Shock Simulations

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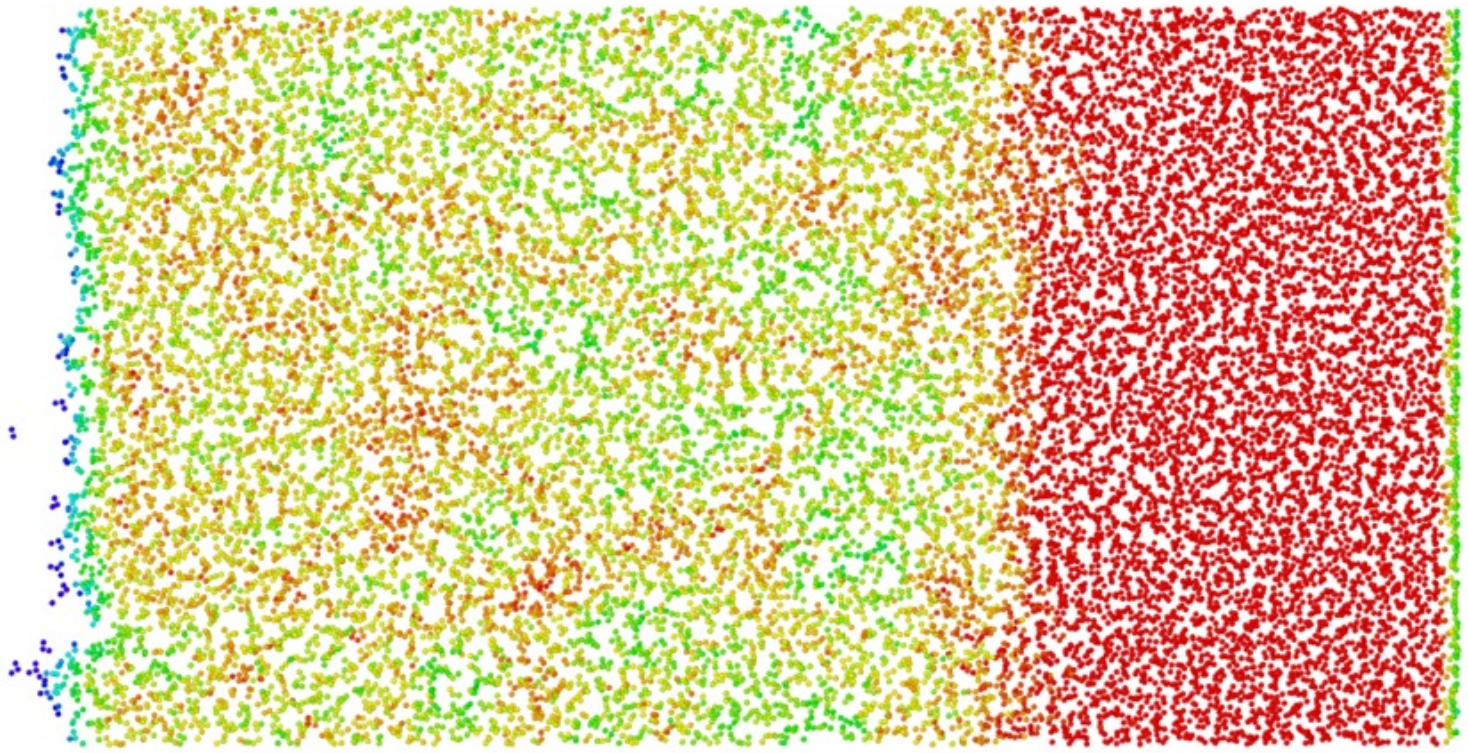


Materials Genome Innovation for Computational Software

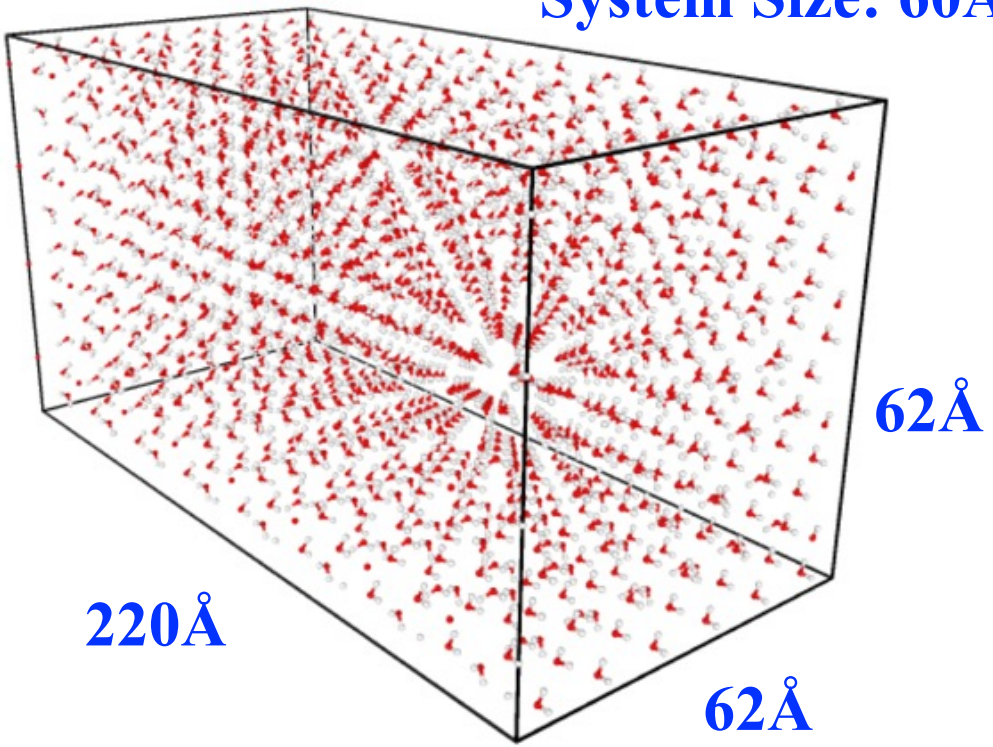
U.S. DEPARTMENT OF ENERGY | Office of Science

