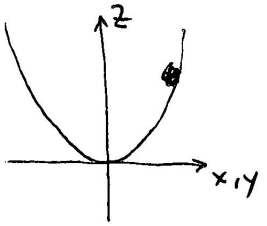
CONSTRAINTS

Consider a particle constrained to move on a surface of equation $\sigma(\vec{r})=0$

For instance

a particle that moves inside a paraboloid

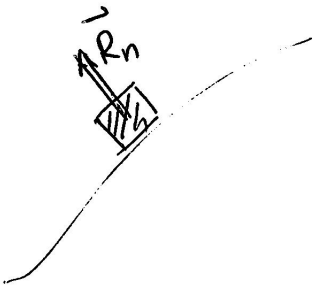


$$\sigma = z - a(x^2+y^2)$$

We wish to solve the Newton's equation with the "constraint" that the the particle position always satisfies $\sigma(r(t))=0$ for any t.

IMPORTANT: NO FRICTION: holonomic constraint

Classical mechanics



If a particle is constrained to move on a surface, there is a constraining force $\vec{R}_n$ such that

a) $|R_n|$ is not known and is determined by the dynamics

b) $\vec{R}_n$ is perpendicular to the surface (REMEMBER: no friction)

Newton's equation $m\bar{a} = \bar{F} + \bar{R}_n$

$\bar{F}$ all external forces: known as a function of $\vec{r}$

(2)

If $\sigma(r(t)) = 0$, the gradient $\nabla\sigma$ is by definition orthogonal to the surface: $\nabla\sigma$ is PARALLEL TO $\bar{R}_n$

$$\bar{R}_n = \lambda(t)\, \nabla\sigma(t)$$

sign of $\lambda(t)$: fixes the direction (up/down) of $\bar{R}_n$

$|\lambda(t)|$: related to $|R_n|$, as such unknown.

Newton: $m\bar{a} = F + \lambda\nabla\sigma$

Verlet algorithm in the presence of constraints

If we use position-Verlet

$$r(t+\Delta t) = 2r(t) - r(t-\Delta t) + \frac{1}{m}\left(F(t) + \lambda(t)\nabla\sigma(t)\right)\Delta t^2$$

We cannot apply directly this equation as $\lambda(t)$ is not known.

Practical approach

(a) Compute

$$r^{(0)} = 2r(t) - r(t-\Delta t) + \frac{1}{m} F(t) \Delta t^2$$

(b) Now, we have $r(t+\Delta t) = r^{(0)} + \frac{1}{m} \lambda(t) \nabla \sigma(t) \Delta t^2$

We require the particle to belong to the surface for $t+\Delta t$, so that we require

$$\sigma\left[r^0 + \frac{1}{m} \lambda(t) \nabla \sigma(t) \Delta t^1\right] = 0 \qquad (*)$$

We solve this equation for $\lambda(t)$

(c) Finally, $r(t+\Delta t)$ can be computed.

The nontrivial part of the algorithm is the solution of the nonlinear equation $(*)$

For a single constraint, standard methods for solving nonlinear equations can be used

In the presence of a large number of constraints recursive algorithms are typically used

A recursive algorithm:

Set $\lambda = \lambda(t-1)$ [this is already a reasonable approximation if Δt is small]

$$\vec{k} = \frac{1}{m} \vec{\nabla}\sigma(t)\Delta t^2$$

Define the desired precision δ on the solution (we are happy if $|\sigma(r(t+\Delta t))| < \delta$)

the iterative algorithm.

- ; begin loop
- compute $\mu = - \dfrac{\sigma(\vec{r}_0^{\,0} + \lambda \vec{k})}{\vec{k} \cdot \nabla\sigma(r^0 + \lambda\vec{k})}$
- update $\lambda \to \lambda + \mu$
- if $|\sigma(r^0 + \lambda\vec{k})| > \delta$ goto ; begin loop
- $r(t+\Delta t) = r^0 + \lambda\vec{k}$

The idea of the algorithm is the following: We have an estimate of $\lambda(t)$ that we simply call λ. How can we improve it?

We write $\lambda^{\text{imp}} = \lambda + \mu$ and insert in the equation

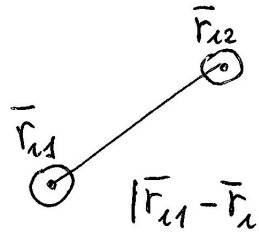
$$\sigma(\vec{r}^{\,0} + (\lambda+\mu)\vec{k}) = 0 \quad . \text{ Expand in } \mu$$

$$\sigma(r^0 + \lambda\vec{k}) + \mu\vec{k} \cdot \nabla\sigma(r^0 + \lambda\vec{k}) = 0 + O(\mu^2)$$

$$\Rightarrow \quad \mu = - \frac{\sigma(r^0 + \lambda k)}{\vec{k} \cdot \nabla\sigma(r^0 + \lambda\vec{k})}$$

An application: diatomic molecules.

At room temperature, diatomic molecules can be schematized as rigid rods



$|\bar{r}_{i1} - \bar{r}_{i2}|^2 = b^2$ bond length = b

The dynamics of the molecules is thus controlled by a Hamiltonian H with N constraints (N = number of molecules)

$$\sigma_i(\{r_1 \dots r_N\}) = |r_{i1} - r_{i2}|^2 - b^2$$

Thus

$$m\ddot{\vec{r}}_{i1} = \vec{F}_{i1} + \lambda_i \vec{\nabla}_{\vec{r}_{i1}} \sigma_i$$

$$m\ddot{\vec{r}}_{i2} = \vec{F}_{i2} + \lambda_i \vec{\nabla}_{\vec{r}_{i2}} \sigma_i$$

forces due to the constraint

λ_i = unknown parameter. (there are N unknowns)

Dynamics: completely analogous to the one discussed before, but

N equations $\quad |r_{i1}(t+\Delta t) - r_{i2}(t+\Delta t)|^2 - b^2 = 0$

to be solved SIMULTANEOUSLY to obtain the N constants $\lambda_i(t)$