Efficient time discretisations of parabolic PDEs

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Part I joint with Conall Kelly : UWI

- Motivation & Taming
- Adaptivity introduction
- General framework for adaptivity & convergence
- Extensions and numerics

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- Motivation & Taming
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Part II joint with Utku Erdoğan : **formerly** Uşak University

- New exponential integrator(s)
- Homotopy
- Application to SPDEs

Non-convergence: [Hutzenthaler, Jentzen, Kloeden 2011].

$$\text{SDE} \qquad dX = f(X)dt + g(X)dW.$$

Euler-Maruyama method:

$$X_{n+1}^N = X_n^N + \Delta t f(X_n^N) + g(X_n^N)(W((n+1)\Delta t) - W(n\Delta t)).$$

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  not globally Lipschitz + polynomial growth condition then
  Non-convergence of $\mathbb{E}\|X(t) - X_n\|^2$

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The associated Euler map with stepsize Δt for deterministic Eq.

$$x_{n+1} = x_n - \Delta t x_n |x_n|^2$$

- stable equilibrium solution at 0
- unstable two-cycle at $\left\{\pm\sqrt{2/\Delta t}\right\}$.

So the basin of attraction of the zero solution is $|x_0| < \sqrt{2/\Delta t}$.

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- Outside of the basin of attraction : oscillation and growth !

Tamed Euler-Maruyama methods

[Hutzenthaler, Jentzen, Kloeden], [Hutzenthaler,Jentzen], [Gyongy, Sabanis, Siska], etc

- Idea : introduce higher order perturbation of the flow

Drift-tamed Euler-Maruyama

$\Delta W_{n+1} = (W((n+1)\Delta t) - W(n\Delta t))$

$$Y_{n+1}^N = Y_n^N + \frac{\Delta t}{1 + \Delta t \|f(Y_n^N)\|} f(Y_n^N) + g(Y_n^N)\Delta W_{n+1}$$

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Moment bounds

$$\sup_{n\in\mathbb{N}} \sup_{n\in\{0,1,\dots,N\}} \mathbb{E}[\|Y_n^N\|^p] < \infty. \tag{1}$$

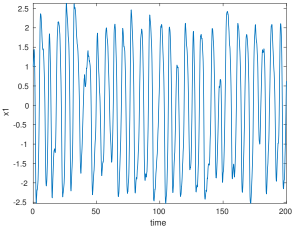
Strong convergence

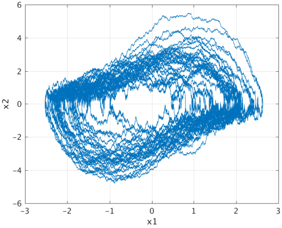
$$\left(\mathbb{E}\left[\sup_{t\in[0,T]} \|X(t) - \bar{Y}_t^N\|^p\right]\right)^{1/p} \leq C_p \Delta t^{1/2}$$

- but use a finite Δt in computations.

Perturbation - large step Δt

- VdPol equation : True $\Delta t = 10^{-4}$





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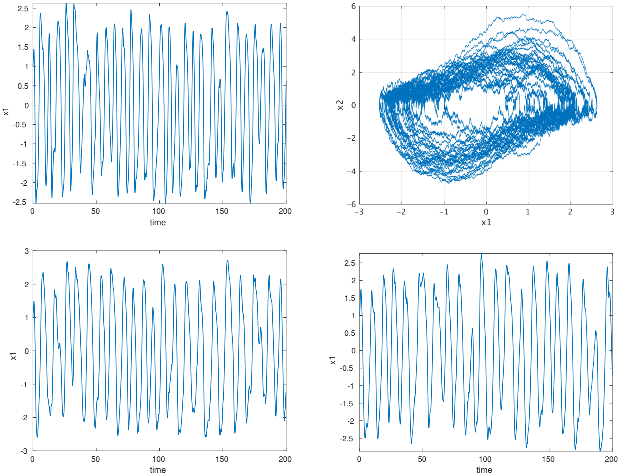

