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The adjoint advection-diffusion equation in stationary and time dependent problems: a reciprocity relation (**)

dedicated to the memory of Giulio Di Cola

1 - Introduction

Let us consider a passive tracer released in a water basin. The dispersion process of the tracer is assumed to obey an advection-diffusion problem, described by equations (1). Both stationary and time dependent adjoint problems associated to (1) have been formulated. The stationary adjoint problem is defined in the usual manner (e.g., see Axelsson and Barker, 1984, p. 122). The adjoint problem is here interpreted as a model for an advection-diffusion process of a tracer called the «adjoint tracer». The construction of such a model enables one to find the tracer concentration in an assigned number of points of the definition domain by solving, according to the boundary conditions, a simplified transport equation, with a subsequent integration which takes into account the initial conditions. In particular, the adjoint procedure is that usually applied for solving the advection-diffusion equation by means of probabilistic methods (e.g. backward Monte Carlo and random flights methods). This work was inspired by the papers of A. De Matteis on the phenomenological interpretation and on the solution of the stationary adjoint particle transport equation by Monte Carlo methods (De Matteis, 1974; De Matteis and Simonini, 1978-a; De Matteis and Simonini, 1978-b). The adjoint Boltzman

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equation is there interpreted as a transport equation of particles called «adjunctons», a term used by Irving (1970).

In section **2** we state the basic assumptions and equations of the Eulerian formulation of the advection-diffusion problems considered in this paper. In section **3** we introduce both stationary and time dependent adjoint problems, and their phenomenological interpretation is given. In section **4** the strategies to solving advection-diffusion problems by means of Monte Carlo methods are described.

2 - Eulerian formulation of advection-diffusion problems

Let Ω be a bounded open and connected set of R^3 representing a semi-enclosed water basin. The boundary Γ of Ω is assumed to be sufficiently smooth; moreover, $\Gamma = \Gamma_s \bigcup \Gamma_f$, where Γ_s are the solid boundaries and Γ_f are the fluid boundaries. Without a real loss of generality, we assume that the air-water interface is approximated by a rigid lid; thus, this boundary is included in the solid boundaries. The large scale mean velocity field $\boldsymbol{b}(\boldsymbol{x}) = (b_1(\boldsymbol{x}),\ b_2(\boldsymbol{x}),\ b_3(\boldsymbol{x}))$, $\boldsymbol{x} = (x_1, x_2, x_3)$, in Ω is assumed to be stationary, divergence free and with zero normal component to Γ_s: $\nabla \cdot \boldsymbol{b} = 0$ in Ω, $\boldsymbol{b} \cdot \boldsymbol{n} = 0$ on Γ_s, where $\boldsymbol{n}$ is the outward normal unit vector to Γ. We define the parts Γ_{f-} and Γ_{f+} of Γ_f of inflow and outflow respectively: $\boldsymbol{b} \cdot \boldsymbol{n} < 0$ on Γ_{f-}, $\boldsymbol{b} \cdot \boldsymbol{n} > 0$ on Γ_{f+}. The action of the small scale turbulent flow is described by an eddy diffusivity diagonal matrix A, with $diagonal(A) = (a_1, a_2, a_3)$.

Let $u(t, \boldsymbol{x})$ and $f(\boldsymbol{x})$ be the concentration and a possible source of a passive tracer in Ω, respectively. We include also a possible elimination process of the tracer, with decay constant $\lambda \geq 0$. The tracer dispersion process is assumed to obey the following advection-diffusion problem

$$
\begin{aligned}
&\partial u/\partial t + \mathcal{L} u = f \ \ in \ \ \Omega_T = (t_0, t_1] \times \Omega, \\
&(-A \nabla u + \boldsymbol{b} u) \cdot \boldsymbol{n} = b^* u \ \ on \ \ \Gamma_T = (t_0, t_1] \times \Gamma, \\
&u(t_0, \boldsymbol{x}) = u_0(\boldsymbol{x}) \ \ in \ \ \overline{\Omega} = \Omega \bigcup \Gamma,
\end{aligned}
\tag{1}
$$

where $T = t_1 - t_0 > 0$, $\mathcal{L}$ is the elliptic operator

$$
\mathcal{L} = \nabla \cdot (-A \nabla + \boldsymbol{b}) + \lambda , \tag{2}
$$

