

# 1 Introduction

## 1.1 Examples of N-body systems

(slides on molecular dynamics and gravitational dynamics)

## 1.2 Basic notation

Consider a  $N$ -body system in which each body is represented by a point particle with position

$$\mathbf{r}_i = (r_{ix}, r_{iy}, r_{iz})^\top$$

Here we will generally consider “real-world” systems where the particles are located in three-dimensional Euclidean space,  $\mathbf{r}_i \in \mathbb{R}^3$ . Nothing prevents us from considering other spaces, such as two-dimensional spaces. Most equations will not change qualitatively when working in different dimensions, only a factors that depend on the dimensionality will be different. If the system is dynamic, these positions also depend on time, i.e.  $\mathbf{r}_i(t) = (r_{ix}(t), r_{iy}(t), r_{iz}(t))^\top$ , but we will consider that in the next section. For simplicity of notation, we write all positions of the  $N$ -body system in a single  $3N$ -dimensional vector

$$\mathbf{r} = (\mathbf{r}_1, \dots, \mathbf{r}_N)^\top \in \Omega_r.$$

Here,  $\Omega_r$  is the *configuration space* or *position space* of the system and its elements  $\mathbf{r}$  are the possible *configurations* of the system. If our system is dynamic we can furthermore assign a velocity to each particle

$$\mathbf{v}_i = (v_{ix}, v_{iy}, v_{iz})^\top$$

and write the entire velocity vector of the system as

$$\mathbf{v} = (\mathbf{v}_1, \dots, \mathbf{v}_N)^\top.$$

In dynamical systems each particle can be assigned a mass  $m_i$ . It is often more convenient to use the momentum instead of the velocity. The momentum is defined by

$$\mathbf{p}_i = m_i \mathbf{v}_i = (m_i v_{ix}, m_i v_{iy}, m_i v_{iz})^\top \in \Omega_p.$$

where  $\Omega_p$  is the *momentum space* which contains all possible momentum vectors of the system. It is sometimes convenient to define the mass matrix

$$\mathbf{M} = \text{diag}(m_1, m_1, m_1, m_2, m_2, m_2, \dots, m_N, m_N, m_N)$$

with which we can write

$$\mathbf{p} = \mathbf{M}\mathbf{v}.$$

## 1.3 Energy and Force

**Forces** are fundamental aspects of physical systems. Let

$$\mathbf{f}(\mathbf{r}) = (f_x(\mathbf{r}), f_y(\mathbf{r}), f_z(\mathbf{r}))$$

be the force acting on a particle at position  $\mathbf{r}$ . Here we will be interested especially in *conservative forces*. A force is conservative when it meets any of these three equivalent conditions:

1. The force can be written as the negative gradient of a **potential**,  $\Phi$

$$\mathbf{f}(\mathbf{r}) = -\nabla\Phi(\mathbf{r})$$

where  $\Phi$  is a scalar.

2. The curl of  $\mathbf{f}$  is the zero vector:

$$\nabla \times \mathbf{f} = \mathbf{0}$$

3. The net work done by the force when moving a particle in a cyclical path is zero:

$$W = \oint \langle \mathbf{f}, d\mathbf{r} \rangle = 0$$

In classical mechanics, if we treat all masses explicitly, forces are conservative. Nonconservative forces can arise by considering only a subset of the masses and treating the other ones implicitly, i.e. by some statistical method. Friction and non-elastic material stress, and general relativity are nonconservative.

Here we are especially interested in the first formulation: The force can be written as the negative gradient of a potential  $\Phi$ . This is a very powerful concept: The force is a relatively complex object:  $\mathbf{f}(\mathbf{r})$  is a vector field, i.e. it is defined by a vector (in our case in  $\mathbb{R}^3$ ) at every configuration  $\mathbf{r}$ . For conservative forces, it is sufficient to know a scalar field  $\Phi$ , i.e. a scalar at every configuration  $\mathbf{r}$ , and we can derive the force field from it by taking the gradient at every configuration needed.