Fixed step approximations : $\Delta t = 0.0838$ and $\Delta t = 0.1269$
Relative Errors in frequency: ≈ 0.21 & ≈ 0.28

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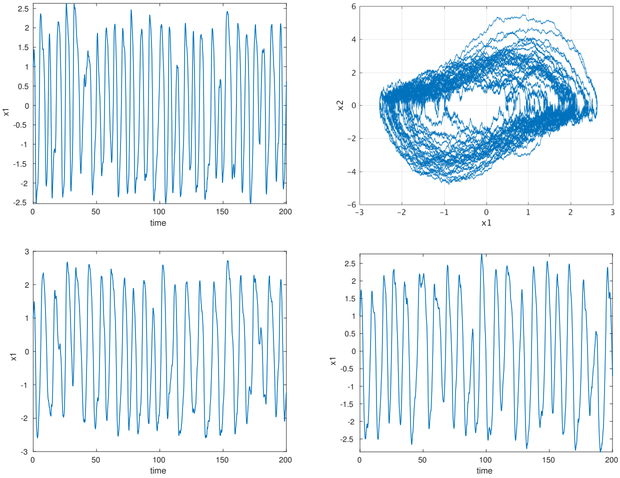

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- Adapt the step. Relative Errors : ≈ 0.09 & ≈ 0.18

SPDE: same issues apply

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$$du = \left[\epsilon u_{xx} + u - u^3\right] dt + \sigma dW,$$

$\epsilon = 0.01$, $\sigma = 0.5$
Discretized in space: (Eg FEM)

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Large system of SDEs with additive noise.

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Sample solution at $T = 5$. $\Delta t_{ref} = 5 \times 10^{-4}$. 100 SDEs

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- RMS L^2 Error using Fixed step $\Delta t = 0.004555$: 0.157084

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- Alternative: fully implicit - expensive.

Explicit Adaptive step : A General Framework

$$dX(t) = f(X(t))dt + g(X(t))dW(t), \quad t > 0,$$

Let $(\mathcal{F}_t)_{t\geq 0}$ be the natural filtration of W.
Suppose $f : \mathbb{R}^d \to \mathbb{R}^d$ is continuously differentiable.

$$\|Df(x)\| \leq c(1 + \|x\|^c), \qquad \|f(x)\| \leq c_1(1 + \|x\|^{c+1})$$

and a one-sided Lipschitz condition with constant $\alpha > 0$:

$$\langle f(x) - f(y), x - y \rangle \leq \alpha \|x - y\|^2.$$

For diffusion term : global Lipschitz

$$\|g(x) - g(y)\|_F \leq \kappa \|x - y\|.$$

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- Unique strong solution on $[0, T]$, on the filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\geq 0}, \mathbb{P})$.

For each $p > 0$ there is $C = C(p, T, X(0)) > 0$ such that

$$\mathbb{E} \sup_{s\in[0,T]} \|X(s)\|^p \leq C.$$

EM with adaptive step

Euler-type method for SDE over a random mesh $\{t_n\}_{n\in\mathbb{N}}$ on $[0, T]$

$$Y_{n+1} = Y_n + \Delta t_{n+1} f(Y_n) + g(Y_n)\left(W(t_{n+1}) - W(t_n)\right)$$

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- $\{\Delta t_n\}_{n\in\mathbb{N}}$ sequence random timesteps: Δt_{n+1} determined by Y_n.
- Let $\{t_n := \sum_{i=1}^{n} \Delta t_i\}_{n=1}^{N}$ with $t_0 = 0$, t_n a $(\mathcal{F}_t)$-stopping time.

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Define discrete-time filtration $\{\mathcal{F}_{t_n}\}_{n\in\mathbb{N}}$ by

$$\mathcal{F}_{t_n} = \{A \in \mathcal{F} \,:\, A \cap \{t_n \leq t\} \in \mathcal{F}_t\}, \quad n \in \mathbb{N}.$$

Suppose that each Δt_n is $\mathcal{F}_{t_{n-1}}$-measurable.

