Numerical stability and accuracy considerations for the solution of Lagrangian stochastic particle dispersion model equations

Brian N. Bailey
USDA-ARS, Corvallis, OR
bailebri@oregonstate.edu

Abstract

Based on the classical Langevin equation for molecular diffusion, Lagrangian stochastic dispersion models are a popular method for stochastic particle dispersion. The theoretical consistency in that they agree with their corresponding boundary layer. Pioneering work in the 1980’s led to the formulation of Lagrangian stochastic dispersion models. Numerical stability and w^2-based schemes are a popular method for stochastic particle dispersion. Based on the classical Langevin equation for molecular diffusion, particle velocity dictated the degree to which the second law of thermodynamics or questionable results. The present work identifies the source of such results. The present work identifies the source of such results. Our modeling task is to generate an ensemble of particles whose velocity statistics agree with these specified Eulerian equations.

Background

Lagrangian Stochastic Dispersion Modeling

Langevin velocity equation - First consider 1D steady isotropic Gaussian turbulence

\[
\frac{dv}{dt} = \frac{C_f}{2\sigma^2} \frac{dv}{dt} + \frac{1}{2} w^2 + \frac{1}{2} \sigma^2 + (C_f)^2 \sigma \Delta W
\]

Nomenclature:
- \( v \): particle velocity
- \( \sigma^2 \): velocity dispersion rate
- \( C_f \): “universal” constant

Implicity, we assume a Gaussian velocity pdf.

\[
\sigma(v) = \frac{\sigma(v)}{\sigma(v) + \sigma(v)} \exp \left( -\frac{v^2}{2\sigma^2} \right)
\]

To test the models, a simple artificial turbulence field was generated:

\[
\sigma^2(z) = 1.1 + \sin(z)
\]

Our modeling task is to generate an ensemble of particles whose velocity statistics agree with these specified Eulerian equations and Eq. 2.

“Toy” Problem

Figure 1. Input profiles for ‘exact’ test case. (a) velocity variance, (b) velocity dispersion rate, (c) concentration (100,000 particles total).

The source of rogue trajectories

Forward Euler scheme

Rogue trajectories arise from an unstable numerical integration scheme.

This can be remedied by:
1. Reducing the timestep
2. Using a stable numerical integration scheme
For real flows, a minuscule timestep often cannot be afforded.

Unconditionally stable schemes

Re-write using the total derivative

\[
\frac{d}{dt} \frac{d}{dt} + \frac{1}{2} \frac{d}{dt} \sigma^2 + \frac{1}{2} \sigma^2 + (C_f)^2 \sigma \Delta W
\]

Isotropic turbulence model

\[
\sigma^2(v) = \frac{C_f}{2\sigma^2} \sigma^2 + \frac{1}{2} \sigma^2 + (C_f)^2 \sigma \Delta W
\]

Generalization to anisotropic turbulence (Thomson’s “simplest” model)

\[
\sigma^2(v) = \frac{C_f}{2\sigma^2} \sigma^2 + \frac{1}{2} \sigma^2 + (C_f)^2 \sigma \Delta W
\]

R^2 - stress tensor (Reynolds or eddy diff)

\[
\Delta \left( \frac{C_f}{2\sigma^2} \sigma \Delta W \right)
\]

\[ \sigma \] must be realizable (positive semidefinite)

\[ R > 0; R_{ij} > 0, R_{ij} = R_{ji} > 0, \epsilon_{ij} > 0 \]

\[ \epsilon_{ij}/R = 0 \]

Eulerian profiles

In the end, our goal is not really to satisfy the well-mixed condition. Rather, it is to match the Eulerian profiles specified as inputs! (See Fig. 1, Eq. 2)

Recommendations

- It is preferable to use an implicit scheme in all scenarios I have encountered to date (assuming Gaussian turbulence).
- If the general anisotropic model is used, it is critical that the stress tensor be realizable.
- See the paper below for a procedure that ensures stability.
- The adequacy of the timestep should be assessed by comparing computed Eulerian profiles to those specified as inputs (see Fig. 5).

Web


Supplemental material: Code, test cases, and input data.

My website: people.oregonstate.edu/~bailebri

References


Acknowledgements

The authors wish to acknowledge financial support from the US Environmental Protection Agency (EPA) through the Air and Waste Management Agency’s National Air Modeling Clearinghouse (NAMC)/Modeling and Assessment Office (MAO) Grant 72013503215. This work was completed while the authors were employed by the NAMC/MAO.

22nd Symposium on Boundary Layers and Turbulence • Salt Lake City, UT • June 20-24, 2016