Numerical analysis of the DMC method in a simple case.

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Structure of the talk

The Born-Oppenheimer approximation

For most applications, systems of limited size (e.g. molecules) are described by

- M nuclei with electric charges $z_k \in \mathbb{N}^*$ and positions $\bar{x}_k \in \mathbb{R}^3$, $k \in \{1, \ldots, M\}$.
  slow variables $\rightarrow$ modelled by classical mechanics.
- N electrons with positions $x_i \in \mathbb{R}^3$, $i \in \{1, \ldots, N\}$ and charge -1.
  Very light particles.
  fast variables $\rightarrow$ modelled by (nonrelativistic) quantum mechanics.

In the Born-Oppenheimer approximation, for electronic computations, the nuclei positions are supposed to be constant.

Electronic state

To simplify, we leave the spin variables aside.
Electronic state $\rightarrow$ modelled by the Hamiltonian

$$H = -\sum_{i=1}^{N} \frac{1}{2}\Delta_{x_i} - \sum_{i=1}^{N}\sum_{k=1}^{M} \frac{z_k}{|x_i - \bar{x}_k|} + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|}$$

where the positions $\bar{x}_k$ of the nuclei are supposed to be fixed.
Electronic ground state energy :

$$E_0 = \inf \left\{ \langle \psi, H\psi \rangle, \quad \psi \in D(H), \int_{\mathbb{R}^{3N}} |\psi|^2 = 1 \right\} \tag{1}$$

with

$$D(H) = \left\{ \psi \in \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3) \quad , \quad H\psi \in \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3) \right\}$$

Electronic state

Antisymmetrized tensor product space

$$\bigwedge_{i=1}^{N} L^2(\mathbb{R}^3) = \{\psi \in L^2((\mathbb{R}^3)^N) : \forall \sigma \in \mathcal{S}_n,\ \forall x \in (\mathbb{R}^3)^N,\ \psi(x_\sigma) = (-1)^{\varepsilon(\sigma)}\psi(x)\}$$

with $x_\sigma = (x_{\sigma(1)}, \ldots, x_{\sigma(N)})$ for $x = (x_1, \ldots, x_N)$ and $\varepsilon(\sigma)$ signature of σ.

Justified by

- exchangeability of the electrons (in terms of the density $|\psi|^2$: $|\psi(x_\sigma)|^2 = |\psi(x)|^2$)
- Pauli's exclusion principle for fermions ($|\psi|^2$ vanishes when two positions x_i are equal)

Ground state properties

Ground state = element ψ_0 of $D(H)$ which minimizes the energy (1)

$$< \psi_0, H\psi_0 >= E_0 \text{ with } \|\psi_0\|_2 = 1.$$

Theorem 1

- *When $N \leq Z = \sum_{k=1}^{M} z_k$ (neutral molecule or positive ion), then H is self-adjoint in $D(H)$ and there exists a ground state ψ_0 (Zhislin 1960).*
- *Any ground state ψ_0 belongs to $C^\theta(\mathbb{R}^{3N})$ for $\theta \in (0,1)$ and to $C^\infty(\mathbb{R}^{3N} \setminus \Gamma)$ where*

$$\Gamma = \{(x_1, \ldots, x_N) \in (\mathbb{R}^3)^N : \exists i \neq j \text{ s.t. } x_i = x_j \text{ or } \exists i, k \text{ s.t. } x_i = \bar{x}_k\}.$$

Any ground state ψ_0 solves the Euler-Lagrange equation

$$H\psi_0 = E_0\psi_0. \tag{2}$$

The Tiling property

For any continuous function ψ on $\mathbb{R}^{3N}$, we define

$$U = \mathbb{R}^{3N} \setminus \psi^{-1}(0).$$

For $\sigma \in \mathcal{S}_N$ and $x = (x_1, \ldots, x_N) \in (\mathbb{R}^3)^N$, we set $x_\sigma = (x_{\sigma(1)}, \ldots, x_{\sigma(N)})$. When ψ is antisymmetric, for any connected component $\mathcal{C}$ of U and $\forall \sigma \in \mathcal{S}_N$,

$$\sigma(\mathcal{C}) = \{x_\sigma : x \in \mathcal{C}\}$$

is also a connected component of U.

Theorem 2

- *Any ground state ψ_0 satisfies the tiling property : for any connected component $\mathcal{C}$ of $U_0 = \mathbb{R}^{3N} \setminus \psi_0^{-1}(0)$, $U_0 = \bigcup_{\sigma \in \mathcal{S}_N} \sigma(\mathcal{C})$ (Ceperley 91).*
- *Moreover, for any connected component $\mathcal{C}$ of U_0,*

$$E_0 = E_{\mathcal{C}} \stackrel{\text{def}}{=} \inf \left\{ \frac{1}{2} \int_{\mathcal{C}} |\nabla \psi|^2 + \int_{\mathcal{C}} V \psi^2, \ \psi \in H_0^1(\mathcal{C}), \ \int_{\mathcal{C}} \psi^2 = 1 \right\}.$$

