Averaging for SPDEs: strong and weak order

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Workshop: Hybrid dynamical systems simulation and applications to molecular dynamics

We study multiscale systems of SPDEs

$$dX^{\epsilon}(t) = \left(AX^{\epsilon}(t) + F(X^{\epsilon}(t), Y^{\epsilon}(t))\right) dt$$

$$dY^{\epsilon}(t) = \frac{1}{\epsilon}(BY^{\epsilon}(t) + G(X^{\epsilon}(t), Y^{\epsilon}(t)))dt + \frac{1}{\sqrt{\epsilon}}dW(t)$$

$$X^{\epsilon}(0) = x, Y^{\epsilon}(0) = y$$

in $H = L^2(0,1)$, on $[0,T]$.
W: **cylindrical Wiener process** on H.
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Problems:

- Give an order of convergence, in strong and weak sense.
- Application: HMM scheme.
- Comparison with the SDE case.

Existing results

- Finite dimensional case:
  R. Z. Khasminskii, *On an averaging principle for Itô stochastic differential equations*, Kybernetica (1968).
  W. E, D. Liu, E. Vanden-Eijnden, *Analysis of Multiscale Methods for Stochastic Differential Equations*, Communications on Pure and Applied Mathematics (2005).

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- Infinite dimensional case:
  S. Cerrai, M. Freidlin, *Averaging principle for a class of SPDEs*, Probability Theory & Related Fields (2009).
  S. Cerrai, *A Khasminskii type averaging principle for stochastic reaction-diffusion equations*, Annals of Applied Probability (2009).

Linear coefficients (1)

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Spectral properties:

$$Ae_k = -\lambda_k e_k \text{ for all } k \in \mathbb{N}$$

$$\lambda := \inf_{k \in \mathbb{N}} \lambda_k > 0, \lambda_k \sim Ck^2.$$

$$Bf_k = -\mu_k f_k \text{ for all } k \in \mathbb{N}$$

$$\mu := \inf_{k \in \mathbb{N}} \mu_k > 0, \mu_k \sim C'k^2.$$

We can define semi-groups $(e^{tA})_{t \geq 0}$ and $(e^{tB})_{t \geq 0}$.

Linear coefficients (2)

Definition

For $\alpha \in [0,1]$,

$$(-A)^{\alpha} x = \sum_{k=0}^{\infty} \lambda_k^{\alpha} x_k e_k$$

with domain

$$D(-A)^{\alpha} = \left\{ x \in H; \sum_{k=0}^{+\infty} (\lambda_k)^{2\alpha} |x_k|^2 < +\infty \right\};$$

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Regularization properties: for $0<s<t$

$$|e^{tA}x|_{(-A)^{\alpha}}\leq C_{\alpha}t^{-\alpha}|x|_H$$

$$|e^{tA}x-e^{sA}x|_H\leq\begin{cases}C\frac{(t-s)^{\delta}}{s^{\delta}}|x|_H\\ C(t-s)^{\delta}|x|_{(-A)^{\delta}}.\end{cases}$$

Nonlinear coefficients

- $F : H^2 \to H$ is $\mathcal{C}_b^2$.
- $U : H^2 \to \mathbb{R}$ is $\mathcal{C}_b^3$.
- $G(x, y) := \nabla_y U(x, y)$.

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Strict dissipativity assumption:

$$L_G := \sup_{x,y_1,y_2 \in H} \frac{|G(x,y_1) - G(x,y_2)|}{|y_1 - y_2|} < \mu.$$

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Additional assumption:

There exists $\alpha > 0$, $0 \leq \gamma < \frac{1}{4}$, $C > 0$ such that for every $x \in H$ and $y_1, y_2 \in D((-B)^\gamma)$

$$|(-A)^\alpha (F(x,y_1) - F(x,y_2))| \leq C |(-B)^\gamma (y_1 - y_2)|.$$

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$W(t) = \sum_k \beta_k(t) q_k$ is **cylindrical Wiener process** on H.
This series does not converge in H, but only in K such that the imbedding $\Psi : H \subset K$ is **Hilbert-Schmidt**:

$$|\Psi|^2_{\mathcal{L}_2(H,K)} := \sum_{k=0}^{+\infty} |\Psi(q_k)|^2_K < +\infty.$$

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$$\int_0^T \Psi(s)dW(s) := \sum_{k,l}\int_0^T < \Psi(s)q_k, r_l > d\beta_k(s)r_l$$

is well-defined for $\Psi \in L^2(\Omega\times[0,T];\mathcal{L}_2(H,K))$.

