

# **NPT Dynamics, Minimization and Elastic Constants for Triclinic Cells**

New LAMMPS features briefs  
LAMMPS Users' Workshop @ CSRI  
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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 introduced the periodic cell matrix as additional coordinates. They also expressed the strain energy in terms of this matrix:

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

$$E_{strain} = \boldsymbol{\sigma}_t : \boldsymbol{\epsilon} = \frac{1}{2} V_0 \text{Tr} \mathbf{h}_0^{-1} \boldsymbol{\sigma}_t \left( \mathbf{h}_0^{-1} \right)^t \mathbf{h}^t \mathbf{h}$$

## New $NVT$ , $NpT$ , $NpH$ , $N\sigma T$ Fixes

- Nose-Hoover chain thermostat for particle velocities
- Nose-Hoover chain thermostat for barostat “velocities”
- Barostat coupling styles:
  - Isotropic
  - Anisotropic
  - Triclinic (Parrinello-Rahman)
- Barostat “pressure” styles
  - Scalar hydrostatic pressure
  - Tensorial non-hydrostatic stress
- Martyna-Tobias-Klein correction to Nose-Hoover barostat

## New NVT, NPT, NPH Fixes

*NVT* Ensemble

```
fix 1 all nvt temp 300.0 300.0 100.0
```

*NpT* Ensemble

```
fix 1 water npt temp 300.0 300.0 100.0 &  
iso 0.0 0.0 1000.0
```

*NpH* Ensemble, anisotropic orthorhombic box

```
fix 1 water nph aniso 0.0 0.0 1000.0
```

*NpT* Ensemble, Parrinello-Rahman

```
fix 2 jello npt temp 300.0 300.0 100.0 &  
tri 5.0 5.0 1000.0
```

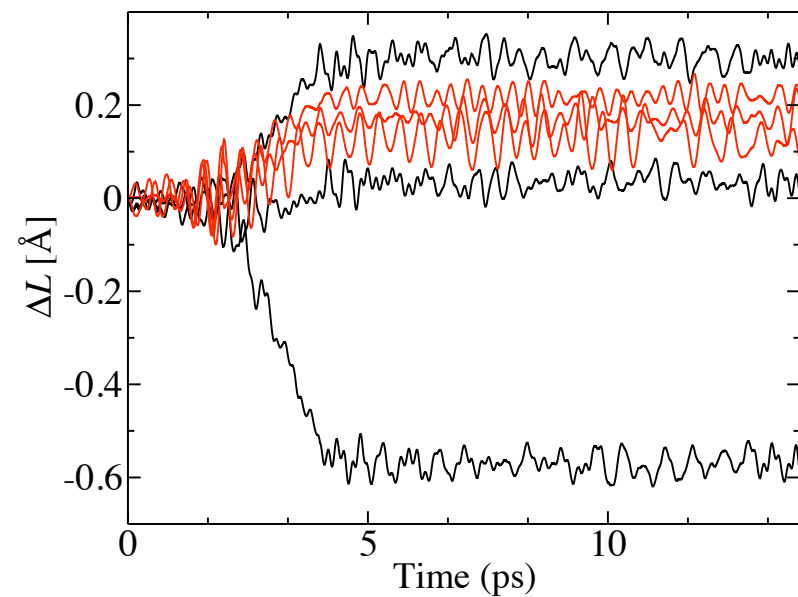
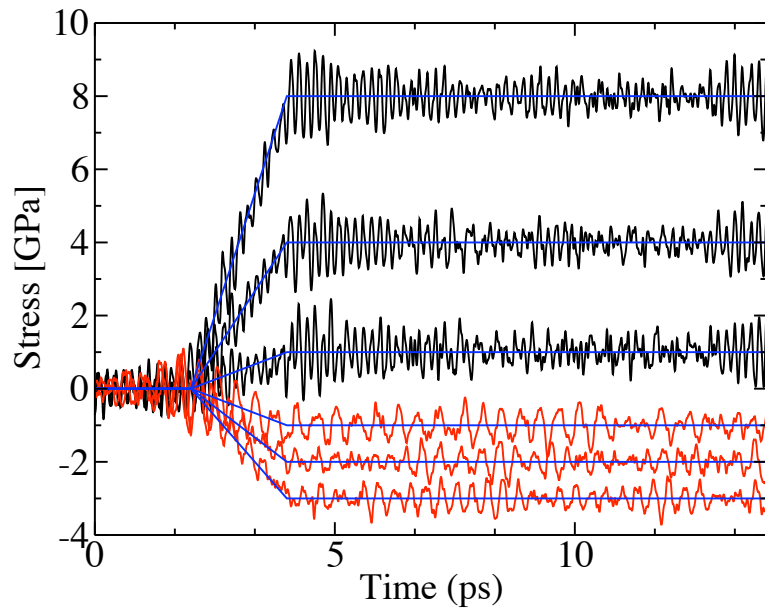
## New NVT, NPT, NPH Fixes