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Let Δt_n satisfy $\Delta t_{\text{min}} < \Delta t_n < \Delta t_{\text{max}}$ where

$$\Delta t_{\text{max}} = \rho \Delta t_{\text{min}} \qquad 0 < \rho \in \mathbb{R}$$

- Δt_{min} ensures finite number of time steps over $[0, T]$.

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$$\Delta t_{\max} = \rho \Delta t_{\min} \qquad 0 < \rho \in \mathbb{R}$$

- $\Delta t_{\min}$ ensures finite number of time steps over $[0, T]$.
- $\Delta t_{\max}$ prevents stepsizes from becoming too large.

Convergence as $\Delta t_{\max} \to 0$.

Adaptive timestepping scheme

$$Y_{n+1} = Y_n$$
$$+\Delta t_{n+1}\left[f(Y_n)\mathcal{I}_{\{\Delta t_{n+1}>\Delta t_{\min}\}} + \frac{f(Y_n)}{1+\Delta t_{\min}\|f(Y_n)\|}\mathcal{I}_{\{\Delta t_{n+1}=\Delta t_{\min}\}}\right]$$
$$+ g(Y_n)\left(W(t_{n+1}) - W(t_n)\right), \quad n = 0, \ldots, N-1.$$

- Each $W(t_{n+1}) - W(t_n)$ is a Wiener increment taken over a random step of length Δt_{n+1} which itself may depend on Y_n.

Adaptive timestepping scheme

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- However, if Δt_{n+1} is an $\mathcal{F}_{t_n}$-stopping time then $W(t_{n+1})-W(t_n)$ is $\mathcal{F}_{t_n}$-conditionally normally distributed with

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\begin{aligned}
\mathbb{E}\left[\|W(t_{n+1})-W(t_n)\| \middle| \mathcal{F}_{t_n}\right] &= 0, \quad a.s. \\
\mathbb{E}\left[\|W(t_{n+1})-W(t_n)\|^2 \middle| \mathcal{F}_{t_n}\right] &= h_{n+1}, \quad a.s.
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$$\mathbb{E}\left[\|W(t_{n+1}) - W(t_n)\|^2\middle|\mathcal{F}_{t_n}\right] = h_{n+1}, \quad a.s.$$

- In practice : replace Wiener increments with i.i.d. $\mathcal{N}(0,1)$ random variables denoted $\{\xi_n\}_{n=1}^N$, scaled at each step by the $\mathcal{F}_{t_n}$-measurable random variable $\sqrt{\Delta t_{n+1}}$.

Admissible steps

- *Admissible timestepping strategy* if whenever

$\Delta t_{\text{min}} \leq \Delta t_n \leq \Delta t_{\text{max}}$,

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- Lemma : Let $\delta \le \Delta t_{\max}$, and c be the constant in bound on Df. $\{\Delta t_n\}_{n\in\mathbb{N}}$ is admissible if, for each $n = 0, \ldots, N-1$, one of the following holds

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(i) $\Delta t_{n+1} \leq \delta/\|f(Y_n)\|$;
(ii) $\Delta t_{n+1} \leq \delta/(1 + \|Y_n\|^{1+c})$;
(iii) $\Delta t_{n+1} \leq \delta\|Y_n\|/\|f(Y_n)\|$;
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Proof.

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Proof. e.g. for (i) we can apply $\rho = \Delta t_{\max}/\Delta t_{\min}$

$$\|f(Y_n)\|^2 \le \left(\frac{\delta}{\Delta t_{n+1}}\right)^2 \le \frac{\Delta t_{\max}^2}{\Delta t_{\min}^2} = \rho^2,$$

and so $R_1 = \rho^2$ and $R_2 = 0$.