$b^* = b^*(\boldsymbol{x})$, $\boldsymbol{x} \in \Gamma$, specifies the behaviour of the tracer at the boundaries, and $u_0(\boldsymbol{x}) \geq 0$ is the initial distribution of the tracer. The boundary condition in (1) is illustrated in Buffoni et al. 1996, 1997. Note that if $b^* \geq \boldsymbol{b} \cdot \boldsymbol{n}$ on Γ, then the unique classical solution to (1), is positive: $u(t, \boldsymbol{x}) > 0$ in Ω (e.g. Pao, 1992, p. 54). Under

some regularity conditions on the initial state $u_0(\boldsymbol{x})$, the classical solution is in class $\mathcal{C} = C(\overline{\Omega}_T) \cap C^{1,2}(\Omega_T)$.

We assume a zero flux of the tracer through Γ_s and a net tracer outflux from the basin through Γ_f, thus

$$b^* = 0 \text{ on } \Gamma_s, \qquad b^* \geqslant \max[0, \boldsymbol{b}\cdot\boldsymbol{n}] \text{ on } \Gamma_f. \tag{3}$$

In particular, here we will illustrate the case when (i) there is either zero flux or a small tracer outflux due to turbulent processes on the inflow boundary Γ_{f-}, and (ii) the tracer leaves the basin only under the action of advection on the outflow boundary Γ_{f+}; i.e.,

$$b^* = 0 \text{ on } \Gamma_s; \qquad b^* = \varepsilon \geqslant 0 \text{ on } \Gamma_{f-}; \qquad b^* = \boldsymbol{b}\cdot\boldsymbol{n} > 0 \text{ on } \Gamma_{f+}. \tag{4}$$

3 - The advection-diffusion adjoint problem

3.1 - *The stationary problem*

Let us consider the steady state problem associated to (1)

$$\begin{aligned} &\mathcal{L}u = f \text{ in } \Omega, \\ &(-A\nabla u + \boldsymbol{b}u)\cdot\boldsymbol{n} = b^* u \text{ on } \Gamma. \end{aligned} \tag{5}$$

Problem (5) is called the direct problem. We recall that by repeated application of integration by parts, we obtain the identity

$$\int_\Omega \tilde{u}(\mathcal{L}u)\, d\Omega = \int_\Omega (\tilde{\mathcal{L}}\,\tilde{u})\, u d\Omega + \int_\Gamma (A\nabla\tilde{u}\cdot\boldsymbol{n} + b^*\tilde{u})\, u d\Gamma, \tag{6}$$

$\forall \tilde{u}$, $u \in C^2(\overline{\Omega})$, with u satisfying the boundary condition in (5), $\mathcal{L}$ defined in (2) and $\tilde{\mathcal{L}}$ given by

$$\tilde{\mathcal{L}} = \nabla\cdot(-A\nabla - \boldsymbol{b}) + \lambda. \tag{7}$$

If we make the boundary integral in (6) vanish by associating a new set of boundary conditions with $\tilde{\mathcal{L}}$, then $\tilde{\mathcal{L}}$ is called the adjoint of $\mathcal{L}$ (e.g. Axelsson and

Barker, 1984, p. 122). Thus, the adjoint problem associated to (5) is written as

$$\begin{aligned} &\tilde{\mathcal{L}}\,\tilde{u} = f \text{ in } \Omega\,, \\ &-A\nabla\tilde{u}\cdot\boldsymbol{n} = b^*\tilde{u} \text{ on } \Gamma\,. \end{aligned} \tag{8}$$

The boundary condition in (8) may be written in terms of the flux as $(-A\nabla\tilde{u} - \boldsymbol{b}\tilde{u})\cdot\boldsymbol{n} = \tilde{b}^*\tilde{u}$, where $\tilde{b}^* = b^* - \boldsymbol{b}\cdot\boldsymbol{n}$. From the boundary conditions in (5) and (8) we can identify the type of flux on Γ_f for u and $\tilde{u}$, in relation to the parameter b^*. We obtain the following table