Fortunately it gets even simpler, because for many physical systems,  $\Phi$  has a relatively simple mathematical form, or at least we have a relatively simple mathematical model which approximates reality well.

**Example 1: Gravity.** Consider a system of 2 masses, e.g. earth and moon. The ideal gravitational force of point mass  $m_2$  at position  $\mathbf{r}_2$  due to point mass  $m_1$  at position  $\mathbf{r}_1$  is given by:

$$\mathbf{f}_2(\mathbf{r}) = -G \frac{m_1 m_2}{|\mathbf{r}_{12}|^2} \hat{\mathbf{r}}_{12}$$

where  $G = 6.674 \times 10^{-11} (\text{Nm/kg})^2$  is the gravitational constant,

$$\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$$

is the vector pointing from object 1 to object 2, and the corresponding normal vector is

$$\hat{\mathbf{r}}_{12} = \frac{\mathbf{r}_{12}}{|\mathbf{r}_{12}|}.$$

Obviously, the component at mass 1 is

$$\mathbf{f}_1(\mathbf{r}) = -G \frac{m_1 m_2}{|\mathbf{r}_{21}|^2} \hat{\mathbf{r}}_{21},$$

i.e. of equal magnitude but pointing in the opposite direction. This is also necessary because forces must be balanced. If the bodies are close relative to their diameters, then we cannot treat them as point masses, but the above force must be obtained as an integral over all mass elements of the two bodies. Gravitational forces are conservative, and the gravitational potential for two point masses is

$$\Phi(\mathbf{r}) = G \frac{m_1 m_2}{|\mathbf{r}_{12}|},$$

such that  $\mathbf{f}(\mathbf{r}) = -\nabla \Phi(\mathbf{r})$  is fulfilled. Note that we have the boundary condition  $\lim_{|\mathbf{r}_{21}| \rightarrow \infty} \Phi(\mathbf{r}) = 0$ , such that the integration constant is zero. The force felt by mass  $i$  within an  $N$ -body system of masses is given by:

$$\mathbf{f}_i(\mathbf{r}) = -m_i G \sum_{j \neq i} \frac{m_j}{|\mathbf{r}_{ji}|^2} \hat{\mathbf{r}}_{ji},$$

and the total potential energy of the system is given by

$$\Phi(\mathbf{r}) = G \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{m_i m_j}{|\mathbf{r}_{ij}|},$$

While the gravitational force is the weakest of all forces, it is very long ranged. The interaction energy decays as  $1/|\mathbf{r}_{12}|$ , i.e. it is still active when strong short-ranged forces, such as the nuclear forces, have decayed.

**Example 2: Molecular dynamics.** In molecular systems, the gravitational force is so minor that it can be neglected. At these lengthscales electrodynamic forces play the main role. The simplest type

of interaction is the Coulomb interaction between charged particles, such as ions. Two point charges  $q_1$  and  $q_2$  at positions  $\mathbf{r}_1$  and  $\mathbf{r}_2$  have the interaction potential

$$\Phi_{\text{Coulomb}}(\mathbf{r}) = \frac{q_1 q_2}{k_e |\mathbf{r}_{12}|}$$

where

$$k_e = \frac{1}{4\pi\epsilon_0} = \frac{c_0^2\mu_0}{4\pi} = c_0^2 \times 10^{-7} \text{ H} \cdot \text{m}^{-1} = 8.987 \times 10^9 \text{ Nm}^2\text{C}^{-2}$$

is Coulomb's constant. The above expression is using the Maxwell relation and contains other constants, such as the speed of light  $c_0$ , the magnetic permeability of vacuum  $\mu_0$ , and electric permittivity of vacuum  $\epsilon_0$ . So the Coulomb energy is unfavorable (positive) if charges have equal sign and favorable (negative) if they have opposite sign. Like the gravitational energy, it goes as  $1/|\mathbf{r}_{12}|$ , so it is long ranged, but its magnitude is many orders of magnitude larger than the gravitational force for molecular systems, such that we usually neglect the gravitational force at this scale.