Numerical computation of the ground state energy

Difficult problem because

- dimension $3N$ with N large,
- antisymmetry condition due to the fermionic nature of electrons

Some numerical methods:

- Hartree-Fock methods *(variational approximation : restriction of $D(H)$ to Slater determinants $\det(\phi_i(x_j))$)*,
- Density Functional Theory *(Thomas-Fermi, Kohn-Sham)*,
- Quantum Monte Carlo methods *(Variational Monte Carlo, Diffusion Monte Carlo)*.

see E. Cancès, M. Defranceschi, W. Kutzelnigg, C. Le Bris and Y. Maday, Computational Quantum Chemistry: a Primer, *Handbook of Numerical Analysis, volume X (2003).*

Trick : Schrödinger in complex time

Add a ficticious time variable : $\phi(t,x) = e^{-tH}\psi_I(x)$ solves

$$\begin{cases} \partial_t \phi = -H\phi = \frac{1}{2}\Delta\phi - V\phi \\ \phi(0,.) = \psi_I(.) \in D(H) \end{cases}$$

with $V(x) = -\sum_{i=1}^{N}\sum_{k=1}^{M}\frac{z_k}{|x_i - \bar{x}_k|} + \sum_{1\leq i<j\leq N}\frac{1}{|x_i - x_j|}$.

If E_0 isolated single eigenvalue for H associated with eigenstate ψ_0 ($\|\psi_0\|_2 = 1$) and $< \psi_I, \psi_0 > \neq 0$, then

$$\phi(t,x) = e^{-tH}\psi_I(x) \sim e^{-E_0 t} < \psi_I, \psi_0 > \psi_0(x) \ (t \text{ large})$$

$$\Rightarrow E_0 = -\lim_{t\to+\infty}\frac{1}{t}\log|\phi(t,x)|\,. \tag{3}$$

Feynman-Kac interpretation

If (W_t) Brownian motion in $\mathbb{R}^{3N}$, for $r \in [0,t]$,

$$d_r e^{-\int_0^r V(x+W_s)ds}\phi(t-r,x+W_r) = e^{-\int_0^r V(x+W_s)ds}\Big(\nabla_x\phi(t-r,x+W_r).dW_r + \underbrace{\Big[-\partial_t\phi+\frac{1}{2}\Delta\phi-V\phi\Big]}_{0}(t-r,x+W_r)dr\Big).$$

Therefore

$$e^{-\int_0^t V(x+W_s)ds}\psi_I(x+W_t) = \phi(t,x)+\int_0^t e^{-\int_0^r V(x+W_s)ds}\nabla_x\phi(t-r,x+W_r).dW_r$$

and $\phi(t,x) = \mathbb{E}\left(\psi_I(x+W_t)e^{-\int_0^t V(x+W_s)ds}\right)$.

By (3),

$$\Rightarrow E_0 = -\lim_{t\to+\infty}\frac{1}{t}\log\left|\mathbb{E}\left(\psi_I(x+W_t)e^{-\int_0^t V(x+W_s)ds}\right)\right|$$

Variance reduction

$$E_0 = -\lim_{t\to+\infty} \frac{1}{t} \log \left| \mathbb{E}\left(\psi_I(x+W_t) e^{-\int_0^t V(x+W_s)ds} \right) \right|$$

Problem : large fluctuations of V in the exponential factor $\Rightarrow$ variance too large.
Need of variance reduction.

Principle of the Diffusion Monte Carlo method (importance sampling)

- choose $\psi_I \in D(H)$ as close as possible to the ground state ψ_0,
- modify the dynamics of the Brownian motion by adding the drift term $\frac{\nabla\psi_I}{\psi_I}$,
- replace V by $E_L = \frac{H\psi_I}{\psi_I}$ in the exponential factor (when $\psi_I = \psi_0$, $E_L = E_0$ constant).

The Diffusion Monte Carlo method

Yields very good results and is widely used in the chemistry community.

TABLE I. Atomization energies (kcal/mol) for the 55 molecules in the G1 set (Refs. 1, 2). Diffusion Monte Carlo (DMC) calculations and experimental (Expt.) results are listed. For DMC, statistical error bars are given in parentheses. Experimental errors are listed in parentheses (a dash indicates no error was available).

Molecule	DMC	Expt.
LiH	55.3(2)	56.00(1)
BeH	43.0(2)	46.90(1)
CH	79.5(2)	79.90(2)
CH_2 ($^3B_1$)	181.9(4)	179.6(4)
CH_2 ($^1A_1$)	169.7(4)	170.6(4)
CH_3	290.9(2)	289.3(2)
CH_4	395.0(2)	392.5(1)
NH	78.2(4)	79.0(4)
NH_2	169.2(4)	170.0(3)
NH_3	276.5(2)	276.7(1)
OH	101.2(3)	101.4(3)
H_2O	219.4(2)	219.35(1)
HF	135.9(2)	135.2(2)
SiH_2 ($^1A_1$)	145.5(2)	144.4(2)

J.C. Grossman, J. Chem. Phys., 117 (2002).