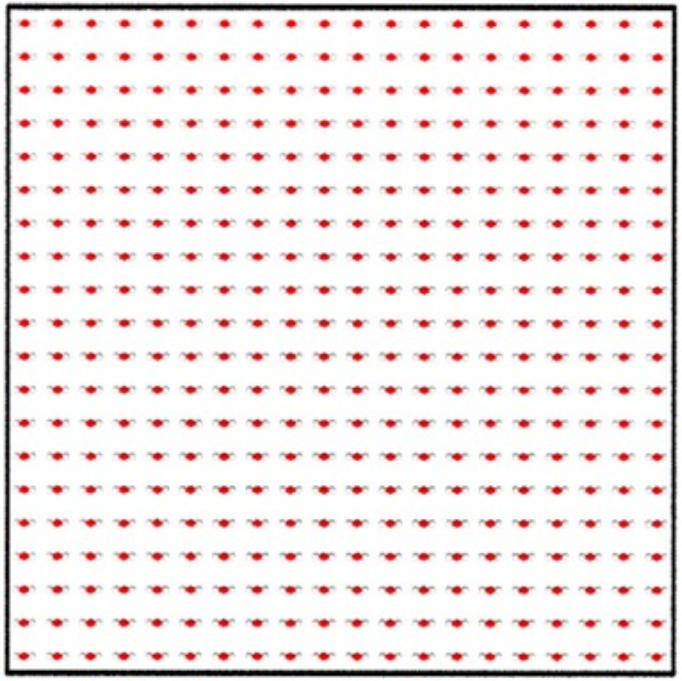
Outline

- Shock simulation setup in water
- Analysis of the simulation result

Step 1a: Create water system and define force field

System Size: 60Å×60Å×220Å

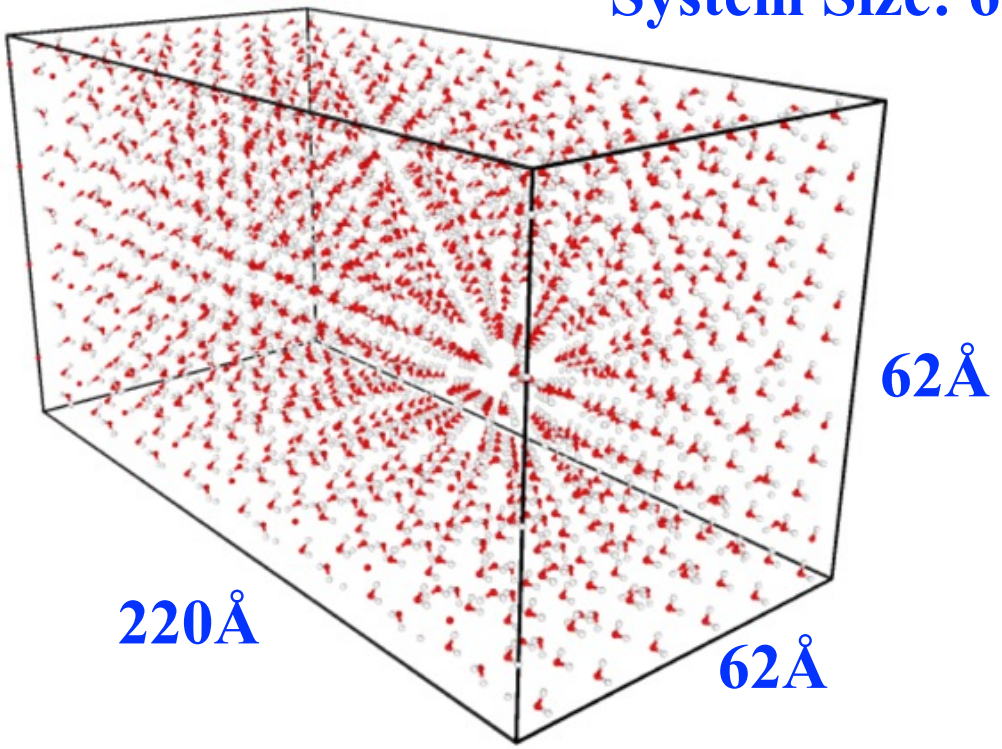


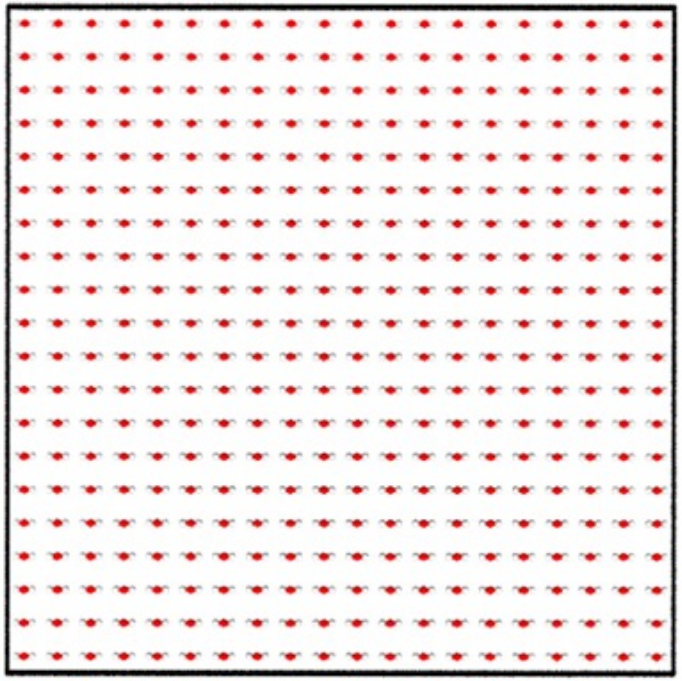


```
unit            real
Boundary        p p p
read_data       water.data
```

Step 1b: Create water system and define force field

System Size: 62Å×62Å×220Å





```
pair_style      lj/cut/tip4p/long 2 1 1 1 0.1546 8.50
kspace_style    pppm/tip4p 1.0e-5
```

Step 2: Heat the system to 300K in NVT

2a. Initialize velocities of atoms at 10K

2b. Heat to 300K and 1 atm in NPT