Admissible steps

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  Proof. e.g. for (i) we can apply $\rho = \Delta t_{\max}/\Delta t_{\min}$
$$\|f(Y_n)\|^2 \leq \left(\frac{\delta}{\Delta t_{n+1}}\right)^2 \leq \frac{\Delta t_{\max}^2}{\Delta t_{\min}^2} = \rho^2,$$
  and so $R_1 = \rho^2$ and $R_2 = 0$.
  So could use $\quad \Delta t_{n+1} = \max\left(\frac{1}{\|f(Y_n)\|}, \frac{\|Y_n\|}{\|f(Y_n)\|}\right)$.

Theorem: Strong Convergence

Let $(X(t))_{t\in[0,T]}$ be solution of the SDE
Let $\{Y_n\}_{n\in\mathbb{N}}$ be solution found with explicit admissible timestepping strategy $\{\Delta t_n\}_{n\in\mathbb{N}}$
Initial value $Y_0 = X_0$.
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$$\mathbb{E}\left[\|X(T) - Y_N\|^2\right] \leq C\Delta t_{\max}$$

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1. Conditional expectation, conditional form Ito isometry
2. Taylor expand f and g :

There are a.s. finite and $\mathcal{F}_{t_n}$-measurable random variables $\bar{K}_1, \bar{K}_2 > 0$, and constants $K_1, K_2 < \infty$,

$$\mathbb{E}\left\|\int_{t_n}^{t_{n+1}} R_z(s, t_n, X(t_n))ds\right\| \Big|\mathcal{F}_{t_n} \leq \bar{K}_1 \Delta t_{n+1}^{3/2}, \quad a.s.$$

$$\mathbb{E}\left\|\int_{t_n}^{t_{n+1}} R_z(s, t_n, X(t_n))ds\right\|^2 \Big|\mathcal{F}_{t_n} \leq \bar{K}_2 \Delta t_{n+1}^{2}, \quad a.s.$$

$$\mathbb{E}[\bar{K}_1] \leq K_1, \quad \text{and} \quad \mathbb{E}[\bar{K}_2] \leq K_2.$$

Define the error sequence $\{E_n\}_{n\in\mathbb{N}}$ by $E_{n+1} := Y_{n+1} - X(t_{n+1})$

$$E_{n+1} = E_n + \int_{t_n}^{t_{n+1}} f(Y_n) - f(X(s))ds + \int_{t_n}^{t_{n+1}} g(Y_n) - g(X(s))dW(s).$$

Then

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&\mathbb{E}\left[\|E_{n+1}\|^2 \middle| \mathcal{F}_{t_n}\right] \\
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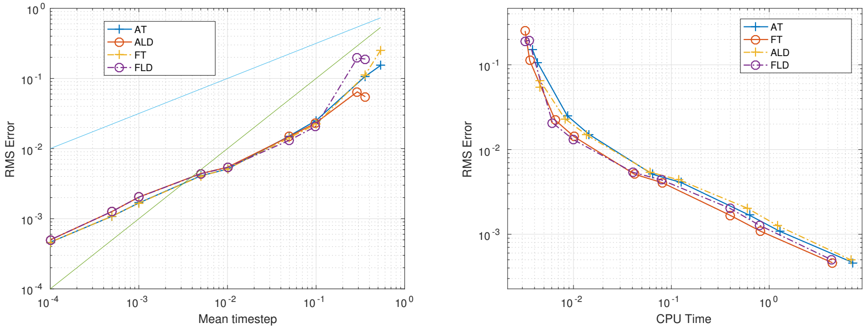
4. Sum, take expectation (Tower property) & discrete Gronwall

Numerical convergence

SDE : SGL equation Multiplicative

$$dX(t) = \left(\left(\eta + \frac{1}{2}\sigma^2\right) X(t) - \lambda X(t)^3\right) dt + \sigma X(t) dW(t)$$



$\rho = 100$. $\eta = 0.1$, $\lambda = 2$ and $\sigma = 0.5$. $T = 2$.