The DMC method

Let

$$E(t) \stackrel{\text{def}}{=} \frac{< e^{-tH}\psi_I, H\psi_I >}{< e^{-tH}\psi_I, \psi_I >}$$

By spectral decomposition,

$$E(t) \sim \frac{E_0 < \psi_I, \psi_0 >^2 e^{-E_0 t}}{< \psi_I, \psi_0 >^2 e^{-E_0 t}} \to E_0 \text{ as } t \to +\infty.$$

For $f(t,x) = \psi_I(x) e^{-tH} \psi_I(x) = \psi_I(x)\phi(t,x)$ and $E_L = \frac{H\psi_I}{\psi_I}$,

$$E(t) = \frac{< f(t,.), E_L(.) >}{< f(t,.), 1 >}.$$

Probabilistic interpretation of $E(t)$

The function $f(t,x) = \psi_I(x)e^{-tH}\psi_I(x) = \psi_I(x)\phi(t,x)$ solves

$$\partial_t f = \frac{1}{2}\Delta f - \nabla.(bf) - E_L f, \quad f(0,.) = \psi_I^2(.) \tag{4}$$

where $b = \frac{\nabla\psi_I}{\psi_I}$ and $E_L = \frac{H\psi_I}{\psi_I} = -\frac{1}{2}\frac{\Delta\psi_I}{\psi_I} + V$. Assume $\|\psi_I\|_2 = 1$.

- Without the term $-E_L f$, (4) Fokker-Planck equation for the density of X_t solving

$$dX_t = dW_t + b(X_t)dt, \quad X_0 \sim \psi_I^2(x)dx. \tag{5}$$

- With this term, $h(t,x)$ defined by

$$\forall g : \mathbb{R}^{3N} \to \mathbb{R}, \quad \int_{\mathbb{R}^{3N}} g(x)h(t,x)dx = \mathbb{E}\left(g(X_t)e^{-\int_0^t E_L(X_s)ds}\right)$$

solves (4).

Probabilistic interpretation of $E(t)$

One expects $E(t)$ to be equal to

$$\frac{< h(t,.), E_L(.) >}{< h(t,.), 1 >} = \frac{\mathbb{E}\left(E_L(X_t) e^{-\int_0^t E_L(X_s)ds}\right)}{\mathbb{E}\left(e^{-\int_0^t E_L(X_s)ds}\right)} \stackrel{\text{def}}{=} E^{DMC}(t).$$

Variance reduction :

- if ψ_I close to the ground state ψ_0, $E_L = \frac{H\psi_I}{\psi_I} \sim \frac{H\psi_0}{\psi_0} = E_0$ fluctuates less than V,
- the drift $b = \nabla \log(|\psi_I|)$ drives the process X_t solving (5) where $|\psi_I|$ (and hopefully $|\psi_0|$) is large.

$b = \frac{\nabla\psi_I}{\psi_I}$ and $E_l = \frac{H\psi_I}{\psi_I}$ both explode near the nodal surface $\psi_I^{-1}(0)$ which is not empty because of the antisymmetry of ψ_I (ex: $\{x : x_1 = x_2\} \subset \psi_I^{-1}(0)$)$\Rightarrow$ previous interpretation formal.
Questions : $E(.) = E^{DMC}(.)$? $E^{DMC}(t) \rightarrow_{t\rightarrow+\infty} E_0$?

The fixed node approximation

Theorem 3

Assume that $U_I = \mathbb{R}^{3N} \setminus \psi_I^{-1}(0)$ *has a finite number of connected components. Under some technical assumptions on* V *and* ψ_I*, as* $t \to +\infty$*,* $E^{DMC}(t)$ *converges exponentially to*

$$E_0^{DMC} = \inf\{< \psi, H\psi >: \psi \in D(H),\ \|\psi\|_2 = 1,\ \psi_I^{-1}(0) \subset \psi^{-1}(0)\}.$$

In addition, $E_0^{DMC} \geq E_0$ *with equality iff* $\psi_I^{-1}(0) \subset \psi_0^{-1}(0)$ *where* ψ_0 *ground state of* H*.*
(Cancès, Jourdain, Lelièvre, M3AS 2006)

The zeros of ψ_I ($\{x : \psi_I(x) = 0\}$) are called the nodes of $\psi_I \to$ Fixed Node Approximation.

Elements of proof

Step 1 : $\forall x \in \mathbb{R}^{3N} \setminus \psi_I^{-1}(0)$, the SDE

$$X_t^x = x + W_t + \int_0^t b(X_s^x) ds$$

admits a unique solution.
In addition, $\forall t \geq 0,\ \psi_I(x)\psi_I(X_t^x) > 0$.

Step 2 : As $b = \frac{\nabla \psi_I}{\psi_I}$, $\frac{1}{2}\nabla \psi_I^2 - b\psi_I^2 = 0$ and $\psi_I^2(x)dx$ reversible measure for the SDE. Hence

$$\forall g : \mathbb{R}^{3N} \to \mathbb{R},\ \int_{\mathbb{R}^{3N}} g(x)h(t,x)dx \stackrel{\text{def}}{=} \mathbb{E}\left(g(X_t)e^{-\int_0^t E_L(X_s)ds}\right)$$

$$= \int_{\mathbb{R}^{3N}} g(x)\psi_I^2(x)\mathbb{E}\left(e^{-\int_0^t E_L(X_s^x)ds}\right)dx.$$

Hence $h(t,x) = \psi_I^2(x)\mathbb{E}\left(e^{-\int_0^t E_L(X_s^x)ds}\right)$.