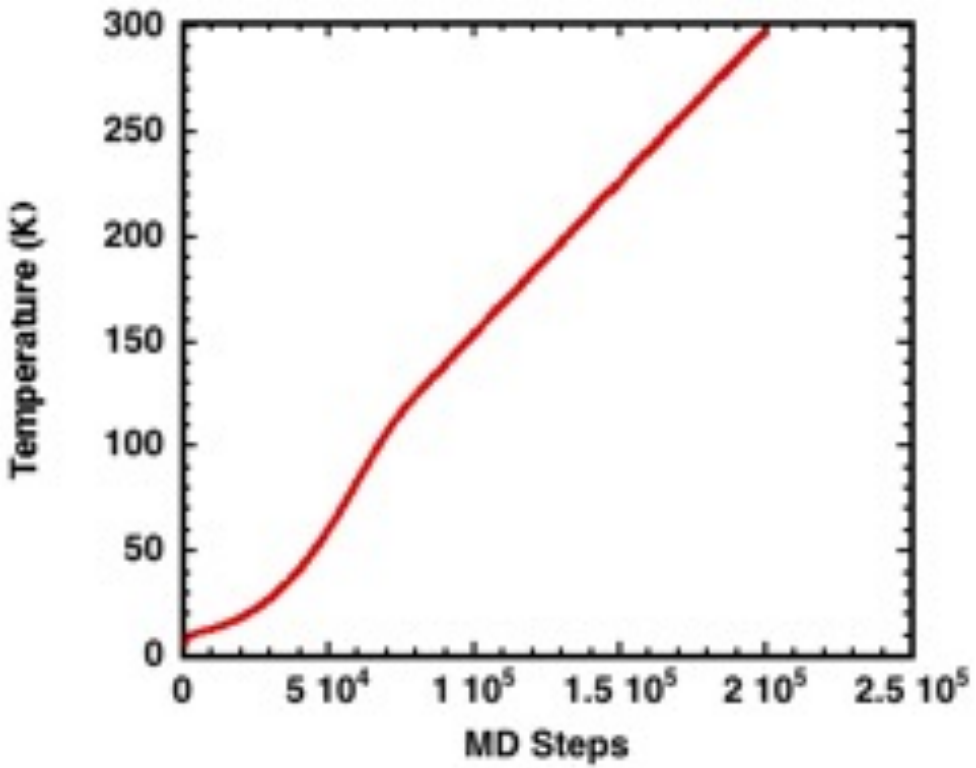
```
Velocity    all create 10.00 156 mom yes rot yes dist gaussian
fix         1 all npt temp $T1 $T2 100.0 iso $P1 $P2 1000
timestep    2.0 fs
run         50000
```

Step 2: Heat the system to 300K in NVT

2a. Initialize velocities of atoms at 10K
2b. Heat to 300K using Nose-Hoover thermostat

Velocity	**all create 10.00 156 mom yes rot yes dist gaussian**
fix	**1 all npt temp $T_1 $T_2 100.0 iso $P_1 $P_2 1000**
timestep	**2.0 fs**
run	**50000**

Temperature profile during heating



Step 3: Relax the system in NVE

Relax the system so that temperature and energy becomes constant

```
fix         1 all nve
timestep    2.0fs
run         50000
```

