Assessment of Different Thermostating Techniques in the Simulation of Molecular Lubrication

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Context and Problematic

- Molecular Dynamics modeling of nano-scale lubrication
  \( h \sim 1-6 \text{ nm} , \ P \sim 0.1 - 2 \text{ GPa} , \ v \sim 1-100 \text{ m/s} , \ T \sim 30 - 200 \text{ °C} \)

- Energy is:
  - added by compression and surface sliding (mechanical form)
  - dissipated by a thermostat (thermal form)

- What temperature to impose? And where?

- Friction is strongly related to the dissipation method in MD

Sliding Boundary Thermostat

- Phantom Molecules method

- Variable Boundary Temperature

Operating conditions

Lubricant: \( \text{n-hexadecane} \)
Surfaces: \( \text{Au (111)} \)
\( v = \pm 100 \text{ m/s} \)
\( h = 2.4 \text{ nm} \)
\( P = 500 \text{ MPa} \)

SBT: \( T(\text{surf}) = 300 \text{ K} \)
Phantom: \( T(\text{bulk}) = 300 \text{ K} \)
VBT: \( T(\infty) = 300 \text{ K} \)

Boundary temperature evolution

\( T_w(t) = 300 \text{ K} \)
Steady state

\( \zeta = 8 \times 10^8 \text{ s}^{-1} \)

Temperature Profiles

Summary

<table>
<thead>
<tr>
<th>Dissipation Method</th>
<th>Temperature rise (K)</th>
<th>Shear Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SBT</td>
<td>0</td>
<td>57.8</td>
</tr>
<tr>
<td>Phantom</td>
<td>32.1</td>
<td>84.7</td>
</tr>
<tr>
<td>VBT</td>
<td>30.5</td>
<td>82.3</td>
</tr>
</tbody>
</table>

- At low shear rates, the thermostat does not influence the friction
- At high shear rates, classical SBT thermostat over-estimate the dissipation and thus the friction
- A new method (VBT) for correctly dissipating energy from the molecular system is developed
- This method gives coherent with another advanced method from the literature (Phantom) but allows modeling more complex situations such as irregular solid structures