Elements of proof

$h(t,x) = \psi_I^2(x)\mathbb{E}\left(e^{-\int_0^t E_L(X_s^x)ds}\right)$. Therefore

$$E^{DMC}(t) \stackrel{\text{def}}{=} \frac{< h(t,.), \frac{H\psi_I}{\psi_I} >}{< h(t,.), 1 >} = \frac{< \chi(t,.), H\psi_I >}{< \chi(t,.), \psi_I >}$$

where $\chi(t,x) = \psi_I(x)\mathbb{E}\left(e^{-\int_0^t E_L(X_s^x)ds}\right)$ vanishes on $\psi_I^{-1}(0)$.

As $E(t) = \frac{<e^{-tH}\psi_I, H\psi_I>}{<e^{-tH}\psi_I, \psi_I>}$ and $e^{-tH}\psi_I$ does not vanish on $\psi_I^{-1}(0)$, in general

$$E^{DMC}(t) \neq E(t).$$

Elements of proof

Step 3 : For each connected component $\mathcal{C}$ of $\mathbb{R}^{3N} \setminus \psi_I^{-1}(0)$,

$$x \in \mathcal{C} \implies \forall t \geq 0,\ X_t^x \in \mathcal{C}$$

Consequence : the restriction of $\chi(t,x)$ to $\mathbb{R}_+ \times \mathcal{C}$ unique solution of

$$\partial_t u = -Hu = \frac{1}{2}\Delta u - Vu,\ u(0,x) = 1_{\mathcal{C}}(x)\psi_I(x),\ u = 0 \text{ on } \partial\mathcal{C}.$$

Let

$$E_{\mathcal{C}} = \inf\{< \psi, H\psi >_{\mathcal{C}} : \psi \in H_0^1(\mathcal{C}), \|\psi\|_{L^2(\mathcal{C})} = 1\}.$$

$E_{\mathcal{C}}$ is attained for some $\psi_{\mathcal{C}}$ positive on $\mathcal{C}$.

$$E^{DMC}(t) = \frac{\sum_{\mathcal{C}} < H\psi_I, \chi(t,.) >_{L^2(\mathcal{C})}}{\sum_{\mathcal{C}} < \psi_I, \chi(t,.) >_{L^2(\mathcal{C})}} \underset{\sim}{t\to+\infty} \frac{\sum_{\mathcal{C}} E_{\mathcal{C}} < \psi_I, \psi_{\mathcal{C}} >^2_{L^2(\mathcal{C})} e^{-E_{\mathcal{C}} t}}{\sum_{\mathcal{C}} < \psi_I, \psi_{\mathcal{C}} >^2_{L^2(\mathcal{C})} e^{-E_{\mathcal{C}} t}}.$$

As $\forall \mathcal{C}, < \psi_I, \psi_{\mathcal{C}} >^2_{L^2(\mathcal{C})} \neq 0$, $\lim_{t\to+\infty} E^{DMC}(t) = \min_{\mathcal{C}} E_{\mathcal{C}}$.

Elements of proof

Step 4: $\min_{\mathcal{C}} E_{\mathcal{C}} = E_0^{DMC}$

$\leq$: minimization component by component $\leq$ global minimization

$\geq$: let $\psi_{\mathcal{C}_0} \in H_0^1(\mathcal{C}_0)$ with $\|\psi_{\mathcal{C}_0}\|_{L^2(\mathcal{C}_0)} = 1$ be such that $< \psi_{\mathcal{C}_0}, H\psi_{\mathcal{C}_0} >_{\mathcal{C}_0} = \min_{\mathcal{C}} E_{\mathcal{C}}$.
Since $\mathcal{C}_0$ connected component of $\mathbb{R}^{3N} \setminus \psi_I^{-1}(0)$ with ψ_I antisymmetric, one can extend $\psi_{\mathcal{C}_0}$ into a function ψ antisymmetric on $\mathbb{R}^{3N}$ such that

$$\begin{cases} \psi_I^{-1}(0) \subset \psi^{-1}(0) \\ < \psi, H\psi >= \|\psi\|_2^2 < \psi_{\mathcal{C}_0}, H\psi_{\mathcal{C}_0} >_{\mathcal{C}_0} . \end{cases}$$

Remark 4

If ψ_I satisfies the tiling property, one can check that for any connected component $\mathcal{C}$ of $\mathbb{R}^{3N} \setminus \psi_I^{-1}(0)$, $E_{\mathcal{C}} = E_0^{DMC}$. Working with a single component is enough to compute E_0^{DMC}.

