Concepts and Algorithms of Scientific and Visual Computing

–Constraint Methods–

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Constraint Optimization

Maximize a function $f : \mathbb{R}^2 \to \mathbb{R}, (x, y) \mapsto f(x, y)$ under the consideration of the constraint $g(x, y) = 0$.

Following the curve defined by $g(x, y) = 0$, we pass contour lines of f. A common point (x, y) can only be a solution of the optimization problem, if our motion is tangential to f at (x, y). Otherwise, the function value could be easily increased by moving forward or backward without violating the constraint.

Therefore, the gradients should be arranged in parallel at the maximum, i.e.

$$\nabla f(x, y) + \lambda \nabla g(x, y) = 0$$

with a so-called Lagrange multiplier λ.

Constrained System

We consider a system of N particles at positions $\mathbf{q}_1, \ldots, \mathbf{q}_N$ with masses $m_1, \ldots, m_N$ and k holonomic constraints, i.e. for $l \in \{1, \ldots, k\}$:

$$\sigma_l(t) := \left\| \mathbf{q}_{l\alpha}(t) - \mathbf{q}_{l\beta}(t) \right\|^2 - d_l^2 = 0,$$

and equations of motions

$$m_i \partial_t^2 \mathbf{q}_i(t) = -\partial_{\mathbf{q}_i} \left(V(\mathbf{q}_i(t)) + \sum_{l=1}^{k} \lambda_l \sigma_l(t) \right).$$

An appropriate time integration scheme is given by

$$\mathbf{q}_i(t + \Delta t) = \hat{\mathbf{q}}_i(t + \Delta t) + \frac{1}{m_i} \sum_{l=1}^{k} \lambda_l \partial_{\mathbf{q}_i} \sigma_l(t) \Delta t^2$$

for $i \in \{1, \ldots, N\}$, in which the $\hat{\mathbf{q}}_i$'s denote the uncorrected positions.

Lagrange Multiplier

We have to determine the Lagrange multiplier λ_k, such that the constraints are fulfilled at time $t+\Delta t$. This leads to the system of non-linear equations

$$\sigma_j(t+\Delta t) = \left\| \hat{\mathbf{q}}_{j\alpha}(t+\Delta t) - \hat{\mathbf{q}}_{j\beta}(t+\Delta t) + \sum_{l=1}^{k} \lambda_l \Delta t^2 \left(\frac{\partial_{\mathbf{q}_{j\alpha}} \sigma_l(t)}{m_{j\alpha}} - \frac{\partial_{\mathbf{q}_{j\beta}} \sigma_l(t)}{m_{j\beta}} \right) \right\|^2 - d_j^2 = 0$$

with k unknown Lagrange multipliers $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_k)^\mathsf{T}$.

The system can be solved with Newton's method

$$\hat{\boldsymbol{\lambda}}^{(\ell+1)} \leftarrow \hat{\boldsymbol{\lambda}}^{(\ell)} - \mathbf{J}_\sigma^{-1} \hat{\boldsymbol{\sigma}}(t+\Delta t)$$

with $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_k)^\mathsf{T}$ and Jacobi matrix $\mathbf{J}$.

Jacobi Matrix

The Jacobi matrix $\mathbf{J}$ given by

$$\mathbf{J} = \begin{pmatrix} \partial_{\lambda_1}\sigma_1 & \dots & \partial_{\lambda_k}\sigma_1 \\ \vdots & \ddots & \vdots \\ \partial_{\lambda_1}\sigma_k & \dots & \partial_{\lambda_k}\sigma_k \end{pmatrix}$$

usually has a sparse block structure.

For $\hat{\boldsymbol{\lambda}}^{(0)} = \mathbf{0}$, the situation can be simplified to

$$J_{ij} = \partial_{\lambda_i}\sigma_j\big|_{\lambda=0} = 2(\hat{\mathbf{q}}_{j\alpha} - \hat{\mathbf{q}}_{j\beta})\left(\frac{\partial_{\mathbf{q}_{j\alpha}}\sigma_i}{m_{j\alpha}} - \frac{\partial_{\mathbf{q}_{j\beta}}\sigma_i}{m_{j\beta}}\right)$$

and

$$\lambda_i = -\mathbf{J}^{-1}\left(\left\|\hat{\mathbf{q}}_{j\alpha}(t+\Delta t) - \hat{\mathbf{q}}_{j\beta}(t+\Delta t)\right\|^2 - d_j^2\right).$$

Position Update

After each iteration we have to update the uncorrected positions according to

$$\hat{\mathbf{q}}_i(t+\Delta t) \leftarrow \hat{\mathbf{q}}_i(t+\Delta t) + \sum_{l=1}^{k} \lambda_l \partial_{\mathbf{q}_i} \sigma_l.$$

Then we set $\hat{\boldsymbol{\lambda}} = \mathbf{0}$ and repeat the whole procedure until a sufficient small error is achieved.