TABLE 1. – *Type of flux on Γ_f for the direct and adjoint problems.*

	b^*	$F = b^* u$	$\tilde{F} = (b^* - \boldsymbol{b}\cdot\boldsymbol{n})\,\tilde{u}$
Γ_{f-}	$= 0$	zero flux	adv. flux
Γ_{f+}	$= \boldsymbol{b}\cdot\boldsymbol{n}$	adv. flux	zero flux
Γ_{f-}	> 0	diff. flux	(diff.+adv.) flux
Γ_{f+}	$> \boldsymbol{b}\cdot\boldsymbol{n}$	(diff.+adv.) flux	diff. flux

Table 1 shows that the type of the flux F on $\Gamma_{f+,-}$ is the same of that of the flux $\tilde{F}$ on $\Gamma_{f-,+}$. Combining the previous results, we thus have

Proposition 1. *The direct problem* (5) *and its adjoint* (8) *describe stationary dispersion processes in Ω characterized by: the same eddy diffusivity matrix A; the large scale mean velocity field $\boldsymbol{b}$ and $-\boldsymbol{b}$, respectively; the same source distribution f in Ω. The equality $\int_\Omega d\Omega f(u - \tilde{u}) = 0$ holds true.*

As a typical example, the boundary conditions for u and $\tilde{u}$ and their fluxes at the boundaries F and $\tilde{F}$, defined in table 1, for the special case characterized by (4) are summarized in the following table

TABLE 2. – *Boundary conditions* (b.c.) *for u and $\tilde{u}$ and fluxes at the boundaries F, $\tilde{F}$* (*defined in table* 1) *for the special case characterized by* (4).

	b.c. for u, F	b.c. for $\tilde{u}$, $\tilde{F}$
Γ_s	$-A\nabla u\cdot\boldsymbol{n} = 0,\ F = 0$	$-A\nabla\tilde{u}\cdot\boldsymbol{n} = 0,\ \tilde{F} = 0$
Γ_{f-}	$-A\nabla u\cdot\boldsymbol{n} + (\boldsymbol{b}\cdot\boldsymbol{n} - \varepsilon)\,u = 0,\ F = \varepsilon u$	$-A\nabla\tilde{u}\cdot\boldsymbol{n} - \varepsilon\tilde{u} = 0,\ \tilde{F} = -\boldsymbol{b}\cdot\boldsymbol{n}\tilde{u} + \varepsilon\tilde{u}$
Γ_{f+}	$-A\nabla u\cdot\boldsymbol{n} = 0,\ F = \boldsymbol{b}\cdot\boldsymbol{n}u$	$-A\nabla\tilde{u}\cdot\boldsymbol{n} - \boldsymbol{b}\cdot\boldsymbol{n}\tilde{u} = 0,\ \tilde{F} = 0$

3.2 - *The time dependent problem*

Let $\tau(t) \in C^1(t_0, t_1)$ satisfy

$$\tau(t_0) = t_1, \qquad \tau(t_1) = t_0, \qquad d\tau/dt < 0 \,. \tag{9}$$

In particular we can choose $\tau(t) = t_0 + t_1 - t$, so that $d\tau/dt = -1$. The variable τ is called the «adjoint time». Let $u(t, \boldsymbol{x}), \tilde{u}(\tau, \boldsymbol{x}) \in \mathcal{C}$, and let

$$I = \int_{t_0}^{t_1} dt \int_{\Omega} d\Omega\, \tilde{u}(\partial u/\partial t + \mathcal{L} u) \,. \tag{10}$$

Taking into account that $\tilde{u}\,\partial u/\partial t = \partial(\tilde{u}\,u)/\partial t - u\partial\tilde{u}/\partial\tau \; d\tau/dt$ and the identity (6), the integral I may be written as

$$\begin{aligned} I = \int_{\Omega} d\Omega [\tilde{u}\,u]_{t_0}^{t_1} + \int_{t_0}^{t_1} dt \Bigg[\int_{\Omega} d\Omega (-d\tau/dt \;\; \partial\tilde{u}/\partial\tau + \tilde{\mathcal{L}}\tilde{u})\, u \\ + \int_{\Gamma} d\Gamma (A\nabla\tilde{u}\cdot\boldsymbol{n} + b^*\tilde{u})\, u \Bigg] . \end{aligned} \tag{11}$$

