Short i-PI tutorial

ICTP Trieste

Riccardo Petraglia
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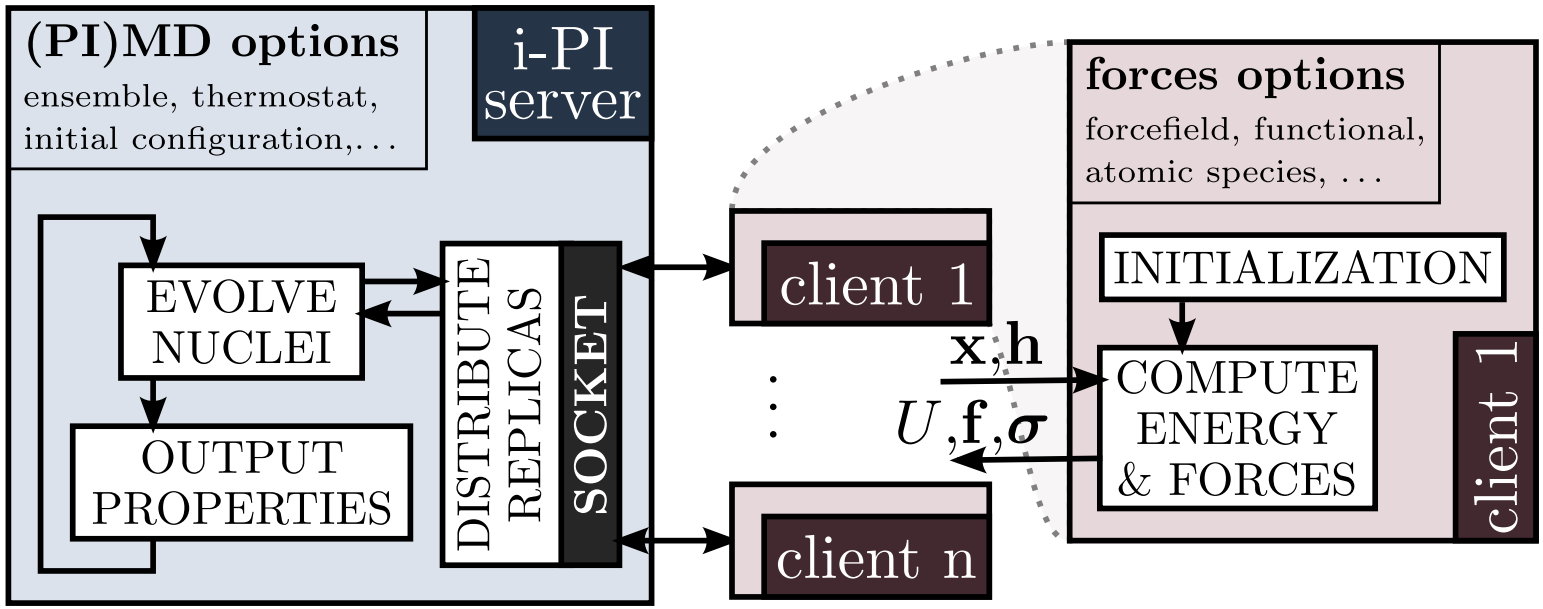
What is i-PI?

- Universal force engine interface
- Written in Python
- (not-only) with *ab-initio* force-evaluators

How i-PI works



Goal

Decouple the problem of evolving the ionic positions and the problem of computing the inter-atomic forces.

- i-PI and force calculator on different machine
- Crash-safe mechanism
- Faster than a “script” interface
- Easy to parallelize with many replicas

A look at the i-PI input

```
<simulation verbosity='medium'>
  <output prefix='npt-ice'>
    <properties stride='20' filename='out'>
        [ step, time{picosecond}, conserved{electronvolt},
        temperature{kelvin}, kinetic_cv{electronvolt}, potential{electronvolt},
        pressure_cv{megapascal}, volume, cell_h]
    </properties>
    <trajectory stride='20' filename='xc' format='xyz' cell_units='angstrom'> x_centroid{angstrom}</trajectory>
    <trajectory stride='20' filename='pos' format='xyz' cell_units='angstrom'> positions{angstrom}</trajectory>
  </output>
  <total_steps>50000</total_steps>
  <ffsocket name='force-provider' mode='unix'>
    <address>e3-1</address>
  </ffsocket>
  <system>
    <initialize nbeads='6'>
      <file mode='xyz'> ice.xyz </file>
      <velocities mode='thermal' units='kelvin'> 200 </velocities>
    </initialize>
    <forces><force forcefield='force-provider'/></forces>
    <ensemble>
      <temperature units='kelvin'> 200 </temperature>
      <pressure units='megapascal'> 10 </pressure>
    </ensemble>
    <motion mode='dynamics'>
      <dynamics mode='npt'>
        <barostat mode='isotropic'>
          <tau units='femtosecond'> 200</tau>
          <thermostat mode='langevin'>
            <tau units='femtosecond'> 100</tau>
          </thermostat>
          <h0> [ 25.6156, 0, 0, 0, 29.5783, 0, 0, 0, 27.8867 ]</h0>
        </barostat>
        <thermostat mode='langevin'>
          <tau units='femtosecond'> 100 </tau>
        </thermostat>
        <timestep units='femtosecond'> 0.25 </timestep>
      </dynamics>
    </motion>
  </system>
</simulation>
```

A look at the i-PI input

XYZ header

```
288
# position{atomic_units} CELL{abcABC}: 25.6156 29.5783 27.8867 90.0 90.0 90.0 cell{atomic_units}
O -10.5426 -11.8121 -10.8042
H -9.46578 -11.2505 -9.49096
H -12.2037 -11.442 -10.107
O -6.48712 -9.20624 -9.18277
H -6.09367 -9.24663 -7.44746
H -6.16664 -7.43114 -9.58718
```

PDB header

```
TITLE cell{atomic_units} position{atomic_units}
CRYST1    10.00    10.00    10.00  90.00  90.00  90.00 P 1           1
ATOM      1   H    1     1       0.610   10.47   6.053  0.00  0.00           0
ATOM      2   H    1     1       1.600   12.78   7.266  0.00  0.00           0
ATOM      3   O    1     1       0.064   12.23   6.458  0.00  0.00           0
```

Let's start the tutorial. . .

. . . remember I am here to answer your questions. . .