Chapter 1: Overview

1.1 Basic input information

Specific the type of simulation in the script by a set of keywords.

- CREATE: random generation of grains in the simulation cell with given grain size distribution, e.g. FRACTAL, UNIFORM, VOLUME. It will produce a very loose sample.
- EVOLVE: this can include procedures as pre-compaction, pre-shearing, and actual simulation processes.

Input and export directories.

Boundary conditions

Simulation types

- CONDUCTION
- PRODUCTION
- EXPANSION

Mechanical properties

- MODULE_N
- FRICTION
- TANG_CONSTANT
- ROLL_CONSTANT

Thermal properties

- CONDUCTIVITY
- SPECIFIC_HEAT
- THER_EXPANSION

Liquid phase properties

- GRAVITY
- MAX_SCAN
- MIN_SCAN
- SURFACE_TENSION

Simulation time and output control

- T_INIT
- T_END
- SAVE_BEGIN
- SAVE_PERIOD

Listing 1.1: "Typical script for input parameters."

```
./SD_parallel<<!
EVOLVE
./data/prepack-p001   51
./data/g1e-3_s0109 1
PERIODIC_SHEAR
CONDUCTION     NO
PRODUCTION     NO
EXPANSION      NO
NORMAL_STRESS  0.001
SHEAR_RATE     0.0
MODULE_N       1000
FRICTION       0.5
TANG_CONSTANT  1
ROLL_CONSTANT  1
CONDUCTIVITY   1
SPECIFIC_HEAT  100
THER_EXPANSION 0.000001
COMP_FRACTION  1.0
WETTING
GRAVITY        0.001
MAX_SCAN       0.9
MIN_SCAN       0.1
SURFACE_TENSION 0.01
T_INIT         0
T_END          4000
SAVE_BEGIN     0
SAVE_PERIOD    10
NO_MORE_TASK
!
```