# IMD version 3

**Minimal Demo** (with LAMMPS)

- MD simulation of Lennard-Jones liquid (Argon) (runs on remote server)
  → sends crds, velo, force, box for system every 10 steps

- Jupyter Notebook with MDAnalysis (runs locally)
  → receives crds, velo, force, box for system
  → prints info for atom 42

# Streaming Molecular Dynamics

```
## Setup
units metal
boundary p p p #periodic boundary condition for all three faces
atom_style atomic #style of atoms to be used in simulation
log    logfile.txt #write the log info to this text file

## Create Box
region forbox block 0 57.7 0 57.7 0 57.7 units box
create_box 1 forbox
lattice fcc 5.77

## Create atoms & define interactions
create_atoms 1 region forbox  basis 1 1 basis 2 1 basis 3 1 basis 4 1 units box
mass 1 39.948
pair_style lj/cut 10
pair_coeff  1 1 0.01006418 3.3952

## Create atom group for argon atoms
group ar type 1

write_data topology.data

## Prepare MD simulation
timestep  0.001
velocity all create 300 102939 dist gaussian mom yes rot yes
fix 1 all nve

dump traj all xyz 1000 traj.xyz

## IMD settings
# https:&docs.lammps.org/fix_imd.html
fix 2 all imd 8888 version 3 &
time on &
coordinates on &
velocities on &
forces on &
box on &
unwrap off &
nowait off &
trate 10

## Run MD sim
run 100000

unfix 1
#End
```

**Example:**

LAMMPS
Large-scale Atomic/Molecular Massively Parallel Simulator

www.lammps.org

MD ANALYSIS

**Trajectory File Output**

```
dump traj all xyz 1000 traj.xyz
```

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**Example:**

LAMMPS
Large-scale Atomic/Molecular Massively Parallel Simulator

MD ANALYSIS

**IMD settings**

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