A Stochastic Evaluation Of The Spatial Moments Of A Contaminant Plume In Porous Media

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ABSTRACT

In a previous report (cf. Dean[6]), a method of deriving statistical moment information was developed using a Hilbert space version of Itô's formula. This approach was used to develop a system of partial differential equations in which the first and second moments of the concentration distribution appear as independent variables. It was shown there that the system of moment equations appearing in Graham and McLaughlin[8] can be derived in this manner. The present report expands on some of the material presented in Dean[5] and provides a method of determining the statistical moments of a contaminant plume from the usual spatial moment formulations. Specifically, the Lagrangian concept of computing along the particle path of a fluid particle is used to develop a transformation, Equation[9], that transforms a function $g(\vec{x}) \in L^1(\Re^d)$ defined on all of $\Re^d$, an Eulerian concept, to a function $g(\vec{X}_T(t,\omega;\vec{x}_0,t_0))$, defined along the fluid particle trajectory, $\vec{X}_T(t,\omega;\vec{x}_0,t_0)$, a Lagrangian concept. The transformation is then used to convert the 0, 1 and 2 Eulerian spatial moments to their Lagrangian counterparts.

1 Particle Concentration Field

Consider a fluid particle with mass given by m_{fp}. Suppose that the particle begins its journey at the spatial point $\vec{x}_0$ at time t_0.

Porosity, n, represents the portion of the total volume available to hold fluid. The rest is solid material. So, if we have a total volume of V, the concentration, C, is given by

$$C = \frac{m_{fp}}{V}$$

provided the total volume is available to hold the fluid. But, since only a portion of the total volume is available to hold fluid and this portion is given by nV, the concentration is given by

$$C = \frac{m_{fp}}{nV}$$

For simplicity, we assume that $V \equiv 1$ and that the particle starts its journey at spatial point $\vec{x}_0$ at time t_0. Then, the concentration field associated with the fluid particle can be represented as

$$C_{fp}(\vec{x},t,\omega) = \frac{m_{fp}}{n}\delta\left(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0)\right) \qquad \vec{x} \in \Re^d \tag{1}$$

where $\vec{X}_T(t,\omega;\vec{x}_0,t_0)$[1] represents the position of the fluid particle at time t assuming that it started at $\vec{x}_0$ at time t_0. The δ-function picks the $\vec{x} \in \Re^d$ that corresponds to the position of the particle's trajectory at time t, given that it started at $\vec{x}_0$ at time t_0. $\delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))$ is an example of a *generalized random field* or *generalized random process*. By fixing t and ω, the fluid particle trajectory, $\vec{X}_T(t,\omega;\vec{x}_0,t_0)$ represents a point in $\Re^d$, By fixing t and letting $\omega \in \Omega$, then $\vec{X}_T(t,\omega;\vec{x}_0,t_0)$ represents a distribution of points in $\Re^d$. Hence, from Equation[1] the expected concentration is given by

$$\begin{aligned}
\mathbf{E}\left[C_{fp}(\vec{x},t;\vec{x}_0,t_0)\right] &= \int_{\Re^n} C_{fp}p(\vec{X}_T,t;\vec{x}_0,t_0)d\vec{X}_T \\
&= \int_{\Re^n} \frac{m_{fp}}{n}\delta(\vec{x} - \vec{X}_T)p(\vec{X}_T,t;\vec{x}_0,t_0)d\vec{X}_T \\
&= \frac{m_{fp}}{n}p(\vec{x},t;\vec{x}_0,t_0)
\end{aligned} \tag{2}$$

[1] In order to simplify notation, this will often be written as $\vec{X}_T(t;\vec{x}_0,t_0)$

where $p(\vec{X}_T, t; \vec{x}_0, t_0)$ is the conditional probability density of the position of the fluid particle given that it started at position $\vec{x}_0$ at time t_0. This type of representation appears frequently in the literature (for axample, Dagan and Neuman[3]). This equation says that the expected concentration is determined by the probability density function of the trajectory.

Similarly, we can write

$$\begin{aligned}
\mathbf{E}\left[C_{fp}(\vec{x}, t; \vec{x}_0, t_0)\right] &= \mathbf{E}\left[\frac{m_{fp}}{n}\delta\left(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)\right)\right] \\
&= \frac{m_{fp}}{n}\mathbf{E}\left[\delta\left(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)\right)\right]
\end{aligned} \tag{3}$$

Comparing Equation[2] and Equation[3] it follows that

$$\mathbf{E}\left[\delta\left(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)\right)\right] = p(\vec{x}, t; \vec{x}_0, t_0)$$

This equation can be used to theoretically determine a probability that the fluid particle will be in a neighborhood of a specified $\vec{x} \in \Re^d$ at time t, given that it started at $\vec{x}_0$ at time t_0. For example, if $B \in \mathcal{B}$, B is compact, such that $\vec{x} \in B$, then the probability that the trajectory $\vec{X}_T(t; \vec{x}_0, t_0)$ is in a B neighborhood of the point $\vec{x}$ given that it started at $\vec{x}_0$ at t_0 is given by

$$\begin{aligned}
\int_B \mathbf{E}\left[\delta(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0))\right] d\vec{x} &= \int_B p(\vec{x}, t; \vec{x}_0, t_0)\, d\vec{x} \\
&= P(B, t; \vec{x}_0, t_0) \\
&= P\{\vec{X}_T(t; \vec{x}_0, t_0) \in B\}
\end{aligned} \tag{4}$$

Figure 1 is intended to represent the fluid particle concentration field. The solid line represents the particle's *Expected Path* and the periodically placed curves represent the time dependent probability density functions of the particle's trajectory.

The Fubini theorem, Burrill[2], states that if $(\Omega_1, \mathcal{F}_1, \mu_1)$ and $(\Omega_2, \mathcal{F}_2, \mu_2)$ are σ-finite measure spaces and if g is a $(\mu_1 \times \mu_2)$-measurable function defined on $\Omega_1 \times \Omega_2$ which is integrable, then

$$\int_{\Omega_1 \times \Omega_2} g\; d(\mu_1 \times \mu_2) = \int \int_{\Omega_1 \times \Omega_2} g\; d\mu_1 d\mu_2 = \int \int_{\Omega_1 \times \Omega_2} g\; d\mu_2 d\mu_1$$

