# Use MW2

# User documentation

Reference user documentation is hosted on the MW2 GitLab's wiki

https://gitlab.maisondelasimulation.fr/amarinla/mw2/wikis/home

# Input Files

# Input Files

- data.inpt
  - initial positions
  - initial velocities
  - initial forces
  - intial charges (+ history)
  - thermostat history
  - box dimension
- runtime.inpt
  - species definitions
  - interactions parameters
  - electrode charges computation parameters
  - ...
- default file name can be modified via command line option

```
./mw --input=runtime_XXX.inpt --data=data_XXX.inpt
```

# data.inpt - Header section

```
istep
n_ions n_xyz_step n_vel_step n_for_step
n_atoms n_xyz_step n_qelec_step
th_chain_length n_th_step
```

# data.inpt - Data section (1/3)

```
x(1,1) y(1,1) z(1,1)
...
x(n_ions,1) y(n_ions,1) z(n_ions,1)
...
x(n_ions,n_xyz_step) y(n_ions,n_xyz_step) z(n_ions,n_xyz_st
vx(1,1) vy(1,1) vz(1,1)
...
vx(n_ions,1) vy(n_ions,1) vz(n_ions,1)
...
vx(n_ions,n_vel_step) vy(n_ions,n_vel_step) vz(n_ions,n_vel
fx(1,1) fy(1,1) fz(1,1)
...
fx(n_ions,1) fy(n_ions,1) fz(n_ions,1)
...
fx(n_ions,n_for_step) fy(n_ions,n_for_step) fz(n_ions,n_for
```

# data.inpt - Data section (2/3)

```
x(1,1) y(1,1) z(1,1)
...
x(n_atoms,1) y(n_atoms,1) z(n_atoms,1)
q(1,1)
...
q(n_atoms,1)
...
q(n_atoms, n_qelec_step)
```

# data.inpt - Data section (3/3)

```
zeta(1,1) ... zeta(chain_length,1)
...
zeta(1,n_th_step) ... zeta(th_chain_length,n_th_step)
vzeta(1,1) ... vzeta(th_chain_length,1)
...
vzeta(1,n_th_step) ... vzeta(th_chain_length,n_th_step)
Gzeta(1,1) ... Gzeta(th_chain_length,1)
...
Gzeta(1,n_th_step) ... Gzeta(th_chain_length,n_th_step)
box_lengthx box_length_y box_length_z
```

# runtime.inpt - File format

ASCII configuration file based on 'keyword value' syntax

- Keywords are all in lower cases.
- One or more space/tab characters indicate the end of a keyword, parameters. This means that string parameters cannot have space in them, use undescore instead.
- There must be at most one keyword per line.
- The parameters associated to the keyword must be on the same line as the keyword.
- Blank lines and indentation are allowed in the configuration file, but not mandatory. They should be used to increase the readability.
- Comments are introduced by a '#' or '!' character and continue until the end of the line.
- The order of the keywords does not matter, however keywords belonging to the same block must be grouped together.

# runtime.inpt - Parameters Examples

```
# This is a comment
# Comment can be on there own line
int_parameter1 1       # or inlined
real_parameter1 1.0
true_parameter1 True
string_parameter1 One Two # 2 words

# You can add spaces to increase readability (or not)
int_parameter2 2
  real_parameter2           2.0
    string_parameter2 two

# Some keywords require multiple parameters.
# Leave at least one space character between parameters
many_parameters 1 2.0 three False
```

# runtime.inpt - Block Examples

```
# Sometimes parameters are grouped by block
# Block are introduced by a keyword without parameter
# Indentation is recommended to increase readability
block1_keyword
  block1_int  1
  block1_real 1.0

# if you don't use indentation, things get messy
# nonblock_parameter does not belong to block2 but
# only the documentation can tell you about this
block2_keyword
block2_int 2
block2_real 2.0
nonblock_parameter something_else
```