Properties:

$$\mathbb{E}\int_0^T \Psi(s)dW(s) = 0$$

$$\mathbb{E}|\int_0^T \Psi(s)dW(s)|_K^2 = \mathbb{E}\int_0^T |\Psi(s)|^2_{\mathcal{L}_2(H,K)}ds.$$

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If $v \in H$, $< v, W(t) >$ exists and the **space-time white noise** property holds:

$$\mathbb{E} < v_1, W(t) >< v_2, W(s) >= t \wedge s < v_1, v_2 > .$$

Basic properties of solutions

The **stochastic convolution** $W^B(t) = \int_0^t e^{(t-s)B} dW(s)$ is well-defined; it is the unique mild solution of

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Proposition

For any $\epsilon > 0$, $T > 0$, $x \in H$, $y \in H$, our system admits a unique ***mild solution*** (X^ϵ, Y^ϵ):

$$X^\epsilon(t) = e^{tA}x + \int_0^t e^{(t-s)A} F(X^\epsilon(s), Y^\epsilon(s))ds$$

$$Y^\epsilon(t) = e^{\frac{t}{\epsilon}B}y + \frac{1}{\epsilon}\int_0^t e^{\frac{(t-s)}{\epsilon}B} G(X^\epsilon(s), Y^\epsilon(s))ds$$

$$+\frac{1}{\sqrt{\epsilon}}\int_0^t e^{\frac{(t-s)}{\epsilon}B} dW(s).$$

On the fast process

If $x \in H$, the fast equation with frozen slow component is:

$$dY_x(t,y) = (BY_x(t,y) + G(x, Y_x(t,y)))dt + dW(t)$$
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For any $t \geq 0$, $y, z \in H$,

$$|Y_x(t,y) - Y_x(t,z)| \leq Ce^{-ct}|y-z| \text{ as }.$$

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Consequences:

- It has a unique invariant probability measure:

$$\mu^x(dy) = \frac{1}{Z(x)} e^{2U(x,y)} \nu(dy). \tag{1}$$

- Exponential mixing: for ϕ Lipschitz continuous,

$$|\mathbb{E}\phi(Y_x(t,y)) - \int \phi(z)\mu^x(dz)| \leq C(1+|x|+|y|)e^{-ct}.$$

The averaged equation

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$$\overline{F}(x) = \int_H F(x,y)\mu^x(dy).$$

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The averaged equation is:

$$d\overline{X}(t) = (A\overline{X}(t) + \overline{F}(\overline{X}(t)))dt,$$

with initial condition $\overline{X}(0) = x \in H$.
It admits a unique mild solution:

$$\overline{X}(t) = e^{tA}x + \int_0^t e^{(t-s)A}\overline{F}(\overline{X}(s))ds.$$

Strong and weak order of convergence

Theorem (Strong-order)

For any $0 < r \ll 1$, *for any* $T > 0$, *if* $x \in D(A)$, *and* $y \in H$, *then for any* $\epsilon > 0$ *and any* $0 \leq t \leq T$

$$\mathbb{E}|X^\epsilon(t) - \overline{X}(t)| \leq C\epsilon^{1/2-r}. \tag{2}$$

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Theorem (Weak-order)

For any $0 < r \ll 1$*, for any* $\phi : H \to \mathbb{R}$ *of class* $\mathcal{C}_b^2$*,* $T > 0$*, if* $x \in D(A)$*,* $y \in D(B)$*, then for any* $\epsilon > 0$ *and* $0 \leq t \leq T$

$$|\mathbb{E}[\phi(X^\epsilon(t))] - \mathbb{E}[\phi(\overline{X}(t))]| \leq C\epsilon^{1-r}. \tag{3}$$

Proof of the strong-order result (1)

Idea: introduction of a parameter δ and of auxiliary processes $(\tilde{X}^\epsilon, \tilde{Y}^\epsilon)$.
On $[k\delta, (k+1)\delta]$, with $0 \leq k \leq N := \lfloor \frac{T_0}{\delta} \rfloor$, we define

$$d\tilde{X}^\epsilon(t) = (A\tilde{X}^\epsilon(t) + F(X^\epsilon(k\delta), \tilde{Y}^\epsilon(t)))dt$$

$$d\tilde{Y}^\epsilon(t) = \frac{1}{\epsilon}(B\tilde{Y}^\epsilon(t) + G(X^\epsilon(k\delta), \tilde{Y}^\epsilon(t)))dt + \frac{1}{\sqrt{\epsilon}}dW(t),$$

with $\tilde{X}^\epsilon(0) = x$, $\tilde{Y}^\epsilon(0) = y$, and a continuity assumption at any $k\delta$.