Computation of $E^{DMC}(t)$ in practice

Use of particles (called walkers by physicists). Evolution of the position $\tilde{X}_t^i$ of the i-th particle at time t by

- a time-discretization of $dX_t^i = dW_t^i + b(X_t^i)dt$.
  In general, Euler scheme :

$$\bar{X}_{t+\delta t}^i = \bar{X}_t^i + W_{t+\delta t}^i - W_t^i + b(\bar{X}_t^i)\delta t,$$

- rejection of the new position until $\psi_I(\bar{X}_{t+\delta t}^i)\psi_I(\bar{X}_t^i) > 0$ (otherwise particle i crosses a nodal surface of ψ_I between t and $t+\delta t$). This does not prevent multiple crossings,
- use of a Metropolis-Hastings acceptation/rejection step to ensure that the distribution of $\tilde{X}_{t+\delta t}^i$ is close to $\psi_I^2(x)dx \rightarrow$ improves the integrability of $E_L(\tilde{X}_{t+\delta t}^i) = \frac{H\psi_I}{\psi_I}(\tilde{X}_{t+\delta t}^i)$. Introduction of an effective time to handle the possibility of staying at the same place in the approximation of the exponential weight $e^{-\int_0^t E_L(X_s)ds}$ (*Umrigar, Nightingale, Runge J. Chem. Phys. 1993*).

Computation of $E^{DMC}(t)$ in practice

$$E^{DMC}(t) = \frac{\mathbb{E}\left(E_L(X_t)e^{-\int_0^t E_L(X_s)ds}\right)}{\mathbb{E}\left(e^{-\int_0^t E_L(X_s)ds}\right)}.$$

In order to control the variance, replication of the particles with high exponential weight and killing of the particles with low weight.

- In general, the number of particles is not preserved during the replication/killing steps,
- Also implementations with constant number of walkers (*Assaraf, Caffarel, Khelif Phys. Rev. E 2000*).

Numerical analysis in a simplified case

- dimension : $3N \to 1$,
- antisymmetry $\to$ oddness,
- $H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\alpha^2 x^2}{2} + \theta x^4$ with $\alpha, \theta > 0$
- $\psi_I = \sqrt{2\alpha}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} x e^{-\frac{\alpha^2 x^2}{2}}$ odd ground state of $H_0 = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{\alpha^2}{2}x^2$ (energy : $\frac{3\alpha}{2}$)
- $b = \frac{\psi_I'}{\psi_I} = \frac{1}{x} - \alpha x$
- $E_L = \frac{H\psi_I}{\psi_I} = \frac{H_0\psi_I}{\psi_I} + \theta x^4 = \frac{3\alpha}{2} + \theta x^4$
- For the SDE $dX_t = dW_t + \left(\frac{1}{X_t} - \alpha X_t\right) dt$, possibility to simulate according to the conditional law of X_{s+r} given X_s and to the reversible measure $21_{\{x>0\}}\psi_I^2(x)dx$ (initialization).

Simplification : even if b is explosive at 0, no simultaneous explosion of E_L. One-dimensional model $\to$ does not take into account explosions at points where two particles coincide.

Numerical analysis

For $E_L = \frac{3\alpha}{2} + \theta x^4$, computation of

$$E^{DMC}(T) = \frac{\mathbb{E}\left(E_L(X_T)e^{-\int_0^T E_L(X_s)ds}\right)}{\mathbb{E}\left(e^{-\int_0^T E_L(X_s)ds}\right)} = \frac{3\alpha}{2} + \theta \underbrace{\frac{\mathbb{E}\left(X_T^4 e^{-\theta\int_0^T X_s^4 ds}\right)}{\mathbb{E}\left(e^{-\theta\int_0^T X_s^4 ds}\right)}}_{E^D(T)}$$

Time discretization of the integral: $K \in \mathbb{N}^*$ steps

Lemma 5

For $K \in \mathbb{N}^*$,

$$\left| E^D(T) - \underbrace{\frac{\mathbb{E}\left(X_T^4 e^{-\frac{\theta T}{K}\sum_{k=1}^K X_{kT/K}^4}\right)}{\mathbb{E}\left(e^{-\frac{\theta T}{K}\sum_{k=1}^K X_{kT/K}^4}\right)}}_{E_K^D(T)} \right| \leq \frac{C_T}{K}.$$

Particle approximation

- $(X_0^i)_{1\leq i\leq N}$ i.i.d. according to $2\psi_I^2(x)1_{\{x>0\}}dx$
- To control variance, ν resampling of the particles over $[0,T]$: $l=\frac{K}{\nu}$ number of discretization steps and $\Delta t=\frac{T}{\nu}$ time between two resampling.
  For $0\leq n\leq \nu-1$, to obtain $(X^i_{(n+1)\Delta t})_{1\leq i\leq N}$ from $(X^i_{n\Delta t})_{1\leq i\leq N}$
  - Mutation step :simulation of $\xi_n=((X^i_{n\Delta t+\frac{T}{K}},\ldots,X^i_{n\Delta t+\frac{lT}{K}})_{1\leq i\leq N})$ according to SDEs driven by independent Brownian motions
  - Selection step : conditionally to the result, generation of $(X^i_{(n+1)\Delta t})_{1\leq i\leq N}$ indep. and s.t. the following consistency equality holds

$$\mathbb{E}\left(\frac{1}{N}\sum_{i=1}^N \delta_{X^i_{(n+1)\Delta t}}\middle|\xi_n\right)=\sum_{j=1}^N \rho^j\delta_{X^j_{n\Delta t+\frac{lT}{K}}} \quad \text{with } \rho^j=\frac{e^{-\frac{\theta T}{K}\sum_{k=1}^l (X^j_{n\Delta t+\frac{kT}{K}})^4}}{\sum_{i=1}^N e^{-\frac{\theta T}{K}\sum_{k=1}^l (X^i_{n\Delta t+\frac{kT}{K}})^4}}$$

