Recall the generalized Markovian description of Langevin dynamics:

\[ \dot{x} = -M \frac{\partial H}{\partial x} + kT \frac{\partial}{\partial x} M + \sqrt{2kT} \xi(t) \]

\[ \tilde{M} \tilde{M}^* = (M + M^*)/2 \]

where \( M(x) \) is the mobility tensor.

\[ M = \Gamma^{-1} \]

\( \Gamma \) = friction tensor

\[ D = (kT)M \]

\( D \) = diffusion tensor

Remember that the spurious drift depends on the stochastic integral convention.
As a particular (important) example, consider Brownian dynamics for a collection of colloidal particles suspended in a fluid.

Denote \( q = \{ q_1, q_2, \ldots, q_N \} \) the positions (configuration) of the particles, and \( V(q) \) the interaction potential (effective).

Under additivity assumptions, mobility/friction is the Oseen tensor from hydrodynamics:

\[
M_{ij} = \frac{1}{6\pi \eta a} \left\{ \frac{3}{4} \frac{a}{r_{ij}} \left( 1 + \frac{r_{ij}}{2} \right) \right\}, \quad i \neq j
\]

\[
1 \quad i = j
\]

Particle indexes
Our previous analysis of drift suggests that numerical methods can avoid the evaluation of $\partial q \cdot M(q)$ by using a **backward Euler** method for the **anti-Ito** or "isothermal" SODE:

$$q^i = -M \cdot \partial q V + \sqrt{2kT \cdot M} \cdot W(t)$$

To avoid an implicit method, we can use an explicit **predictor-corrector** method.

**BAD IDEA!**

Explicit

"Backward" Euler

NOT consistent
In the Fixman algorithm one can evaluate the term $M \partial_{q} V$ at midpoint to improve the deterministic order of accuracy to second-order, though the formal order of accuracy (weak sense) remains one.

How to construct $\tilde{M}$ from $M$?

All that matters at this stage is that $\tilde{M} \tilde{M}^{*} = M$.

\[
\begin{cases}
\tilde{M} = \tilde{M}^{*} = M^{1/2} \quad \text{(matrix square root)} \\
\tilde{M} = \text{lower triangular square (Cholesky factorization)} \\
\tilde{M} = \text{non-square (physics?)}
\end{cases}
\]
So far we proposed the algorithm based on "Backward Euler", which we can condense to leading order as:

\[ q(t + \Delta t) = q^n + M(q^n) \cdot \frac{\partial V}{\partial q^n} \Delta t + \sqrt{2 \Delta t (\kappa_I)} \cdot \tilde{M} \left[ q^n + \sqrt{2 \Delta t (\kappa_I)} \tilde{M}(q^n) \tilde{W} \right] \tilde{W}, \]

We already checked that this is correct in one dimension, but how about the multi-variable case?

Let's check the drift due to the multiplicative noise explicitly:
"Spurious" drift:

\[ \Delta q_k = \sqrt{2A_t(kt)} \mathcal{E}_{\tilde{M}_{ik}} \tilde{W}_i \sqrt{2A_t(kt)} (\tilde{M} \tilde{W}) \tilde{W} \]

\[ \Rightarrow \frac{\langle \Delta q_k \rangle}{2A_t(kt)} = \mathcal{E}_{\tilde{M}_{ik}} \tilde{M}_{ij} \langle \tilde{W}_j \tilde{W}_e \rangle = \mathcal{E}_{\tilde{M}_{ik}} \tilde{M}_{ij} \delta_{je} = \mathcal{E}_{\tilde{M}_{ikj}} \tilde{M}_{ij} \]

What we want to get is

\[ \frac{1}{2} \left( \frac{\partial}{\partial q} \cdot M \right)_k = \frac{1}{2} \mathcal{E}_{\tilde{M}_{ik}} \tilde{M}_{ik} \]
\[ \frac{1}{2} \frac{\partial}{\partial q_i} M_{ik} = \frac{1}{2} \frac{\partial}{\partial q_i} (\tilde{M}_{ij} \tilde{M}_{kj}) = \]

\[ = \frac{1}{2} \left[ \frac{\partial \tilde{M}_{ij}}{\partial q_i} \tilde{M}_{kj} + \tilde{M}_{ij} \frac{\partial \tilde{M}_{kj}}{\partial q_i} \right] \]

Compare this to previous

Except for a single variable, this does not seem to match.