The operator $-d\tau/dt \; \partial/\partial\tau + \tilde{\mathcal{L}}$ in the second integral of the right side of (11) is called the adjoint operator of the direct operator $\partial/\partial t + \mathcal{L}$. Assume now that $\tilde{u}(\tau, \boldsymbol{x})$ satisfy the following advection-diffusion problem

$$\begin{aligned} & -d\tau/dt \;\; \partial\tilde{u}/\partial\tau + \tilde{\mathcal{L}}\tilde{u} = f \;\text{ in }\; \Omega_T, \\ & -A\nabla\tilde{u}\cdot\boldsymbol{n} = b^*\tilde{u} \;\text{ on }\; \Gamma_T, \\ & \tilde{u}(t_0, \boldsymbol{x}) = \tilde{u}_0(\boldsymbol{x}) \;\text{ in }\; \overline{\Omega} \,. \end{aligned} \tag{12}$$

Problem (12) is called the adjoint (backward) problem associated to the direct (forward) problem defined in (1). It follows

Proposition 2. *Assume* (9), *then* (12) *is a well posed problem and the solution* $\tilde{u}(\tau, \boldsymbol{x})$ *to* (12) *is positive in* Ω. *Thus, problem* (12) *describes a non stationary dispersion process in* Ω *characterized by: the same eddy diffusivity matrix* A *and velocity field* $-b$ *of the stationary adjoint problem* (8); *a time variable* τ, *the «adjoint time», which is a decreasing function of the time variable* t *of the direct problem* (1).

The relation between the solutions $u(t, \boldsymbol{x})$ and $\tilde{u}(\tau, \boldsymbol{x})$ to (1) and (12), respectively, is described by

Theorem 1. *Assume* $f=0$ *in* (1) *and* (12). *Let the Green functions, solutions to* (1) *and* (12) *with initial conditions given by*

$$u(t_0, \boldsymbol{x}) = \delta(\boldsymbol{x}-\boldsymbol{y}), \qquad \tilde{u}(t_0, \boldsymbol{x}) = \delta(\boldsymbol{x}-\boldsymbol{y}), \tag{13}$$

be denoted by

$$U(t, \boldsymbol{x}; t_0, \boldsymbol{y}), \quad \textit{for } t > t_0; \qquad \tilde{U}(\tau, \boldsymbol{x}; t_0, \boldsymbol{y}), \quad \textit{for } \tau > t_0. \tag{14}$$

Then,

$$\tilde{u}(t_1, \boldsymbol{y}) = \int_{\Omega} d\Omega U(t_1, \boldsymbol{x}; t_0, \boldsymbol{y})\, \tilde{u}(t_0, \boldsymbol{x}), \tag{15}$$

$$u(t_1, \boldsymbol{y}) = \int_{\Omega} d\Omega\, \tilde{U}(t_1, \boldsymbol{x}; t_0, \boldsymbol{y})\, u(t_0, \boldsymbol{x}). \tag{16}$$

Furthermore,

$$\tilde{U}(t_1, \boldsymbol{x}; t_0, \boldsymbol{y}) = U(t_1, \boldsymbol{y}; t_0, \boldsymbol{x}). \tag{17}$$

Proof. Under the assumption that $u(t, \boldsymbol{x})$ and $\tilde{u}(\tau, \boldsymbol{x})$ are solutions to (1) and (12), respectively, from (10) and (11) it follows that

$$\begin{aligned} &\int_{\Omega} d\Omega[\tilde{u}(t_0, \boldsymbol{x})\, u(t_1, \boldsymbol{x}) - \tilde{u}(t_1, \boldsymbol{x})\, u(t_0, \boldsymbol{x})] \\ &\qquad + \int_{t_0}^{t_1} dt \int_{\Omega} d\Omega f(u - \tilde{u}) = 0\,. \end{aligned} \tag{18}$$

By letting in (18) $f=0$ and $u=U$ we obtain (15). Analogously, by letting $\tilde{u}=\tilde{U}$ we obtain (16).