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```
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```
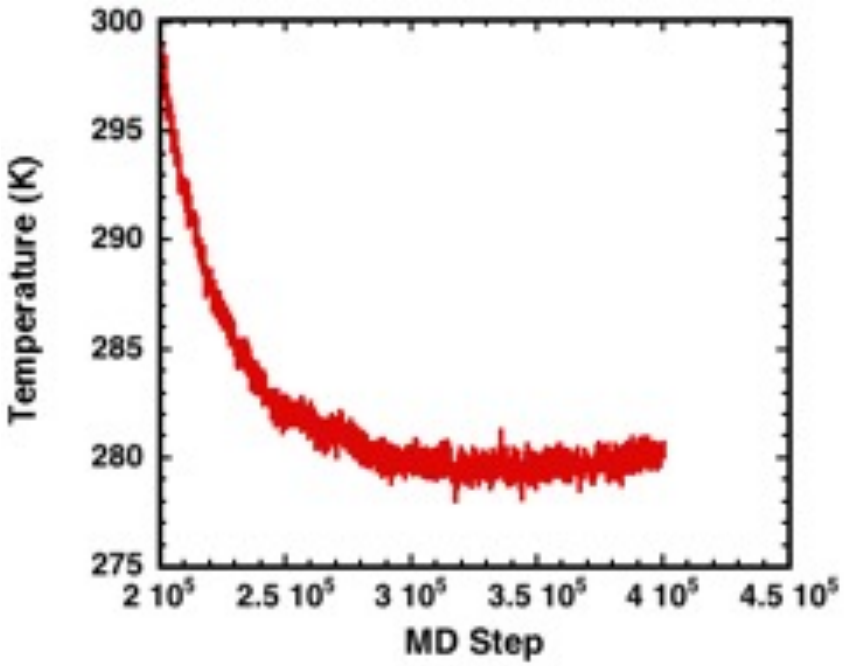
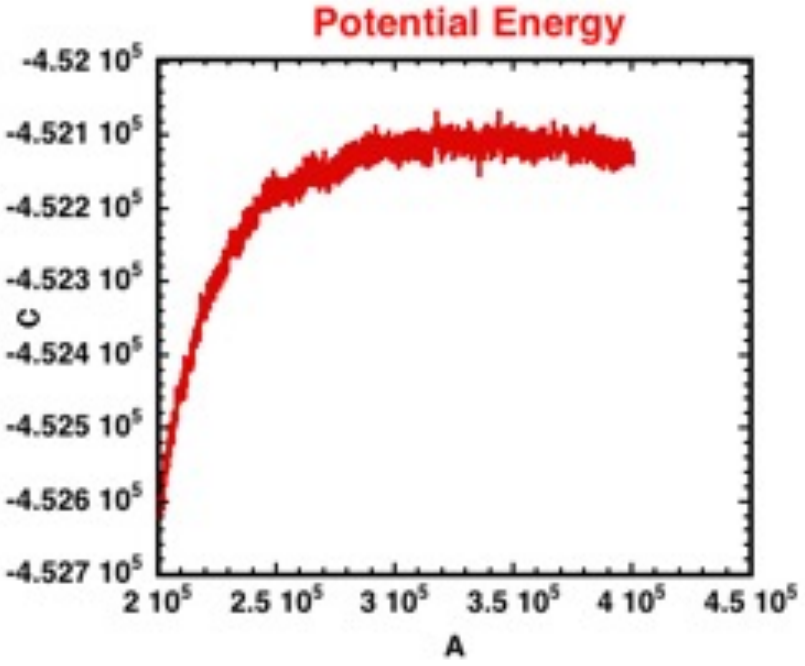
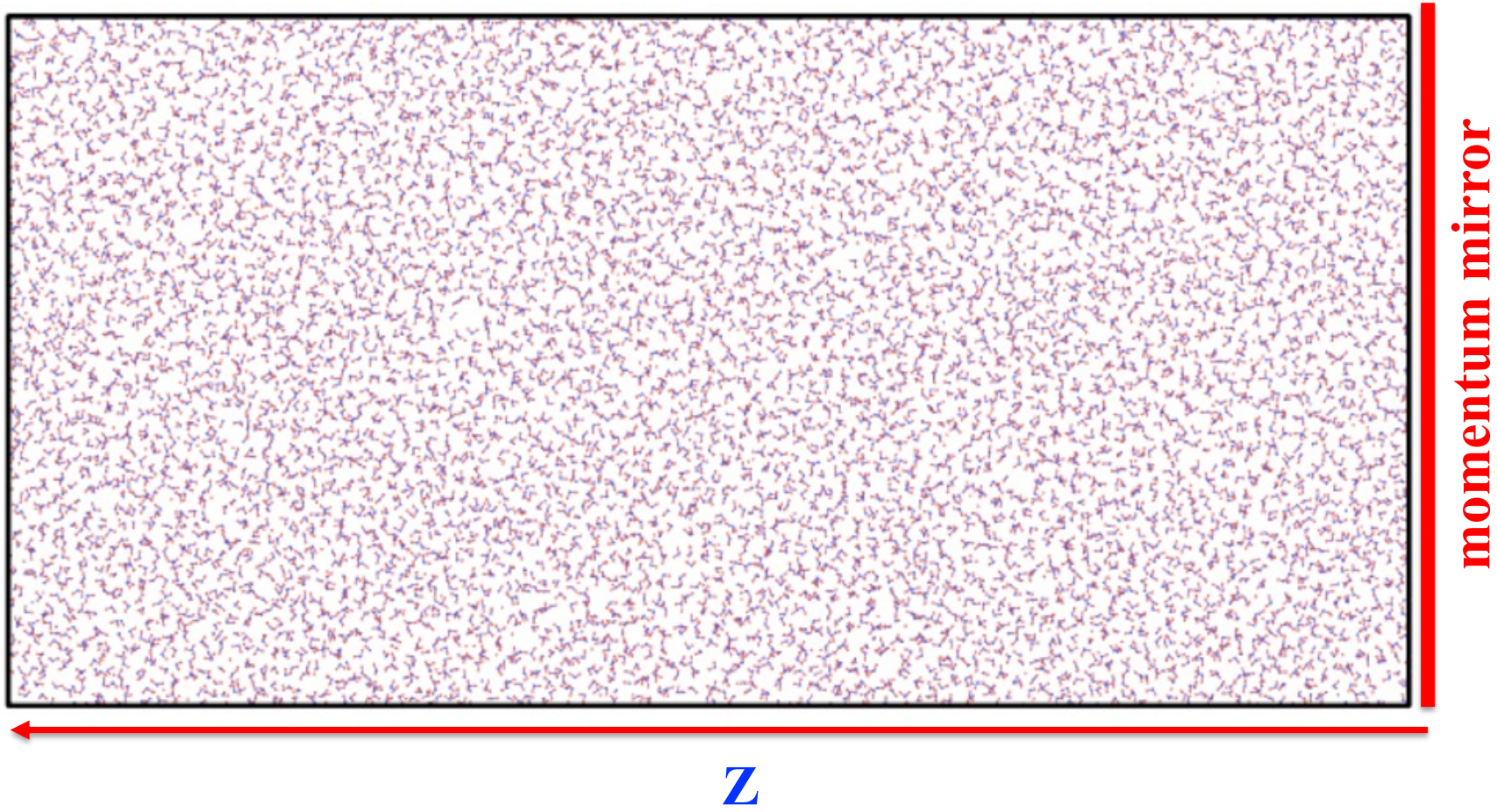