Numerical convergence

SDE : SGL equation Additive

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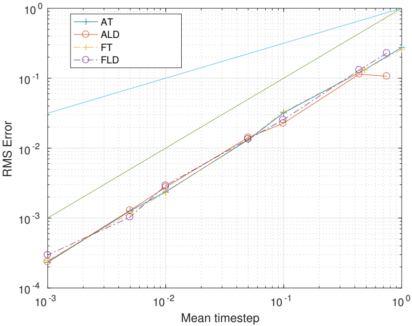

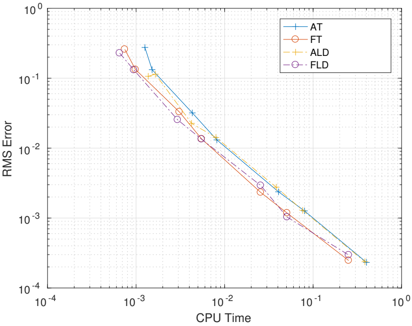

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$$\langle Y_n, f(Y_n)\rangle + \frac{1}{2}\Delta t_{n+1}\|f(Y_n)\|^2 \le \alpha\|Y_n\|^2 + \beta, \quad n = 0, \ldots, N-1,$$

One sided linear bound $\langle x, f(x)\rangle \le \alpha\|x\|^2 + \beta$, for $\alpha, \beta > 0$

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Additional upper and lower bounds on each timestep

Introduction of a convergence parameter $\delta \leq 1$.

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(i) corresponds to admissible step $\Delta t_{n+1} \leq \delta\|Y_n\|/(\|f(Y_n)\|)$;
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- Included in the framework of our proof.

Extensions:

$$\text{SDEs} \qquad dX = [AX + f(X)]\,dt + g(X)dW.$$

- Semi-implicit Euler–Maruyama

$$(I - \Delta t_{n+1} A) Y_{n+1} = Y_n + \Delta t_{n+1} f(Y_n) + g(Y_n)\,(W(t_{n+1}) - W(t_n))$$

More suitable for SPDEs - eg finite differences in space.

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- Assume f, g satisfy local Lipschitz condition and

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Mild solution

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Suppose $\Delta t_{\max} = \rho\Delta t_{\min}$, $\Delta t = Ch$ for some $c, \rho > 0$

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$$\left(\mathbb{E}\left[\|X(T) - Y_N\|^2\right]\right)^{1/2} \leq C(\Delta t_{\max}^{1/2} + h^2).$$

(Trace class noise).

Numerical results : Semi-Implicit adaptive time stepping

$$du = \left[\epsilon u_{xx} + u - u^3\right] dt + \sigma dW$$

AT = Adaptive Tamed : $\Delta t_{\min} \leq \Delta t_n \leq 1/\|f(X_n)\| \leq \Delta t_{\max}$
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H^r	Adpt Method	Error Adapt	Error TAMED	Δt_{mean}
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H^r	Adpt Method	Error Adapt	Error TAMED	Δt_{mean}
$H^{-1/2}$	AT	0.038935	0.034863	0.001730
$H^{-1/2}$	AM	0.152562	0.235331	0.028505
L^2	AT	0.013265	0.025524	0.003500
L^2	AM	0.050701	0.178778	0.041565
$H^{1/2}$	AT	0.005988	0.028424	0.004220
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Reference solution fixed step tamed method with $\Delta t = 0.0005$.
100 realizations.

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H^1	AM	0.021265	0.167884	0.046780

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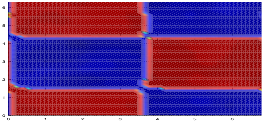
2D SPDEs additive noise. Semi-implicit solver.

$$du = \left[\epsilon \Delta u + u - u^3\right] dt + \sigma dW$$

Adpt Method	Error Adapt	Error Fixed	Δt_{mean}
AT	0.032576	0.209977	0.250000
AM	0.001032	0.017541	0.006200



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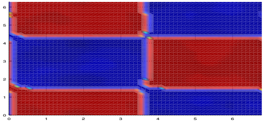

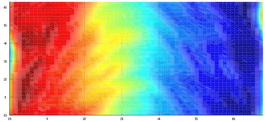

$$\text{vorticity} \quad u := \nabla \times \mathbf{v}$$

$$du = [\varepsilon \Delta u - (\mathbf{v} \cdot \nabla) u] + \sigma dW \qquad \Delta \psi = -u$$

$\psi(t, \mathbf{x})$ is scalar stream function, and $\mathbf{v} = (\psi_y, -\psi_x)$.