Moreover, the concentration $u(t_1, \boldsymbol{y})$ may be expressed in terms of the Green function $U(t_1, \boldsymbol{y}; t_0, \boldsymbol{x})$ of the direct problem

$$u(t_1, \boldsymbol{y}) = \int_{\Omega} d\Omega U(t_1, \boldsymbol{y}; t_0, \boldsymbol{x})\, u(t_0, \boldsymbol{x}). \tag{19}$$

Thus, from equations (16) and (19), and taking into account that $u(t_0, \boldsymbol{x})$ is an arbitrary non negative function, it follows the equality (17). ■

Remark. $U(t_1, \boldsymbol{y}; t_0, \boldsymbol{x})$ and $\widetilde{U}(t_1, \boldsymbol{x}; t_0, \boldsymbol{y})$ are density functions normalized to a unitary source. They can be interpreted as the transition probabilities of the tracer from the point $\boldsymbol{x}$ at time $t = t_0$ to the point $\boldsymbol{y}$ at time $t = t_1$, and of the «adjoint tracer» from the point $\boldsymbol{y}$ at time $\tau = t_0$ to the point $\boldsymbol{x}$ at time $\tau = t_1$, respectively. Equalities of the type (17) are known as reciprocity relations. A reciprocity theorem has been derived by Davison (1958) when treating of the stationary one energy group integral equation of neutron transport. Relations of this type have been applied in the solution of particle transport problems by means of Monte Carlo methods (Maynard, 1961; De Matteis and Simonini, 1978-a).

4 - Solution of advection-diffusion problems by Monte Carlo methods

By virtue of the probabilistic interpretation of $U(t_1, \boldsymbol{y}; t_0, \boldsymbol{x})$ and $\widetilde{U}(t_1, \boldsymbol{x}; t_0, \boldsymbol{y})$, procedures for computing $u(t_1, \boldsymbol{y})$ given by the integral forms (16) and (19) by means of Monte Carlo methods can be formulated. These numerical schemes are called backward and forward procedures, and will be described in some details in the following.

Appropriate discrete equations of (1) in the r-dimensional space ($r = 1, 2, 3$) can be written, which make possible to define transition probabilities from a grid point of the definition domain to a contiguous one, so as to realize a stochastic solving procedure for the integral forms (16) and (19). The discrete space equations are obtained by means of the finite volume method, or box integration method (Varga, 1965, p. 181), and hold for a_i and b_i space dependent. Discretization of the time variable is performed by forward differencing, and evalauting the term λu at time $t + \Delta t$, where Δt is the time step size. In what follows, for sake of simplicity, a constant step size Δx_i is assumed along the $i - th$ coordinate axis. For each point $\boldsymbol{x}$ of the grid the discrete equation can be written as

$$
\begin{aligned}
u(t + \Delta t, \boldsymbol{x}) = (1 + \lambda \Delta t)^{-1} \Big[& \sum_{i=1}^{r} a_i^{+} \, u(t, x_1 + \delta_{1i} \Delta x_i, \ldots, x_r + \delta_{ri} \Delta x_i) \\
& + \sum_{i=1}^{r} a_i^{-} \, u(t, x_1 - \delta_{1i} \Delta x_i, \ldots, x_r - \delta_{ri} \Delta x_i) + a \; u(t, \boldsymbol{x}) + f(t, \boldsymbol{x}) \, \Delta t \Big],
\end{aligned}
\tag{20}
$$

where

$$
a_i^{+} = q_i^{+} (1 - p_i^{+}), \qquad a_i^{-} = q_i^{-} (1 + p_i^{-}), \qquad a = 1 - \sum_{i=1}^{r} (q_i^{+} + q_i^{-}),
\tag{21}
$$

with

$$
\begin{aligned}
&q_i^+(\boldsymbol{x}) = \Delta t/\Delta x_i^2\, a_i(x_1 + \delta_{1i}\Delta x_i/2, \ldots, x_r + \delta_{ri}\Delta x_i/2)\\
&q_i^-(\boldsymbol{x}) = \Delta t/\Delta x_i^2\, a_i(x_1 - \delta_{1i}\Delta x_i/2, \ldots, x_r - \delta_{ri}\Delta x_i/2)\\
&p_i^+(\boldsymbol{x}) = b_i(\boldsymbol{x})\,\Delta x_i/[2a_i(x_1 + \delta_{1i}\Delta x_i/2, \ldots, x_r + \delta_{ri}\Delta x_i/2)]\\
&p_i^-(\boldsymbol{x}) = b_i(\boldsymbol{x})\,\Delta x_i/[2a_i(x_1 - \delta_{1i}\Delta x_i/2, \ldots, x_r - \delta_{ri}\Delta x_i/2)]
\end{aligned}
\tag{22}
$$