# Blue Energy Tutorial

# Blue Energy system

- Species
  - $2 \times 3649$ atoms of carbon electrodes
  - 10489 SPC/E water molecules
  - 95 Na and 95 Cl ($\approx 30 g.L^{-1}$)
  - $2 \times 400$ atoms of carbon walls
- Box
  - 2D periodic boundary conditions
  - $4.4\mathrm{nm} \times 4.4\mathrm{nm} \times 19.7\mathrm{nm}$
  - Volume of box $377\mathrm{nm}^3$
  - Width of an electrode $\approx 4.4\mathrm{nm}$
- Interactions
  - Coulomb + Lennard-Jones
- Thermostat
  - temperature: 298 K

# runtime.inpt - global parameters

```
# Global simulation parameters
# ----------------------------
timestep  41.341      # 10 fs
num_steps 1000000     # 1 000 000 * 10 fs = 10 ns

temperature  298.0    # 25 C

num_pbc   2
```

- `timestep` in atomic units ($1\mathrm{au} = 2.4\ 10^{-17}\mathrm{s}$)
- `temperature` in K

# thermostat parameters

```
# Thermostat
# ----------
thermostat
   relaxation_time 1000
   max_iteration   50
   tolerance       1.0e-17
   chain_length    5
```

- Thermostat is used if this block is present
- All parameters are optional and the default value are shown here
- `relaxation_time` corresponds to $\omega^{-1}$ in the equations

# Ion species parameters

```
# Ion species definition
# ----------------------
ions

  ion_type
    name   O                    # name of the species
    count  10489                # number of species
    charge -0.8476              # permanent charge on the ions
    mass   15.996               # mass in amu
    mobile True
```

- `ions` are point charge species which can be mobile or not
- `charge` in atomic unit ($1\mathrm{au} = 1e$)
- `mass` in atomic mass unit (u) (this is not atomic unit! $1\mathrm{au} = 1m_e = 5.488\ 10^{-4}\mathrm{u}$)

# Ion species parameters

```
ion_type
  name   H1                  # name of the species
  count  10489               # number of species
  charge 0.4238              # permanent charge on the ions
  mass   1.0008              # mass in amu
  mobile True

ion_type
  name   H2                  # name of the species
  count  10489               # number of species
  charge 0.4238              # permanent charge on the ions
  mass   1.0008              # mass in amu
  mobile True
```

- The two H sites in the water molecules must be defined as two distinct species

# Ion species parameters

```
ion_type
  name   Na                  # name of the species
  count  95                  # number of species
  charge 1.000               # permanent charge on the ions
  mass   22.990              # mass in amu

ion_type
  name   Cl                  # name of the species
  count  95                  # number of species
  charge -1.000              # permanent charge on the ions
  mass   35.453              # mass in amu
```

- `mobile` is an optional keyword. By default, ions are mobile.

# Ion species parameters

```
ion_type
  name   P                    # name of the species
  count  400                  # number of species
  mass   12                   # mass in amu
  charge 0.000                # fixed charge
  mobile False
```

- Fixed wall neutral particles

# Molecule parameters

```
# Molecule definitions
# --------------------
molecules

  molecule_type
    name  water
    count 10489
    sites O H1 H2

    constraint   O  H1  1.88973  # 0.1 nm
    constraint   O  H2  1.88973  # 0.1 nm
    constraint  H1  H2  3.08589  # HOH = 109.47 °

    constraints_algorithm rattle 1.0e-8 100
```

- constraint distance in au
- rattle parameters are $\epsilon$ and maximum number of iteration.

# Electrodes parameters

```
electrodes
  electrode_charges cg 5.0e-8 100
```

- Compute electrode electrode charges with conjugate gradient
- cg parameters are $\epsilon$ and maximum number of iteration.
- CG converged when $|res| < \sqrt{N} * \epsilon$

# Electrode types parameters

```
electrode_type
  name      C1
  count     3649
  eta       0.955234657
  potential +0.000

electrode_type
  name      C2
  count     3649
  eta       0.955234657
  potential -0.000
```

- `eta` gaussian charge distribution parameter
- `potential` in atomic unit ($1\mathrm{au} = 27.2\mathrm{V}$)