Adpt Method	Error Adapt	Error Fixed	Δt_{mean}
AT	0.008514	0.015214	0.003970
AM	0.009098	0.012038	0.003730

Summary I

1. Proved convergence of adaptivity step method.
2. Showed more accurate simulations for larger steps than fixed step tamed methods. (Although this is not error control).
3. Methods applicable to SPDEs: semi-linear
4. Extension to diffusion term as SDE system.

- No rejection of steps
- Could be used with error control

S(P)DEs and Multiplicative noise : with Utku Erdoğan

]
Consider SDEs of form :

$$d\mathbf{u} = (A\mathbf{u} + \mathbf{F}(\mathbf{u}))\, dt + \sum_{i=1}^{m} (B_i\mathbf{u} + \mathbf{g}_i(\mathbf{u}))\, dW_i(t), \qquad \mathbf{u}(0) = \mathbf{u}_0 \in \mathbb{R}^d,$$

where $W_i(t)$ are iid Brownian motions, $\mathbf{F}, \mathbf{g}_i : \mathbb{R}^d \to \mathbb{R}^d$
Matrices $A, B_i \in \mathbb{R}^{dxd}$, satisfy the following zero commutator conditions

$$[A, B_i] = 0, \quad [B_j, B_i] = 0, \qquad \text{for} \quad i, j = 1 \dots m.$$

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Like exponential integrators : idea is to use exact solution.

For Geometric Brownian motion ...

$$dX = \mu X dt + \sigma X dW$$

then solution

$$X(t) = X(0)\exp((\mu - \sigma^2/2)t + \sigma dW).$$

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Consider the linear homogeneous matrix differential equation

$$d\mathbf{\Phi}_{t,t_0} = A\mathbf{\Phi}_{t,t_0} dt + \sum_{i=1}^{m} B_i \mathbf{\Phi}_{t,t_0} dW_i(t), \qquad \mathbf{\Phi}_{t_0,t_0} = I_d$$

Exact solution:

$$\mathbf{\Phi}_{t,t_0} = \exp\left((A - \frac{1}{2}\sum_{i=1}^{m} B_i^2)(t - t_0) + \sum_{i=1}^{m} B_i (W_i(t) - W_i(t_0)) \right).$$

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We construct general schemes based on this.

Let $\mathbf{u}(t)$ be the solution of

$$d\mathbf{u} = (A\mathbf{u} + \mathbf{F}(\mathbf{u}))\,dt + \sum_{i=1}^{m} (B_i\mathbf{u} + \mathbf{g}_i(\mathbf{u}))\,dW_i(t),$$

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Applying the Ito formula to $\mathbf{Y}(t) = \mathbf{\Phi}_{t,t_0}^{-1}\mathbf{u}$, we obtain

$$\mathbf{u}(t_{n+1}) = \mathbf{\Phi}_{t_{n+1},t_n} \left(\mathbf{u}(t_n) + \int_{t_n}^{t_{n+1}} \mathbf{\Phi}_{s,t_n}^{-1} \tilde{f}\,(\mathbf{u}(s))\, ds + \sum_{i=1}^{m} \int_{t_n}^{t_{n+1}} \mathbf{\Phi}_{s,t_n}^{-1}\mathbf{g}_i(\mathbf{u}(s))dW_i(s)\right)$$

where

$$\tilde{\mathbf{f}}(.) = \mathbf{F}(.) - \sum_{i=1}^{m} B_i\mathbf{g}_i(.).$$

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Different treatment of the integrals above leads to different numerical schemes.

