A fully-compressible nonhydrostatic cell-integrated semi-Lagrangian atmospheric solver with conservative and consistent transport

by

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Abstract

Traditional semi-Lagrangian dynamical solvers are widely used in current global numerical weather prediction (NWP) and climate models, but are known to lack inherent mass-conserving properties. Some newer approaches utilize a cell-integrated (conservative) semi-Lagrangian (CISL) semi-implicit solver, which is inherently mass-conserving. However, existing CISL semi-implicit solvers lack consistent formulation among the discrete continuity equation and other discrete conservation equations for scalar tracers such as water vapour and air pollutants. Such inconsistency can lead to spurious generation or removal of scalar mass.

In this dissertation, a new cell-integrated semi-Lagrangian (CISL) semi-implicit nonhydrostatic solver is presented with consistent discrete mass conservation equations for air and all tracers, and which preserves the shape of tracer-mass distribution. The discretization does not depend on a mean reference state, but maintains the same framework as typical semi-implicit CISL solvers, where a linear Helmholtz equation is constructed and a single application of the cell-integrated transport scheme is needed for scalar transport.

Tests of this new solver are made for a series of increasingly complex flow scenarios. The initial testbed utilizes the hydrostatic, incompressible, shallow-water equations, for which the new solver is shown to be numerically stable. It maintains accuracy comparable to other existing solvers even for a highly nonlinear unstable jet. The second suite of tests are for nonhydrostatic two-dimensional (x-z) fully compressible flows in the atmosphere as governed by the moist Euler equations, which compare well to several idealized benchmark test cases from the literature. The third flow scenario is complex orography, where the nonhydrostatic equations are transformed to use a terrain-following height coordinate. Results from test cases of dry and moist flows over idealized mountain shapes are presented. In summary, the prototype development work presented in this dissertation shows that the proposed CISL nonhydrostatic solver with conservative and consistent transport may be a desirable candidate for a dynamical core in comprehensive global NWP and climate models.
Preface

The main body of this dissertation is composed of work from two accepted journal papers (Chapters 2 and 3) and one submitted (Chapter 4).

Chapter 1
I wrote this chapter with editing provided by Prof. Stull.

Chapter 2

- I designed the proposed formulation for consistent transport in a cell-integrated semi-Lagrangian semi-implicit shallow-water model with Dr. W.C. Skamarock.

- I analyzed the effectiveness of the consistent transport scheme in CSLAM-SW.

- I provided most of the machinery and tools needed in the CSLAM-SW solver (including discretizing the system, the elliptic solver, trajectory computations, and marriage of solver components to the existing CSLAM transport scheme).

- Dr. P.H. Lauritzen provided the CSLAM transport scheme.

- Dr. J.B. Klemp provided the Eulerian solver that was used for comparison purposes (which I modified from using a flux-form leapfrog explicit time-stepping scheme to an advective leapfrog semi-implicit scheme to provide a fair comparison with CSLAM-SW).

- I wrote the manuscript with editing provided by the co-authors and four anonymous reviewers. I prepared most of the figures for this publication; Dr. P.H. Lauritzen provided Fig. 2.1 and Dr. W.C. Skamarock provided Fig. 2.2.

Chapter 3
• I extended the design of CSLAM-SW for a nonhydrostatic system to formulate CSLAM-NH.

• I analyzed and compared the results from CSLAM-NH with an existing Eulerian nonhydrostatic solver (see below).

• As in Chapter 2, I provided most of the machinery needed in the nonhydrostatic solver (including the coupling of an existing microphysics scheme to the solver and other components that I adapted from the code I developed in CSLAM-SW).

• Dr. J.B. Klemp provided the Eulerian nonhydrostatic solver, used for comparison purposes, and the Kessler microphysics scheme.

• I wrote the manuscript with editing provided by the co-authors and three reviewers. I prepared all the figures (except for Fig. 3.1, which is the same as Fig. 2.1 that was provided by Dr. P.H. Lauritzen) for this publication, with labelling touch-ups by Dr. W.C. Skamarock.

Chapter 4
A version of Chapter 4 has been submitted for publication:

• I reformulated CSLAM-NH to use terrain-following height coordinates and an implicit Rayleigh damping layer.

• I provided the modifications to CSLAM-NH for it to work with idealized terrain.

• I designed CSLAM-NH to use an iterative scheme to handle the buoyancy terms implicitly, and in the testing process, I found that recomputation of the trajectories are needed to allow for large time steps over terrain.

