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NPT Dynamics, Minimization and Elastic Constants for Triclinic Cells

New LAMMPS features briefs
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Parrinello-Rahman MD

Invented by :

Parrinello and Rahman, *J. Appl. Phys.* ***52*** 7182 (1981) (1,268 citations up to Feb 2010)

Core Ideas:

1. They proposed extending the Lagrangian operator to include the periodic cell dimensions as additional coordinates. From this operator, equations of motion were derived.

2. They included a general expression for strain energy contribution ot potential energy:

$$E = U + P_t \left(V - V_0\right) + E_{strain}$$

$$E_{strain} = \frac{1}{2} V_0 \mathrm{Tr} \mathbf{h}_0^{-1} \sigma_t \left(\mathbf{h}_0^{-1}\right)^t \mathbf{h}^t \mathbf{h}$$

Parrinello-Rahman Box Dynamics

```
fix 1 all   nvt     temp 300.0 300.0 100.0

fix 1 water npt     temp 300.0 300.0 100.0 \
                    iso 0.0 0.0 1000.0

fix 2 jello npt     temp 300.0 300.0 100.0 \
                    tri 5.0 5.0 1000.0

fix 3 ice   nph     temp 273.15 273.15 \
                    x 1.0 1.0 0.5 \
                    y 2.0 2.0 0.5 \
                    z 3.0 3.0 0.5 \
                    yz 0.1 0.1 0.5 \
                    xz 0.2 0.2 0.5 \
                    xy 0.3 0.3 0.5 \
                    nreset_ref 1000
```

Triclinic Cell Relaxation

P = 0

```
fix 1 all   box/relax   xyz 0.0 vmax 0.001
```

L_{xx} , L_{yy} fixed, P_{zz} = 1000 atm.

```
fix 1 water box/relax   aniso NULL NULL 1000.0
```

P = 0, except P_{xy} = 10 atm.

```
fix 3 ice   box/relax   tri 0.0 0.0 0.0 0.0 0.0 10.0 \
            nreset_ref 1000
```