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# A purely Lagrangian method for simulating the shallow water equations on a sphere using smooth particle hydrodynamics

Jesse Capecelatro

*Department of Mechanical Engineering, University of Michigan, Ann Arbor, MI 48109-2125, USA*

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ABSTRACT

It has long been suggested that a purely Lagrangian solution to global-scale atmospheric/oceanic flows can potentially outperform tradition Eulerian schemes. Meanwhile, a demonstration of a scalable and practical framework remains elusive. Motivated by recent progress in particle-based methods when applied to convection dominated flows, this work presents a fully Lagrangian method for solving the inviscid shallow water equations on a rotating sphere in a smooth particle hydrodynamics framework. To avoid singularities at the poles, the governing equations are solved in Cartesian coordinates, augmented with a Lagrange multiplier to ensure that fluid particles are constrained to the surface of the sphere. An underlying grid in spherical coordinates is used to facilitate efficient neighbor detection and parallelization. The method is applied to a suite of canonical test cases, and conservation, accuracy, and parallel performance are assessed.


## 1. Introduction

Accurate and conservative methods for convection-dominated flows in spherical geometries is of key importance in geophysical fluid mechanics. To date, numerical implementations of such flows typically consider an Eulerian, or semi-Lagrangian frame of reference. In a recent review on conservation properties of atmospheric numerical model dynamical cores, Thuburn [1] concludes that it might be possible to obtain a greater number of conservation properties by moving to a fully Lagrangian, rather than Eulerian formulation. In the same year, Alam and Lin [2] proposed a fully Lagrangian atmospheric model for a two-dimensional sea-breeze circulation problem. The authors observed that in comparison to traditional semi-Lagrangian and Eulerian finite-difference models, the fully Lagrangian simulations were more computationally efficient and exhibited higher accuracy when integrated over long time durations. Meanwhile, to the best of our knowledge, a purely Lagrangian method for atmospheric flows in spherical coordinates remains elusive, and a practical and scalable framework has yet to be introduced.

Atmospheric motion is highly turbulent and greatly influences a wide range of important processes, including transport of water vapor and atmospheric dust, the formation of clouds, and heat transfer [3]. Due to the vast scale differences between the horizontal flow and vertical motion, the shallow water equations are typically used as a first step towards the construction of global atmospheric models. A wide range of Eulerian and semi-Lagrangian techniques for the shallow water equations in spherical geometries can be found in the literature (see, e.g., [4–14]). In a spherical coordinate system, lines of constant longitude converge at the poles, resulting in the coordinate system to become singular there. Some of the first attempts to alleviate the issues related to the pole singularity involved limiting the latitude $-85^\circ \le \theta \le 85^\circ$ [4], introducing

*E-mail address:* jcaps@umich.edu.

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filtering at the pole, or solving the equations of motion in Cartesian coordinates on overset grids [15,16]. While overset grid methods have shown great promise in recent years, they typically involve interpolation at grid boundaries that can degrade the global conservation properties of the overall method, require memory-intensive algorithms for parallelization, or replace the pole singularities with multiple weaker singularities at the intersection of grid boundaries [13]. As noted by Williamson [17], the pole problem is not a fundamental problem but rather one of economics. For example, the time step used in explicit finite difference schemes is restricted by the Courant–Fredrich–Levy (CFL) condition based on the wind speed and grid spacing, which becomes excessively small near the poles. To date, a variety of established methods exist that define velocities as fluxes through cell edges rather than zonal and meridional components, and thus avoids the pole singularity altogether (e.g., [18–20]).

