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Parcels 2.2 - An increasingly versatile, open-source Lagrangian ocean simulation tool

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Lagrangian simulations contribute to the study and comprehension of particulate-matter transport, its dissolution and dispersion in the oceans. Parcels is an open-source, Python-based module for Lagrangian ocean simulations. It is a known tool in the oceanographic community that has been applied to a variety of case studies, such as the tracing of microplastics, the backtracking of ocean floor plankton, and the migration of fish. In this module, particles are advected over time according to a selected flow field, where those particles can represent particulate-matter, biota or other objects with physical, hydrodynamic or biogeochemical properties. In this contribution, we present the substantial extensions of Parcels with respect to usability, physics modelling aspects of particle advection, and computational aspects of versatile, scalable and efficient simulations.

Specifically, a suite of simple, concise notebook tutorials are tailored to novice user, covering step-by-step simulation setup instructions, whereas self-contained special-issue tutorials address advanced- and proficient user requirements. The considerable expansion of supported OGCM flow field input formats (e.g. MITgcm, POP and MOM5, among others) is a major interest in Parcels v2.2 for our steadily-growing user base.

The new version further integrates previously-published physics methods into practical lagrangian particle simulations. As such, we implement an analytical advection scheme in addition to existing Runge-Kutta advection schemes. Furthermore, two-dimensional advection-diffusion is upgraded with the Milstein stochastic integration scheme and improved documentation. Those capabilities enable a more consistent modelling of diffusion- and uncertainty-dominated fluid transport processes.

The case studies performed with previous versions indicate increased computational demands. Simulations are run over long decadal time scales as well as over day-periods with sub-second temporal increments, involving multiple basins and global scenarios, while also modelling increasingly complex particle processes. Overall, our developments respond to the big-data requirements of modern oceanographic studies, which include the aspects of (i) high record volume (i.e. large number of particles), (ii) high dimensionality in multi-variate records, (iii) high spatial resolution, (iv) high temporal resolution, (v) high scenario (i.e. case study) variability and (vi) the prevention of numerical error accumulation over long simulation time scales.

The novel features of Parcels v2.2 are illustrated on distinct case studies within our contribution, in order to connect the technical features to their impact on particulate-matter ocean transport studies.