It is necessary to show that a similar result holds for the generalized stochastic process

$$\delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0))$$

It has been shown that

$$\mathbf{E}[\delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0))] = p(\vec{x}, t; \vec{x}_0, t_0)$$

where $p(\vec{x}, t; \vec{x}_0, t_0)$ is the conditional density of the fluid particle given that it started at $\vec{x}_0$ at time t_0. Let $(\Omega, \mathcal{F}, P)$ be a complete probability space and let $(\Re^d, \mathcal{B}, d\vec{x})$ be the Lebesque measure space for $\Re^d$. Let $B \in \mathcal{B}$ be a compact set, then the probability that the trajectory $\vec{X}_T(t, \omega; \vec{x}_0, t_0) \in B$ at time t given that it started at $\vec{x}_0$ at time t_0 is given by

$$\int_B \mathbf{E}\left[\delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_), t_0))\right]\; d\vec{x} = \int_B \int_\Omega \delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0))\; dP d\vec{x} = P\left\{\vec{X}_T(t, \omega; \vec{x}_0, t_0) \in B\right\}$$

Now, let $A = \{\omega \in \Omega : \vec{X}_T(t, \omega; \vec{x}_0, t_0) \in B\}$. In Dean[5] it is shown that

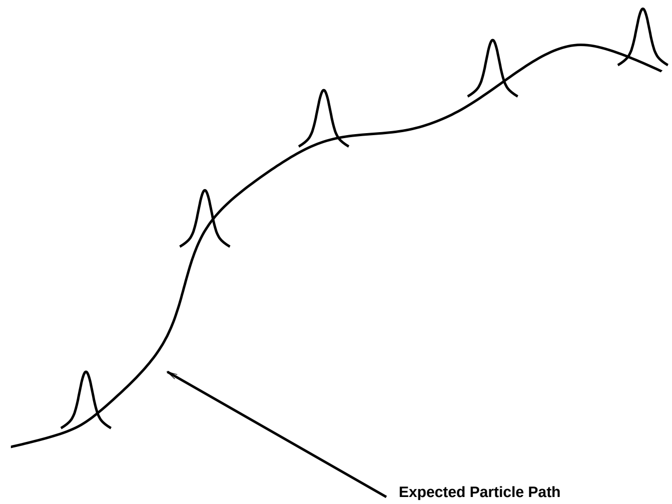

Figure 1

$$\int_{\Omega} \int_{B} \delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0)) \, d\vec{x} dP = P(A) \tag{5}$$

Hence, it follows that

$$\begin{aligned} \int_{B} \mathbf{E} \left[\delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0)) \right] \, d\vec{x} &= \int_{B} \int_{\Omega} \delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0)) \, dP d\vec{x} \\ &= \int_{\Omega} \int_{B} \delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0)) \, d\vec{x} dP \end{aligned} \tag{6}$$

The concentration field of the fluid particle is given by

$$C_{fp}(\vec{x}, t, \omega) = \frac{m_{fp}}{n} \delta \left(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0) \right) \tag{7}$$

where m_{fp} is the mass of the fluid particle, n is the porosity and $\vec{X}_T(t, \omega; \vec{x}_0, t_0)$ is a stochastic process describing the path of the fluid particle. Each $\omega \in \Omega$ yields a sample trajectory of the fluid particle starting at $\vec{x}_0$ at time t_0. Let $t_1 > t_0$, then the set

$$\left\{ \vec{X}_T(t_1, \omega) : \omega \in \Omega \text{ and } \vec{X}_T(t_0, \omega) = \vec{x}_0 \right\}$$

represents the concentration field at time t_1.

Let $g : \Re^d \rightarrow \Re^1$ such that

$$\int_{\Re^d} |g(\vec{x})| \, d\vec{x} < \infty \quad \Rightarrow \quad g(\vec{x}) \in L^1(\Re^d)$$

and let $\phi(\vec{x}) \in C_0^\infty(\Re^d)$ be a test function. Since L^1-convergence implies convergence in measure, a result due to F. Reisz states that any sequence of functions which converges in L^1 to $g(\vec{x})$ has a subsequence that converges a.e. to $g(\vec{x})$, Hewitt and Stromberg[9], Theorem 11.26. Since $C_0^\infty(\Re^d)$ is dense in $L^1(\Re^d)$, $\exists \{\phi_n\} \subset C_0^\infty(\Re^d)$ such that

$$\phi_n(\vec{x}) \xrightarrow{L^1} g(\vec{x})$$

This is also true for L^p, $1 \leq p < \infty$, Adams[1], Theorem 2.19. Hence, it is assumed that a subsequence exists for which $\lim_{n_k \to \infty} \phi_{n_k}(\vec{x}) = g(\vec{x})$ for almost all $\vec{x} \in \Re^d$. Now, for $\vec{X}_T(t; \vec{x}_0, t_0) \in \Re^d$

$$\begin{aligned} \lim_{n_k \to \infty} \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)) \phi_{n_k}(\vec{x}) \, d\vec{x} &= \lim_{n_k \to \infty} \phi_{n_k}(\vec{X}_T(t; \vec{x}_0, t_0)) \\ &= g(\vec{X}_T(t; \vec{x}_0, t_0)) \qquad \text{a.a. } \vec{X}_T(t; \vec{x}_0, t_0) \end{aligned} \tag{8}$$

So, by defining

$$\int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)) g(\vec{x}) \, d\vec{x} = \lim_{n_k \to \infty} \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)) \phi_{n_k}(\vec{x}) \, d\vec{x}$$

it follows that except on a set $C \subset \Re^d$ of measure zero, the statement

$$\int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)) g(\vec{x}) \, d\vec{x} = g(\vec{X}_T(t; \vec{x}_0, t_0)) \tag{9}$$

holds.

2 Moment Calculations

In the computations that follow, it is assumed that the concentration field of the fluid particle at time T is contained in a compact set $B \in \mathcal{B}$. The existence of a probability space $(\Omega, \mathcal{F}, P)$ is assumed, and the behavior of the fluid particle is described by the stochastic process $\vec{X}_T(t, \omega; \vec{x}_0, t_0)$. Fixing $\omega \in \Omega$ generates a sample path of the fluid particle in time. This allows the study of the trajectories of the fluid particle in continuous time. These trajectories, taken together, can be interpreted as a plume described by several fluid particles. The sample paths can be simulated by solving a stochastic differential equation as described in Dean[5].

