The uneasy collaboration of Leonhard Euler (1707-1783) and Joseph Louis de Lagrange (1736-1813) in environmental fluid mechanics

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The tracer and timescale literature is replete with terms like Lagrangian, Eulerian, particle, parcel, tracer, constituent or water type/mass, making it difficult to avoid confusion. Going back to the fundamentals may help find one's way in this jungle.

Water is a mixture of a large number of dissolved or particulate constituents. At any time and position, each of them may be ascribed a concentration. There exist many definitions of the concept of concentration, leading to dimensionless or dimensional quantities, whose values are in various units (e.g. kg/kg, kg/m^3, mol/l, etc.), of which some of them are somewhat ambiguous (e.g. ppm). Each concentration, irrespective of its specific definition, obeys a reactive transport equation (e.g. de Groot and Mazur 1962), i.e. a parabolic partial differential equation in which reactions (e.g. radioactive decay, chemical reactions, etc.), if any, are taken into account as well as transport processes, i.e. advection, (molecular and turbulent) diffusion and settling, if appropriate (e.g. Nihoul 1981, Deleersnijder 2019). A dissolved, inert (i.e. not subject to any reaction) constituent is often termed a tracer, which, strictly speaking, is a misuse of words. Indeed, according to Baretta-Bekker et al. (1998) a tracer is a (dissolved) substance that is used to help identify transport pathways. Since there is a huge number of constituents, it may be convenient to focus on groups of constituents, i.e. aggregates, whose concentrations may bee seen to obey equations similar to those pertaining to individual constituents, which is why many use the word "constituent" (or a similar term) even if the substance under consideration actually is an aggregate (e.g. salt). Obviously, the water is the aggregate consisting of all the constituents. Under the Boussinesq approximation, its density (kg/m^3) is considered constant.

The reactive transport equation may be solved numerically in the Eulerian framework whatever the very nature of the concentration to be dealt with. Then, this variable is to be discretised in time and space. The main difficulty lies in the representation of advection: preventing spurious oscillations and negative values from occurring without introducing an unacceptably-high amount of numerical diffusivity is far from trivial. Although this issue has been addressed in countless studies (e.g. Thuburn 1997, El Soueidy et al. 2009), no entirely satisfactory scheme has been worked out. Positive and conservative time-integration, first- or higher-order accurate, have been developed for reactive terms, some of which were inspired by the so-called "Patankar trick" (e.g. Patankar 1980, Burchard et al. 2003, Kopecz and Meister 2019, Öffner and Torlo 2020). The discretisation of diffusive terms is rather straightforward, except for anisotropic diffusion (Beckers et al. 2000).

In the Lagrangian approach, the substance under study, is split into so-called particles, i.e. material points having zero volume and a non-zero mass. Each particle contains many ions, molecules, sediment particles, plankton cells, etc. The motion of particles is to be simulated numerically by means of a time marching procedure. During each time increment, the displacement of every particle is the sum of a deterministic drift and a stochastic component, related to diffusive processes. The velocity included in the deterministic term consists of the

fluid velocity and corrective terms taking into account the space variations of the diffusivity or the diffusivity tensor (e.g. Hunter et al. 1993, Visser 1997, Visser 2008, Spivakovskaya et al. 2007a) and the water column depth for two-dimensional, depth-integrated modelling (Heemink 1990, Dimou and Adams 1993, Spagnol et al. 2002). Lagrangian methods are generally superior to Eulerian ones for the representation of advection. They also allow representing rather easily dispersive phenomena others than those modelled by means of harmonic diffusion (e.g. Visser 2008, van Sebille et al. 2018). However, a poorly-documented shortcoming of Lagrangian methods lies in the fact that a large number of particles must be seeded into the domain of interest to obtain accurate concentration fields, possibly requiring greater computational resources than their Eulerian counterparts to achieve the same level of accuracy. What is worse, estimating a priori the minimum number of particles needed is not as straightforward as one would like. Useful guidelines, however, exist (Silverman 1986, Spivakovskaya et al. 2007a).

Well designed Eulerian and Lagrangian schemes must result in concentration estimates converging to the exact solution as the space and time increments decrease for the former methods, and as the time resolution and the number of particles are increased for the latter. Therefore, discrepancies between Eulerian and Lagrangian simulation results are always due to numerical inaccuracies (or an erroneous implementation) and, hence, must not be ascribed to supposedly irreconcilable differences between the two approaches.

The rate at which concentrations ensuing from Eulerian and Lagrangian simulations converge to each other may be slow due in part to difficulties with the discretisation of advection terms for Eulerian schemes and the representation of the impact of large gradients of the diffusivity or diffusivity tensor in Lagrangian techniques. The latter issue may be addressed, to a certain degree, by having recourse to sophisticated time steppings (Stijnen et al. 2006, Spivakovskaya et al. 2007b, Gräwe and Wolff 2010, Gräwe et al. 2012, Shah et al. 2013). Such discretisations, which can be derived from stochastic Taylor expansions, have also been seen to be much more computationally efficient than the most widely used Lagrangian scheme (e.g. Shah et al. 2011, Gräwe et al. 2012, Shah et al. 2013), which actually is a simple Euler-forward time-discretisation of the stochastic differential equation associated with the Eulerian advection-diffusion equation.

Water may be split into several water types, components or masses (though the word “type” is likely to be more appropriate in this instance), which can be treated as inert tracers (e.g. Cox 1989, Hirst 1999, Deleersnijder et al. 2001, Goosse et al. 2001, Haine and Hall 2002, Deleersnijder 2009, de Brye et al. 2012). Obviously, the diagnostic strategy must be designed in such a way that the sum of all the water type concentrations be equal to a constant at any time and location. As for any other constituent or aggregate, every water type may viewed as being made up of (water) particles, which should not be confused with water parcels.

A water parcel is an elemental volume, i.e. a volume whose typical size is much smaller than the smaller length scale of the processes under study. Its velocity is that of the mixture, i.e. the mass-weighted average of the velocities of the molecules contained in it. Because of diffusive processes, a water parcel does not always contain the same molecules. Under the Boussinesq approximation, the volume of a water parcel is constant over time, but its shape is

not. Its total mass is also considered constant, but the masses of its constituents change as time passes. Clearly, the concept of water parcel refers to a mathematical notion that is unrelated to that of particle. In other words, distinguishing a material particle from a water parcel is not a mere matter of vocabulary.

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