If charges are opposite, then the energy goes to  $-\infty$  when the distance goes to 0. That is obviously a problem, because in reality two atoms cannot just collapse. When molecules are close, there are other forces that are also relevant. The attractive van der Waals force, or dispersion force, and the repulsive Pauli exclusion. Often, the energy of these components is qualitatively modeled by the Lennard-Jones potential:

$$\Phi_{\text{LJ}}(\mathbf{r}) = 4\epsilon_{12} \left[ \left( \frac{\sigma_{12}}{|\mathbf{r}_{12}|} \right)^{12} - \left( \frac{\sigma_{12}}{|\mathbf{r}_{12}|} \right)^6 \right]$$

where  $\epsilon_{12}$  is the well depth at the minimum and  $\sigma_{12}$  is the effective atom radius. The total potential of  $N$  atoms using both ingredients is then given by

$$\Phi(\mathbf{r}) = \sum_{\text{pairs } i,j} \frac{q_i q_j}{k_e |\mathbf{r}_{ij}|} + \sum_{\text{pairs } i,j} 4\epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{|\mathbf{r}_{ij}|} \right)^{12} - \left( \frac{\sigma_{ij}}{|\mathbf{r}_{ij}|} \right)^6 \right].$$

Note that molecular dynamics models use more terms, for example they have terms that affect bond lengths, and angles between bonds and torsions.

In a classical molecular dynamics simulation, the conservative force is given by the gradient  $\mathbf{f}(\mathbf{r}) = -\nabla\Phi(\mathbf{r})$ .

**Kinetic energy:** While the potential energy of the system is often based on a model, the kinetic energy of the system is well defined for an  $N$ -body system. The kinetic energy of each single particle is given by

$$K(\mathbf{v}_i) = \frac{1}{2} m_i |\mathbf{v}_i|^2 = \frac{1}{2m_i} |\mathbf{p}_i|^2 = K(\mathbf{p}_i)$$

For the entire system we have

$$K(\mathbf{p}) = \frac{1}{2} \sum_i \frac{1}{m_i} |\mathbf{p}_i|^2 = \frac{1}{2} \mathbf{p}^\top \mathbf{M}^{-1} \mathbf{p}$$

where we have used the definition of the mass matrix  $\mathbf{M}$  introduced above.

## 1.4 Dynamics

Next we turn to dynamics, i.e. we are interested in how the  $N$ -body system - be it a gravitational system such as a Galaxy, or a molecular system such a protein - evolves in time  $t$ . We have silently assumed that the state variables depend on time, e.g.  $\mathbf{q}(t)$ ,  $\mathbf{p}(t)$ . Now we will make this time dependence explicit. The basic equation needed for the dynamics of  $N$ -body system is Newtons second law, which in scalar variables is  $f = ma$ , where  $f$  is the force,  $m$  is the mass and  $a = dv/dt = d^2x/dt^2$  is the acceleration that is the time derivative of the velocity and the second time derivative of the position. For an  $N$ -body system we employ the vector notation:

$$\mathbf{f} = \mathbf{M}\mathbf{a}$$

with the acceleration

$$\mathbf{a} = \frac{d}{dt} \mathbf{v} = \mathbf{a} = \mathbf{M}^{-1} \frac{d}{dt} \mathbf{p}$$

we get just

$$\mathbf{f} = \frac{d}{dt} \mathbf{p}$$

and using

$$\mathbf{p} = \mathbf{M} \frac{d}{dt} \mathbf{r}$$

we have

$$\mathbf{f} = \mathbf{M} \frac{d^2}{dt^2} \mathbf{r}.$$

Thus we can write:

$$\frac{d^2}{dt^2} \mathbf{r}_i = \frac{\mathbf{f}_i}{m_i}$$

Integrating the equation of motion over  $t$  yields the solution of the dynamical trajectory:

$$\mathbf{p}_i(t) = \mathbf{p}_i(0) + \int_{t'=0}^t \mathbf{f}_i(t') dt' \quad (1)$$

$$\mathbf{r}_i(t) = \mathbf{r}_i(0) + \mathbf{M}^{-1} \int_{t'=0}^t \mathbf{p}_i(t') dt' \quad (2)$$