We assume that the following constraints

$$
|p_i^+| < 1,\ |p_i^-| < 1, \qquad \sum_{i=1}^{r} (q_i^+ + q_i^-) \leqslant 1\,,
$$

hold. It follows that the coefficients a_i^+, a_i^- and a are nonnegative and $a + \sum_{i=1}^{r} (a_i^+ + a_i^-) = 1$. Thus, random walks on the grid of virtual particles can be performed by assuming a_i^+ and a_i^- as transition probabilities from a point $\boldsymbol{x}$ to a contiguous one, and a as rest probability. This probabilistic interpretation of the coefficients of equation (20) will be stated precisely in the following.

(*a*) *Backward solving procedure*

The backward procedure is apt to estimate the concentration of the passive tracer, given by (16), at assigned points and time instants According to this procedure, starting from a detector point at the observation time of interest t, random walks of virtual particles are carried out in the discretized domain going back in time, until the initial time t_0 is achieved or a boundary is reached. The initial and boundary conditions are consequently taken into account (e.g., see Haji-Sheikh and Sparrow, 1967).

Let $t_k = t_0 + k\Delta t$ and $\tau_k = t_0 + t_n - t_k$, $(k = 1, 2, \ldots, n)$. Starting from the point $\boldsymbol{x}$ at the «adjoint time» τ_0, a random walk is followed by assuming a_i^+ and a_i^- as transition probabilities from a residence point $\boldsymbol{x}$ to a contiguous one whose $i-th$ coordinate is given by $x_i + \Delta x_i$ and $x_i - \Delta x_i$, respectively, and a is the rest probability. The basic solving procedure can be sintetized as follows:

$$
\begin{aligned}
&W_0 = 1,\\
&W_k = (1 + \lambda\Delta t)^{-1} W_{k-1},\\
&S_k = W_k\, f(\tau_k, \boldsymbol{x}_k)\,\Delta t,\ k = 1, 2, \ldots, n,\\
&u_s(t_n, \boldsymbol{x}) = W_n\, u(\tau_n, \boldsymbol{x}_n) + \sum_{k=1}^{n} S_k,
\end{aligned}
\tag{23}
$$

where $u(\tau_n, \boldsymbol{x}_n) = u(t_0, \boldsymbol{x}_n)$ is known, W_k is the statistical weight associated to the

virtual particle at the $k-th$ time step, $\boldsymbol{x}_k$ the $k-th$ residence grid point, and $u_s(t_n, \boldsymbol{x})$ the concentration estimator with reference to the $s-th$ virtual particle random walk. The average value of $u_s(t_n, \boldsymbol{x})$ over the total number of random walks processed gives the searched estimate of $u(t_n, \boldsymbol{x})$. If a boundary point is reached at the current time $t_m \leqslant t_n$, its contribution has to be taken into account according to the assigned boundary conditions. Inflow, outflow and reflection conditions, together with their combinations according to appropriate coefficients, can be foreseen. It is worth to underline that several time instants and observation points can be considered in each calculation. It can be noted that the computation time depends on the number of time steps only, whatever may be the number of grid points.

(*b*) *Forward solving procedure*

The forward procedure is worthwile to give a representation of the evolution of the passive tracer on the whole, starting from the source. The concentration of the tracer is computed by using equation (19). According to this procedure, taking into account the initial conditions, random walks of virtual particles are carried out going forward in time starting at the time t_0 from the source spatial distribution of the passive tracer, until the observation time t is achieved or a boundary is reached. In this last case, the boundary conditions are taken into account. (e.g., see Hunter, 1987; Buffoni et al., 1996).