2.1 Total Mass

Since we are dealing with the concentration plume of a single particle, the mass at any time t is given by m_{fp}. In general, the mass is given by the zeroth spatial moment

$$M(t) = \mathbf{E}[M(t)] = \mathbf{E}\left[\int_{\Re^d} nC_{fp}(\vec{x}, t, \omega) \, d\vec{x}\right] \tag{10}$$

Let $A = \left\{\omega \in \Omega : \vec{X}_T(t, \omega; \vec{x}_0, t_0) \in B\right\}$ and let $g(\vec{x}) = \chi_B(\vec{x})$, then except on a set of measure zero

$$\int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t; \vec{x}_0, t_0)) \chi_B(\vec{x}) \, d\vec{x} = \chi_B(\vec{X}_T(t; \vec{x}_0, t_0)) = \begin{cases} 1 & \text{if } \vec{X}_T(t; \vec{x}_0, t_0) \in B \\ 0 & \text{otherwise} \end{cases} = \chi_A(\omega) \tag{11}$$

From Equation[8], Equation[7] and Equation[5],

$$
\begin{aligned}
M(t) &= \int_\Omega \left(\int_{\Re^d} nC_{fp}(\vec{x},t,\omega)\, d\vec{x} \right) dP \\
&= \int_\Omega \int_{\Re^d} m_{fp}\delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))\chi_B(\vec{x})\, d\vec{x}dP \\
&= m_{fp} \int_\Omega \int_B \delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))\, d\vec{x}dP \\
&= m_{fp}\; P(A)
\end{aligned}
$$

But, since all points of the concentration field are in the set B at time t, $A = \Omega$ and

$$
M(t) = m_{fp}\; P(A) = m_{fp}\; P(\Omega) = m_{fp} \tag{12}
$$

2.2 Centroid

The centroid of the concentration field of the fluid particle at time t is the vector given by

$$
\vec{R}(t) = \mathbf{E}\left[\frac{1}{M} \int_{\Re^d} n\vec{x}C_{fp}(\vec{x},t,\omega)\, d\vec{x} \right]
$$

for which the i^{th} compoment is given by

$$
\vec{R}_i(t) = \mathbf{E}\left[\frac{1}{M} \int_{\Re^d} n\vec{x}_iC_{fp}(\vec{x},t,\omega)\, d\vec{x} \right] \qquad i = 1,\cdots,d
$$

Since the concentration field of the fluid particle at time t is assumed to be contained in the compact set $B \in \mathcal{B}$, let $g(\vec{x}) = x_i\chi_B(\vec{x}) \in L^1(\Re^d)$. Note that

$$
\int_{\Re^d} n\vec{x}C_{fp}(\vec{x},t,\omega)\, d\vec{x} = \int_{\Re^d \setminus (B\cap C)} n\vec{x}C_{fp}(\vec{x},t,\omega)\, d\vec{x} + \int_{B\cap C} n\vec{x}C_{fp}(\vec{x},t,\omega)\, d\vec{x}
$$

But, since $B \cap C$ has measure zero, the second integral on the RHS is zero, so that

$$
\int_{\Re^d} n\vec{x}C_{fp}(\vec{x},t,\omega)\, d\vec{x} = \int_{\Re^d \setminus (B\cap C)} n\vec{x}C_{fp}(\vec{x},t,\omega)\, d\vec{x}
$$

The i^{th} component of the centroid is then given by

$$
\begin{aligned}
\vec{R}_i(t) &= \int_\Omega \frac{1}{M(t)} \int_{\Re^d} n\vec{x}_iC_{fp}(\vec{x},t,\omega)\, d\vec{x}dP \\
&= \int_\Omega \frac{1}{M(t)} \int_{\Re^d \setminus (B\cap C)} n\vec{x}_iC_{fp}(\vec{x},t,\omega)\, d\vec{x}dP \\
&= \int_\Omega \int_{\Re^d \setminus (B\cap C)} \delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))\vec{x}_i\chi_B(\vec{x})\, d\vec{x}dP \\
&= \int_\Omega \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))\vec{x}_i\chi_B(\vec{x})\chi_{\Re^d \setminus (B\cap C)}(\vec{x})\, d\vec{x}dP
\end{aligned}
$$

However, using the properties of the indicator function, it follows that

$$
\chi_{\Re^d \setminus (B\cap C)} \cdot \chi_B = (1 - \chi_{B\cap C}) \cdot \chi_B
$$

$$
\begin{aligned}
&= \chi_B - \chi_B \cdot \chi_B \cdot \chi_C \\
&= \chi_B \cdot (1 - \chi_C) \\
&= \chi_{B \setminus C}
\end{aligned}
$$

and the expression for the i^{th} component of the centroid becomes, using Equation[9],

$$
\begin{aligned}
\vec{R}_i(t) &= \int_\Omega \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0)) \vec{x}_i \chi_{B \setminus C}(\vec{x}) \, d\vec{x} dP \\
&= \int_\Omega \vec{X}_{T_i} \chi_{B \setminus C}(\vec{X}_T) \, dP
\end{aligned}
$$

Furthermore, if $g(\vec{x})$ is a Borel function from $\Re^d$ into $\Re^d$, such that

$$\vec{Y} = \vec{g}(\vec{X})$$

and the i^{th} component is given by

$$\vec{Y}_i = \vec{g}_i(\vec{X})$$

and $F_{\vec{X}}(\vec{x})$ is the probability distribution function for $\vec{X}$, then

$$\int_\Omega \vec{Y}_i \, dP = \int_{\Re^d} \vec{g}_i(\vec{X}) \, dF_{\vec{X}} \qquad i = 1, \cdots, d$$

Using these comments, it follows that

$$
\begin{aligned}
\vec{R}_i(t) &= \int_{B \setminus C} \vec{X}_{T_i} \, dF_{\vec{X}_T} \\
&= \int_{B \setminus C} \vec{X}_{T_i} \, dF_{\vec{X}_T} + \int_{B \cap C} \vec{X}_{T_i} \, dF_{\vec{X}_T} \\
&= \int_B \vec{X}_{T_i} \, dF_{\vec{X}_T} \\
&= \int_{\Re^d} \vec{X}_{T_i} \, dF_{\vec{X}_T} \qquad \text{since } \vec{X}_T(t, \omega; \vec{x}_0, t_0) \in B \ \ \forall \, \omega \in \Omega \\
&= \mathbf{E}\left[\vec{X}_{T_i}\right] \qquad (13)
\end{aligned}
$$

2.3 Second Moment

The second spatial moment characterizes the spread around the centroid. It is a matrix with components

$$\mathbf{S}_{ij}(t) = \mathbf{E}\left[\frac{1}{M(t)} \int_{\Re^d} n(\vec{x}_i - \vec{R}_i)(\vec{x}_j - \vec{R}_j) C_{fp}(\vec{x}, t, \omega) \, d\vec{x}\right] \qquad i, j = 1, \cdots, d$$