# Coulomb interactions

```
# Interactions definition
# ----------------------
interactions
  coulomb
    coulomb_rcut        41.29
    coulomb_rtol        1.0e-10
    coulomb_ktol        1.0e-10
```

- `rcut` in atomic unit
- In production, always use maximum value: $r_c = \frac{1}{2}\min(a, b, c)$
- $\frac{1}{|r_c|}\exp(-\alpha^2|r_c|^2) < \epsilon_r$
- $\frac{1}{|k_c|^2}\exp(-\frac{|k_c|^2}{4\alpha^2}) < \epsilon_k$

# Coulomb interactions

```
# Interactions definition
# ----------------------
interactions
  (...)
  lennard-jones
     lj_rcut 41.29
      # LJ interactions parameters (eps,sig) for a pair of
      #                eps in kJ/mol  sig in angstrom
      lj_pair O   O  6.50465E-01    3.16600E+00
      lj_pair O  Na  5.34518E-01    2.87650E+00
      lj_pair O  Cl  5.34517E-01    3.78350E+00
      (...)
```

- `rcut` in atomic unit
- Only half of the pair needs to be defined because symmetry is imposed
- If a pair is not defined, it gets $\epsilon = 0$ and $\sigma = 0$

# Output

```
output
  default      0
  trajectories 10
  charges      1
  restart      1000
  energies     100
  forces       0
```

- periodicity of outputs for each type of file in number of steps
- 0 turns off output
- `trajectories` prints out (x,y,z) and (vx,vy,vz) data for all mobile particles
- `charges` prints charges on all electrode atoms
- `restart` creates data.inpt files
- `energies` prints energies breakdown. Energy is computed only for those timesteps.
- `forces` prints forces breakdown.

# Output files

# Output Files

- Several output files:
  - run.out
  - trajectories.out
  - charges.out
  - forces.out
  - energies.out and energies_breakdown.out
- By default, only *root* does output.

  `./mw --output-rank=[root|all|rank-ids]`
- If *all* or list of rank-ids is provided then rank id is appended to file name: run.out $\rightarrow$ run_000000.out

# run.out - Compilation information

```
MetalWalls 00.00
commit aa88c5e4b405c625bf7902918059ac29e99a3e79

Compiled with Intel Fortran 18. 0. 0 on  Jul 05 2018 at   (
MPI library version 3.1
HOSTNAME: jrl09
F90:       mpif90
F90FLAGS: -g -O2 -xHost -align array64byte
FPPFLAGS: -fpp
LDFLAGS:

GCCcore/.5.5.0
binutils/.2.30
StdEnv
icc/.2018.2.199-GCC-5.5.0
ifort/.2018.2.199-GCC-5.5.0
Intel/2018.2.199-GCC-5.5.0
ParaStationMPI/5.2.1-1
```

# run.out - System information

```
System parameters:
==================

Time step:                4.13410E+01
Number of steps:                   10
Total simulation time:    4.13410E+02

Total number of molecules:                10489
Total number of ions:                     32057
Total number of atoms:                     7298
Total number of degrees of freedom:       63501

(...)
```

- Verify that what the code does is what you intended to do
- All values are in atomic units, except for temperature in K

# run.out - SR-interaction matrices

```
|ewald| Short-Range interaction matrices:
|ewald| ion <-> ion
|ewald| X X X X X X
|ewald| X X X X X X
|ewald| X X X X X X
|ewald| X X X X X X
|ewald| X X X X X X
|ewald| X X X X X X
|ewald| atom <-> atom
|ewald| X O
|ewald| O X
```

- Show which types interacts with each other for coulomb real space interactions
- Here the 2 electrodes only interact with themselves

# run.out - step info

```
|step| step      1
|step| step      1 /     10 in this run.
|step| elapsed time:         ?.?????E+??
|step| temperature:          3.00379E+02 K
|step| Global charge on electrode  1: -6.37052E-03
|step| Global charge on electrode  2:  1.39116E-02
|step| Global charge on electrodes:    7.54109E-03
|cg| number of iterations:            96
|cg| Residual norm:          5.98632E-09
|cg| Residual target:        8.54283E-09
```

