Assessment of Different Thermostating Techniques in the Simulation of Molecular Lubrication

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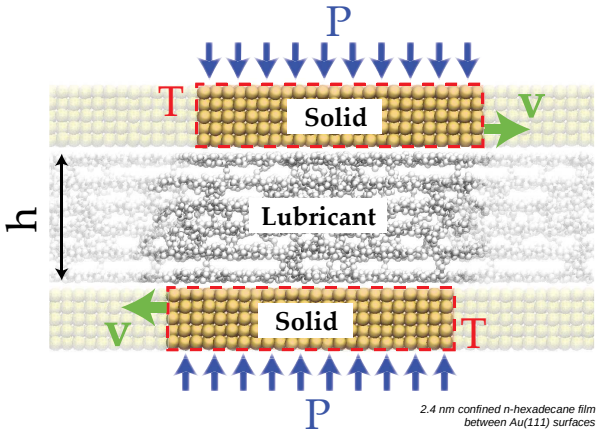
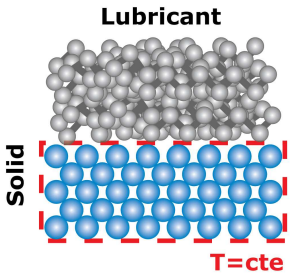
Context and Problematic

- Molecular Dynamics modeling of nano-scale lubrication
  h ~ 1-6 nm , P ~ 0.1 - 2 GPa , v ~ 1-100 m/s , T ~ 30 - 200 °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

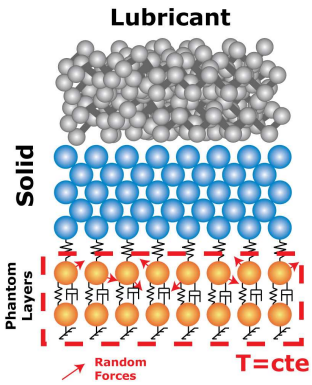


Sliding Boundary Thermostat



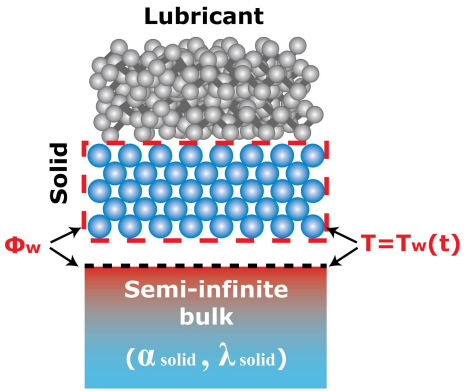
- \+ Computationally efficient and easy to apply
- \+ Works well for low levels of shearing
- − In the high-shear, high-dissipation regime only the lubricant may heat up
- − In these conditions, the method unrealistically over-dissipates energy thus over-estimating the friction

Phantom Molecules method



- \+ Phantom layers are employed to model a semi-infinite solid with bulk thermal properties
- \+ Surface temperature increases naturally due to the generated flux by lubricant shear
- − The method is difficult to apply for complex surface structures
- − Computational efficiency is influenced by the additional phantom atoms and their special interactions

Variable Boundary Temperature



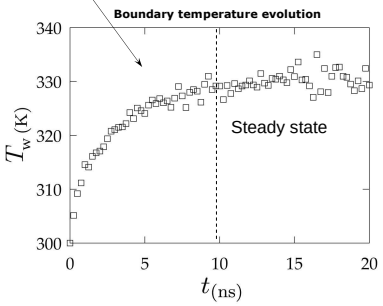
- \+ Surface temperature evolves realistically according to the liberated flux from the confined contact using a direct multi-scale thermal coupling from the molecular to the macroscopic scale
- \+ Computationally efficient since no additional degrees of freedom are required
- \+ The method is easy to apply for complex surface structures

Comparison between the thermostating methods in the high-shear regime

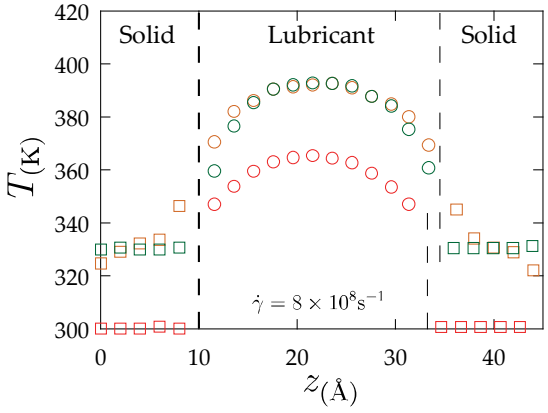
Operating conditions

Lubricant: n-hexadecane
Surfaces: Au (111)
v = ±100 m/s
h = 2.4 nm
P = 500 MPa

SBT:	T(surf)	= 300 K
Phantom:	T(bulk)	= 300 K
VBT:	T(∞)	= 300 K



Temperature Profiles



○/□ Classical Sliding Boundary Thermostat (Langevin)
○/□ Phantom Molecules method
○/□ Variable Boundary Thermostat (Langevin)

Summary

Dissipation Method	Temperature rise (K)		Shear Stress (MPa)
	Surface	Lubricant	
SBT	0	57.8	65.4
Phantom	32.1	84.7	60.6
VBT	30.5	82.3	60.8

- 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

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