By abandoning the notion of a grid, it becomes possible to construct a method with geometric flexibility free of the aforementioned challenges. To this end, particle-based methods have been receiving much attention as an alternative tool for solving partial differential equations (PDEs) on arbitrary geometries. Flyer and Wright [21] demonstrated that the radial basis function (RBF) spatial discretization is capable of solving purely hyperbolic PDEs on a sphere, and outperforms traditional spectral methods in terms of the number of discrete points and time-step size needed to achieve a given accuracy. A key benefit of the RBF method (and in general any particle-based method) is that the algorithmic complexity does not increase with the dimension of the problem. Flyer and Wright [12] later derived the first shallow water model on a sphere using RBFs. However, global RBFs require dense matrix solves that typically cost $\mathcal{O}\left(N^3\right)$ operations to create the differentiation matrices, which is not practical for high resolution or high-dimensional problems. A local RBF-generated finite difference approach was later introduced to alleviate this issue by only considering neighboring particles when constructing the derivative operators [22]. The method was shown to be computationally efficient with spectral-like accuracy that scales with the number of neighboring particles. While this represents a promising new approach for large-scale geophysical modeling, it has to date only been demonstrated using a moderate number of particles on a single CPU. Furthermore, the particles are fixed in space, and thus the benefits of Lagrangian particle methods (e.g., exact treatment of the advection term) cannot be leveraged.

The purpose of the present work is to extend the techniques used with RBF methods to a Lagrangian framework that enables efficient parallelism. By allowing the particles to evolve in a Lagrangian manner, and constructing difference operators using a kernel approximation (as opposed to basis functions that require linear solves), the equations reduce to a smooth particle hydrodynamics (SPH) formulation on a sphere. SPH has received much attention in the past three decades for a wide range of applications (see, e.g., [23] and references therein), though its use for atmospheric flows (and spherical geometries in general) are non-existent.

The development of SPH for the shallow water equations has received much attention in the past two decades [24–30]. The majority of this work focuses on improving stability properties, free surface boundary treatment (though not relevant to the present work), and conservation properties. Frank and Reich [31] showed that SPH applied to the shallow water equations satisfies an exact circulation theorem, which leads to statements of conservation of potential vorticity and generalized enstrophies. While exact mass conservation is intrinsic to the SPH approach, they demonstrated discrete conservation of circulation as well. However, stability becomes a main concern when particles become highly disordered. Ata and Soulaïmani [25] addressed this problem by proposing an artificial dissipation term based on Riemann solvers. Rodriguez-Paz and Bonet [26] presented a corrected variational SPH formulation for shallow water flows to conserve both the total mass and momentum. De Leffe et al. [27] later proposed an algorithm to periodically redistribute the particles in order to improve solution accuracy. Vacondio et al. [30] derived a corrected SPH algorithm to properly account for complex domain topography under the assumption that the particles are equally distributed. Soon after, Xia et al. [29] relaxed this constraint by introducing an improved shock-capturing scheme to yield accurate solutions of the shallow water equations over a non-uniform topography.

Using these ideas, this paper presents an SPH formulation in spherical geometries to model global-scale atmospheric flows. To avoid singularities at the poles, the equations are solved in a Cartesian coordinate system augmented with a Lagrange multiplier that constrains the particles to the surface of the sphere. Difference operators are derived using a kernel approximation that is a function of the great-arc distance between particles. A modified nearest-neighbor detection algorithm is presented using an auxiliary grid in spherical coordinates that allows for accurate detection near the poles. Finally, conservation, accuracy, and computational efficiency are assessed for a range of canonical flows.

## 2. Governing equations

### *2.1. Cartesian form of the shallow water equations on a rotating sphere*

Consider a fluid parcel located on the surface of a sphere of radius $a$ with coordinates $(\lambda, \theta)^{\mathsf{T}}$, where $\lambda \in (0, 2\pi]$ is the longitude and $\theta \in [-\pi/2, \pi/2]$ is the latitude. In a latitude–longitude grid, lines of constant longitude converge at the poles (i.e., $\theta = \pm\pi/2$), requiring special care to avoid excessively small timestep restrictions. To avoid the resulting singularity, the present study considers the three-dimensional Cartesian form of the shallow water equations.

Thus, three components of velocity are solved for, $\boldsymbol{u} = (u, v, w)^{\mathsf{T}}$, with coordinates $\boldsymbol{x} = (x, y, z)^{\mathsf{T}}$. The Cartesian form of the shallow water equations in a frame of reference rotating with angular velocity $\Omega$ are given by