Proof of the strong-order result (2)

- For any $\epsilon > 0$, for any $0 \leq t \leq T$

$$\mathbb{E}|X^\epsilon(t) - \tilde{X}^\epsilon(t)|^2 \leq C\delta^{2(1-r)}$$
$$\mathbb{E}|Y^\epsilon(t) - \tilde{Y}^\epsilon(t)|^2 \leq C\delta^{2(1-r)}.$$

- Estimate: for any $0 \leq t \leq T$

$$\mathbb{E}|\tilde{X}^\epsilon(t) - \overline{X}(t)|^2 \leq C\delta^{2(1-r)} + C(1+\delta^{-r})(1+\frac{1}{1-e^{-c\frac{\delta}{\epsilon}}})\epsilon$$

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- Now we choose $\delta = \delta(\epsilon)$; then

$$\mathbb{E}|X^\epsilon(t) - \overline{X}(t)|^2 \leq C\epsilon^{(1-r')}.$$

Asymptotic expansion (1)

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u^ϵ and $\overline{u}$ are solutions of Kolmogorov equations:

$$\frac{\partial u^\epsilon}{\partial t}(t,x,y) = L^\epsilon u^\epsilon(t,x,y)$$
$$u^\epsilon(0,x,y) = \phi(x)$$

$$\frac{\partial \overline{u}}{\partial t}(t,x,y) = \overline{L}\overline{u}(t,x,y)$$
$$\overline{u}(0,x,y) = \phi(x)$$

Asymptotic expansion (2)

Differential operators are

$$L_1\psi(x,y) = < By + G(x,y), D_y\psi(x,y) > + \frac{1}{2}\mathrm{Tr}(D^2_{yy}\psi(x,y))$$
$$L_2\psi(x,y) = < Ax + F(x,y), D_x\psi(x,y) >$$
$$L^\epsilon = \frac{1}{\epsilon}L_1 + L_2$$
$$\overline{L}\psi(x) = < Ax + \overline{F}(x), D_x\psi(x) > .$$

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Strategy: find an expansion of u^ϵ with respect to the parameter ϵ:

$$u^\epsilon = u_0 + \epsilon u_1 + v^\epsilon,$$

v^ϵ being a residual term.

Asymptotic expansion (3)

By identification with respect to powers of ϵ:

$$L_1 u_0 = 0$$

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u_1 is solution of

$$L_1 u_1(t,x,y) =< \overline{F}(x) - F(x,y), D_x u_0(t,x) > := -\chi(t,x,y).$$

Then $u_1(t,x,y) = \int_0^{+\infty} \mathbb{E}[\chi(t,x,Y_x(s,y))]ds$.

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Therefore

$$\begin{aligned} u^\epsilon(T,x,y) - u^0(T,x,y) &= \epsilon u^1(T,x,y) \\ &+ \epsilon\mathbb{E}[u^1(0,X^\epsilon(T,x,y),Y^\epsilon(T,x,y))] \\ &+ \epsilon\mathbb{E}[\int_0^T (L_2 u_1 - \frac{\partial u_1}{\partial t})(T-t,X^\epsilon(t,x,y),Y^\epsilon(t,x,y))dt]. \end{aligned} \tag{4}$$

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If you can control each term, the proof is done.

The SPDE case

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Remedy: reduction to a finite dimensional problem and proving uniform bounds with respect to dimension.

Reduction to a finite dimensional problem (1)

We use spaces $H_N^{(1)}$ and $H_N^{(2)}$ spanned by the first N eigenvectors of the operators A and B.

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We naturally define orthogonal projectors $P_N^{(1)}$, $P_N^{(2)}$, coefficients F_N, G_N, and processes

$$dX_N^\epsilon(t) = (AX_N^\epsilon(t) + F_N(X_N^\epsilon(t), Y_N^\epsilon(t)))dt$$

$$dY_N^\epsilon(t) = \frac{1}{\epsilon}(BY_N^\epsilon(t) + G_N(X_N^\epsilon(t), Y_N^\epsilon(t)))dt + \frac{1}{\sqrt{\epsilon}}dW_N(t), \tag{5}$$

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\end{aligned}
\tag{5}
$$

We have new invariant measures $\mu_N^x(dy)$, new averaged coefficient $\overline{F_N}$.