Euler type Exponential Integrators

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$$\mathbf{\Phi}_{t_{n+1},t_n} \int_{t_n}^{t_{n+1}} \mathbf{\Phi}_{s,t_n}^{-1} \mathbf{g}_i(\mathbf{u}(s)) dW_i(s) \approx \mathbf{\Phi}_{t_{n+1},t_n} \mathbf{g}_i(\mathbf{u}(t_n)) \Delta W_{i,n}$$

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We obtain our first method *EI0*

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- Capture good properties of both by introducing a homotopy parameter $p \in [0, 1]$.

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Suggest : βB_i and αg_i $\quad p = \dfrac{|\beta|}{|\alpha| + |\beta|}$.

A spectral Galerkin discretisation of an SPDE

$$du = \left[\varepsilon \frac{\partial^2 u}{\partial x^2} + 1 - u\right] dt + \left[\beta u + \alpha \frac{1-u}{1+u^2}\right] dW(t), \qquad u(x,0) = u_0(x),$$

with $x \in [0,1]$ subject to zero Dirichlet boundary conditions.

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Take $W(t)$ to be a Q–Wiener process
Let Q have orthonormal eigenfunctions $\sqrt{2} sin(j\pi x)$
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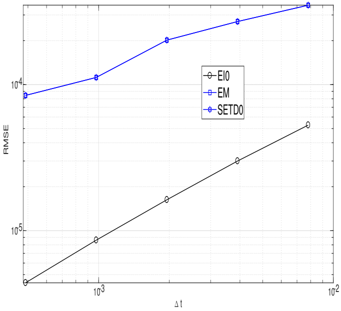
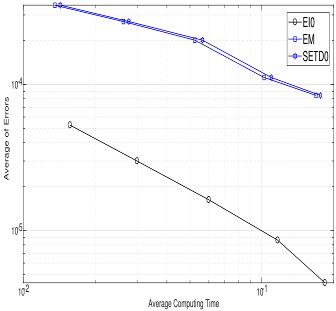
Note : Jentzen and Röckner derived the special case of *EI0* for $\alpha = 0$ as a splitting procedure.

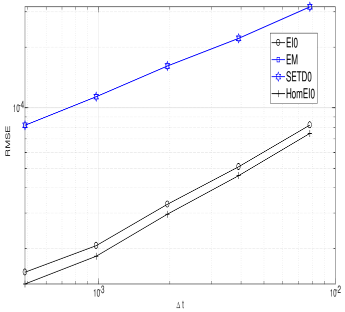
$M = 1000$ samples with $\beta = 1$, $\alpha = 0$.
$\varepsilon = 0.01$, $T = 1$.

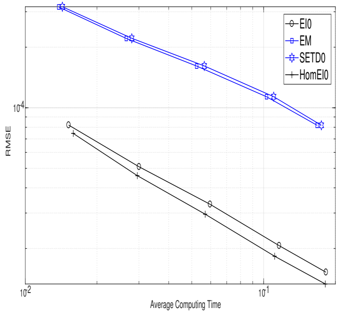




Here *HomEI0* and *EI0* are the same and noise consists of a linear diagonal term.

$M = 1000$ samples with $\beta = 1$, $\alpha = 0.1$





Here see advantage of the homotopy method.

A finite difference discretisation of an SPDE

$$du = \left[\varepsilon \frac{\partial^2 u}{\partial x^2} + 1 - u\right] dt + \left[\beta u + \alpha \frac{1-u}{1+u^2}\right] dW(t), \quad u(x,0) = u_0(x),$$

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where $\mathbf{f}, \mathbf{g} : \mathbb{R}^{J-1} \to \mathbb{R}^{J-1}$ and
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▶ For this finite difference discretisation the commutator conditions do not hold.