Then, as before, with $g(\vec{x}) = (\vec{x}_i - \mathbf{E}[\vec{X}_{T_i}])(\vec{x}_j - \mathbf{E}[\vec{X}_{T_j}])\chi_B(\vec{x})$ and assuming the concentration field of the fluid particle at time t is contained in the compact set $B \in \mathcal{B}$, the second spatial moment is

$$\mathbf{S}_{ij}(t) = \mathbf{E}\left[\frac{1}{M(t)} \int_{\Re^d} n(\vec{x}_i - \mathbf{E}[\vec{X}_{T_i}])(\vec{x}_j - \mathbf{E}[\vec{X}_{T_j}]) C_{fp}(\vec{x}, t, \omega) \, d\vec{x}\right]$$

$$= \mathbf{E}\left[\frac{1}{M(t)}\int_{\Re^d\setminus(B\cap C)} n(\vec{x}_i - \mathbf{E}[\vec{X}_{T_i}])(\vec{x}_j - \mathbf{E}[\vec{X}_{T_j}])C_{fp}(\vec{x},t,\omega)\; d\vec{x}\right]$$

$$= \mathbf{E}\left[\int_{\Re^d\setminus(B\cap C)} \delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))(\vec{x}_i - \mathbf{E}[\vec{X}_{T_i}])(\vec{x}_j - \mathbf{E}[\vec{X}_{T_j}])\chi_B(\vec{x})\; d\vec{x}\right]$$

$$= \mathbf{E}\left[\int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))(\vec{x}_i - \mathbf{E}[\vec{X}_{T_i}])(\vec{x}_j - \mathbf{E}[\vec{X}_{T_j}])\chi_{\Re^d\setminus(B\cap C)}\chi_B(\vec{x})\; d\vec{x}\right]$$

$$= \mathbf{E}\left[\int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))(\vec{x}_i - \mathbf{E}[\vec{X}_{T_i}])(\vec{x}_j - \mathbf{E}[\vec{X}_{T_j}])\chi_{B\setminus C}\; d\vec{x}\right] \quad (14)$$

From Equation[14], the ij^{th} component of the displacement covariance matrix is given by

$$\begin{aligned}
\mathbf{S}_{ij}(t) &= \int_\Omega \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t,\omega;\vec{x}_0,t_0))(\vec{x}_i - \mathbf{E}[\vec{X}_{T_i}])(\vec{x}_j - \mathbf{E}[\vec{X}_{T_j}])\chi_{B\setminus C}(\vec{x})\; d\vec{x}dP \\
&= \int_\Omega (\vec{X}_{T_i} - \mathbf{E}[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}[\vec{X}_{T_j}])\chi_{B\setminus C}(\vec{X}_T)\; dP \\
&= \int_{\Re^d} (\vec{X}_{T_i} - \mathbf{E}[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}[\vec{X}_{T_j}])\chi_{B\setminus C}(\vec{X}_T)\; dF_{\vec{X}_T} \\
&\qquad + \int_{\Re^d} (\vec{X}_{T_i} - \mathbf{E}[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}[\vec{X}_{T_j}])\chi_{B\cap C}(\vec{X}_T)\; dF_{\vec{X}_T} \\
&= \int_{\Re^d} (\vec{X}_{T_i} - \mathbf{E}[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}[\vec{X}_{T_j}])\chi_{B}(\vec{X}_T)\; dF_{\vec{X}_T} \\
&\qquad \text{since } \int_{\Re^d} (\vec{X}_{T_i} - \mathbf{E}[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}[\vec{X}_{T_j}])\chi_{B\cap C}(\vec{X}_T)\; dF_{\vec{X}_T} = 0 \\
&= \int_{\Re^d} (\vec{X}_{T_i} - \mathbf{E}[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}[\vec{X}_{T_j}])\; dF_{\vec{X}_T} \quad \text{since } \vec{X}_T(t,\omega;\vec{x}_0,t_0) \in B \;\; \forall\, \omega \in \Omega \\
&= \mathbf{E}\left[(\vec{X}_{T_i} - \mathbf{E}[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}[\vec{X}_{T_j}])\right] \qquad (15)
\end{aligned}$$

If $\vec{x}$ and $\vec{y}$ represent two points on the particle path, then

$$\rho_{ij}(\vec{x},\vec{y}) = \mathbf{E}\left[\left(\vec{V}_i(\vec{x}) - \mathbf{E}[\vec{V}_i(\vec{x})]\right)\left(\vec{V}_j(\vec{y}) - \mathbf{E}[\vec{V}_j(\vec{y})]\right)\right]$$

Using the kinematic relationship

$$\vec{X}_T(t;\vec{x}_0,t_0) = \int_0^t \vec{V}(\vec{X}_T(t'))dt'$$

it follows that $\mathbf{E}[\vec{X}_T(t;\vec{x}_0,t_0)] = \int_0^t \mathbf{E}[\vec{V}(\vec{X}_T(t'))]dt'$. The convective displacement is given by

$$\begin{aligned}
\vec{X}'_T(t;\vec{x}_0,t_0) &= \vec{X}_T(t;\vec{x}_0,t_0) - \mathbf{E}[\vec{X}_T(t;\vec{x}_0,t_0)] \\
&= \int_0^t \left(\vec{V}(\vec{X}_T(t')) - \mathbf{E}[\vec{V}(\vec{X}_T(t'))]\right) dt'
\end{aligned}$$

So, the displacement covariance is given by

$$\mathbf{S}_{ij}(t) = \int_0^t \int_0^t \rho_{ij}\left(\vec{X}_T(t'), \vec{X}_T(t'')\right) dt'dt''$$

And, by differentiation,

$$\mathbf{D}_{ij} = \frac{1}{2}\frac{d}{dt}\mathbf{S}_{ij} = \int_0^t \rho_{ij}\left(\vec{X}_T(t'), \vec{X}_T(t)\right) dt'$$

In Dean and Russell[7], a Lagrangian numerical framework is proposed for computing the components of the tensor $\mathbf{D}$. The physical domain is subdivided into computational grid blocks, and as time t' increases from 0 to t, the particle moves from its original position at time $t = 0$ to its position at time t, in block (m). As it moves, it traverses different grid blocks on its way to block (m). Figure 2 is an illustration of a particle traversing its way through the computational grid.

Track Of Particle Through A Computational Grid

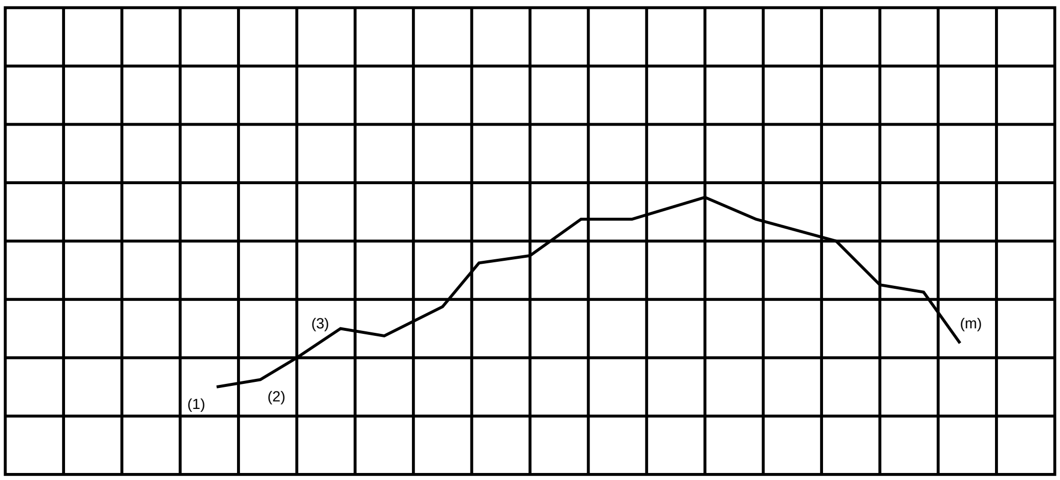

Figure 2

The numerical approximation of the component $\mathbf{D}_{ij}$ is computed using the stochastic properties of the domain in the grid blocks traversed by the fluid particle and the characteristics of the velocity field in those grid blocks. It is given by