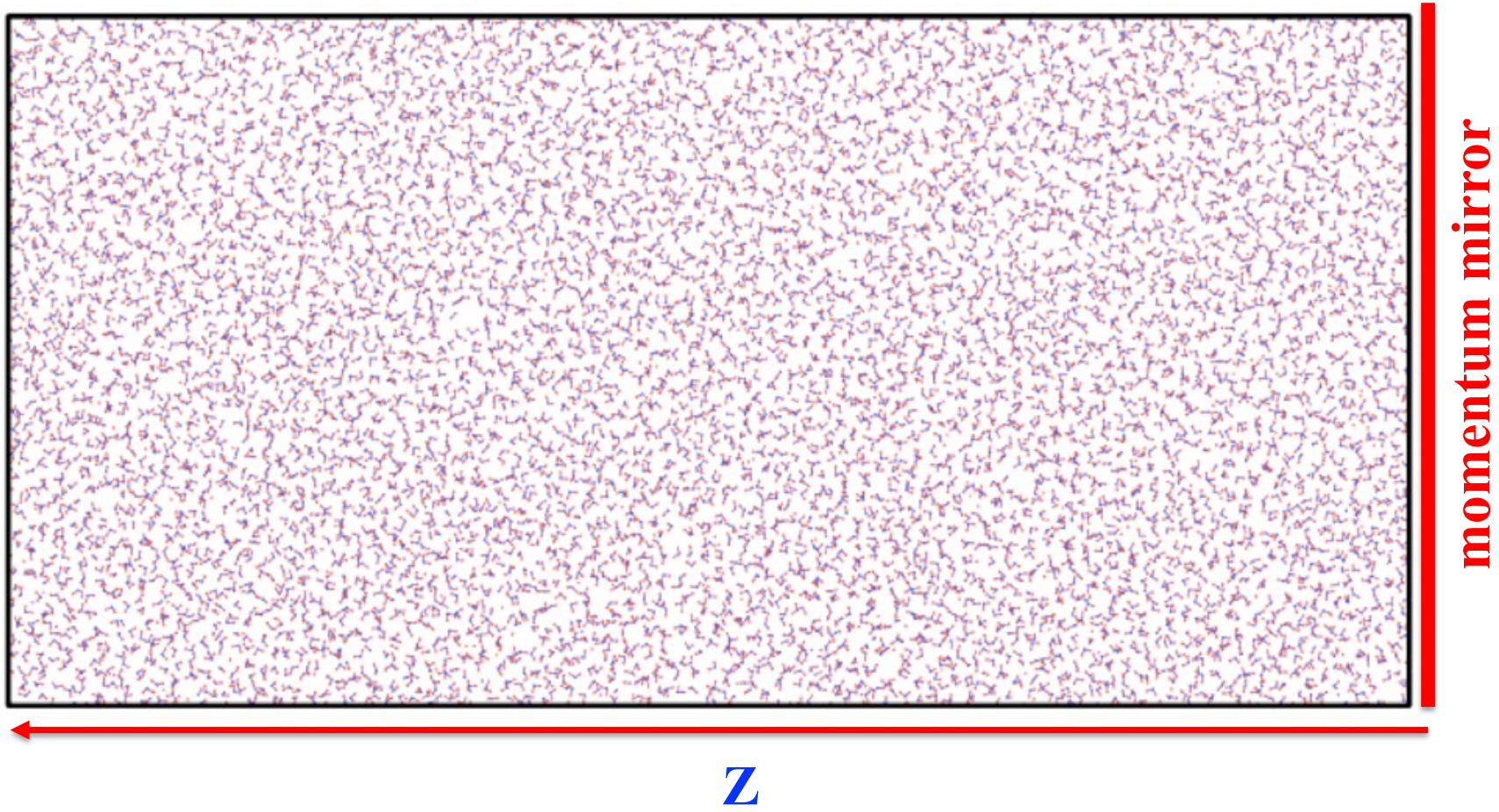
Step 4: Shock Simulation Setup

Remove periodic boundary condition from z direction
Put momentum mirror at Z= 0Å