$N\sigma T$  Ensemble, Parrinello-Rahman

```
fix 3 ice      npt      temp 273.15 273.15 &  
              x 0.0 1.0 0.5 &  
              y 0.0 2.0 0.5 &  
              z 0.0 3.0 0.5 &  
              yz 0.0 0.1 0.5 &  
              xz 0.0 0.2 0.5 &  
              xy 0.0 0.3 0.5
```

# Example: Strained FCC Nickel

```
fix          mynpt all npt &
            pchain 3 tchain 3 mtk yes &
            temp 300.0 300.0 0.1 &
            x      10000.0    10000.0 1.0 &
            y      40000.0    40000.0 1.0 &
            z      80000.0    80000.0 1.0 &
            xy     -10000.0   -10000.0 1.0 &
            xz     -20000.0   -20000.0 1.0 &
            yz     -30000.0   -30000.0 1.0 &
```

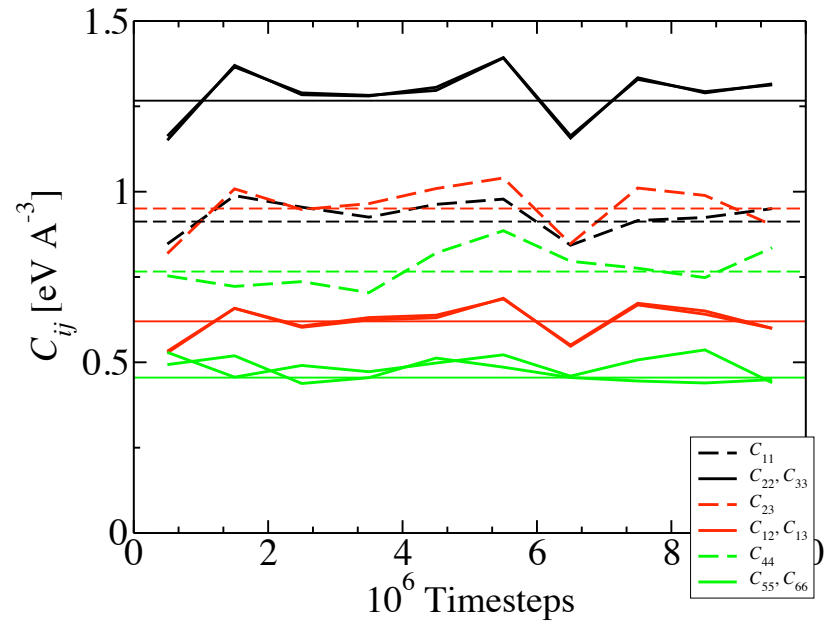
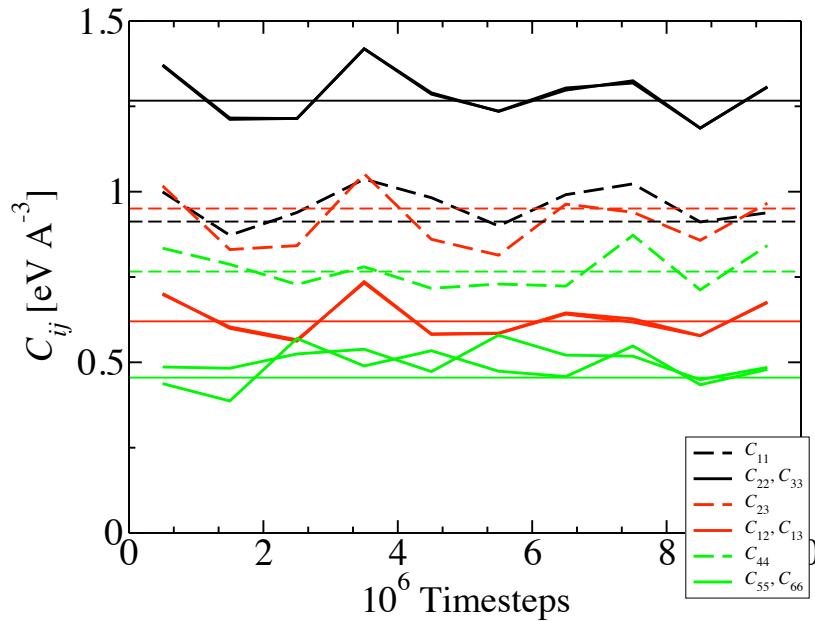