• I analyzed and compared the results from CSLAM-NH with those from the literature, and in one case, I modified the Eulerian solver (provided by Dr. J.B. Klemp for Chapter 3) for comparison with CSLAM-NH.

• I wrote the manuscript and prepared all the figures for this manuscript, with editing provided by the co-authors.

Chapter 5
I drew all the conclusions and wrote this chapter, with editing provided by Prof. Stull.
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Dedicated to my mah mah (grandmother), Low Lam
Chapter 1

Introduction

1.1 The role of a dynamical core in an atmospheric model

Fluid motion in the atmosphere is described by a system of equations that includes the equations of motion, the continuity equation, the thermodynamic equation, water vapour conservation equation, and the ideal gas law. These equations depict how features in the atmosphere evolve and affect weather conditions at the earth’s surface. Analytical solutions are typically not available due to the nonlinearity of the system, so numerical solutions are sought by discretizing the equations in time and space in numerical weather prediction (NWP) computer models. The output from these computer models is a useful tool for meteorologists in the generation of weather forecasts.

An NWP model can be broadly divided into two main components: the model dynamics and the model physics. The “dynamics” include physical processes resolvable at the grid scale of an NWP model and are approximated using a fluid flow solver (also termed the ‘dynamical core’ of the model). These processes include wind evolution, and some of its driving forces such as horizontal and vertical advection of momentum, pressure-gradient force, Coriolis force, and gravitational force. The dynamical core is also responsible for the advection of all scalars (moisture, tracers, etc.) by the Reynolds-averaged winds, and these advective processes are carried out by the transport scheme of the fluid flow solver.

The “physics” component refers to the subgrid-scale physics that are approximated using parameterization schemes. These schemes parameterize physical processes unresolved at the grid cell, such as cloud microphysics, cumulus convection, turbulence, radiative fluxes, and modification of fluxes due to land-surface characteristics. The validity of these physical parameterization schemes, as well as how they are coupled to the dynamics, are ongoing research topics that will not be addressed here. The work presented in this dissertation will focus on the dynamics component of an NWP model, in particular on the development of a prototype solver serving as a viable alternative dynamical core for an NWP model.
Chapter 1: Introduction

1.2 Previous related work

1.2.1 Eulerian vs. Lagrangian advection schemes

The advection (or transport) scheme of a fluid flow solver is responsible for computing the time tendencies due to advection. A simplified one-dimensional passive advection equation for mixing ratio \( q \) in a flow with constant velocity \( U \) is given below:

\[
\frac{\partial q}{\partial t} + U \frac{\partial q}{\partial x} = 0.
\]  

(1.1)

As an example of an Eulerian advection scheme, the upstream method is used to discretize (1.1):

\[
\frac{q_{i}^{t+\Delta t} - q_{i}^{t}}{\Delta t} + U \frac{q_{i}^{t} - q_{i-1}^{t}}{\Delta x} = 0,
\]  

(1.2)

where \( \Delta t \) and \( \Delta x \) are the time step and grid spacing, respectively. The superscripts represent the time level at which the terms are evaluated, and the subscripts denote the position of the grid point. Assuming that values for \( q \) from the previous time step are known, we can solve for \( q_{i}^{t+\Delta t} \).

The stencil of the scheme (1.2) is shown as grey squares, and the numerical domain of dependence is shaded in light grey in Fig. 1.1. If the advection velocity \( U \) translates the parcel beyond this stencil, the scheme violates a numerical stability condition called the Courant-Friedrichs-Lewy (CFL) condition. Qualitatively, the CFL condition “requires that the numerical domain of dependence of a finite-difference scheme include the domain of dependence of the associated partial differential equation” (Durran, 2010). In an Eulerian scheme such as (1.2), the discrete advection scheme poses a limit on the maximum time step by the CFL stability condition.

![Figure 1.1: Numerical domain of dependence the upstream finite difference scheme [adapted from Durran (2010), Fig. 2.1]](image-url)
The simplified passive advection equation in (1.1) can be rewritten as the Lagrangian derivative (also known as the material derivative or the total derivative),

$$\frac{dq}{dt} = 0,$$

(1.3)

which can be solved numerically using

$$\frac{q_A^{t+\Delta t} - q_D}{\Delta t} = 0,$$

(1.4)

where subscript $A$ denotes the arrival position and subscript $D$ denotes the departure location, calculated using the wind speed $U$. In other words, the mixing ratio $q$ is conserved along the trajectory (arrow connecting from $q_D$ to $q_A$ in Fig. 1.2). The Lagrangian transport method allows the elimination of the advection terms by numerically solving for the total derivative. Moreover, the departure location defines the domain of dependence of the continuous problem. Since this point is calculated explicitly, it will always be included in the numerical domain of dependence and therefore, the Lagrangian method is not subject to the CFL condition.

