Tsai stress tensor

Cauchy stress tensor

Virial stress tensor

Spatial averaging
Replace ensemble avg w/ time avg

Does not satisfy the strong law of action-reaction

Materials with internal structure?

Spatial averaging

- IKN pointwise Cauchy stress

\[ \sigma_v(x, t) = \sum_{\alpha, \beta \atop \alpha < \beta} -f_{\alpha \beta} \otimes (x_\alpha - x_\beta) \int_{s=0}^{1} \delta((1 - s)x_\alpha + sx_\beta - x) \, ds \]

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 pointwise stress.
Atomistic stress tensor fields

- **Hardy Cauchy stress**
  \[ \sigma_w = \sigma_{w,v} + \sigma_{w,k}, \]
  \[ \sigma_{w,v}(x, t) = \sum_{\alpha, \beta} -f_{\alpha\beta} \otimes (x_\alpha - x_\beta) b(x, x_\alpha, x_\beta), \]
  \[ \sigma_{w,k}(x, t) = -\sum_\alpha m_\alpha (v_{\alpha}^{\text{rel}} \otimes v_{\alpha}^{\text{rel}}) w(x_\alpha - x) \]
  \[ b(x, x_\alpha, x_\beta) := \int_{s=0}^{1} w((1-s)x_\alpha + sx_\beta - x) \, ds \]
  \[ f_{\alpha\beta} = -\frac{\partial V}{\partial r_{\alpha\beta}} \frac{x_\alpha - x_\beta}{r_{\alpha\beta}} \]

- **Tsai Cauchy stress**
  \[ t(x, n) = \lim_{T \to \infty} \frac{1}{AT} \left[ \int_0^T \sum_{\alpha\beta \in \mathcal{L}} f_{\alpha\beta} \frac{(x_\alpha - x_\beta) \cdot n}{|x_\alpha - x_\beta|} \, dt - \sum_{\alpha \in \mathcal{L}} m_\alpha v_\alpha(t_{\alpha}) (v_\alpha(t_{\alpha}) \cdot n) \right], \]

- **Virial stress**
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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
1.4. Units

The units used by the MDStressLab program are:

- Distance: Å
- Energy: eV
- Time: ps
- Mass: \( \text{eV} \cdot \text{ps}^2/\text{Å}^2 \)

In the next section, the format of the input file to MDStressLab is described.

2. Input file

Below is a sample input file to MDStressLab. This is followed by a detailed explanation of the commands that appear in it.

```markdown
% 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
```

The input file consists of six stages: read, grid, potential, uniqueness, stress and stop. All lines starting with `%` are comments. (However, `%` appearing in the middle of the text is not treated as comments.) Each stage (except `stop`) contains commands and their associated arguments in the following format: `command,value_1,value_2,...`

Each stage (except `stop`) ends with an `end` command. Note that the six stages and their corresponding commands (except the commands in `stress` stage) should be in sequence as the example shows. Violation of the sequence might lead to undefined behavior. The six stages are described separately below.
Each stage (except the commands in the middle of the text) contains commands and their associated arguments in the following format: command,value_1,value_2,...

The six stages are described separately below.

1. **Stage 1**
   - **read**
     - spec,species
     - conf,config

2. **Stage 2**
   - **grid**
     - spec.data

3. **Stage 3**
   - **potential**
     - modl,Pair_LJ_Smooth_Berends,species_Ar_MO_764178710049_000

4. **Stage 4**
   - **uniqueness**
     - project,T

5. **Stage 5**
   - **stress**
     - A1, -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

6. **Stage 6**
   - **stop**
     - hardy,T

Below is a sample input file to demonstrate the use of these stages.

```plaintext
% Read in atomic configuration and species information
read
  spec,species
  conf,config
end
% Set up the grid for computing the atomic interactions
grid
  200 200 300 0 0 0
end
% Define the KIM model used to compute the atomic interactions
potential
  modl,Pair_LJ_Smooth_Berends,species_Ar_MO_764178710049_000
end
% Specify whether to decompose stress into unique and non-unique parts
uniqueness
  project,T
end
% Start and begin stress calculation
stress
  F F T
  A1, -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
end
% Read in atomic configuration and species information
read
  spec,species
  conf,config
end
% Set up the grid for computing the atomic interactions
grid
  200 200 300 0 0 0
end
% Define the KIM model used to compute the atomic interactions
potential
  modl,Pair_LJ_Smooth_Berends,species_Ar_MO_764178710049_000
end
% Specify whether to decompose stress into unique and non-unique parts
uniqueness
  project,T
end
% Start and begin stress calculation
stress
  F F T
  A1, -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
end
% Stop
stop
```

