

Week 1 Molecular Dynamics

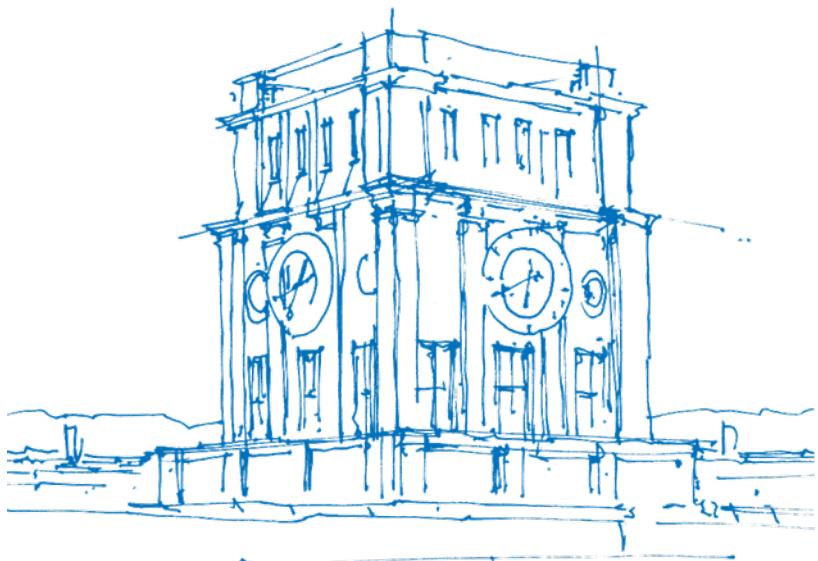
Alex Hocks Jan Hampe Johannes Riemenschneider

Technische Universität München

TUM CIT

Lehrstuhl für wissenschaftliches Rechnen

16. November 2022



TUM Uhrenturm

Example of new input file

```
#Random comments
# xyz-coord      velocity      mass      shape      dimensions      distance
2
0.0 0.0 0.0      0.0 0.0 0.0      1.0
7.0 7.0 7.0      1.0 1.0 1.0      2.0e-8      Cuboid      4          5          6          3.0
# epsilon      sigma
0.1            0.2
```

Structure:

- Comments
- Number of bodies

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Structure:

- Comments
- Number of bodies
- Bodies (with Shape, Dimensions and distance as optional)

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```

Structure:

- Comments
- Number of bodies
- Bodies (with Shape, Dimensions and distance as optional)
- Comments
- Definition of epsilon and sigma (optional)

Input parsing - Definition of Body

```
enum Shape {cuboid, sphere};

struct Body {
    Shape shape;
    Eigen::Vector3d fixpoint;
    Eigen::Vector3d dimensions;
    double distance;
    double mass;
    Eigen::Vector3d start_velocity;
};
```