Although fully Lagrangian schemes allow for larger time steps than Eulerian schemes, they have the disadvantage that the parcels will eventually become unevenly distributed in deformed flows. Features in parts of the domain where parcels are sparse will become under-resolved. To maintain an even resolution, traditional semi-Lagrangian schemes were devised. Semi-Lagrangian schemes use a combination of two reference frames: Eulerian and Lagrangian. For schemes that
use backward trajectories, a new set of parcels is traced back a time step. The arrival grid points are chosen to be on a pre-defined regular Eulerian grid (Fig. 1.2). However, the departure location typically does not coincide with the Eulerian grid (such as the departure point in Fig. 1.2). Since the solution from the previous time step is only known on the Eulerian grid, some interpolation is needed to obtain the value at the departure point. Staniforth and Côté (1991) provides a review on traditional semi-Lagrangian schemes.

1.2.2 Traditional semi-Lagrangian semi-implicit method

Semi-Lagrangian schemes are the most widely used space-time numerical integration scheme in current global NWP and climate models. The popularity of these schemes can be mainly attributed to their lenient numerical stability condition for advection. Larger stable advection time steps help make these numerical models more computationally efficient. The gain in efficiency can then be used to offset any increase in computational time needed in making longer forecasts, using more sophisticated physics schemes, and/or making higher resolution forecasts. In general, terrain and land surface features are better resolved using higher model resolution.

The early work of semi-Lagrangian transport schemes was pioneered by Fjørtoft (1952, 1955), Wiin-Nielsen (1959), Krishnamurti (1962) and Sawyer (1963) for a more accurate representation of advection. Robert (1969) proposed combining an implicit treatment of the terms responsible for fast propagating waves in the atmosphere with an explicit treatment of the advection terms. By implicitly solving the gravity and acoustic wave terms, larger stable time step sizes are allowed as compared to using fully explicit schemes. Later, Robert (1981, 1985) suggested combining the traditional semi-Lagrangian method for the advection terms with the implicit integration of the fast propagating terms, which combines the extended stability of both schemes. This method has since been widely adopted at numerous weather research centres.

At the time of writing this dissertation, the following weather research centres are using semi-Lagrangian transport schemes in their numerical models: the Canadian Meteorological Centre (Côté et al., 1998), the European Centre of Medium-Range Weather Forecasts (ECMWF) (Ritchie et al., 1986; Ritchie et al. 1995), the United Kingdom Meteorological Office (Davies et al., 2005), the Danish Meteorological Institute (Nair and Machenhauer, 2002), the China Meteorological Association (Yang et al., 2008), Météo-France (Bubenová et al., 1995), Hydrometcentre of Russia (RosHydromet, 2011), and the Japan Meteorological Agency (JMA, 2013).

As mentioned, traditional semi-Lagrangian schemes often require some grid-point interpolation to retrieve the value at a departure point. A widely known caveat of traditional semi-Lagrangian schemes is that it does not ensure mass conservation due to grid-point interpolation. The distribution of atmospheric pressure is the main driver for the flow features we see in our weather. As
atmospheric pressure is the weight of air mass above, errors in the transport of the latter will likely have an impact on the prediction of meteorological features. Hence, mass-conserving advection schemes are desirable, which is the motivation for this research.

The following section describes some of the past modelling efforts in ensuring mass conservation in models.

1.2.3 Mass conservation in semi-Lagrangian schemes

Mass fixers

Not all transport schemes inherently conserve mass, but this property can be enforced using *a priori* or *a posteriori* constraints (Rasch and Williamson, 1990a). *A priori* mass-conserving schemes are often formulated with the desirable property inherent in the design of the numerical method, whereas *a posteriori* schemes typically attain mass conservation through an adjustment procedure, and are known as ‘fixers’, following Rasch and Williamson (1990a).