Step 4: Shock Simulation Setup

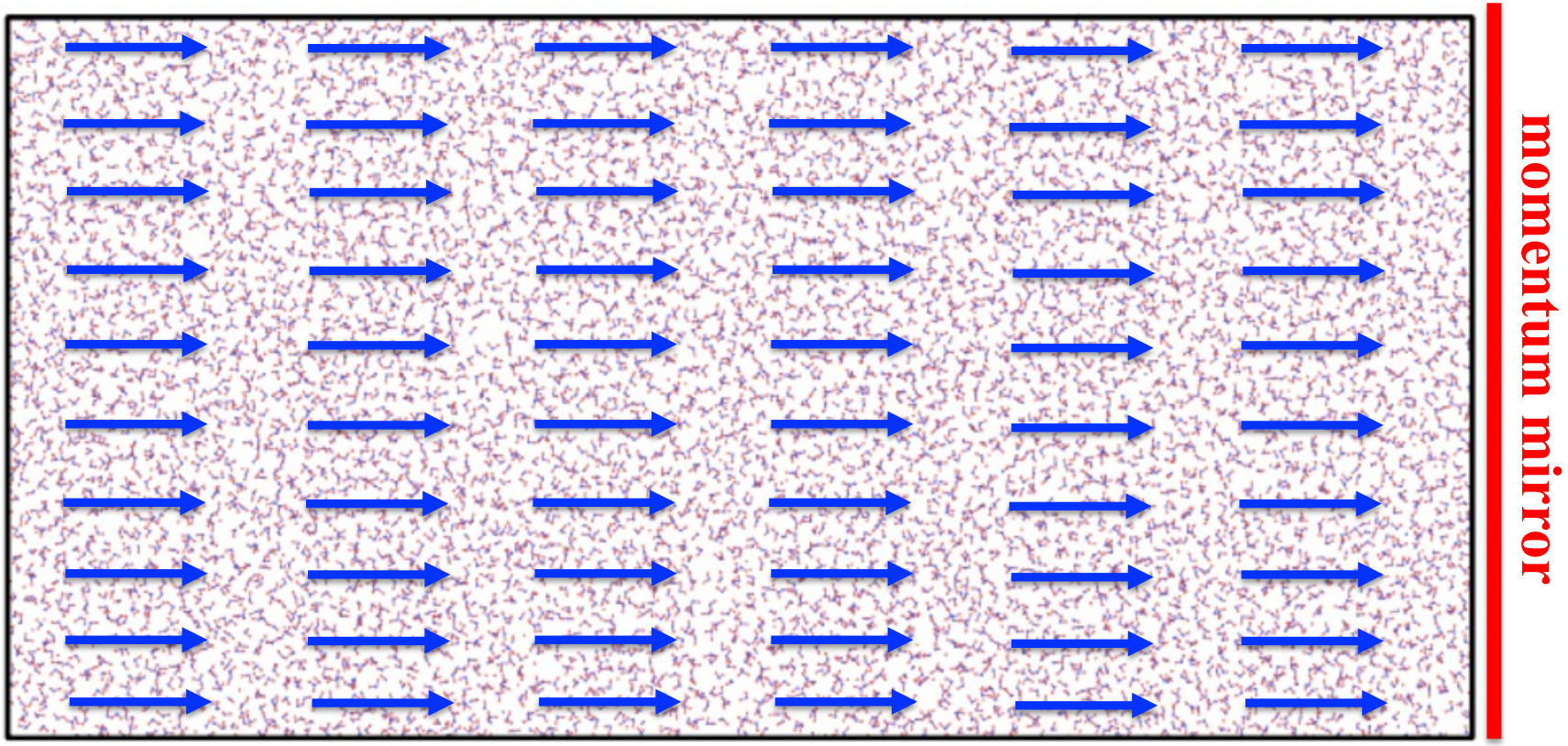
```
change_box      all boundary p p s
fix               wallr all wall/reflect zhi EDGE units box
```



