1 Error ascribed to the stochastic Euler-Method

A rough estimate

$$\frac{(\Delta t)^{1/2} B^{1/2} \{|[B],_{\alpha}^{1/2}|(\Delta t)^{1/2} + |[A],_{\alpha}|(\Delta t)\}}{B^{1/2}(\Delta t)^{1/2} + |A|(\Delta t)} \leq 2\epsilon \tag{1}$$

The term multiplying the curly braces is less than one, so we can have an even more conservative estimate and demand instead

$$\{|[B],_{\alpha}^{1/2}|(\Delta t)^{1/2} + |[A],_{\alpha}|(\Delta t)\} \leq 2\epsilon \tag{2}$$

This can be guaranteed if

$$\Delta t \leq \min\left\{\frac{\epsilon}{|[A],_{\alpha}|}, \left(\frac{\epsilon}{[B],_{\alpha}^{1/2}}\right)^2\right\} \tag{3}$$

As the algorithm works on $\mathbb{R}^3$, where D is a constant, its derivatives are null

$$D,_{\alpha} = 0 \tag{4}$$

so the above estimate reduces to

$$\Delta t \leq \frac{\epsilon}{|[A],_{\alpha}|} \tag{5}$$

The derivatives for the components of the force along the direction of $\hat{\theta}$ are

$$A,_{\theta} = \lambda \sin\theta \tag{6a}$$

$$A,_{\theta} = 3\lambda \sin 2\theta \tag{6b}$$

$$A,_{\theta} = \lambda[10\cos^2 \sin\theta - \sin\theta(3 - 5\cos^2\theta)] \tag{6c}$$

which are bounded by the values

$$|A,_{\theta}| \leq \lambda \tag{7a}$$

$$|A,_{\theta}| \leq 6\lambda \tag{7b}$$

$$|A,_{\theta}| \leq \lambda[10|\cos^2 \sin\theta| + |\sin\theta|(3 + 5\cos^2\theta)] \leq 18\lambda \tag{7c}$$

A very rough criteria would be

$$\Delta t \leq \frac{\epsilon}{18\lambda} \tag{8}$$

So After N steps we would like to have a difference less than a specified tolerance $0 < \epsilon$, we might take a Δt less than

$$\Delta t \leq \frac{\epsilon/N}{18\lambda} \tag{9}$$

For long simulations the Euler Algorithm has a very high computational cost. The error is proportional to Δt. However, this analysis is related to the *strong convergence* analysis not with the *weak convergence* analysis in which we are evaluating our numerical methods. Emphasis is made to the relaxation process rather than with the poor performance that the Langevin dynamics might have when trying to use it to calculate functions of the dynamical variables in the stationary states.

2 Stability Analysis of the stationary states

$$\overline{g(t)} = \frac{1}{\tau}\int_{t_{\min}}^{t_{\min}+\tau} g(\xi)\, d\xi = \frac{1}{(m - k_{\min})}\sum_{k=k_{\min}}^{m} g(t_k) \tag{10}$$

where m is the number of Monte Carlo steps for the simulation. Non-equilibrium time average with respect the equilibrium average

$$\Delta f(t) = f(t) - \langle f \rangle \tag{11}$$

$$t_{\min} = \min_{t\in[0,T]} \{t | f(t) = \langle f \rangle\} \tag{12}$$

and $\tau = m([t_{\min}, T]) = T - t_{\min}$, where $T = m \times dt$

On the one hand, there is the so called *strong error of convergence*, which is a measure in terms of the L^p-norm for random variables. This error is small if for a given initial state and a given sample path of the forcing random noise the corresponding trajectories of the exact solution and the numerical scheme are close to each other.

On the other hand, the *weak error of convergence* is already small if the laws of the exact solution and the numerical scheme almost coincide. Usually, a strongly convergent scheme is also weakly convergent and the strong order of convergence is a lower bound for the weak order of convergence.

From this, we can conclude that for the stationary state, when there is an external force, the moments of the distribution are stationary and the mean absolute error depends more on the ensemble size (N), than on the time step.

