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Comment on the article "An effective particle tracing scheme on structured/unstructured grids in hybrid finite volume/PDF Monte Carlo methods" by Li and Modest

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In a recently published article [1], Li and Modest proposed a predictor/corrector numerical scheme to integrate the stochastic differential equation (SDE) for position which arises in composition PDF model. However, it is shown here that this scheme is not consistent with the SDE.

In the composition PDF model, the location $\mathbf{x} = (x_i)_{i=1,3}$ of a stochastic particle evolves according to the following SDE [2]

$$\mathrm{d}\mathbf{x} = \left(\tilde{\mathbf{u}} + \frac{\nabla \Gamma_{\mathrm{T}}}{\langle\rho\rangle}\right)\mathrm{d}t + \sqrt{2\frac{\Gamma_{\mathrm{T}}}{\langle\rho\rangle}}\mathrm{d}\mathbf{W}. \tag{1}$$

In this equation, $\tilde{\mathbf{u}}$ is the Favre-average mean velocity, Γ_{T} is the turbulent diffusivity and $\langle\rho\rangle$ is the mean density. All these quantities are mean fields and the values entering the equation are taken at particle locations. They are, therefore, functions of the stochastic variable $\mathbf{x}$ (e.g., one has $\tilde{\mathbf{u}}(\mathbf{x})$ and $(\Gamma_{\mathrm{T}}/\langle\rho\rangle)(\mathbf{x})$). The increments of the independent Wiener processes $\mathbf{W} = (W_i)_{i=1,3}$ over an interval of time $\mathrm{d}t$ are Gaussian random variables having the following properties [3–5]

$$\langle \mathrm{d}W_i\rangle = 0, \quad \langle \mathrm{d}W_i\,\mathrm{d}W_j\rangle = \mathrm{d}t\,\delta_{ij} \quad \text{and} \quad \langle(\mathrm{d}W_i)^p(\mathrm{d}W_j)^q\rangle = o(\mathrm{d}t) \quad \text{for } p+q \geqslant 3.$$

The predictor/corrector scheme proposed in the article by Li and Modest consists of two steps, and is written here with a constant time step Δt. We also limit ourselves to stationary mean fields, for the sake of simplicity, since this does not change the argument detailed below.

(a) Predictor step: application of the Euler Scheme (see, Eq. (9) in [1])

$$\hat{x}_i^{n+1} = x_i^n + \left(\widetilde{u}_i(\mathbf{x}^n) + \frac{1}{\langle\rho\rangle}\frac{\partial \Gamma_{\mathrm{T}}}{\partial x_i}(\mathbf{x}^n)\right)\Delta t + \sqrt{2\left(\frac{\Gamma_{\mathrm{T}}}{\langle\rho\rangle}\right)(\mathbf{x}^n)}\Delta W_i. \tag{2}$$

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The increments of the independent Wiener processes are generated by $\Delta W_i = \sqrt{\Delta t}\xi_i$ where $(\xi_i)_{i=1,3}$ is a set of independent standardized Gaussian random variables.

(b) Corrector step: the values of the drift and diffusion coefficients are recalculated based on the predictor value $\hat{\mathbf{x}}^{n+1}$, and the corrector approximation for the new value is (see, Eq. (12) in [1])

$$x_i^{n+1} = x_i^n + \frac{1}{2}\left\{\left[\widetilde{u_i}(\mathbf{x}^n) + \frac{1}{2\langle\rho\rangle}\frac{\partial \Gamma_{\mathrm{T}}}{\partial x_i}(\mathbf{x}^n)\right] + \left[\widetilde{u_i}(\hat{\mathbf{x}}^{n+1}) + \frac{1}{2\langle\rho\rangle}\frac{\partial \Gamma_{\mathrm{T}}}{\partial x_i}(\hat{\mathbf{x}}^{n+1})\right]\right\}\Delta t + \frac{1}{2}\left\{\sqrt{2\frac{\Gamma_{\mathrm{T}}}{\langle\rho\rangle}(\mathbf{x}^n)} + \sqrt{2\frac{\Gamma_{\mathrm{T}}}{\langle\rho\rangle}(\hat{\mathbf{x}}^{n+1})}\right\}\Delta W_i. \tag{3}$$

It is important to note that the same Wiener-process increments are used for both steps.

In order to check the consistency of the scheme, one has to write a Taylor expansion of the coefficients in Eq. (3). To this end we write $\hat{x}_i^{n+1} = x_i^n + \delta x_i^n$, where both the mean and variance of δx_i^n are of order Δt. Then, each coefficients calculated at the predictor location $\hat{\mathbf{x}}^{n+1}$ can be expressed in terms of the values at the previous location $\mathbf{x}^n$. For example, denoting the diffusion coefficient by $b(\mathbf{x}) = \sqrt{2\Gamma_{\mathrm{T}}/\langle\rho\rangle}$, we have

$$b^{n+1} = b^n + \left(\frac{\partial b}{\partial x_k}\right)^n \delta x_k^n + \mathrm{O}(\Delta t), \tag{4}$$

where here and below, the summation convention applies to repeated suffixes. By developing the expressions for the drift and the diffusion coefficients in Eq. (3), we obtain the first-order terms in the Taylor expansion for the corrector:

$$x_i^{n+1} = x_i^n + \left(\widetilde{u_i}(\mathbf{x}^n) + \frac{1}{2\langle\rho\rangle}\frac{\partial \Gamma_{\mathrm{T}}}{\partial x_i}(\mathbf{x}^n)\right)\Delta t + b^n \Delta W_i + \frac{1}{2}\left(\frac{\partial b}{\partial x_k}\right)^n b^n \Delta W_i \Delta W_k + \mathrm{o}(\Delta t). \tag{5}$$