Selection step

Resampling methods which satisfy the assumption

Multinomial sampling : $(X^i_{(n+1)\Delta t})_{1\leq i\leq N}$ conditionally i.i.d. according to $\sum_{j=1}^N \rho^j \delta_{X^j_{n\Delta t+\frac{lT}{K}}}$

Residual sampling : Let $a^j = \lfloor N\rho^j \rfloor$. Choose $X^i_{(n+1)\Delta t} = X^j_{n\Delta t+\frac{lT}{K}}$ for $1+\sum_{m=1}^{j-1} a^m \leq i \leq \sum_{m=1}^{j} a^m$ and choose the remaining $N-\sum_{m=1}^N a^m$ positions i.i.d. according to $\sum_{j=1}^N \frac{N\rho^j - a^j}{N-\sum_{m=1}^N a^m}\delta_{X^j_{n\Delta t+\frac{lT}{K}}}$.

Stratified sampling : for $1\leq i\leq N$ let U^i be i.i.d. $\sim \mathcal{U}[0,1]$ and

$$X^i_{(n+1)\Delta t} = \sum_{j=1}^N 1_{\{\sum_{m=1}^{j-1}\rho^m \leq \frac{i-U^i}{N} \leq \sum_{m=1}^{j}\rho^m\}} X^j_{n\Delta t+\frac{lT}{K}}$$

Stratified reminder sampling : First step in residual sampling + stratified instead of multinomial sampling in the 2^{nd}

Particle approximation

Theorem 6

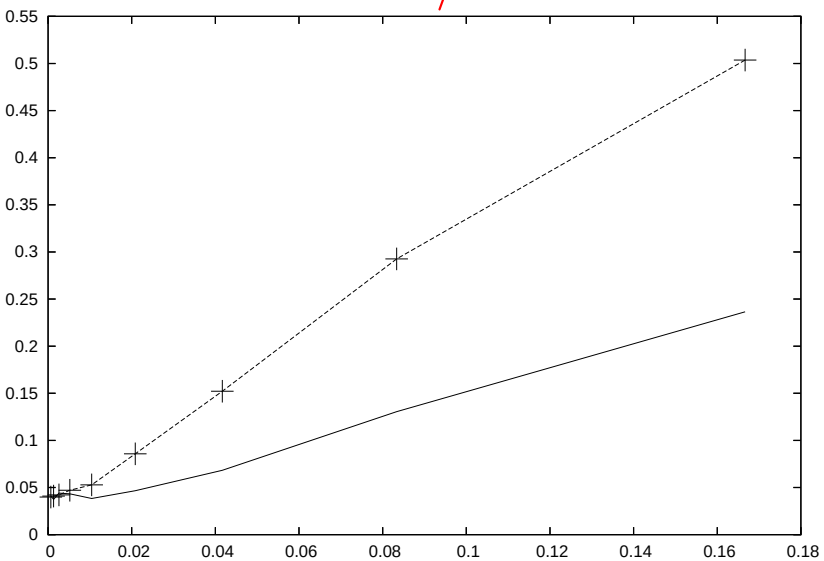
$$\mathbb{E}\left|E^D(T) - \frac{1}{N}\sum_{i=1}^{N}(X^i_{\nu\Delta t})^4\right| \leq \frac{C_\nu}{\sqrt{N}} + \frac{C_T}{K}.$$

(El Makrini, Jourdain, Lelièvre M2AN 2007).

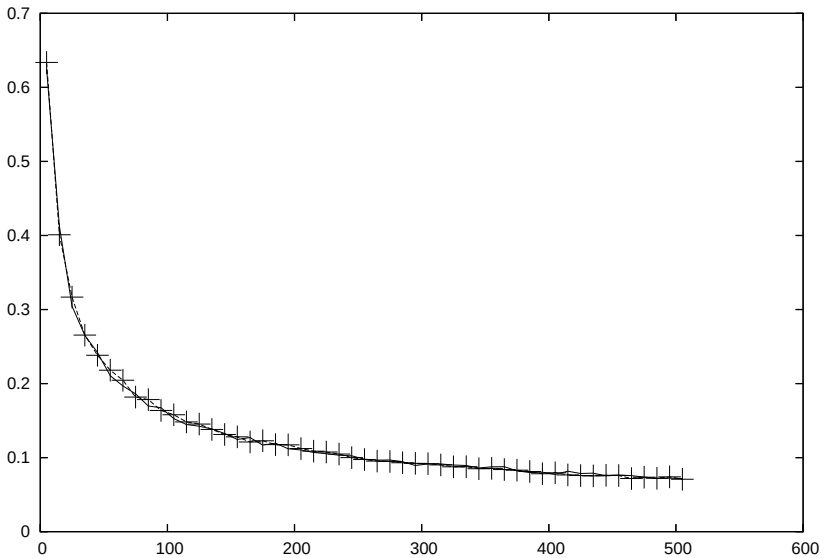
- main contribution w.r.t. *Del Moral et al*: C_ν does not depend on K, E_L unbounded
- for fixed ν and T, convergence as $N, K \to +\infty$
- optimal number ν of resampling?