Reduction to a finite dimensional problem (2)

New averaged equation

$$d\overline{X_N}(t) = (A\overline{X_N}(t) + \overline{F_N}(\overline{X_N}(t)))dt. \tag{6}$$

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New averaged equation

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Lemma

1. *For any fixed* $\epsilon > 0$ *and* $t \geq 0$*, when* $N \to +\infty$

$$\mathbb{E}|X^\epsilon(t) - X_N^\epsilon(t)|^2 + \mathbb{E}|Y^\epsilon(t) - Y_N^\epsilon(t)|^2 \to 0.$$

2. *For any* $t \geq 0$*, when* $N \to +\infty$

$$|\overline{X}(t) - \overline{X_N}(t)| \to 0.$$

Example of estimate

For any t, x, y,

$$\begin{aligned}
|u_1(t,x,y)| &= \Big|\int_0^{+\infty} \mathbb{E}[\chi(t,x,Y_x(s,y))]ds\Big| \\
&\leq \int_0^{+\infty} |\mathbb{E}[\chi(t,x,Y_x(s,y))]|ds \\
&\leq \int_0^{+\infty} Ce^{-cs}(1+|x|+|y|)[y \mapsto \chi(t,x,y)]_{\mathrm{Lip}}ds.
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But $\chi(t,x,y) =< \overline{F}(x) - F(x,y), D_x u_0(t,x) >$; so you need $|D_x u_0(t,x).h|$, for any h.

Since $u_0(t,x) = \phi(\overline{X}(t,x))$, we compute

$$D_x u_0(t,x).h = D\phi(\overline{X}(t,x)).\eta^h(t,x),$$

with

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Conclusion: for any t,x,y

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Description of the numerical method (1)

Aim: approximation of the slow component X^ϵ.

Principle:

- 2 time step size Δt (macrosolver for X) and δt (microsolver for Y): *Heterogeneous Multiscale Method*.
- Instead of looking at $X^\epsilon(t)$, look at $\overline{X}(t)$ (averaging result!).
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More precisely:

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More precisely:

$$X_{n+1} = X_n + \Delta t A X_{n+1} + \Delta t \tilde{F}_n$$
$$X_0 = x.$$

Description of the numerical method (2)

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\begin{aligned}
Y_{n,m+1,j} = Y_{n,m,j} + \frac{\delta t}{\epsilon} B Y_{n,m+1,j} + \frac{\delta t}{\epsilon} G(X_n, Y_{n,m,j}) \\
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$$\tilde{F}_n = \frac{1}{MN} \sum_{j=1}^{M} \sum_{m=n_T}^{N_m} F(X_n, Y_{n,m,j}),$$

with parameters M, n_T, N, $N_m = n_T + N - 1$.

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Initial conditions:

$$Y_{0,0,j} = y$$
$$Y_{n+1,0,j} = Y_{n,N_m,j}.$$

Strong convergence

Theorem

Assume $x \in D(A)$. For any $0 < r \ll 1$, for any $T > 0$, there exists $c, C > 0$ such that for any $0 \leq n \leq N_0 = \lfloor \frac{T}{\Delta t} \rfloor$

$$\mathbb{E}|X_n - X(n\Delta t)| \leq C(\epsilon^{\frac{1}{2}-r} + \Delta t^{1-r}) + C[(\frac{\delta t}{\epsilon})^{1/2-r} + \frac{1}{\sqrt{N\frac{\delta t}{\epsilon} + 1}} e^{-cn_T\frac{\delta t}{\epsilon}}(R + \sqrt{R})] + C\frac{\sqrt{\Delta t}}{\sqrt{M(N\frac{\delta t}{\epsilon} + 1)}},$$

with $R = \frac{\Delta t}{1 - e^{-\frac{c}{2}N_m\frac{\delta t}{\epsilon}}}$.

Weak convergence

Theorem

Assume $x \in D(A)$ and $y \in D(B)$. Let $\Phi : H \to H$ of class $\mathcal{C}_b^2$. For any $0 < r \ll 1$, for any $T > 0$, there exists $c, C > 0$ such that for any $0 \leq n \leq N_0 = \lfloor \frac{T}{\Delta t} \rfloor$

$$
\begin{aligned}
|\mathbb{E}\Phi(X_n) - \mathbb{E}\Phi(X(n\Delta t))| \leq C(\epsilon^{1-r} + \Delta t^{1-r}) \\
+ C[(\frac{\delta t}{\epsilon})^{1/2-r} + \frac{1}{\sqrt{N\frac{\delta t}{\epsilon} + 1}} e^{-cn_T\frac{\delta t}{\epsilon}}(R + R^2)] \\
+ C\frac{\Delta t}{M(N(\frac{\delta t}{\epsilon}) + 1)}.
\end{aligned}
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Conclusion

Proof of a strong order and of a weak order of convergence, as for SDEs.
Weak order is better than strong order.
HMM method can be adapted.

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Proof of a strong order and of a weak order of convergence, as for SDEs.
Weak order is better than strong order.
HMM method can be adapted.
Some limits:

- No noise in the slow equation.
- The strict dissipativity assumption.
- The additional assumption on F.