Thus, given a starting condition  $\mathbf{r}_i(0)$ ,  $\mathbf{p}_i(0)$ , these equations provide the entire dynamical trajectory  $\mathbf{q}_i(t)$ ,  $\mathbf{p}_i(t)$  for any time  $t \in 0^+$ . Since, for Newtonian dynamics we have time-reversibility:

$$\begin{aligned} \mathbf{r}_i(0), \mathbf{p}_i(0) &\rightarrow \mathbf{r}_i(t), \mathbf{p}_i(t) \\ \mathbf{r}_i(t), -\mathbf{p}_i(t) &\rightarrow \mathbf{r}_i(0), \mathbf{p}_i(0) \end{aligned}$$

where  $\rightarrow$  indicates time evolution, we can also go back to any past time  $t \in 0^-$  by inverting the momenta and integrating normally.

Unfortunately, Eqs. (1-2) can only be solved analytically in very few cases. For example, try solving them for an harmonic oscillator, i.e. using the potential  $\Phi(x) = \frac{1}{2}kx^2$ . In general, the integrals are not be analytically tractable for  $N$ -body systems, so we need to employ a numerical integration scheme, in short called **integrator**.

The simplest choice is the **explicit Euler**, which we will only show for pedagogical reasons. Consider approximating the integral with  $S = t/\Delta t$  little steps of length  $\Delta t$ :

$$\begin{aligned} \mathbf{p}(t) &\approx \mathbf{p}(0) + \sum_{n=0}^{S-1} \Delta t \mathbf{p}(n) \\ &= \mathbf{p}(0) + \sum_{n=0}^{S-2} \Delta t \mathbf{f}(n) + \Delta t \mathbf{f}(S-1) \\ &= \mathbf{p}(t - \Delta t) + \Delta t \mathbf{f}(t - \Delta t). \end{aligned}$$

And likewise we can approximate

$$\mathbf{r}_i(t) = \mathbf{r}_i(t - \Delta t) + \Delta t \mathbf{M}^{-1} \mathbf{p}(t - \Delta t).$$

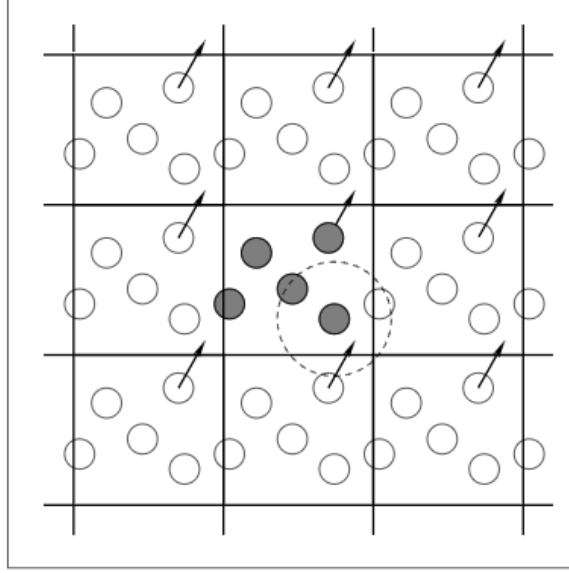
**WARNING:** The explicit Euler scheme is really bad for our purposes (see computer-oriented Mathematics II). It will quickly diverge from the true solution, and worse than that it will be unstable (i.e. lead to an exponential increase of the total energy in the system).