# run.out - time

```
Total elapsed time:  ?.?????E+?? seconds.

Elapsed Times breakdown:
========================
                      average (s)   cumul. (s) fraction (%)
  initialization:  ?.?????E+??  ?.?????E+??         ??.??
  setup:           ?.?????E+??  ?.?????E+??         ??.??
  main loop:       ?.?????E+??  ?.?????E+??         ??.??

Ions->Atoms Coulomb potential
-----------------------------
  long range       ?.?????E+??  ?.?????E+??         ??.??
  k==0             ?.?????E+??  ?.?????E+??         ??.??
  short range      ?.?????E+??  ?.?????E+??         ??.??

(...)
```

# trajectories.out

```
# Trajectories of mobile particles in atomic unit
# ---------------------------------------------
# Length:   1 au = 0.052917721067 nm
# Velocity: 1 au = 2.1876912633e6 m.s^-1
# step         0
#   x          y          z         vx         vy         vz
+7.32E+1 +7.27E+1 +1.42E+1 -1.50E-3 -1.55E-3 -1.34E-3
(...)
```

- Output format truncated to fit in the slide
  - `+7.32E+1` $\rightarrow$ `+7.32191796000000E+001`
- Trajectories are given only for mobile species
- Last 2 header lines are repeated for each output step
- 1 empty line between 2 steps data

# charges.out

```
# Electrode atom charges in atomic unit
# ------------------------------------
# Charge:    1 au = 1.602176565e-19 C = 1 e
# step         0
+7.657118215562047E-004
(...)
```

- Charges are given only for electrode species
- Last header line is repeated for each output step
- 1 empty line between 2 steps data

# forces.out

```
# Forces on mobile particles in atomic unit
# ----------------------------------------
# Force:   1 au = 8.2387225e-8 N = 51.421 eV/angstrom
# step         0
# fx_t     fy_t     fz_t     fx_c     fy_c     fz_c
+1.5E-2 +1.3E-2 -9.6E-3 +1.9E-2 +2.4E-2 +2.0E-3
~    fx_i     fy_i     fz_i     fx_m     fy_m     fz_m
~ -3.9E-3 -1.0E-2 -1.1E-2 +0.0E+0 +0.0E+0 +0.0E+0
```

- Output format truncated to fit in the slide
  - +1.5E-2 $\rightarrow$ +1.59076879578622E-002
  - lines are wrapped
  - t = total, c = coulomb, i = intermolecule, m = intramolecular
- Forces are given only for mobile species
- Last 2 header lines are repeated for each output step
- 1 empty line between 2 steps data

# energies.out

```
# Energy in atomic unit (1 Eh = 2625.499640 kJ/mol)
# ------------------------------------------------
#s    Tot       Kin       Pot      Coul      Intra    Inter    Therm
 0 -1.6E+2   4.4E+1 -2.1E+2 -2.5E+2   0.0E+0   3.7E+1   0.0E+0
```

-1.67458274687477 8E+002

- Output format truncated to fit in the slide
  - `+1.6E+2` → `-1.67458274687477 8E+002`
  - s = step index
- 1 line per step
- energies_breakdown.out adds more detailed information:
  - coulomb energy for sr, lr, self, k=0, intra-molecular
  - intra-molecular for harmonic potentials
  - Fumi-Tosi, Lennard-Jones

# Performances

# Performances - Time to solution (s)

Blue Energy 10 time step

| Machine | Processor | Nodes | MPI ranks | MW1 | MW2 |
|---|---|---|---|---|---|
| Jureca | HSW | 2 | 48 | 87.58 | 31.63 |
| Irene | SKL | 1 | 48 | N/A | 39.01 |

$\times$2.7 performance improvement on Haswell architecture

- Predictor starts only after 6 steps
- On Irene, AVX512 not fully exploited
- TODO: test performance with different cache block sizes and pair block sizes