SHAKE and RATTLE Algorithms

In the SHAKE algorithm, see [Andersen 1983], the non-linear constraint equations are solved using the Gauß-Seidel method approximating the linear system

$$\hat{\boldsymbol{\lambda}} = -\mathbf{J}_{\sigma}^{-1}\hat{\boldsymbol{\sigma}}$$

with Newton's method. The requires a linear runtime $\mathcal{O}(k)$ per iteration.

Combining the SHAKE algorithm with a Verlet time integration scheme, we obtain the RATTLE algorithm, see [Ryckaert 1977].

Molecular Dynamics (MD)

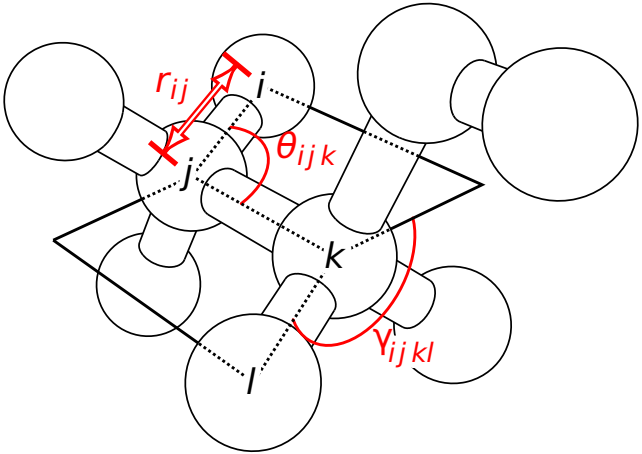

Figure : Example scenario of distance r_{ij}, angle θ_{ijk}, and torsional angle γ_{ijkl} in the case of a trans configuration illustrated using an ethanol molecule.

MD Potentials

A molecular dynamics potential V is typically written as the sum of distinct potentials

$$V = V_{\mathbf{B}} + V_{\mathbf{A}} + V_{\mathbf{T}} + V_{LJC}$$

where the covalent bond potential $V_{\mathbf{B}}$ is given by a simple harmonic potential

$$V_{\mathbf{B}} := \sum_{(i,j)\in\mathbf{B}} \frac{k_{\mathbf{B}_{ij}}}{2}(r_{ij} - \overline{r}_{ij})^2,$$

the angle potential $V_{\mathbf{A}}$ is expressed as

$$V_{\mathbf{A}} := \sum_{(i,j,k)\in\mathbf{A}} \frac{k_{\mathbf{A}_{ijk}}}{2}(\theta_{ijk} - \overline{\theta}_{ijk})^2,$$

the torsional potential $V_{\mathbf{T}}$ is written as

$$V_{\mathbf{T}} := \sum_{(i,j,k,l)\in\mathbf{T}} \sum_{s=1}^{3} k_{\mathbf{T}_{ijkl,s}} \Big(\cos\Big(s\gamma_{ijkl} - \delta_s\Big) + 1\Big).$$

MD Potentials

Finally, the non-bonded Lennard-Jones and Coulomb potential is expressed as

$$V_{LJC} := \sum_{i=1}^{N} \sum_{j=1}^{i-1} 4\epsilon \left(\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right) + \frac{e^2}{4\pi\epsilon_0} \frac{Z_i Z_j}{r_{ij}}.$$

These potentials are parameterized by the harmonic bending constants $k_{\mathbf{B}_{ij}}$, the initial distances $\overline{r}_{ij}$, the angular constants $k_{\mathbf{A}_{ijk}}$, the initial angles $\overline{\theta}_{ijk}$, the torsional constants $k_{\mathbf{T}_{ijkl,s}}$ and phase shifts δ_s, the well-depth ϵ and finite distance values σ_{ij} of the Lennard-Jones potential, see [Lennard-Jones 1924].