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A conservative multi-tracer transport scheme for spectral-element spherical grids

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ABSTRACT

Atmospheric models used for practical climate simulation must be capable handling the transport of hundreds of tracers. For computational efficiency conservative multi-tracer semi-Lagrangian type transport schemes are appropriate. Global models based on high-order Galerkin approach employ highly non-uniform spectral-element grids, and semi-Lagrangian transport is a challenge on those grids. A conservative semi-Lagrangian scheme (SPELT — SPectral-Element Lagrangian Transport) employing a multi-moment compact reconstruction procedure is developed for non-uniform quadrilateral grids. The scheme is based on a characteristic semi-Lagrangian method that avoids complex and expensive upstream area computations. The SPELT scheme has been implemented in the High-Order Method Modeling Environment (HOMME), which is based on a cubed-sphere grid with spectral-element spatial discretization. Additionally, we show the (strong) scalability and multi-tracer efficiency using several benchmark tests. The SPELT solution can be made monotonic (positivity preserving) by combining the flux-corrected transport algorithm, which is demonstrated on a uniform resolution grid. In particular, SPELT can be efficiently used for non-uniform grids and provides accurate and stable results for high-resolution meshes.

1. Introduction

In the past two decades, global spectral methods have dominated in atmospheric modeling. However, the main disadvantage of these methods is that they require expensive non-local communication operations, which prevents them from using the full potential of available massive parallel petascale computers. In recent years, high-order accuracy is being achieved by using finite-element type models, including the spectral-element (SE) or continuous Galerkin and the discontinuous Galerkin (DG) methods (see [31,32,14,26]). These element-based and high-order Galerkin methods have the nice feature that the data for parallel communication is reduced to a minimum due to localized computations. Additionally, element-based methods allow a more flexible choice of domain and local mesh refinement as, for example, spectral methods.

The spectral-element dynamical core [31] based on the High-Order Method Modeling Environment (HOMME) [8] framework is the default dynamical core for the Community Atmosphere Model (CAM, version 5.2 and higher) — CAM-SE. The grid system in HOMME is based on the cubed-sphere geometry resulting from a gnomonic equiangular projection of the sphere. It has been shown in [7] that this approach is highly scalable, up to 170 000 cores on the Oak Ridge LCF Cray XT5 JaguarPF system. However, with a growing number of tracers in today's atmospheric modeling applications transport becomes a

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dominating factor of the total computational costs; for example, more than $O(100)$ tracers are used in the current chemistry version of CAM, and this number is likely to increase in future applications. A native SE transport scheme combined with non-oscillatory features is available in HOMME [15]. Unfortunately, it is computationally prohibitive for a large number of tracers due to three communications per time step and a relatively small time step of the explicit Runge–Kutta based approach [7]. In addition, SE advection is coupled with a hyper-diffusion operator that also increases the computational cost.

Thus the multi-tracer transport is a major computational bottleneck of the HOMME dynamical core for climate simulations. Furthermore, HOMME supports unstructured grids. Therefore it is desirable to have multi-tracer efficient schemes capable of handling such grid system. Conservative semi-Lagrangian methods with moderate Courant numbers can be employed for efficiently handling the multi-tracer problems [11]. Using a moderate Courant number for the semi-Lagrangian advection does not adversely affect the parallel efficiency of the Eulerian host model. But this Courant number can still be chosen several times larger than that for a high-order advection scheme. Recently, a third-order Conservative Semi-LAgrangian Multi-tracer transport scheme (CSLAM [20]) has been integrated in HOMME [11]. This is achieved by overlaying the HOMME SE grids with uniform finite-volume cells. However, the CSLAM scheme is designed for uniform grids and requires a 5×5 reconstruction stencil (as implemented in HOMME), for which extra interpolations are required at the cube corner (ghost cells). In addition, CSLAM relies on computing the upstream (Lagrangian) areas through an intricate process. For that an expensive search algorithm is needed to locate and compute the overlap areas [20]. This implies that for an arbitrary unstructured cubed-sphere grid, implementation of a finite-volume semi-Lagrangian scheme such as CSLAM may be prohibitively complicated.

In order to preserve the parallel efficiency of the host model HOMME, the multi-tracer transport algorithm should depend only on a compact computational stencil and should also be suitable for unstructured grid systems. The multi-moment based finite-volume approach introduced in [34,3] employs a single-cell reconstruction procedure and is well-suited for our application. The upstream overlap-area computation required for the conservative semi-Lagrangian scheme can be avoided by using the characteristic semi-Lagrangian approach, where the fluxes are integrated along the characteristics as shown in [4]. We further extend this approach for arbitrary quadrilateral grids on the cubed sphere by designing a conservative semi-Lagrangian scheme on the spectral-element grid, hereinafter referred to as SPELT — SPectral-Element Lagrangian Transport. For the SPELT scheme the upstream search is reduced to a point search on the cubed sphere and the reconstruction is local, which makes SPELT extremely attractive for arbitrary grids. SPELT is a conservative flux-based scheme (with a monotonic option) and is accurate on arbitrary quadrilateral grids. Moreover, a new algorithm in HOMME shows that SPELT is highly scalable *and* multi-tracer efficient. The performance of SPELT in climate simulations is beyond the scope of this manuscript and will be discussed in a future work [13].

The remainder of the paper is organized as follows: in Section 2 we briefly describe semi-Lagrangian schemes for the transport equation. Section 3 describes our SPELT algorithm, in particular the scheme for arbitrary quadrilateral grids. Section 4 shows the multi-tracer efficiency, scalability and some high-resolution experiments comparing the relative merits of both schemes in HOMME.

2. Tracer transport schemes

The flux-form transport equation for a scalar $\rho(x, y, t)$ in 2D Cartesian (x, y)-plane, without a source or sink, can be written as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (u\rho)}{\partial x} + \frac{\partial (v\rho)}{\partial y} \equiv \frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{F} = 0, \quad t \in (0, T], \tag{1}$$

where (u, v) is the wind velocity vector, $\mathbf{F} = (\rho u, \rho v)$ is the flux, and the initial condition is prescribed as $\rho(x, y, t = 0) = \rho_0(x, y)$. Equivalently, (1) can be cast in the following Lagrangian form:

$$\frac{D}{Dt} \int\limits_{\mathcal{A}(t)} \rho \, d\mathcal{A} = 0, \tag{2}$$

where $D/Dt = \partial_t + u\partial_x + v\partial_y$ is the Lagrangian (material) derivative, $\mathcal{A}$ is the area (volume) in which the fluid density ρ evolves in time along the Lagrangian trajectories (characteristics). However for the non-divergent flow fields, a regular semi-Lagrangian approach, which is not constrained to be conservative, uses the following simple form:

$$\frac{D\rho}{Dt} = 0, \quad \Rightarrow \quad \rho^{n+1} = \left[\rho^n\right]^*, \tag{3}$$

where the second equation indicates a semi-Lagrangian time discretization. Here, ρ^{n+1} is the estimate of ρ at the new time level t^{n+1} from known values ρ^n at time $t^n = n\Delta t$. Usually ρ^{n+1} is computed by an interpolation at the foot of the trajectory (upstream position), in (3) this is denoted as $[\cdot]^*$.

Both forms, (1) and (2), are used for numerical discretization of a conservative transport based on Eulerian and Lagrangian methods, respectively. Conservative finite-volume semi-Lagrangian methods such as the cell-integrated semi-Lagrangian schemes (CISL [25], CSLAM [20]) and other schemes based on incremental remapping [9] employ the Lagrangian form (2). These schemes utilize backward trajectories. The upstream or Lagrangian cell corresponding to the arrival cell (or