N	$O(dt)$	$\overline{\Delta\vert\theta(t)\vert}$	$\overline{\Delta \mathrm{Var}[\theta(t)]}$	$\overline{\Delta\langle \mathbf{n}(t)\cdot\mathbf{n}(0)\rangle}$
100	10^{-3}	0.0455	0.0383	0.0397
1000	10^{-3}	0.0173	0.0109	0.0146
10,000	10^{-3}	0.0047	0.0046	0.0042
100	10^{-2}	0.0649	0.0407	0.0553
1000	10^{-2}	0.0159	0.0125	0.0134
10,000	10^{-2}	0.0058	0.0040	0.0048
100	10^{-1}	0.0532	0.0419	0.0450
1000	10^{-1}	0.0175	0.0129	0.0147
10,000	10^{-1}	0.0053	0.0041	0.0045

Table 1: Free diffusion fluctuations around the stationary states for different time steps dt and ensembles of different size N. In all this simulations we took $D = 1$.

N	$O(dt)$	$\overline{\Delta\vert\theta(t)\vert}$	$\overline{\Delta \mathrm{Var}[\theta(t)]}$	$\overline{\Delta\theta^3(t)}$	$\overline{\Delta\theta^4(t)}$
100	10^{-3}	0.0566	1.4220	0.5525	1.6731
1000	10^{-3}	0.0184	1.4274	0.1636	0.4792
10,000	10^{-3}	0.0141	1.4282	0.1296	0.3825
100	10^{-2}	0.2189	1.3772	2.0189	5.9430
1000	10^{-2}	0.0907	1.4168	0.8259	2.4256
10,000	10^{-2}	0.0025	1.4246	0.0443	0.1504
100	10^{-1}	0.1982	1.3469	1.6401	4.6619
1000	10^{-1}	0.0477	1.3812	0.6576	2.1147
10,000	10^{-1}	0.0133	1.3833	0.0908	0.4465

Table 2: Stationary fluctuations around the stationary state for the interaction proportional to $Y_2^0(\theta,\phi)$, for different time steps dt and ensembles of different size N. In all this simulations we took $D = 0.1$.

3 Force of constraint

The component of the external force along the direction perpendicular to the surface to which the motion is contrained is

$$\mathbf{F}_{\perp} = [\mathbf{n}(\mathbf{r}) \cdot \mathbf{F}(\mathbf{r})]\mathbf{n}(\mathbf{r}) \tag{13}$$

where the unit normal is given by

$$\mathbf{n}(\mathbf{r}) = \frac{\nabla\sigma(\mathbf{r})}{|\nabla\sigma(\mathbf{r})|}. \tag{14}$$

So the component parallel to the surface is

$$\mathbf{F}_{\parallel} = \mathbf{F} - \mathbf{F}_{\perp} = \mathbf{F} - [\mathbf{n}(\mathbf{r}) \cdot \mathbf{F}(\mathbf{r})]\mathbf{n}(\mathbf{r}) \tag{15}$$

3.0.1 Gauss' principle of least constrain

Equation of an holonomic constraint can be cast as

$$\sigma(\mathbf{r}) = 0 \tag{16}$$

The equations of motion satisfy

$$m\ddot{\mathbf{r}} = \mathbf{F}(t) + \lambda\nabla\sigma \tag{17}$$

where λ is an undefined parameter, and the last term represents the force of constraint. If we take the time derivative of the equation of constraint

$$\nabla\sigma \cdot \dot{\mathbf{r}} = 0 \tag{18}$$

If we take again the time derivative of this equation and use $\ddot{\mathbf{r}}$ from Newton's equation 17, we can find an expression for λ

$$\lambda = \frac{\nabla\nabla\sigma \cdot \cdot \dot{\mathbf{r}}\dot{\mathbf{r}} + \nabla\sigma \cdot \mathbf{F}/m}{|\nabla\sigma|^2/m} \tag{19}$$

Where $\nabla\nabla\sigma \cdot \cdot \dot{\mathbf{r}}\dot{\mathbf{r}}$ denotes full contraction of the two tensors $\nabla\nabla\sigma$ and $\dot{\mathbf{r}}\dot{\mathbf{r}}$ Substituing this value in 17

$$m\ddot{\mathbf{r}} = \mathbf{F}(t) - \frac{\nabla\nabla\sigma \cdot \cdot \dot{\mathbf{r}}\dot{\mathbf{r}} + \nabla\sigma \cdot \mathbf{F}/m}{|\nabla\sigma|^2/m}\nabla\sigma \tag{20}$$

As we can appreciate the force of constrain is always pointing into the center of $\mathbb{S}^2$, the same happens with the projection of any vector with a magnitude greater than one into $\mathbb{S}^2$.