$$\mathbf{D}_{ij} = \sum_{k=0}^{m-1} \mathbf{E}\left[\left(\hat{\mathbf{K}}^{(k+1)}\mathbf{E}\left[\vec{V}^{(k+1)}\right]\Delta t_{k+1}\right)_i \left(\hat{\mathbf{K}}^{(m)}\mathbf{E}\left[\vec{V}^{(m)}\right]\right)_j\right]$$

where $\hat{\mathbf{K}} = (\mathbf{K} - \mathbf{E}[\mathbf{K}])\mathbf{E}[\mathbf{K}]^{-1}$. The indexes in parentheses denote the computational block number, $\mathbf{K}$ denotes the hydraulic conductivity matrix on the block, $\mathbf{E}[\vec{V}]$ is the expected velocity on the block and Δt is the time the particle spends in the block during its traverse.

2.4 L^2 Approach

Let $\{\phi_n\} \subset C_0^\infty(\Re^d)$ be a sequence of test functions. When the space $C_0^\infty(\Re^d)$ is equipped with a special topology, $C_0^\infty((\Re^d)$ becomes the space of test functions, denoted $\mathcal{D}(\Re^d)$. Denote by $< \cdot, \cdot >$ the duality pairing on the space $\left(\mathcal{D}(\Re^d)\right)' \times \mathcal{D}(\Re^d)$, where $\left(\mathcal{D}(\Re^d)\right)'$ is the dual of $\mathcal{D}(\Re^d)$, so that in the scalar sense

$$< \cdot, \cdot >: \left(\mathcal{D}(\Re^d)\right)' \times \mathcal{D}(\Re^d) \longrightarrow \Re^1$$

The intention here is to define something similar in the Hilbert space sense. It is to introduce a special *generalized random process* which according to Hida[10], " ...is understood to be a family $\{X(\xi, \omega) : \xi \in E\}$ of random variables on a probability space $(\Omega, \mathcal{B}, P)$ with parameter set a certain function space E ...such that for almost all ω, $X(\xi, \omega)$ is a continuous linear functional in ξ ...".

Since the type of measure space that is considered is one in which the total measure is unity, the following results are available:

- L^q-convergence $\Rightarrow$ L^p-convergence, if $q > p \geq 1$.
- L^p-convergence $\Rightarrow$ convergence in probability.
- Convergence in probability $\Rightarrow$ the existence of an almost everywhere convergent subsequence.

Let $L^2(\Omega, \mathcal{F}, P)$ represent the Hilbert space of random variables with inner product given by

$$(X, Y) = \mathbf{E}\left[|XY|\right]$$

and mean squared norm given by

$$\|X\|_{L^2(P)} = \left(\mathbf{E}\left[|X|^2\right]\right)^{\frac{1}{2}} = \left(\int_\Omega |X|^2 \, dP\right)^{\frac{1}{2}} < \infty$$

Since $P(\Omega) = 1$, it follows that if $1 \leq p < q$ and $X \in L^q(P)$, then by Hölder's inequality

$$\int_\Omega |X(\omega)|^p \, dP \leq \left\{\int_\Omega (|X(\omega)|^p)^{\frac{q}{p}} \, dP\right\}^{\frac{p}{q}} \left\{\int_\Omega 1^{1-\frac{q}{p}} \, dP\right\}^{1-\frac{p}{q}}$$

Hence,

$$\|X(\omega)\|_{L^p(P)} = \left(\int_\Omega |X(\omega)|^p \, dP\right)^{\frac{1}{p}} \leq \left(\int_\Omega |X(\omega)|^q \, dP\right)^{\frac{1}{q}} = \|X(\omega)\|_{L^q(P)} \tag{16}$$

Therefore, $X(\omega) \in L^p(\Omega)$ and

$$L^q(P) \subset L^p(P)$$

For the present application, let $q = 2$ and $p = 1$.

Since $\mathcal{D}(\Re^d)$ is dense in $L^2(\Re^d)$, which is complete, assume that for $g \in L^2(\Re^d)$

$$g(\vec{x}) = (m^2) \lim_{n\to\infty} \phi_n(\vec{x}) \tag{17}$$

for $\{\phi_n\} \subset \mathcal{D}(\Re^d)$.

Define $\delta(\psi)(t, \omega)$ such that

$$\delta(\psi)(t, \omega) = \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0))\psi(\vec{x}) \, d\vec{x} = \psi\left(\vec{X}_T(t, \omega; \vec{x}_0, t_0)\right)$$

where $\psi(\vec{x}) \in \mathcal{D}(\Re^d)$. $\delta(\vec{x} - \vec{X}_T(t, \omega; \vec{x}_0, t_0))$ then represents a *generalized random field* or a *generalized random process*. By fixing $\hat{\omega} \in \Omega$, the *sample path*

$$\delta(\psi)(t, \hat{\omega}) = \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(t, \hat{\omega}; \vec{x}_0, t_0))\psi(\vec{x}) \, d\vec{x} = \psi\left(\vec{X}_T(t, \hat{\omega}; \vec{x}_0, t_0)\right)$$

is obtained. By fixing $\hat{t} \in [0, \infty)$, yields the *random variable*

$$< \omega, \psi > \equiv \delta(\psi)(\hat{t}, \omega) = \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0))\psi(\vec{x}) \, d\vec{x} = \psi\left(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0)\right) \tag{18}$$

where ω is identified with $\delta(\vec{x} - \vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0))$ so that ω can be considered an element of $\mathcal{S}'$. This defines that action of ω on ψ.

The following will require, (see Burrill[2]),

Fatou's lemma: If $\{g_\nu\}$ is a sequence of nonnegative measurable functions and if (a.e.)$\liminf_\nu g_\nu = g$, then

$$\int_E g\ d\mu \leq \liminf_\nu \int_E g_\nu\ d\mu \qquad \square$$

Fix $t = \hat{t}$. In order to simplify notation, let $\mathcal{S} = \mathcal{D}(\Re^d)$ and $\mathcal{S}' = (\mathcal{D}(\Re^d))'$. Let $\mathcal{B}(\mathcal{S}')$ represent the Borel subsets of $\mathcal{S}'$.

