Stochastic Diffusion Equation

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1 Temporal Integrators

This is taken from [1].

In this section we consider a relatively general system of Langevin equations for the coarse-grained variable $\boldsymbol{x}(t)$ in the Ito interpretation,

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{L}(\boldsymbol{x})\boldsymbol{x} + \boldsymbol{g}(\boldsymbol{x}) + \boldsymbol{K}(\boldsymbol{x})\boldsymbol{\mathcal{W}}(t), \tag{1}$$

which is a generalization of the constant additive noise equation considered in [2]. Such an equation may arise, for example, by considering a time-dependent temperature in the fluctuating Navier-Stokes equation. Here $\boldsymbol{\mathcal{W}}(t)$ denotes a collection of independent white-noise processes, formally identified with the time derivative of a collection of independent Brownian motions (Wiener processes) $\boldsymbol{\mathcal{B}}(t)$, $\boldsymbol{\mathcal{W}} \equiv d\boldsymbol{\mathcal{B}}/ds$, $\boldsymbol{g}(\boldsymbol{x})$ denotes all of the terms handled explicitly (e.g., advection or external forcing), and the term $\boldsymbol{L}(\boldsymbol{x})\boldsymbol{x}$ denotes terms that will be handled semi-implicitly (e.g., diffusion) for stiff systems (large spread in the eigenvalues of $\boldsymbol{L}$). In general, $\boldsymbol{L}(\boldsymbol{x})$ may depend on $\boldsymbol{x}$ since the transport coefficients (e.g., viscosity) may depend on certain state variables (e.g., concentration). Note that the equation (1) also includes the case where $\boldsymbol{L}(\boldsymbol{x}, t)$ and $\boldsymbol{g}(\boldsymbol{x}, t)$ depend explicitly on time, as can be seen by considering an expanded system of equations for $\boldsymbol{x} \to (\boldsymbol{x}, t)$.

1.1 Explicit Midpoint Scheme

A fully explicit midpoint predictor-corrector scheme is

$$\begin{aligned}
\boldsymbol{x}^{p,n+\frac{1}{2}} =& \boldsymbol{x}^n + \frac{\Delta t}{2}\left(\boldsymbol{L}^n\boldsymbol{x}^n + \boldsymbol{g}^n\right) + \sqrt{\frac{\Delta t}{2}}\boldsymbol{K}^n\boldsymbol{W}_1^n \\
\boldsymbol{x}^{n+1} =& \boldsymbol{x}^n + \Delta t\left(\boldsymbol{L}^{p,n+\frac{1}{2}}\boldsymbol{x}^{p,n+\frac{1}{2}} + \boldsymbol{g}^{p,n+\frac{1}{2}}\right) + \sqrt{\frac{\Delta t}{2}}\boldsymbol{K}^n\left(\boldsymbol{W}_1^n + \boldsymbol{W}_2^n\right).
\end{aligned} \tag{2}$$

Note that for linearized fluctuating hydrodynamics we know we get second-order weak accuracy if we set the noise amplitude in the corrector be $\boldsymbol{K}^{p,n+\frac{1}{2}}$ [1], but, unfortunately, this is not consistent with an Ito interpretation of the original equation.

There are, however, alternatives, that are still consistent with the Ito interpretation. For example,

$$\begin{aligned}
\boldsymbol{x}^{p,n+\frac{1}{2}} =& \boldsymbol{x}^n + \frac{\Delta t}{2}\left(\boldsymbol{L}^n\boldsymbol{x}^n + \boldsymbol{g}^n\right) + \sqrt{\frac{\Delta t}{2}}\boldsymbol{K}^n\boldsymbol{W}_1^n \\
\boldsymbol{x}^{n+1} =& \boldsymbol{x}^n + \Delta t\left(\boldsymbol{L}^{p,n+\frac{1}{2}}\boldsymbol{x}^{p,n+\frac{1}{2}} + \boldsymbol{g}^{p,n+\frac{1}{2}}\right) + \sqrt{\frac{\Delta t}{2}}\left(\boldsymbol{K}^n\boldsymbol{W}_1^n + \boldsymbol{K}^{p,n+\frac{1}{2}}\boldsymbol{W}_2^n\right)
\end{aligned} \tag{3}$$

works also, but, unfortunately, the analysis in [1] does not apply and so it is not clear if this scheme will be second-order weakly accurate. Note that the scheme can be written in the form of stepping to the midpoint first, and then *continuing* the step from the midpoint to the end from there; this is what Mattingly and Andersen do [3]. So the decision would be whether to regenerate the stochastic fluxes for the second half of the time step. The option (2) means generate stochastic fluxes only once per time step, and option (3) means generate new ones at the midpoint.