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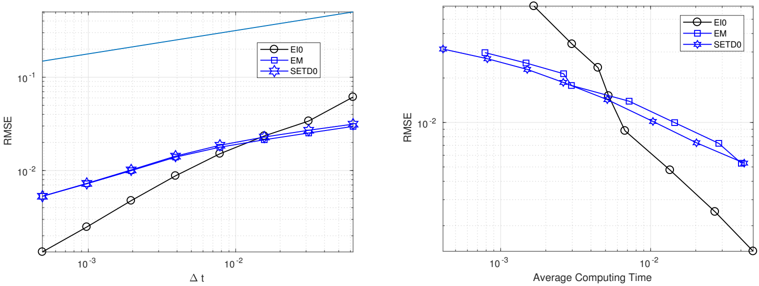
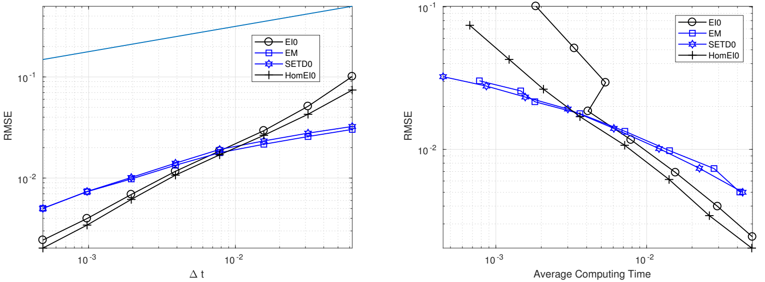
Not covered by theory ...

$\beta = 0.5$, $\alpha = 0$, $T = 1$ and $M = 1000$ samples.



Still see improvement - even though commutivity conditions not met.
(No nonlinearity in noise).

$\beta = 0.5$, $\alpha = 0125$, $T = 1$ and $M = 1000$ samples.



Still see improvement - even though commutivity conditions not met.
(AND nonlinearity in noise).

Theorem for SDEs

Theorem

For commutative matrices and for globally Lipschitz drift and diffusion and let $\mathbf{u}_n$ *be approximation to the solution of our SDE using EI0. For* $T > 0$, *there exists* $K > 0$ *such that*

$$\sup_{0 \le t_n \le T} \|\mathbf{u}(t_n) - \mathbf{u}_n\|_{L^2(\Omega, \mathbb{R}^d)} \le K \Delta t^{1/2}. \quad (3)$$

Proof :
(Also for Milstein version.)

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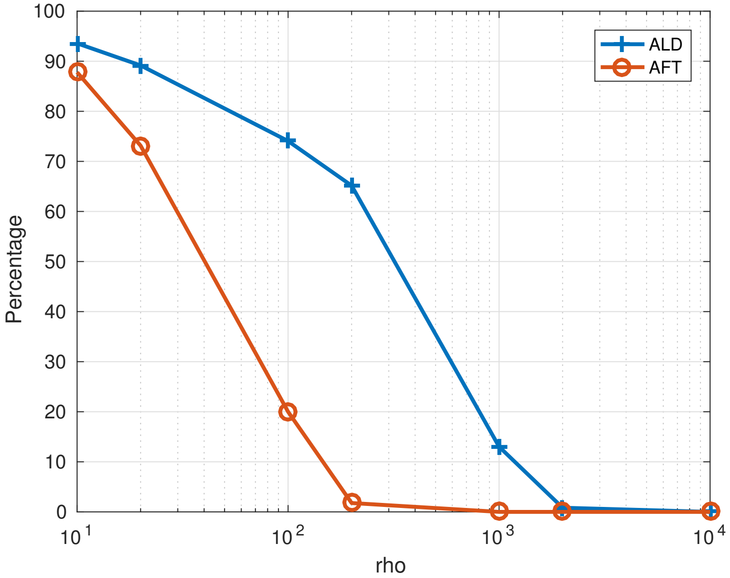
Thank You.

Role of $\rho = \Delta t_{\max}/\Delta t_{\min}$



Here $\Delta t_{\max} = 2$ and so $\Delta t_{\min} = 0.2, \dots, 0.0002$.