So our "backward explicit Euler" algorithm is actually not consistent.

Do not use it!
Instead, rewrite the Langevin equation as

\[ \dot{q} = -M \cdot \frac{\partial V}{\partial q} + \sqrt{2kT} \cdot \mathbf{W}(t) \]

where

\[ \mathbf{NN}^* = M^{-1} = \Gamma \leftrightarrow \text{symmetric} \]

This is equivalent to what we wrote before since all that matters is the noise covariance (think FPE):

\[ (MN)(MN)^* = MNN^*M = M \]

At first glance this requires both \( M \) and \( M^{-1} \), which complicates things..
Fixman proposed the following mid-point explicit predictor-corrector alg:

\[ q^{n+1} = q^n + M(q^n) \cdot \frac{\partial V}{\partial q^n} \Delta t + \sqrt{2 \Delta t (h_t)} M(q^n) \cdot N \cdot W \]

\[ q^{n+1/2} = \frac{1}{2} (q^n + q^{n+1}) \quad \text{(mid point)} \]

\[
\begin{cases}
q^{n+1} = q^n + M(q^{n+1/2}) \cdot \frac{\partial V}{\partial q^{n+1/2}} \Delta t + \\
\sqrt{2 \Delta t (h_t)} \cdot M(q^{n+1/2}) \cdot N \cdot W
\end{cases}
\]

same as predictor.
Is this algorithm now consistent?

To leading order, we are doing

\[ q^{n+1} = q^n + M(q^n) \cdot \frac{\partial V}{\partial q^n} \Delta t + \sqrt{2 \Delta t (kT) \cdot M \left[ q^n + \frac{\Delta t (kT)}{2} M(q^n) \cdot N(q^n) \cdot \tilde{W} \right]} \]

Now the extra drift is

\[ N(q^n) \cdot \tilde{W}^n \]

\[ \Delta q_k = \sqrt{2 \Delta t (kT)} \frac{\partial M_{k,l}}{\partial q_i} \cdot \sqrt{\frac{\Delta t (kT)}{2} (MN \tilde{W})_i \cdot (N \tilde{W})_l} \]

\[ = \Delta t (kT) \frac{\partial M_{k,l}}{\partial q_i} M_{i,j} N_{j,m} \tilde{W} \cdot m N_{l,n} \tilde{W} \cdot n \]
\[
\frac{\langle \Delta q_{ij} \rangle}{(kT) \Delta t} = \frac{\partial M_{kl}}{\partial q_{ij}} M_{ij} (N_{jm} N_{lm}) = \frac{(NN^*)_{jl}}{kT} \left( \frac{\partial}{\partial q_{ij}} \right) (\hat{b}_{il})
\]

\[
= \frac{\partial M_{kl}}{\partial q_{ij}} M_{ij} (M^{-1})_{jl} = \frac{\partial M_{kl}}{\partial q_{ij}} (\hat{b}_{il})
\]

\[
= \frac{\partial M_{ki}}{\partial q_{ij}} = \frac{\partial M_{ik}}{\partial q_{ij}} = \left( \frac{\partial}{\partial q_{ij}} M \right)_k
\]

So indeed the extra drift is

\[
kT \left( \frac{\partial}{\partial q_{ij}} M \right) \text{ as it should be.}
\]

but maybe there are other ways also...
Recall that for additive noise (no dependence in stochastic term) or for Langevin dynamics there is no problem with extra drift terms, and the "mobility" matrix $M$ is rather simple:

$$H = \frac{m\dot{q}^2}{2} + V(q) = \frac{p^2}{2m} + V(q)$$

$$\Rightarrow \frac{\partial H}{\partial t} = \begin{bmatrix} \partial V/\partial q \\ \dot{p}/m = \dot{q} \end{bmatrix} \text{ where } z = (q, p)$$
\[ \dot{z} = \begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \text{be/ve} \\ \text{be/ve} \end{bmatrix} \]