# Elastic Constants, Nickel, $P_{xx} = -5$ GPa, $T = 300$ K

```

fix                               mynpt all npt &
temp 300.0 300.0 0.5 &
x      -50000 -50000 2.0 &
y      0      0 2.0 &
z      0      0 2.0 &
xy     0      0 2.0 &
xz     0      0 2.0 &
yz     0      0 2.0 &
pchain 0 mtk yes &
nreset_ref 0 &
    
```

$$C_{ijkl}^{-1} = S_{ijkl} = \beta V_0 \langle \varepsilon_{ij} \varepsilon_{kl} \rangle$$



# 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
```

Non-hydrostatic target stress tensor

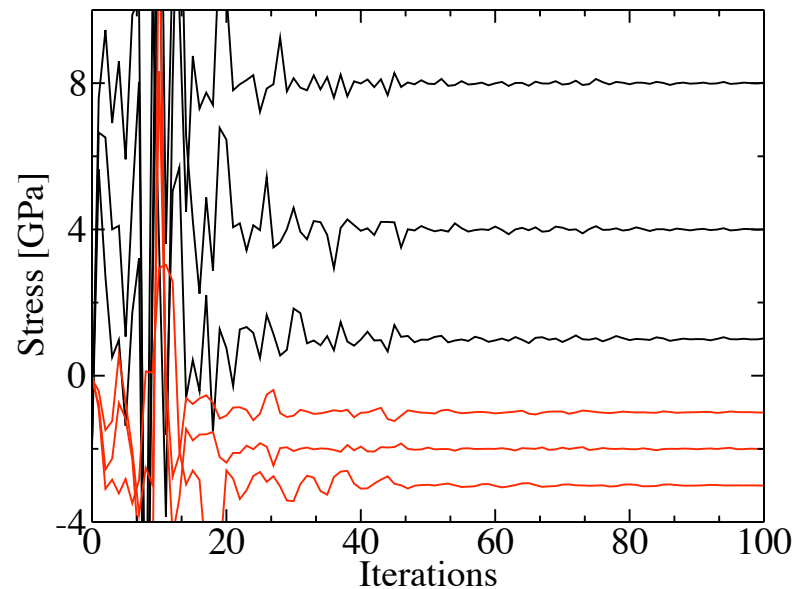
```
fix 3 ice box/relax tri 10.0 20.0 30.0 0.0 0.0 10.0 &  
nreset_ref 1000
```



# Triclinic Cell Relaxation

Non-hydrostatic target stress tensor

```
fix 1 all box/relax tri 10000.0 40000.0 80000.0 &  
-10000.0 -20000.0 -30000.0 &  
nreset_ref 10  
  