In the development of the different terms coming from the discrete form of the drift coefficient in the corrector approximation, Eq. (3), all the additional terms are at least of the order $\Delta t^{3/2}$ and are thus negligible with respect to Δt. The last term in Eq. (5) comes from the development of the diffusion coefficient. The quantity $\Delta W_i \Delta W_k$ has mean $\delta_{ik}\Delta t$ and variance $\mathrm{o}(\Delta t)$. Consequently, to first order in Δt, Eq. (5) yields

$$x_i^{n+1} = x_i^n + \left(\widetilde{u_i}(\mathbf{x}^n) + \frac{1}{2\langle\rho\rangle}\frac{\partial \Gamma_{\mathrm{T}}}{\partial x_i}(\mathbf{x}^n)\right)\Delta t + \sqrt{2\frac{\Gamma_{\mathrm{T}}}{\langle\rho\rangle}(\mathbf{x}^n)}\Delta W_i + \frac{1}{2}\left(\frac{\partial(\Gamma_{\mathrm{T}}/\langle\rho\rangle)}{\partial x_i}\right)(\mathbf{x}^n)\Delta t + \mathrm{o}(\Delta t). \tag{6}$$

By manipulating the gradient terms, we can re-express this result as:

$$x_i^{n+1} = x_i^n + \left(\widetilde{u_i}(\mathbf{x}^n) + \frac{1}{\langle\rho\rangle}\frac{\partial \Gamma_{\mathrm{T}}}{\partial x_i}(\mathbf{x}^n)\right)\Delta t + \sqrt{2\frac{\Gamma_{\mathrm{T}}}{\langle\rho\rangle}(\mathbf{x}^n)}\Delta W_i + \frac{\Gamma_{\mathrm{T}}}{2}\left(\frac{\partial(1/\langle\rho\rangle)}{\partial x_i}\right)(\mathbf{x}^n)\Delta t + \mathrm{o}(\Delta t). \tag{7}$$

From this Taylor expansion, we can draw the following conclusions:

1. The proposed P/C scheme is *not consistent* with the stochastic differential equation, Eq. (1) but instead it converges to the different stochastic differential equation

$$\mathrm{d}\mathbf{x} = \left(\tilde{\mathbf{u}} + \frac{\nabla\Gamma_{\mathrm{T}}}{\langle\rho\rangle} + \frac{\Gamma_{\mathrm{T}}}{2}\nabla\left(\frac{1}{\langle\rho\rangle}\right)\right)\mathrm{d}t + \sqrt{2\frac{\Gamma_{\mathrm{T}}}{\langle\rho\rangle}}\mathrm{d}\mathbf{W}. \tag{8}$$

The difference is quite important since the numerical scheme introduces a deterministic term and thus produces a spurious drift in the variable-density case.

2. In the constant-density case, the proposed P/C scheme is consistent. However, pursuing the Taylor expansion to include higher-order terms shows that the scheme is only first-order accurate in the weak sense and not of second order as claimed. (We have performed numerical tests to confirm this finding.)

In the Li and Modest article, reference is made to a second-order scheme introduced by Welton and Pope [6]. However, the stochastic model considered by Welton and Pope is for the joint variables of particle location and velocity, and the system of equations has a different structure and properties. The equation system considered by Welton and Pope is:

$$d\mathbf{x}(t) = \mathbf{U}(t)\,dt, \tag{9}$$

$$d\mathbf{U}(t) = \mathbf{D}(\mathbf{x}(t), \mathbf{U}(t), t)\,dt + B(\mathbf{x}(t), t)\,d\mathbf{W}(t). \tag{10}$$

In this case, the complete stochastic process $\mathbf{Y} = (\mathbf{x}, \mathbf{U})$ is a six-dimensional vector and the diffusion matrix for $\mathbf{Y}$ can be written (using block notation) as

$$b(t, \mathbf{x}, \mathbf{U}) = \begin{bmatrix} 0 & 0 \\ 0 & B(t, \mathbf{x}) \end{bmatrix}. \tag{11}$$

The fact that B does not depend on $\mathbf{U}$ is essential. Indeed, it is seen that $(\partial b_{ij}/\partial y_k)$ is only non-zero when $1 \leqslant k \leqslant 3$ and when $3 \leqslant i,j \leqslant 6$. And, in that case, we have $b_{kj} = 0$ since there is no white-noise term in the particle equation. Thus, *for that special case*, a simple P/C is indeed consistent. The same structure of the diffusion matrix is also crucial to show that the P/C is, in that case, a second-order weak numerical scheme. However, the composition PDF model Eq. (1) does not have these same properties, and so the P/C scheme proposed by Welton and Pope cannot be applied directly to devise a second-order scheme for Eq. (1).

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