Chapter 2

Definitions and Units

2.1 Notation

The following conventions for mathematical typesetting are used throughout this document:

Item	Notation	Example
Vector	Bold italic	$\boldsymbol{r}_i$
Vector Length	Italic	r_i

We define the *lowercase* subscripts i, j, k and l to denote particles: $\boldsymbol{r}_i$ is the *position vector* of particle i, and using this notation:

$$\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i \tag{2.1}$$

$$r_{ij} = |\boldsymbol{r}_{ij}| \tag{2.2}$$

The force on particle i is denoted by $\boldsymbol{F}_i$ and

$$\boldsymbol{F}_{ij} = \text{force on } i \text{ exerted by } j \tag{2.3}$$

Please note that we changed notation as of version 2.0 to $\boldsymbol{r}_{ij} = \boldsymbol{r}_j - \boldsymbol{r}_i$ since this is the notation commonly used. If you encounter an error, let us know.

2.2 MD units

GROMACS uses a consistent set of units that produce values in the vicinity of unity for most relevant molecular quantities. Let us call them *MD units*. The basic units in this system are nm, ps, K, electron charge (e) and atomic mass unit (u), see Table 2.1.

Consistent with these units are a set of derived units, given in Table 2.2.

The **electric conversion factor** $f = \frac{1}{4\pi\varepsilon_o} = 138.935\,485(9)$ kJ mol^{-1} nm e^{-2}. It relates the mechanical quantities to the electrical quantities as in

$$V = f\frac{q^2}{r} \quad \text{or} \quad F = f\frac{q^2}{r^2} \tag{2.4}$$

Quantity	Symbol	Unit
length	r	nm $= 10^{-9}$ m
mass	m	u (atomic mass unit) $= 1.6605402(10)\times10^{-27}$ kg
		($1/12$ the mass of a ^{12}C atom)
		$1.6605402(10) \times 10^{-27}$ kg
time	t	ps $= 10^{-12}$ s
charge	q	e = electronic charge $= 1.60217733(49) \times 10^{-19}$ C
temperature	T	K

Table 2.1: Basic units used in GROMACS. Numbers in parentheses give accuracy.

Quantity	Symbol	Unit
energy	E, V	kJ mol^{-1}
Force	$\boldsymbol{F}$	kJ mol^{-1} nm^{-1}
pressure	p	kJ mol^{-1} nm^{-3} $= 10^{30}/N_{AV}$ Pa
		$1.660\,54 \times 10^{6}$ Pa $= 16.6054$ bar
velocity	v	nm ps^{-1} $= 1000$ m s^{-1}
dipole moment	μ	e nm
electric potential	Φ	kJ mol^{-1} $e^{-1} = 0.010\,364\,272(3)$ Volt
electric field	E	kJ mol^{-1} nm^{-1} $e^{-1} = 1.036\,427\,2(3) \times 10^{7}$ V m^{-1}

Table 2.2: Derived units

Electric potentials Φ and electric fields $\boldsymbol{E}$ are intermediate quantities in the calculation of energies and forces. They do not occur inside GROMACS. If they are used in evaluations, there is a choice of equations and related units. We strongly recommend following the usual practice of including the factor f in expressions that evaluate Φ and $\boldsymbol{E}$:

$$\Phi(\boldsymbol{r}) = f \sum_j \frac{q_j}{|\boldsymbol{r} - \boldsymbol{r}_j|} \tag{2.5}$$

$$\boldsymbol{E}(\boldsymbol{r}) = f \sum_j q_j \frac{(\boldsymbol{r} - \boldsymbol{r}_j)}{|\boldsymbol{r} - \boldsymbol{r}_j|^3} \tag{2.6}$$

With these definitions, $q\Phi$ is an energy and $q\boldsymbol{E}$ is a force. The units are those given in Table 2.2: about 10 mV for potential. Thus, the potential of an electronic charge at a distance of 1 nm equals $f \approx 140$ units ≈ 1.4 V. (exact value: 1.439965 V)

Note that these units are mutually consistent; changing any of the units is likely to produce inconsistencies and is therefore *strongly discouraged*! In particular: if Å are used instead of nm, the unit of time changes to 0.1 ps. If kcal mol^{-1} (= 4.184 kJ mol^{-1}) is used instead of kJ mol^{-1} for energy, the unit of time becomes 0.488882 ps and the unit of temperature changes to 4.184 K. But in both cases all electrical energies go wrong, because they will still be computed in kJ mol^{-1}, expecting nm as the unit of length. Although careful rescaling of charges may still yield consistency, it is clear that such confusions must be rigidly avoided.

In terms of the MD units, the usual physical constants take on different values (see Table 2.3). All quantities are per mol rather than per molecule. There is no distinction between Boltzmann's constant k and the gas constant R: their value is $0.008\,314\,51$ kJ mol^{-1} K^{-1}.

Symbol	Name	Value
N_{AV}	Avogadro's number	$6.022\,136\,7(36) \times 10^{23}$ mol^{-1}
R	gas constant	$8.314\,510(70) \times 10^{-3}$ kJ mol^{-1} K^{-1}
k_B	Boltzmann's constant	*idem*
h	Planck's constant	$0.399\,031\,32(24)$ kJ mol^{-1} ps
$\hbar$	Dirac's constant	$0.063\,507\,807(38)$ kJ mol^{-1} ps
c	velocity of light	$299\,792.458$ nm ps^{-1}

Table 2.3: Some Physical Constants

Quantity	Symbol	Relation to SI
Length	r*	r σ^{-1}
Mass	m*	m M^{-1}
Time	t*	t σ^{-1} $\sqrt{\epsilon/M}$
Temperature	T*	k$_B$T ϵ^{-1}
Energy	E*	E ϵ^{-1}
Force	F*	F σ ϵ^{-1}
Pressure	P*	P $\sigma^3\epsilon^{-1}$
Velocity	v*	v $\sqrt{M/\epsilon}$
Density	ρ^*	N σ^3 V^{-1}

Table 2.4: Reduced Lennard-Jones quantities

2.3 Reduced units

When simulating Lennard-Jones (LJ) systems, it might be advantageous to use reduced units (*i.e.*, setting $\epsilon_{ii} = \sigma_{ii} = m_i = k_B = 1$ for one type of atoms). This is possible. When specifying the input in reduced units, the output will also be in reduced units. The one exception is the *temperature*, which is expressed in $0.008\,314\,51$ reduced units. This is a consequence of using Boltzmann's constant in the evaluation of temperature in the code. Thus not T, but k_BT, is the reduced temperature. A GROMACS temperature $T = 1$ means a reduced temperature of $0.008\ldots$ units; if a reduced temperature of 1 is required, the GROMACS temperature should be 120.2717.

In Table 2.4 quantities are given for LJ potentials:

$$V_{LJ} = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{2.7}$$