\text{skew-adjoint Louisvile operator}

\[ - \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \gamma \\ 0 & \gamma & 0 \end{bmatrix} \begin{bmatrix} \text{be/ve} \\ \text{be/ve} \\ \text{be/ve} \end{bmatrix} = \frac{\partial H}{\partial z} \]

\text{"irreversible" self-adjoint friction operator}

\[ + \begin{bmatrix} 0 \\ \sqrt{2kTg} \end{bmatrix} \tilde{W}(t) \]

\[ \tilde{M} \text{, with } \tilde{M} \tilde{M}^* \equiv M \]
Recall the FPE for Langevin dynamics:

\[
\frac{\partial P}{\partial t} = - \nabla \cdot \mathbf{X} P = -(X_1 + X_2 + X_3 + X_4) P
\]

\[
\begin{align*}
X_1 &= \frac{\mathbf{P} \cdot \mathbf{v}}{m} \quad \text{(advection)} \\
X_2 &= -\frac{\mathbf{P} \cdot \mathbf{v}}{\mathbf{P}} \quad \text{(constant force acceleration)} \\
X_3 &= -\frac{\mathbf{P}}{m} \frac{\partial}{\partial P} \quad \text{(constant friction)} \\
X_4 &= -\frac{e^2}{m} \frac{\partial}{\partial P} \quad \text{(noise)}
\end{align*}
\]

In general, \( \mathbf{P} = \mathbf{P}(\mathbf{q}) \).
Recall that for Hamiltonian dynamics (MD) we desired symplectic integrators and constructed them using operator splitting and the Trotter factorization.

\[
P(\Delta t) = e^{-\mathbf{A} \Delta t} P(0)
\]

Strang splitting

\[
\approx e^{-\mathbf{A}_2 \Delta t/2} e^{-\mathbf{A}_\beta \Delta t} e^{-\mathbf{A}_2 \Delta t/2} P(0)
\]

where \( \mathbf{A} = \mathbf{A}_2 + \mathbf{A}_\beta \)
For this to work as written the two pieces $Y_2$ and $Y_3$ should ideally be exactly solvable so that

$$e^{-\lambda_2 \Delta t}\quad \text{and} \quad e^{-\lambda_3 \Delta t}$$

are exact.

This suggests the splitting

$$\begin{cases} Y_2 = Y_1 \\ Y_3 = Y_2 + Y_3 + Y_4 \end{cases}$$

(streaming advection)

We already showed how to do this.
Explicitly:

\[ q^{n+1} = q^n + \frac{p^n}{m} \Delta t \quad (\text{this is } \tau \Delta t) \]

\[ p^{n+1} = p^n - \lambda \Delta t + m \frac{1}{\sqrt{2}} \frac{\partial F(q^n)}{\partial q^n} (1 - e^{-\lambda \Delta t}) \]

\[ + \sqrt{m kT (1 - e^{-2\lambda \Delta t})} \cdot N(0,1) \]

where \( \lambda = \frac{g}{m} \)

This is the so-called quasi-symplectic stochastic Verlet algorithm.
Another option is to do the splitting

\[
\begin{cases}
Y_2 = Y_1 + Y_2 & \text{(Hamiltonian dynamics)} \\
\text{use any second-order symplectic integrator}
\end{cases}
\]

\[
\begin{cases}
Y_\beta = Y_3 + Y_4 & \text{(irreversible dynamics)} \\
\text{use previous formula with } F = 0
\end{cases}
\]

Both splittings give quasi-symplectic integrators (Jacobian not unity but constant), but it seems there is no common agreement on which one is "best".