A more stable and energy-conserving integrator is the **velocity Verlet** method, which works as follows:

$$\begin{aligned} \mathbf{p}\left(t + \frac{\Delta t}{2}\right) &= \mathbf{p}(t) + \frac{\Delta t}{2} \mathbf{f}(t). \\ \mathbf{r}\left(t + \frac{\Delta t}{2}\right) &= \mathbf{r}(t) + \Delta t \mathbf{M}^{-1} \mathbf{p}\left(t + \frac{\Delta t}{2}\right). \\ \mathbf{p}(t + \Delta t) &= \mathbf{p}\left(t + \frac{\Delta t}{2}\right) + \frac{\Delta t}{2} \mathbf{f}(t + \Delta t). \end{aligned}$$

## 1.5 Boundary conditions

Periodic boundary conditions:



(Figure taken from <http://www.wabi.snv.jussieu.fr/jompo/Public/PSF/IntroductionMolecularDynamics.pdf>)

## 1.6 Stochastic dynamics and statistical mechanics

The classical mechanics using Newton's equation of motion described above is the mechanics of a **closed system**. A closed system is characterized by the **conservation of total energy in time**, i.e.:

$$H(\mathbf{r}, \mathbf{p}) = \Phi(\mathbf{r}) + K(\mathbf{p})$$

is constant - the fraction of potential and kinetic energy changes over time, but the total energy doesn't. Such a system is also said to be in the **microcanonical ensemble**. A microscopical ensemble, as it is closed, is also deterministic - given an initial setting for  $(\mathbf{r}(0), \mathbf{p}(0))$ , the entire trajectory in the future and past is determined.

Especially microscopic systems, such as molecular systems, are usually not closed, but rather exchange energy (e.g. heat or particles) with their surrounding medium. In such systems, we are thus usually interested in other ensembles. The simplest case is the **canonical ensemble**, which is characterized by constant volume, temperature and number of particles. Imagine a container of fixed size, with boundaries that prevent particles from entering or leaving. However that container is kept at a constant temperature, and to do so it must exchange heat with the environment. The **temperature** can be defined *via* the mean kinetic energy  $K/N$ , by:

$$T = \frac{2}{3k_B} \frac{K}{N}$$

$k_B$  is the Boltzmann constant. Note that the temperature is an ensemble property, i.e. the number of particles  $N$  must be very large in order to speak about temperature in a meaningful way.

From a statistical viewpoint, you can relate the microcanonical and the canonical ensemble in the following way. Imagine a distribution of microcanonical systems, each with a constant total energy  $H(\mathbf{r}, \mathbf{q})$ . The correct distribution turns out to be the Boltzmann distribution, i.e. for each pair  $(\mathbf{r}, \mathbf{q})$  we have the following probability of occurring in the ensemble:

$$\mathbb{P}(\mathbf{r}, \mathbf{q}) \propto \exp\left(-\frac{H(\mathbf{r}, \mathbf{q})}{k_B T}\right).$$

This is the reason for the name microcanonical, as it could be considered as a part of the canonical ensemble.

However, this is a purely statistical viewpoint in practice we usually can't afford to simulate a large set of microcanonical simulations and weigh them. Instead we run only one simulation, but instead of keeping the energy constant, we couple the simulation to a **thermostat**, which has the purpose of allowing  $H(\mathbf{r}, \mathbf{q})$  to fluctuate over time, in such a way that  $\mathbb{P}(\mathbf{r}, \mathbf{q})$  is sampled from the Boltzmann distribution. Since we cannot simulate an infinite number of particles, we can in practice not keep the temperature  $T$  exactly constant, but it will rather also fluctuate around a fixed mean temperature. However the main property is to ensure that  $\mathbb{P}(\mathbf{r}, \mathbf{q})$  is sampled correctly.