Bochner-Minlos Theorem: Let $C(\xi)$ be a characteristic functional on $\mathcal{S}$. Then there exists a unique probability measure μ on $(\mathcal{S}', \mathcal{B}(\mathcal{S}'))$ such that

$$C(\xi) = \int_{\mathcal{S}'} e^{i<\omega,\xi>}\ d\mu(\omega) \qquad \square$$

Expectation with respect to the probability measure μ is denoted by $\mathbf{E}_\mu$. Let

$$C(\xi) = \exp\left[i < m, \xi > -\frac{1}{2}\|\xi\|_{L^2(\Re^d)}\right] \tag{19}$$

where m is a continuous linear functional on $\mathcal{S}$,

$$m : \mathcal{S} \to \Re^1$$

The characteristic functional [19] determines the measure space $(\mathcal{S}', \mathcal{B}(\mathcal{S}), \mu)$ on which there is a system of Gaussian random variables $\{< \omega, \xi >: \xi \in \mathcal{S}\}$ with mean $< m, \xi >$ and variance $\|\xi\|^2_{L^2(\Re^d)}$.

The L^2-completion of the space $(\mathcal{S}', \mathcal{B}(\mathcal{S}), \mu)$ is denoted $L^2(\mu)$. Since $\{< \omega, \xi >: \xi \in \mathcal{S}\}$ is a Gaussian system, the even order moments are given by

$$\int_{\mathcal{S}'} |< \omega, \xi > - < m, \xi >|^{2n}\ d\mu(\omega) = \frac{(2n)!}{2^n n!}\|\xi\|^{2n}_{L^2(\Re^d)} \qquad n = 1, 2, \cdots \tag{20}$$

From Equation[17], $\{\phi_n\} \to g$ in $L^2(\Re^d)$ where $\{\phi_n\} \subset \mathcal{D}(\Re^d)$, and from Equation[20] with $n = 1$,

$$\begin{aligned}\int_{\mathcal{S}'} |< \omega - m, \phi_n - \phi_m >|^2\ d\mu &= \int_{\mathcal{S}'} |< \omega, \phi_n - \phi_m > - < m, \phi_n - \phi_m >|^2\ d\mu \\ &= \|\phi_n - \phi_m\|^2_{L^2(\Re^d)} \to 0 \quad \text{as } m, n \to 0\end{aligned}$$

Since $< \omega - m, \phi_n - \phi_m >= (< \omega, \phi_n > - < m, \phi_n >) - (< \omega, \phi_m > - < m, \phi_m >)$, it follows that $\{< \omega, \phi_n > - < m, \phi_n >\}_{n=1}^\infty$ is a Cauchy sequence in $(\mathcal{S}', \mathcal{B}(\mathcal{S}'), \mu)$. Let $h_n(\omega) =< \omega, \phi_n > - < m, \phi_n >$, then

$$\mu\{\omega : |h_n(\omega) - h_m(\omega)| \geq \epsilon\} \leq \frac{1}{\epsilon^2}\int_{\mathcal{S}'} |h_n(\omega) - h_m(\omega)|^2\ d\mu$$

So, $\{h_n(\omega)\}$ is a Cauchy sequence in measure. Hence, there is a subsequence $\{h_{n_k}\}$ such that

$$\lim_{k\to\infty} h_{n_k}(\omega) =< \omega, h > \qquad \text{a.e. } \omega \in \mathcal{S}'$$

$$\Rightarrow \qquad \lim_{k\to\infty} |h_{n_k}(\omega)|^2 = |< \omega, h >|^2 \qquad \text{a.e. } \omega \in \mathcal{S}'$$

By Fatou's lemma,

$$\begin{aligned}\int_{\mathcal{S}'} |< \omega, h >|^2 \; d\mu &\leq \liminf_{n_k \to \infty} \int_{\mathcal{S}'} |h_{n_k}(\omega)|^2 \; d\mu \\ &= \sup_{n_k} \inf_{\nu \geq n_k} \int_{\mathcal{S}'} |h_\nu(\omega)|^2 \; d\mu \qquad (21)\end{aligned}$$

Assuming that $\int_{\mathcal{S}'} |h_{n_k}(\omega)|^2 \; d\mu < \infty, \forall \; n_k$, and given $\epsilon > 0, \exists \; \nu_0$ such that

$$\int_{\mathcal{S}'} |h_{n_k}(\omega) - h_{\nu_0}(\omega)|^2 \; d\mu < \epsilon \qquad n_k > \nu_0$$

Using the inequality

$$\begin{aligned}|h_{n_k}(\omega)|^2 &= |h_{n_k}(\omega) - h_{\nu_0}(\omega) + h_{\nu_0}(\omega)|^2 \\ &\leq 4\,|h_{n_k}(\omega) - h_{\nu_0}(\omega)|^2 + 4\,|h_{\nu_0}(\omega)|^2\end{aligned}$$

it follows that

$$\int_{\mathcal{S}'} |h_{n_k}(\omega)|^2 \; d\mu \leq 4\epsilon + 4 \int_{\mathcal{S}'} |h_{\nu_0}(\omega)|^2 \; d\mu = K < \infty \qquad \text{for } \; n_k > \nu_0$$

Since K is an upper bound for these integrals,

$$\sup_{n_k} \int_{\mathcal{S}'} |h_{n_k}(\omega)|^2 \; d\mu < \infty \;\; \Rightarrow \;\; \sup_{n_k} \inf_{\nu \geq n_k} \int_{\mathcal{S}'} |h_{n_k}(\omega)|^2 \; d\mu < \infty$$

Equation[21] then gives

$$\int_{\mathcal{S}'} |< \omega, h >|^2 \; d\mu < \infty \qquad (22)$$

so that $|< \omega, h >|^2$ is integrable. The sequence $\{h_n(\omega)\}$ is a Cauchy sequence in mean square, and for each n

$$\lim_{k \to \infty} |h_n(\omega) - h_{n_k}(\omega)|^2 = |h_n(\omega) - < \omega, h >|^2 \qquad \text{a.e. } \; \omega \in \mathcal{S}'$$

again by Fatou's lemma,

$$\int_{\mathcal{S}'} |h_n(\omega) - < \omega, h >|^2 \; d\mu \leq \liminf_{n_k \to \infty} \int_{\mathcal{S}'} |h_n(\omega) - h_{n_k}(\omega)|^2 \; d\mu$$