Numerical results

$1/K$



N

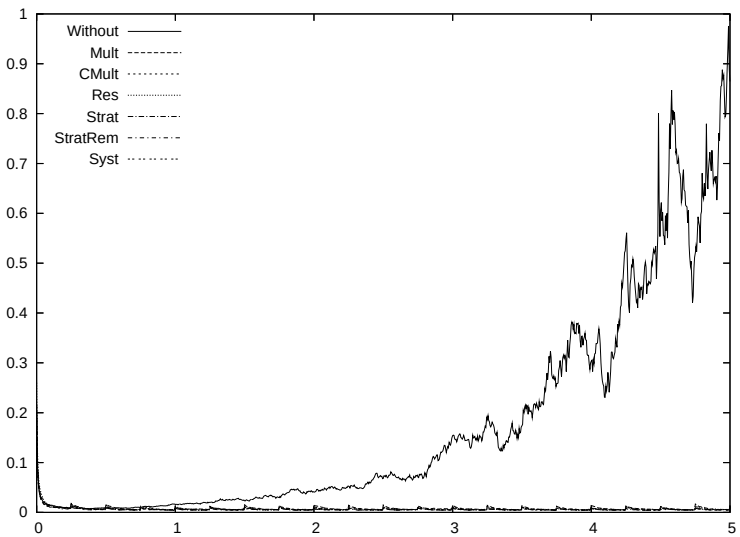


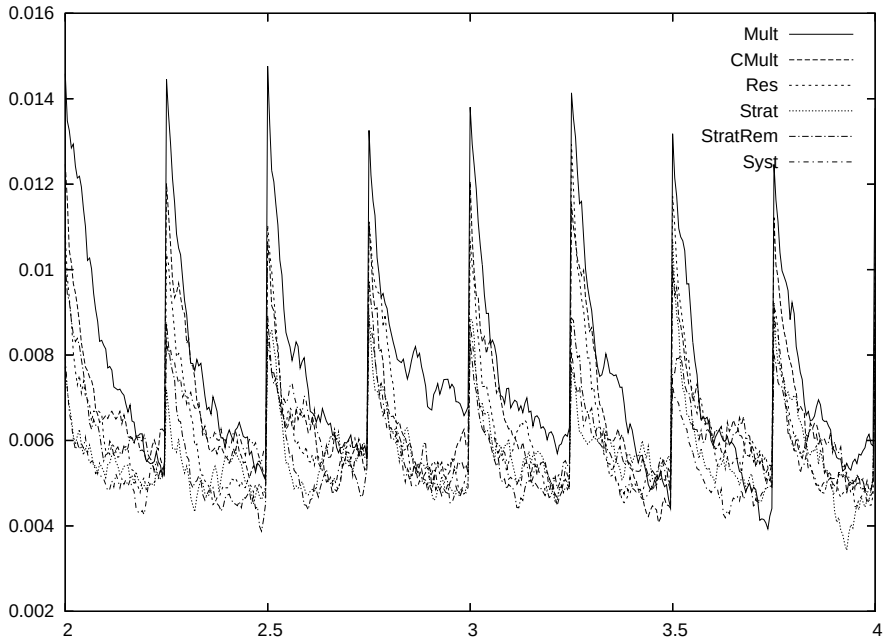
Expectation of the absolute value of the error (reference energy computed by a spectral method) w.r.t.

- the number K of discretization steps ($N = 5000$, $\nu = 30$ multinomial resampling, $\theta = 2$, $T = 5$, 300 independent realizations)
- the number N of particles ($\nu = 50$ multinomial resampling, $\theta = 0.5$, $T = 5$, $K = 1000, 2000$ independent realizations).

Exact simulation of the SDE (dotted curves)/ use of a discretization scheme proposed by *Alfonsi, MCMA 2006 (solid curves).*