Step 5: Shock Simulation in water

Give all atoms 1 km/sec velocity along +Z direction

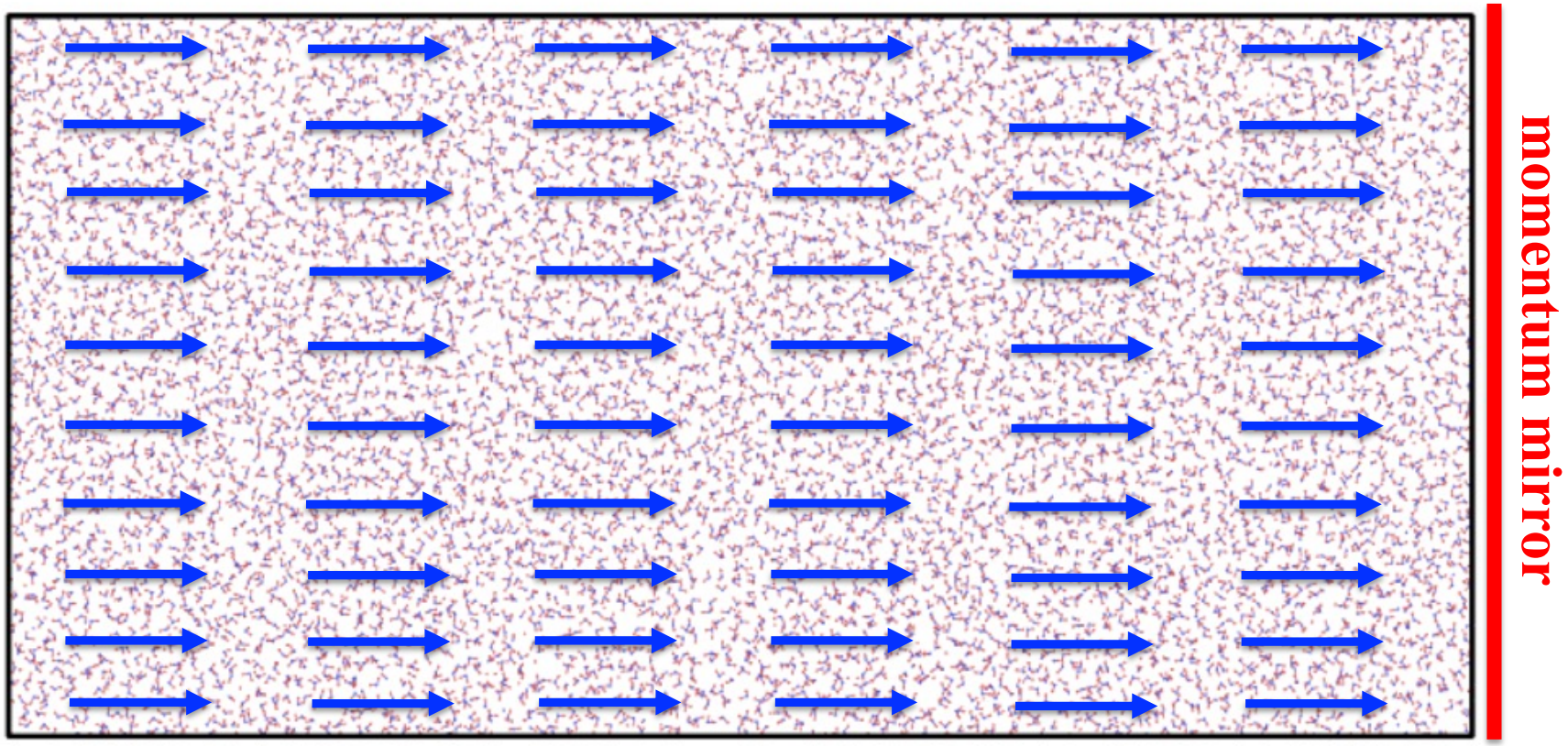
velocity all set NULL NULL 1Km/sec



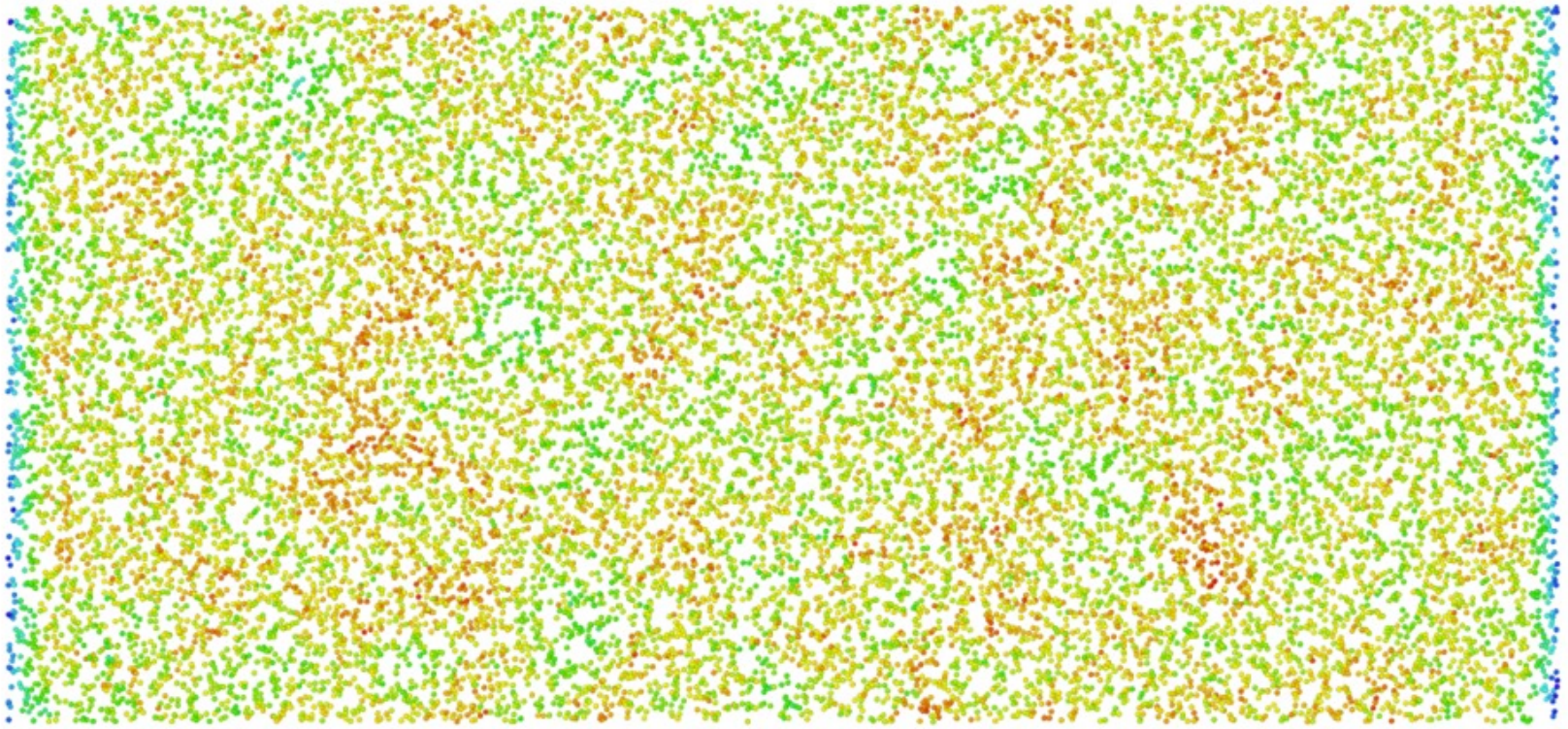
Step 5: Shock Simulation in water

Reduce time-step to 0.1fs and run under NVE for 60000 steps

```
timestep   0.1fs
run        10000
```