# Performances - Strong Scaling

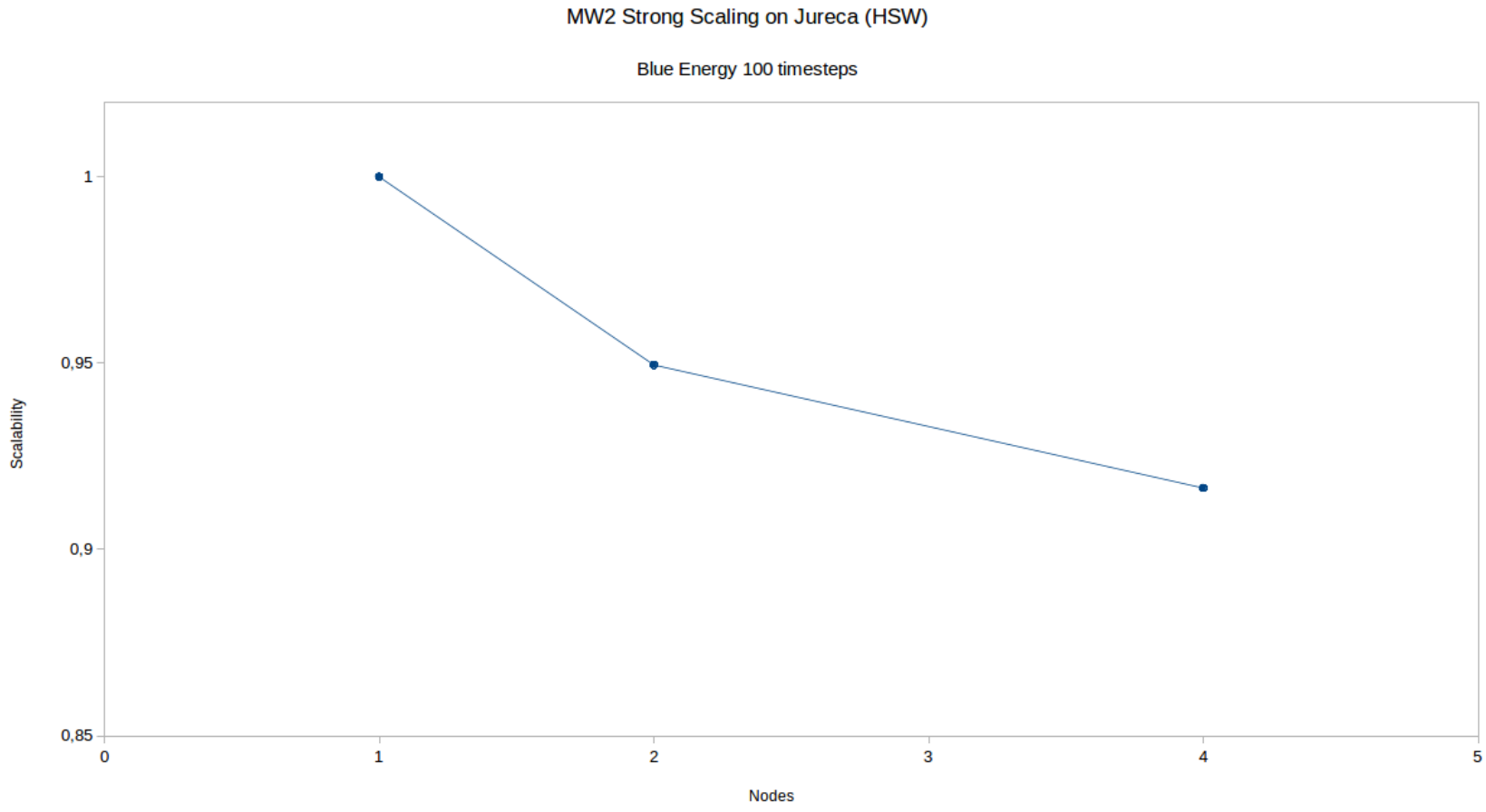


Figure 1: MW2 Scalability

- 91% strong scaling at 4 nodes (96 MPI ranks)