**Stochastic Dynamics:** There are many different thermostats and other coupling algorithms (barostates, chemostats, etc.). Here we will briefly discuss two commonly used integration schemes that include a thermostat, i.e. these are full algorithms to simulate molecular dynamics in the  $NVT$  ensemble. The first scheme is multidimensional Langevin dynamics

$$\mathbf{M} \frac{d^2}{dt^2} \mathbf{r} = \mathbf{f}(\mathbf{r}) - \Gamma(\mathbf{r}) \frac{d}{dt} \mathbf{r} + \mathcal{D}(\mathbf{r}) \boldsymbol{\eta}(t)$$

where  $\Gamma$  is the matrix of Stokes friction coefficients and  $\mathcal{D}$  is the matrix of noise intensities.  $\boldsymbol{\eta}(t)$  is a vector of uncorrelated Gaussian random numbers. Note the first part of the equation is equal to Newtonian dynamics, and the function of the last two terms is to act as a thermostat. While the above form is quite general, we can in practice often choose a relatively simply form for the friction and noise coefficients, namely:

$$\mathbf{M} \frac{d^2}{dt^2} \mathbf{r} = \mathbf{f}(\mathbf{r}) - \gamma \mathbf{M} \frac{d}{dt} \mathbf{r} + \sqrt{2k_B T \gamma} \mathbf{M}^{\frac{1}{2}} \boldsymbol{\eta}(t)$$

where  $\gamma$  is an isotropic friction constant. If we simulate all particles that are physically meaningful for our system - such as explicitly-solvated molecular dynamics, we choose  $\gamma$  relatively small, because the particles should not feel "real" friction in addition to the particles they actually collide with, so the whole purpose of  $\gamma$  is to couple our system to the heat bath, and we want to avoid slowing down our system artificially. Note that for  $\gamma = 0$ , we recover Newtonian dynamics.

In the overdamped limit, the equation can be written as the overdamped Langevin, or Smoluchowski, or Brownian dynamics equation:

$$\frac{d}{dt} \mathbf{r} = \gamma^{-1} \mathbf{M}^{-1} \mathbf{f}(\mathbf{r}) + \sqrt{\frac{2k_B T}{\gamma}} \mathbf{M}^{-\frac{1}{2}} \boldsymbol{\eta}(t)$$

Note that in the overdamped limit the motion is no longer inertial, which is why the accelerations do not appear anymore. Under certain circumstances we can use the so-called fluctuation dissipation theorem and write

$$\frac{d}{dt} \mathbf{r} = \frac{1}{k_B T} \mathbf{D} \mathbf{f}(\mathbf{r}) + \sqrt{2\mathbf{D}}^{\frac{1}{2}} \boldsymbol{\eta}(t)$$

where  $\mathbf{D} = \text{diag}(d_{1x}, d_{1y}, d_{1z}, \dots, d_{Nx}, d_{Ny}, d_{Nz})$  is a diagonal matrix of diffusion coefficients. Note that if we have dynamics of rigid bodies that are not just point particles,  $\mathbf{D}$  will not be diagonal, but rather be replaced by a diffusion tensor.

## 1.7 Monte Carlo simulation

Let us reconsider the Boltzmann distribution, and insert the definitions of potential and kinetic energy:

$$\begin{aligned} \mathbb{P}(\mathbf{r}, \mathbf{q}) &\propto \exp \left( -\frac{\Phi(\mathbf{r})}{k_B T} - \frac{K(\mathbf{p})}{k_B T} \right) \\ &\propto \exp \left( -\frac{\Phi(\mathbf{r})}{k_B T} \right) \exp \left( -\frac{K(\mathbf{p})}{k_B T} \right). \end{aligned}$$

Now we're not interested in the statistics of momenta anymore, so we integrate them out:

$$\mathbb{P}(\mathbf{r}) \propto \exp \left( -\frac{\Phi(\mathbf{r})}{k_B T} \right).$$

The integral over the momentum term results in a constant (the partition sum of momenta), but it can be ignored for our purpose. In short we just average over momenta for each position  $\mathbf{r}$ . Now we are interested in sampling this probability density. A conceptually simple algorithm is Monte Carlo simulation. Here we show a very simple version of Metropolis Monte Carlo. We proceed in the following steps:

1. Start with initial configuration  $\mathbf{r}^{(0)}$  and set  $k = 0$ .
2. For  $k = 1, \dots, K$ :
  - (a) Sample random vector  $\boldsymbol{\eta} \in \mathbb{R}^N$  with  $\eta_i \sim \mathcal{N}(0, \sigma^2)$ , i.e. an isotropic multivariate Gaussian distribution with variances  $\sigma^2$ .
  - (b) Propose new configuration  $\mathbf{r}' = \mathbf{r}^{(k)} + \boldsymbol{\eta}$ .
  - (c) Accept new configuration with probability

$$p_{\text{acc}} = \min \left\{ 1, \exp \left( -\frac{\Phi(\mathbf{r}') - \Phi(\mathbf{r}^{(k)})}{k_B T} \right) \right\}$$

If accepted, set  $\mathbf{r}^{(k+1)} = \mathbf{r}'$ , otherwise  $\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)}$ .

This algorithm will in the long run sample from the correct probability density  $\mathbb{P}(\mathbf{r})$ . The algorithm can be modified in many different ways. In particular, we have a lot of freedom in designing Monte-Carlo moves (2a-b). Instead of adding random vectors from a symmetric distribution, we could propose very different steps, and as long as we can evaluate the probability of proposing a given step, we can always account for that in the acceptance step (2c). This more general variant is called Metropolis-Hastings Monte Carlo. We will not go deeper into this subject right now, but just mention that Monte Carlo methods are used ubiquitously in the computational sciences, and it is extremely useful to know this technology.

## 1.8 Optimization

Now we shall be interested in the question which system coordinates are most probable, i.e. we want to know what are the configurations  $\mathbf{r}$  for which  $\mathbb{P}(\mathbf{r})$  is maximum? So instead of running dynamics, we could use the following algorithm:

1. Start with initial configuration  $\mathbf{r}^{(0)}$  and set  $k = 0$ .
2. Increment  $k = 1, \dots, K$  until convergence criterion met:
  - (a) Move configuration  $\mathbf{r}^{(k)} \rightarrow \mathbf{r}^{(k+1)}$  in such a way that  $\Phi(\mathbf{r}^{(k+1)}) \leq \Phi(\mathbf{r}^{(k)})$ .
3. Return  $\mathbf{r}^{(K)}$ ,  $\Phi(\mathbf{r}^{(K)})$ .

So we just minimize the energy, because that would maximize the probability density. Clearly, there are many ways to implement (2a), e.g. gradient descent, conjugate gradient, Newton methods etc. (see Numerics II).

In complex systems, the energy landscape  $\Phi(\mathbf{r})$  will have many local minima, so the result will depend very much on the initial configuration  $\mathbf{r}^{(0)}$ , and we will usually have to repeat this algorithm many times with different initial configurations in order to find a good energy minimum. Even then, this algorithm becomes in practice untractable for high-dimensional systems because they tend to have very rugged energy landscapes and an astronomical number of irrelevant local energy minima. Another way to deal with this problem may be to reduce the dimension, i.e. to replace the full (atomistic) coordinates  $\mathbf{r}$  with some effective or coarse-grained coordinates in which the energy landscape is “smoother”. Finding appropriate coarse-grained models for many-body problems in particular domains of science is a whole area of computational sciences by itself.