Step 6: Shock Simulation in water



Shock Simulation Hands-on:

Copy the shock simulation hands-on to your staging directory.

```
cp –r ~magics35/magics/shock-demo.tar.gz   .
tar xvfz shock-demo.tar.gz

cd shock-demo
ls
```

```
a.out           dumpshock.nve     job.pbs      temp.atoms
calTemp_F.f90   forcefield.tip4p  log.lammps   water.restart
Density.txt     in.shock          relax
```

Shock Simulation Hands-on:

Go to the folder shock-demo and submit a job for 10000 steps

- **qsub job.pbs**

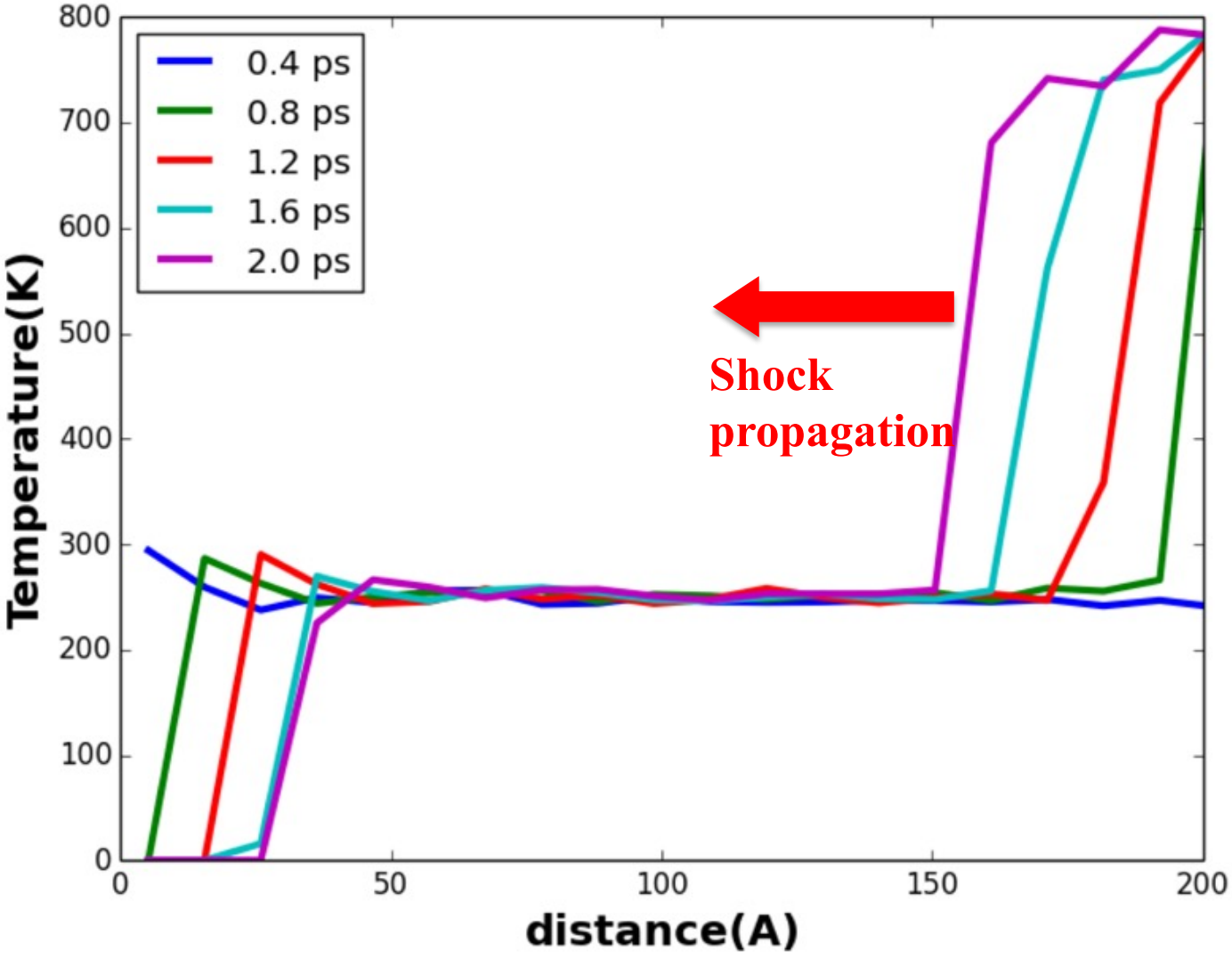
File description:

in.waterrelax (in relax folder) : creates a relaxed configuration

in.shock : does shock simulation and takes input.restart as input data which is generated by in.relax

Note: water.restart is already generated for you by running in.*waterrelax *from relax folder

Step 7: Temperature profile



Computational Challenges in Shock Simulation

Issue 1: Most interaction potential are fitted for low temperature and pressure
Example : SB potential for RDX is attractive at very small interatomic distance

Solution: Add repulsive wall in interaction potential at small distance

Computational Challenges in Shock Simulation

Issue 2: Due to the change in density of atoms inside simulation box during simulation, you simulation will speed will slow down

Solution: Dynamic Load balancing