A sample species file is given below.

```plaintext
A1 0.0027964393
Ar 0.0041406102
Si 0.0029111119
```

A sample configuration file is shown below.

```plaintext
3 58260
1000.00 1000.00 26.46 1000.00 1000.00 26.46
F F T
```

Note that the order of the atomic positions in the final configuration should be identical to the order of the atomic positions in the initial configuration. The species file contains masses of different species of atoms. The format of the species file is as follows:

```plaintext
<Species_n> <Position_n>_i <Velocity_n>_i
```

The subscripts of the element name. A snippet of a configuration file of Aluminum atoms is shown below.

```plaintext
Al -129.658 -148.180 2.6460 0.00 0.00 0.00
Ar 0.0041406102
Si 0.0029111119
```

```plaintext
3 58260
1000.00 1000.00 26.46 1000.00 1000.00 26.46
F F T
```

In this stage, the state of the system is read as an input from a configuration file and a species file. The two files are specified using the commands read spec,species and read conf,config, respectively. For example, in the input file shown above, the mass fields for Aluminum, Argon, and Silicon are indicated as follows:

```plaintext
A1 0.0027964393
Ar 0.0041406102
Si 0.0029111119
```

The configuration and species files are specified using the commands read spec,species and read conf,config, respectively. For example, in the input file shown above, the mass fields for different species are indicated as follows:

```plaintext
A1 0.0027964393
Ar 0.0041406102
Si 0.0029111119
```

A snippet of a configuration file of Aluminum atoms is shown below.

```plaintext
Al -129.658 -148.180 2.6460 0.00 0.00 0.00
Ar 0.0041406102
Si 0.0029111119
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1000.00 1000.00 26.46 1000.00 1000.00 26.46
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Ar 0.0041406102
Si 0.0029111119
```
% Read in atomic configuration and species information
read
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   conf,config
end

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end

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

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uniqueness
   project,T
end

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

stop
% 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
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end

% Specify whether to decompose stress into unique and non-unique parts
uniqueness
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stress
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  tsai,F
  hardy,T
end
stop

---

1.4. Units

The units used by the MDStressLab program are:

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- Energy: eV
- Time: ps
- Mass: eV · ps^2/Å^2

In the next section, the format of the input file to MDStressLab is described.
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Example

\[-t_x \quad H \quad t_x\]

\[H \quad y \quad R \quad z\]

\[\text{Exact}\]

\[\text{Hardy}\]

\[\text{Virial}\]

\[\text{Tsai}\]

\[\sigma_{11}\]
Role of the averaging domain
Comparison with LAMMPS

\[ \sigma_{11}[\text{eV/Å}^3] \]

\[ x[\text{Å}] \]
Helmholtz-Hodge-Beltrami decomposition

- Non-uniqueness due to force decomposition

\[ f_\alpha = \sum_{\alpha, \beta} f_{\alpha \beta} \]

Results from a QM calculation

- Decomposition of interatomic forces using rigidity theory

\[ (f_{\alpha \beta}) = (f_{\alpha \beta})^\parallel + (f_{\alpha \beta})^\perp \]

Extension-independent

Extension-dependent

\[ \left(\sigma_c\right)_{xx}/\bar{t}_x \]

\[ \left(\sigma_c^\parallel\right)_{xx}/\bar{t}_x \]

\[ \left(\sigma_c^\perp\right)_{xx}/\bar{t}_x \]

\[ \begin{array}{ccc}
0.00 & +1.00 & +2.00 & +3.00 \\
\end{array} \]

\[ \begin{array}{ccc}
0.00 & +1.00 & +2.00 & +3.00 \\
\end{array} \]

\[ \begin{array}{ccc}
-0.20 & 0.00 & +0.20 \\
\end{array} \]
Helmholtz-Hodge-Beltrami decomposition

\[ R = 12.0 \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]

\[ R = 7.5 \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]

\[ R = 5 \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]

\[ R = 4.5 \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]

\[ R = 4.0 \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]

\[ R = 3.5 \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]
\[ \frac{(\sigma_{w,v})_{xx}}{\sigma_{\infty}} \]
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


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.