min_modify dmax 1.0e-2 line quadratic  
minimize 0.0 1.0e-10 100 200
```



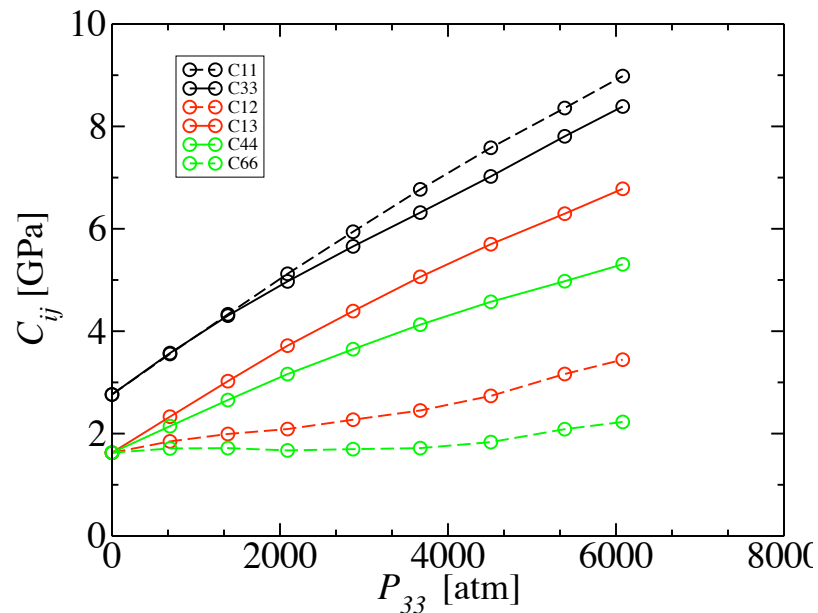
# Elastic Constants, $T = 0$

## LJ FCC crystal uniaxial strain

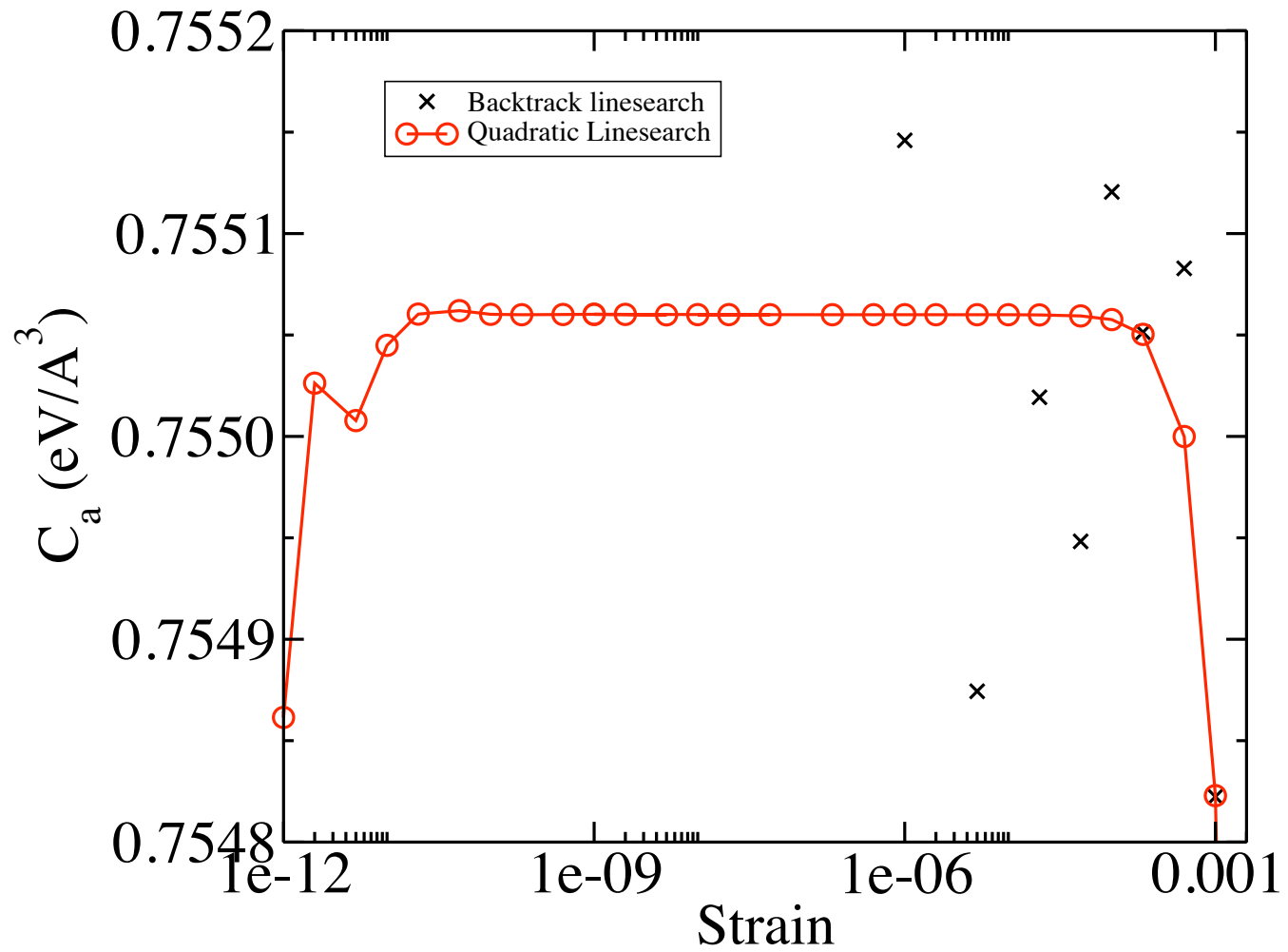
variable dneg equal  $-\{\text{up}\} * \{\text{ylen}\}$   
 displace\_box all xy delta  $\{\text{dneg}\}$

:

variable C66neg equal  $(\{\text{pxy}\} - \{\text{pxy0}\}) / \{\text{up}\}$



# Effect of Linesearch on Elastic Constant



# Summary

- Nose-Hoover chain thermostats
- Parrinello-Rahman dynamics for  $NpT$  and  $N\sigma T$
- Triclinic Box Relaxation for target  $p$  or  $\sigma$
- Elastic constants:
  - $T=0$ ,  $p \neq 0$  or  $\sigma \neq 0$  easy
  - $T > 0$  hard