Also, for $\epsilon > 0$, $\exists \, \nu_0$ such that

$$\int_{\mathcal{S}'} |h_n(\omega) - h_{n_k}(\omega)|^2 \; d\mu < \epsilon$$

for $n \geq \nu_0$ and $n_k \geq \nu_0$, which yields

$$\int_{\mathcal{S}'} |h_n(\omega) - < \omega, h >|^2 \; d\mu \leq \sup_{n_k} \inf_{\nu \geq n_k} \int_{\mathcal{S}'} |h_n(\omega) - h_\nu(\omega)|^2 \; d\mu$$

But, for $\nu \geq n_k \geq \nu_0$,

$$\inf_{\nu \geq n_k} \int_{\mathcal{S}'} |h_n(\omega) - h_\nu(\omega)|^2 \; d\mu < \epsilon \qquad \Rightarrow \qquad \int_{\mathcal{S}'} |h_n(\omega) - < \omega, h >|^2 \; d\mu \leq \epsilon$$

Hence,

$$\{h_n(\omega)\} \xrightarrow{m^2} < \omega, h > \tag{23}$$

From Equation[17], for $g(\vec{x})$ in $L^2(\Re^d)$

$$g(\vec{x}) = (m^2) \lim_{n\to\infty} \phi_n(\vec{x})$$

for $\{\phi_n\} \subset \mathcal{S}$. Since $\Re^1$ is complete in the $|\cdot|$ metric, and m is a continuous linear functional, the mean of g is defined as

$$< m, g >= \lim_{n\to\infty} < m, \phi_n > \tag{24}$$

Since $\int_{\mathcal{S}'} < \omega, \xi > \; d\mu = \mathbf{E}_\mu[< \omega, \xi >] =< m, \xi >$, this means that

$$\mathbf{E}_\mu \left[< \omega, g >\right] = \lim_{n\to\infty} \mathbf{E}_\mu \left[< \omega, \phi_n >\right] \tag{25}$$

Furthermore,

$$\begin{aligned}
\int_{\mathcal{S}'} |< \omega, \phi_n > -(< \omega, h > + < m, g >)|^2 \; d\mu &= \int_{\mathcal{S}'} |< \omega, \phi_n > -(< \omega, h > + < m, g >) \\
&\qquad - < m, \phi_n > + < m, \phi_n >|^2 \; d\mu \\
&\le \int_{\mathcal{S}'} |(< \omega, \phi_n > - < m, \phi_n >) - < \omega, h > \\
&\qquad - (< m, g > - < m, \phi_n >)|^2 \; d\mu \\
&\le 4 \int_{\mathcal{S}'} |(< \omega, \phi_n > - < m, \phi_n >) - < \omega, h >|^2 \; d\mu \\
&\qquad + 4 \int_{\mathcal{S}'} |< m, g > - < m, \phi_n >|^2 \; d\mu
\end{aligned}$$

from Equation[23] and Equation[24] both of the integrals on the right go to zero as $n \to \infty$.

Next define

$$< \omega, g >=< \omega, h > + < m, g >= (m^2) \lim_{n\to\infty} < \omega, \phi_n > \qquad \text{in } L^2(\mu) \tag{26}$$

But, since $\phi_n \in \mathcal{D}(\Re^d)$, it follows from Equation[18] that

$$< \omega, \phi_n >= \int_{\Re^d} \delta(\vec{x} - \vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0))\phi_n(\vec{x}) \; d\vec{x} = \phi_n(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0))$$

Hence, from Equation[25],

$$\mathbf{E}_\mu \left[< \omega, g >\right] = \lim_{n\to\infty} \mathbf{E}_\mu \left[\phi_n(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0))\right] \tag{27}$$

From Equation[22] and Equation[24], and since μ is a finite measure,

$$\begin{aligned}
\int_{\mathcal{S}'} |< \omega, g >|^2 \; d\mu &= \int_{\mathcal{S}'} |< \omega, h > + < m, g >|^2 \; d\mu \\
&\le 4 \int_{\mathcal{S}'} |< \omega, h >|^2 \; d\mu + 4 \int_{\mathcal{S}'} |< m, g >|^2 \; d\mu \\
&< \infty
\end{aligned}$$

It then follows from Equation[16] that

$$\| < \omega, g > \|_{L^1(\mu)} \leq \| < \omega, g > \|_{L^2(\mu)} < \infty$$

Since m^p-convergence implies convergence in measure, it follows from Equation[26] that

$$< \omega, g >= (\mu) \lim_{n \to \infty} < \omega, \phi_n >$$

which means that there is a subsequence $\{\phi_{n_k}\}_{k=1}^{\infty} \subset \mathcal{D}(\Re^d)$ such that

$$< \omega, g >= \lim_{k \to \infty} < \omega, \phi_{n_k} >= \lim_{k \to \infty} \phi_{n_k}(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0)) \quad \text{a.a. } \omega \in \mathcal{S}'$$

If the set of exceptional values of ω is denoted N, $N \subset \mathcal{S}'$ with $\mu(N) = 0$, then

$$< \omega, g >= \lim_{k \to \infty} < \omega, \phi_{n_k} >= \lim_{k \to \infty} \phi_{n_k}(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0)) \quad \text{on } \mathcal{S}' \setminus N$$

For $\epsilon > 0$, $\exists\, N_\epsilon > 0$ such that for $n_k > N_\epsilon$

$$\begin{aligned} |\,| < \omega, \phi_{n_k} > | - | < \omega, g > |\,| &\leq | < \omega, \phi_{n_k} > - < \omega, g > | < \epsilon \\ \Rightarrow \quad | < \omega, \phi_{n_k} > | &< | < \omega, g > | + \epsilon \quad \text{on } \mathcal{S}' \setminus N \end{aligned}$$

Since $< \omega, g > \in L^1(\mu)$ and $\mu(\mathcal{S}') = 1$, by the Dominated Convergence Theorem,

$$\lim_{n_k \to \infty} \int_{\mathcal{S}' \setminus N} \phi_{n_k}(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0))\, d\mu = \int_{\mathcal{S}' \setminus N} < \omega, g > \, d\mu$$

And, since $\mu(N) = 0$, it follows that

$$\lim_{n_k \to \infty} \mathbf{E}_\mu \left[\phi_{n_k}(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0)) \right] = \mathbf{E}_\mu [< \omega, g >] \tag{28}$$

Now, from Equation[17], $\exists$ a subsequence $\{\phi_{n_k}\}_{k=1}^{\infty}$ such that

$$\phi_{n_k}(\vec{x}) \to g(\vec{x}) \qquad (\lambda)\text{a.e. } k \to \infty$$

where λ represents Lebesque measure. This means that for $\epsilon > 0$, $\exists\; N_\epsilon > 0$ such that for $n_k > N_\epsilon$,

$$|\,|\phi_{n_k}(\vec{x})| - |g(\vec{x})|\,| \leq |\phi_{n_k}(\vec{x}) - g(\vec{x})| < \epsilon \quad (\lambda) \text{ a.e.}$$