In [3], for special classes of SODEs where the driving noise is a sum of one-dimensional multiplicative noise processes (stochastic diffusion equations do not belong to this class per se but it may be that doing this helps even for diffusion), a second-order integrator is proposed where the noise amplitude in the second half of the time step is computed to satisfy

$$\tilde{\boldsymbol{K}}\tilde{\boldsymbol{K}}^{\star} = \max\left[0,\ 2\left(\boldsymbol{K}^{p,n+\frac{1}{2}}\right)\left(\boldsymbol{K}^{p,n+\frac{1}{2}}\right)^{\star} - \boldsymbol{K}^{n}\left(\boldsymbol{K}^{n}\right)^{\star}\right],$$

giving the scheme

$$\begin{aligned}
\boldsymbol{x}^{p,n+\frac{1}{2}} =& \boldsymbol{x}^{n} + \frac{\Delta t}{2}\left(\boldsymbol{L}^{n}\boldsymbol{x}^{n} + \boldsymbol{g}^{n}\right) + \sqrt{\frac{\Delta t}{2}}\boldsymbol{K}^{n}\boldsymbol{W}_{1}^{n} \\
\boldsymbol{x}^{n+1} =& \boldsymbol{x}^{n} + \Delta t\left(\boldsymbol{L}^{p,n+\frac{1}{2}}\boldsymbol{x}^{p,n+\frac{1}{2}} + \boldsymbol{g}^{p,n+\frac{1}{2}}\right) + \sqrt{\frac{\Delta t}{2}}\left(\boldsymbol{K}^{n}\boldsymbol{W}_{1}^{n} + \tilde{\boldsymbol{K}}\boldsymbol{W}_{2}^{n}\right)
\end{aligned} \tag{4}$$

In our stochastic diffusion code, this would correspond to setting the value of n on the faces, when computing the second half of the step, to be

$$2\boldsymbol{n}_{\text{face}}^{p,n+\frac{1}{2}} - \boldsymbol{n}_{\text{face}}^{n},$$

and then generating the stochastic fluxes using these values on the faces of the grid. Should be easy to implement an sounds worth trying out.

1.2 Implicit Trapezoidal Integrator

A semi-implicit trapezoidal predictor-corrector scheme is

$$\begin{aligned}
\boldsymbol{x}^{p,n+1} &= \boldsymbol{x}^{n} + \frac{\Delta t}{2}\boldsymbol{L}^{n}\left(\boldsymbol{x}^{n} + \boldsymbol{x}^{p,n+1}\right) + \Delta t\,\boldsymbol{g}^{n} + \sqrt{\Delta t}\,\boldsymbol{K}^{n}\boldsymbol{W}^{n} \\
\boldsymbol{x}^{n+1} &= \boldsymbol{x}^{n} + \frac{\Delta t}{2}\left(\boldsymbol{L}^{n}\boldsymbol{x}^{n} + \boldsymbol{L}^{p,n+1}\boldsymbol{x}^{n+1}\right) + \sqrt{\Delta t}\,\boldsymbol{K}^{n}\boldsymbol{W}^{n} \\
&+ \Delta t\begin{cases} \frac{1}{2}(\boldsymbol{g}^{n} + \boldsymbol{g}^{p,n+1}) & \text{(trapezoidal) or} \\ \boldsymbol{g}\left(\frac{\boldsymbol{x}^{n}+\boldsymbol{x}^{p,n+1}}{2}\right) & \text{(midpoint)} \end{cases}.
\end{aligned} \tag{5}$$

This requires solving a linear system involving the matrix $\boldsymbol{L}$ so it requires multigrid. In the linearized context one can get second-order weak accuracy by setting the noise amplitude in the corrector to $\left(\boldsymbol{K}^{n} + \boldsymbol{K}^{p,n+1}\right)/2$ but this is not consistent with the Ito Interpretation.