## 1.9 Computation

Before moving on, let us recap the essential computational steps necessary to simulate or optimize  $N$ -body systems using the methods above. We can summarize all algorithms that employ simple particle-pair potentials as follows:

1. Start with initial state  $\mathbf{r}^{(0)}$  or  $(\mathbf{r}^{(0)}, \mathbf{p}^{(0)})$ .
2. For  $k = 1, \dots, K$ :
  - (a) Dynamics (stochastic or deterministic): Compute forces  $\mathbf{f}$  with

$$\mathbf{f}_i(\mathbf{r}^{(k-1)}) = \nabla_i \Phi(\mathbf{r}^{(k-1)}) = \sum_j \mathbf{f}_{ji}(\mathbf{r}^{(k-1)})$$

where  $\mathbf{f}_{ij}(\mathbf{r})$  is the force from particle  $j$  onto particle  $i$ . Then update

$$\mathbf{r}^{(k)} = F \left\{ \mathbf{r}^{(k-1)}, \mathbf{f}(\mathbf{r}^{(k-1)}) \right\}$$

- (b) Monte-Carlo or Optimization: Compute energy  $\Phi(\mathbf{r}^{(k)})$  with

$$\Phi(\mathbf{r}^{(k)}) = \sum_{\text{pairs } i, j} \mathbf{f}_{ji}(\mathbf{r}^{(k)})$$

where  $\mathbf{f}_{ij}(\mathbf{r})$  is the force from particle  $j$  onto particle  $i$ . Then update

$$\mathbf{r}^{(k)} = F \left\{ \mathbf{r}^{(k-1)}, \Phi(\mathbf{r}^{(k)}), \Phi(\mathbf{r}^{(k-1)}) \right\}$$

The main insight is that no matter which algorithm we will be using, and no matter if we need energies or forces, we will have to compute on the order of  $N^2$  interaction terms between  $N$  particles. Since the number of time or iteration steps  $K$  can be huge, and the number of particles can be very large (e.g.  $K = 10^{12}$  and  $N = 10^6$  for molecular dynamics), the computational effort is going to be immense. In order to keep the computational cost under control, it is elementary that we use all possible tricks available to reduce this computational cost. In most of this lecture we will focus on methods to reducing the computational cost per iteration from  $\mathcal{O}(N^2)$  to lower complexities, such as  $\mathcal{O}(N^{3/2})$ ,  $\mathcal{O}(N \ln N)$  or even  $\mathcal{O}(N)$ .

## 1.10 The four fundamental forces and interactions

In physics we generally distinguish four fundamental forces or interactions. Let's briefly review these before investigating some forces in more detail:

(taken from <http://www.phy.duke.edu/~kolena/modern/forces.html>)

### Weak (nuclear) interaction:

The interaction range  $r$  can be roughly estimated by assuming that during their lifetime  $\tau$  particles move with 71% of the speed of light  $c$  in the laboratory frame (Lorentz factor  $\gamma = 1.41$ ):  $r \approx \gamma v \tau \approx c \tau$ . With a lifetime of  $3 \times 10^{-25}$  s, this results in an interaction range of 0,09 femtometer. A proton has a diameter of approximately one femtometer.

### Strong (nuclear) interaction:

(taken from [https://en.wikipedia.org/wiki/Strong\\_interaction](https://en.wikipedia.org/wiki/Strong_interaction))

In particle physics, the strong interaction is the mechanism responsible for the strong nuclear force (also called the strong force, nuclear strong force), and is one of the four known fundamental interactions, the others are electromagnetism, the weak interaction and gravitation. At the range of  $10^{-15}$  m (femtometer), the strong force, is approximately 137 times stronger than electromagnetism, a million times stronger than the weak interaction and 1038 times stronger than gravitation.

The strong interaction is observable at two ranges: on a larger scale (about 1 to 3 femtometers (fm)), it is the force that binds protons and neutrons (nucleons) together to form the nucleus of an atom. On



the smaller scale (less than about 0.8 fm, the radius of a nucleon), it is the force (carried by gluons) that holds quarks together to form protons, neutrons, and other hadron particles.

**Electromagnetic interaction:**

Long-ranged, especially the charge-charge interaction. Can become short-ranged in the practical sense of computation (see below) if we consider special cases, such as the van der Waals force or higher multipole interactions. Can be both attractive and repulsive

**Gravity:**

Long-ranged, but of weak absolute magnitude. If bodies are charged, will be dominated by electromagnetic interactions. Is always attractive.