If $G \subset \Re^d$ is the exception set, $\lambda(G) = 0$, and if the distribution function for the random variable $\vec{X}_T(\omega)$, $F_{\vec{X}_T}$, is absolutely continuous, then the induced measure, $\mu_{\vec{X}_T}$ is absolutely continuous with respect to Lebesque measure, $\mu_{\vec{X}_T} \ll \lambda$, hence,

$$|\phi_{n_k}(\vec{x})| \leq |g(\vec{x})| + \epsilon \quad (\mu_{\vec{X}_T})\text{a.e.}$$

And,

$$\phi_{n_k}(\vec{x}) \to g(\vec{x}) \quad (\mu_{\vec{X}_T})\text{a.e.}$$

Consequently, if $\int_{\Re^d} (|g(\vec{x})| + \epsilon)\; d\mu_{\vec{X}_T} < \infty$, the Dominated Convergence Theorem can be used to conclude that

$$\int_{\Re^d} \phi_{n_k}(\vec{x})\, d\mu_{\vec{X}_T} \to \int_{\Re^d} g(\vec{x})\, d\mu_{\vec{X}_T} \tag{29}$$

In order to complete this discussion, the following Definition and Theorem from Burrill[2] are required:

Definition: A mapping S is a *measurable transformation* if the inverse image of a measurable set is measurable.

Given two measure spaces $(\Omega_1, \mathcal{E}_1, \mu_1)$ and $(\Omega_2, \mathcal{E}_2, \mu_2)$, a set function can be defined on the σ-algebra $\mathcal{E}_2$ as

$$\phi(E) = \mu_1\left(S^{-1}(E)\right) \qquad E \in \mathcal{E}_2$$

The following theorem then holds:

Theorem: Let S be a measurable transformation from $(\Omega_1, \mathcal{E}_1, \mu_1)$ into $(\Omega_2, \mathcal{E}_2, \mu_2)$. Then for any

$$h : \Omega_2 \to \Re^*$$

$$\int_{\Omega_1} h \circ S \, d\mu_1 = \int_{\Omega_2} h \, d\phi$$

if h is non-negative or h is integrable with respect to ϕ.

The random variable $\vec{X}_T(\omega)$ performs the following measurable transformation:

$$\vec{X}_T : (\mathcal{S}', \mathcal{B}(\mathcal{S}'), \mu) \to \left(\Re^d, \mathcal{B}(\Re^d), \lambda\right)$$

and the measure $\mu_{\vec{X}_T}$ is defined as

$$\mu_{\vec{X}_T}(E) = \mu\left(\vec{X}_T^{-1}(E)\right) \qquad E \subset \Re^d$$

The probability measure $\mu_{\vec{X}_T}$ determines the probability of all events involving the random variable $\vec{X}_T(\omega)$.

Hence, if $f : \Re^d \to \Re^*$ and f is integrable with respect to $\mu_{\vec{X}_T}$, then

$$\int_{\mathcal{S}'} f(\vec{X}_T(\omega)) \, d\mu = \int_{\Re^d} f(\vec{x}) \, d\mu_{\vec{X}_T} \tag{30}$$

If the functions ϕ_{n_k} and g are integrable with respect to $\mu_{\vec{X}_T}$, then from Equation[28],

$$\begin{aligned}
\mathbf{E}_\mu[< \omega, g >] &= \lim_{n_k \to \infty} \mathbf{E}_\mu\left[\phi_{n_k}(\vec{X}_T(\omega))\right] \\
&= \lim_{n_k \to \infty} \int_{\mathcal{S}'} \phi_{n_k}(\vec{X}_T(\omega)) \, d\mu \\
& \qquad\qquad \text{from Equation[30]} \\
&= \lim_{n_k \to \infty} \int_{\Re^d} \phi_{n_k}(\vec{x}) \, d\mu_{\vec{X}_T} \\
& \qquad\qquad \text{from Equation[29]} \\
&= \int_{\Re^d} g(\vec{x}) \, d\mu_{\vec{X}_T} \\
& \qquad\qquad \text{from Equation[30]} \\
&= \int_{\mathcal{S}'} g(\vec{X}_T(\omega)) \, d\mu
\end{aligned}$$

From which it follows that

$$\mathbf{E}_\mu\left[< \omega, g >\right] = \mathbf{E}_\mu\left[g(\vec{X}_T(\hat{t}, \omega; \vec{x}_0, t_0))\right] \tag{31}$$

2.4.1 Total Mass

Again, let B be a compact set that contains the entire plume, and let $A = \{\omega \in \mathcal{S}' : \vec{X}_T(\hat{t}, \omega : \vec{x}_0, t_0 \in B\}$, then with $g(\vec{x}) = \chi_B(\vec{x})$ it follows from Equation[31]

$$\begin{aligned}
\mathbf{E}_\mu[< \omega, g >] &= \mathbf{E}_\mu\left[\chi_B(\vec{X}_T(\omega))\right] \\
&= \mathbf{E}_\mu\left[\chi_A(\omega)\right] \\
&= \mu(A)
\end{aligned}$$

2.4.2 Centroid

Let $g(\vec{x}) = x_i \chi_B(\vec{x})$, then

$$\begin{aligned}
\mathbf{E}_\mu[< \omega, g >] &= \mathbf{E}_\mu\left[\vec{X}_{T_i}\chi_B(\vec{X}_T(\omega))\right] \\
&= \mathbf{E}_\mu\left[\vec{X}_{T_i}\chi_A(\omega)\right] \\
&= \mathbf{E}_\mu\left[\vec{X}_{T_i}\right]
\end{aligned}$$

which is the same as Equation[13].

2.4.3 Second Moment

Let $g(\vec{x}) = (x_i - \mathbf{E}_\mu[\vec{X}_{T_i}])(x_j - \mathbf{E}_\mu[\vec{X}_{T_j}])\chi_B(\vec{x})$, then

$$\begin{aligned}
\mathbf{E}_\mu[< \omega, g >] &= \mathbf{E}_\mu\left[(\vec{X}_{T_i} - \mathbf{E}_\mu[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}_\mu[\vec{X}_{T_j}])\chi_B(\vec{x})\right] \\
&= \int_A (\vec{X}_{T_i} - \mathbf{E}_\mu[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}_\mu[\vec{X}_{T_j}])\, d\mu \\
&= \mathbf{E}_\mu\left[(\vec{X}_{T_i} - \mathbf{E}_\mu[\vec{X}_{T_i}])(\vec{X}_{T_j} - \mathbf{E}_\mu[\vec{X}_{T_j}])\right]
\end{aligned}$$

which is the same as Equation[15].

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