2 Fluctuating Multispecies Diffusion Equation

The equation we want to solve is just the diffusion portion of the general multispecies equations [4]

$$\partial_t\left(\rho\boldsymbol{w}\right) = \boldsymbol{\nabla}\cdot\left(\rho\boldsymbol{W}\left(\boldsymbol{\chi}\boldsymbol{\nabla}\boldsymbol{x} + \sqrt{\frac{2}{n}}\,\boldsymbol{\chi}_{\frac{1}{2}}\boldsymbol{\mathcal{Z}}\right)\right), \tag{6}$$

where we assumed an ideal mixture, $\boldsymbol{\Gamma} = \boldsymbol{I}$. Observe that density is conserved by diffusion and therefore it is not changed and we can assume $\rho = \rho_0$ is spatially constant to write

$$\partial_t \boldsymbol{w} = \boldsymbol{\nabla} \cdot \left(\boldsymbol{W}\boldsymbol{\chi}\boldsymbol{\nabla}\boldsymbol{x} + \sqrt{\frac{2}{n}}\,\boldsymbol{W}\boldsymbol{\chi}_{\frac{1}{2}}\boldsymbol{\mathcal{Z}} \right). \tag{7}$$

To apply the temporal integrators above we define

$$\boldsymbol{L}(\boldsymbol{x})\boldsymbol{x} \equiv \boldsymbol{\nabla} \cdot (\boldsymbol{D}\boldsymbol{\nabla}\boldsymbol{w})$$

where $\boldsymbol{D}$ is a diagonal matrix, and then we simply define the remainder to be the nonlinear part

$$\boldsymbol{g}(\boldsymbol{x}) \equiv \boldsymbol{\nabla} \cdot (\boldsymbol{W}\boldsymbol{\chi}\boldsymbol{\nabla}\boldsymbol{x}) - \boldsymbol{\nabla} \cdot (\boldsymbol{D}\boldsymbol{\nabla}\boldsymbol{w}),$$

and the noise amplitude is

$$\boldsymbol{K}(\boldsymbol{x}) \equiv \boldsymbol{\nabla} \cdot \sqrt{\frac{2}{n}}\,\boldsymbol{W}\boldsymbol{\chi}_{\frac{1}{2}}.$$

2.1 Dilute Solutions

We are interested here in the case when there is one solvent species for which $x_{N_s} \to 1$ and all other solute species are in trace quantities. In this limit we can take the off-diagonal MS diffusion coefficients (recall the diagonal are zero) to be defined by [5]

$$D_{kN_s} = D_k \text{ for } k < N_s$$

$$D_{ij} = \frac{D_i D_j}{D_{N_s}} \text{ for } (i \neq j) < N_s,$$

where D_i is the tracer diffusion coefficient of a molecule of species i in the solvent of species N_s (therefore D_{N_s} is the self-diffusion coefficient of the solvent molecules). In this limit, one gets that the different species equations are decoupled and the mass fluxes are simply

$$\boldsymbol{F}_k = -\rho \frac{m_k D_k}{m_{N_s}} \boldsymbol{\nabla} x_k \text{ for } k < N_s.$$

In this limit we get $\bar{m} = m_{N_s}$ so the relation between mole and number fractions becomes

$$x_k = \frac{\bar{m}}{m_k} w_k = \frac{m_{N_s}}{m_k} w_k,$$

which gives the usual formula $\boldsymbol{F}_k = -\rho D_k \boldsymbol{\nabla} w_k$.

This means that in this limit of tracer reactants we get the familiar uncoupled Fickian equations for the mole fractions of the tracer species (so here now $\boldsymbol{x}$ does not include $x_{N_s} = 1 - \boldsymbol{1}^T\boldsymbol{x}$).

$$\partial_t x_k = \boldsymbol{\nabla} \cdot \left(D_k \boldsymbol{\nabla} x_k + \sqrt{\frac{2 D_k x_k}{n}}\,\boldsymbol{\mathcal{Z}} \right),$$

which can also be written in terms of the number densities for each of the tracer species as the familiar stochastic diffusion equation [6]

$$\partial_t n_k = \boldsymbol{\nabla} \cdot \left(D_k \boldsymbol{\nabla} n_k + \sqrt{2 D_k n_k}\,\boldsymbol{\mathcal{Z}} \right).$$

References

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