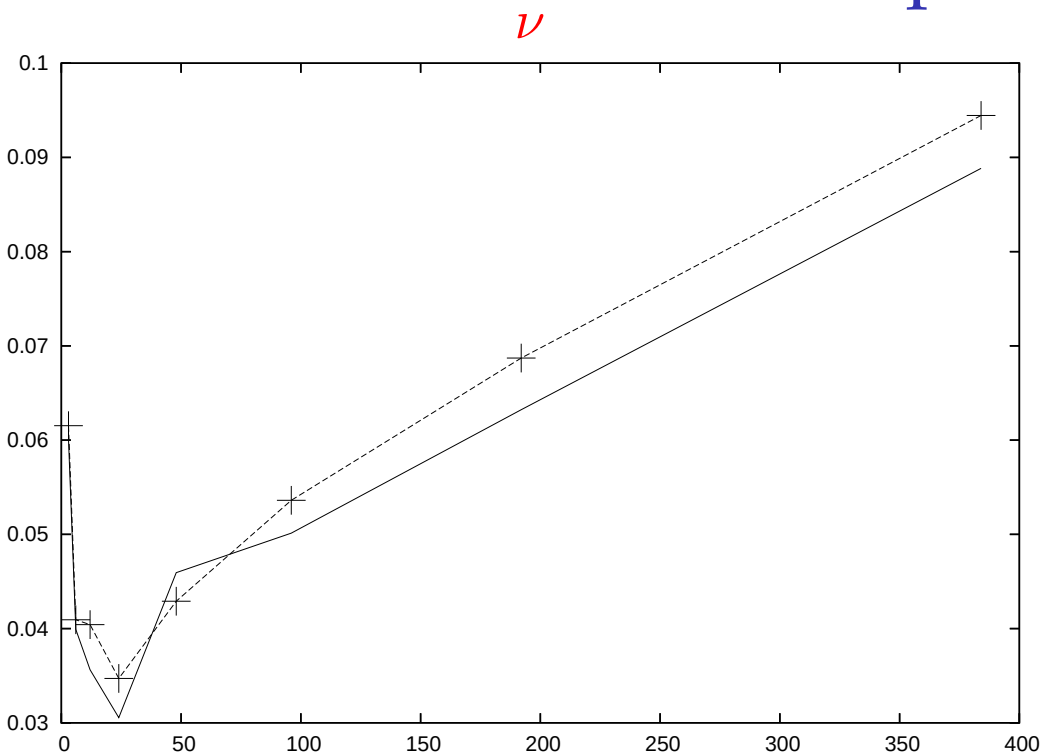
Comparison of the resampling methods





Evolution of the variance (computed over 200 indep. simulations) with time : $N = 1000$, $T = 5$, $K = 1000$, $\nu = 20$, $\theta = 2$.

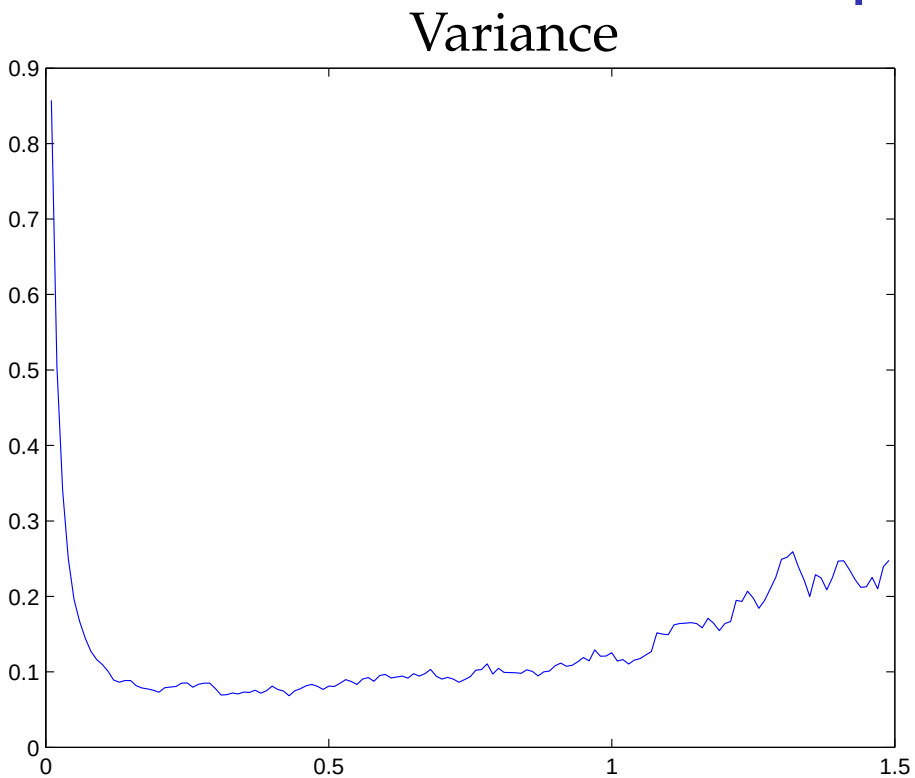
Choice of the number ν of selection steps



Expectation of the absolute value of the error (reference energy computed by a spectral method) w.r.t. the number ν of selection steps (multinomial resampling, $N = 5000$, $T = 5$, $K = 1000$, $\theta = 2$, 300 independent realizations)

$\nu_* = 25$ optimal !

Choice of the number ν of selection steps



Evolution of the variance without resampling with time T (same parameters)

Minimal for $t_* \sim 0.25$. $T/t_* = 20$ close to $\nu_* = 25$.

Suggests to compute t_* (without resampling, variance easily estimated over a few independent particles) and choose $\nu = T/t_*$.