Starting from the point $\boldsymbol{x}_0$ at time t_0 a random walk is followed by assuming a_i^+ and a_i^- as transition probabilities from a residence point $\boldsymbol{x}$ to a contiguous one whose $i-th$ coordinate is given by $x_i - \Delta x_i$ and $x_i + \Delta x_i$, respectively, and a is the rest probability. The solving procedure can now be so summarized:

$$
\begin{aligned}
&V_0 = u(t_0, \boldsymbol{x}_0), \\
&S_{k-1} = (1 + \lambda \Delta t)^{-1} f(t_{k-1}, \boldsymbol{x}_k)\, \Delta t, \\
&V_k = (1 + \lambda \Delta t)^{-1} V_{k-1} + S_{k-1},\ k = 1, 2, \ldots, n, \\
&u_s(t_n, \boldsymbol{x}) = V_n
\end{aligned}
\tag{24}
$$

where, as before, V_k is the statistical weight and $\boldsymbol{x}_k$ is the $k-th$ visited grid point. Smooth velocity fields are assumed. If a random walk ends at a point $\boldsymbol{x}$ at time t_n, $u_s(t_n, \boldsymbol{x})$ is an estimator of $u(t_n, \boldsymbol{x})$. The average value over the walks processed of the total density belonging to each final point will give an estimate of the passive tracer concentration in that point at time t_n.

The evolution of the dispersion process is represented as follows. Assume that a set of N_0 grid points $\boldsymbol{x}_0^1, \boldsymbol{x}_0^2, \ldots, \boldsymbol{x}_0^{N_0}$, be representative of the source, with initial

concentrations $u_0^1, u_0^2, \ldots, u_0^{N_0}$. Let, moreover, $t_1, t_2, \ldots$ be the observation times. An evolution of the initial distribution of the tracer is realized so that N_0 grid points will give rise at time t_1 to N_1 points, and so on:

$$\boldsymbol{x}_0^1, \boldsymbol{x}_0^2, \ldots, \boldsymbol{x}_0^{N_0} \Rightarrow^{t_1} \boldsymbol{x}_1^1, \boldsymbol{x}_1^2, \ldots, \boldsymbol{x}_1^{N_1} \Rightarrow^{t_2} \ldots$$

with corresponding concentrations

$$u_0^1, u_0^2, \ldots, u_0^{N_0} \Rightarrow^{t_1} u_1^1, u_1^2, \ldots, u_1^{N_1} \Rightarrow^{t_2} \ldots$$

(*c*) *Remarks on the implementation of MonteCarlo simulations*

When a Monte Carlo simulation, as previously described, is performed, the time and spatial step sizes should be chosen in such a way to make the rest probability as small as possible. Moreover, to make the method worth to be used, as usually done in Monte Carlo simulation of particle transport problems, analytical estimates (e.g., in the treatment of the boundary conditions) and variance reducing techniques can profitably be adopted. As an example, in the backward solving procedure the so called splitting technique could be used, which allows the grid points of the definition domain to be better explored. According to this device, at assigned times the virtual particle is splitted in more particles which are independently followed. Statistical weight factors will take the device into account.

As regard the number of random walks to be run, it obviously depends on the particular problem to be solved. However, in the backward procedure it can be said that a few thousands of them could be enough to obtain percentage standard deviations of few per cent.

To avoid to follow inessential virtual particles, when the concentration associated to a particle falls below a cut-off value, the walk is interrupted. To avoid losses of concentrations, the so called russian roulette game can be played. If V_c is the cut-off value and V_k is the actual value of the concentration, being $V_k < V_c$, with probability V_k/V_c the concentration is restored to V_c, otherwise it is lost.

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Abstract

Both stationary and time dependent adjoint problems associated to advection-diffusion problems are formulated. The adjoint problem is then interpreted as a model for an advection-diffusion process of a tracer called the «adjoint tracer». The construction of such a model is a sine qua non condition for the integration of the adjoint advection-diffusion equation by means of probabilistic methods. A reciprocity relation relating direct and adjoint transition probability density functions is derived. Strategies to solving advection-diffusion problems by means of Monte Carlo methods are illustrated.

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