

Week 1 Molecular Dynamics

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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:

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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;
} ;
```