Different *a posteriori* adjustment procedures have been devised to overcome the lack of mass conservation in semi-Lagrangian schemes. Priestley (1993) developed a mass restoration scheme that minimizes the local mass change in one time step by constraining the interpolation coefficients in the solution of a monotonic semi-Lagrangian transport scheme. Moorthi et al. (1995) applied an adjustment formula such that the entire model surface pressure field (equivalent to mass) is multiplied by a constant factor that preserves the global mean surface pressure at its initial value. Williamson and Rasch (1994) enforced a conservation fixing step after the advection calculation, and restores global mass conservation selectively over regions more strongly affected by the advection scheme. These schemes, albeit carried out in a rather ad-hoc manner, can all maintain global mass conservation.

Inherently conservative transport

Recently, stricter approaches of ensuring mass conservation in semi-Lagrangian schemes have been devised. These schemes are referred to as conservative semi-Lagrangian transport schemes, also known as cell-integrated semi-Lagrangian (CISL) schemes (Rancic, 1992; Nair and Machenhauer, 2002; Zerroukat et al., 2002; Lauritzen et al., 2010). In essence, these schemes are finite-volume methods that utilize the fact that the integral mass over a control volume is conserved along its trajectory. The problem then reduces to a remapping problem from an Eulerian arrival grid to a Lagrangian departure grid (for a backward-in-time scheme). The three main steps to a CISL scheme are: (i) departure cell approximation, (ii) subgrid-cell reconstruction of the field on the Eulerian grid,
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and (iii) remapping of the field onto the Lagrangian grid. These are explained as follows.

(i) There are multiple ways to define the discrete Lagrangian departure cell over which the integration of the mass field is carried out. A rigorous approach is to trace the vertices of the Eulerian arrival grid cell back to their departure locations, which define the corners of the departure cell (e.g. Rancic, 1992; Lauritzen et al., 2010). The departure cell edges can then be approximated as straight lines, forming irregular quadrilaterals. This set of irregular quadrilateral cells form a grid that typically does not coincide with the Eulerian arrival grid (similar idea to that shown for traditional schemes in Fig. 1.2).

Another approximation is to compute the mass over an approximated area of the discrete departure cell. The area of the discrete departure cell is approximated with edges parallel to the coordinate axes to simplify the remapping procedure (e.g. Nair and Machenhauer, 2002). The horizontal positions of the vertical cell edges coincide with the midpoints between the computed departure points of the arrival grid cell vertices. The vertical positions of the horizontal cell edges are defined by those of the departure cell vertices. This approximation leads to a computational departure cell with more sides (generally eight, but possibly fewer in some special circumstances), but the departure cell is now made up of rectangular areas that align with the Eulerian grid.

(ii) Since the Lagrangian departure grid cells typically do not coincide with the Eulerian grid cells, a reconstruction of the subgrid-cell distribution of the transported variable is needed. A subgrid-cell reconstruction function provides a best fit continuous function based on known Eulerian cell-averaged values. Fig. 1.3 shows an example of a quasi-biparabolic fit (the smooth surface, elevated in the figure for clarity) of the Eulerian cell-averaged values (columns). The function is then integrated over the Lagrangian departure cell (as opposed to using interpolation as in traditional semi-Lagrangian schemes).

Various subgrid-cell reconstruction methods have been reported in the literature: piecewise constant method, piecewise linear method, piecewise parabolic method, and even higher-order methods such as the piecewise cubic method and piecewise quartic method. The lower the order of accuracy of the method, the more inherently damping the scheme. However, more reconstruction coefficients are required in higher-order methods, which can become expensive to compute. To reduce the cost associated with the computation of the coefficients, Nair and Machenhauer (2002) introduced an extension of the quasi-biparabolic method of Rancic (1992) (shown in Fig. 1.3) and used only five of the nine coefficients in a fully two-dimensional piecewise biparabolic fit. The method has been shown to still give accurate representation despite the simplification, and also has the benefit of a straightforward implementation of shape-preserving filters (next section).

(iii) Given the departure cell position and the reconstruction function, the final step is to carry out the remapping of the transported variable from the Eulerian arrival grid to the Lagrangian departure
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Figure 1.3: Reconstruction of the subgrid-cell distribution using the piecewise quasi-biparabolic reconstruction method of Rancic (1992). The columns represent known Eulerian cell-averaged values and the smooth surface represents the quasi-biparabolic reconstruction function (elevated in the figure for clarity).

grid. One approach is to do the remapping of the mass field from one grid to another using a cascade approach, i.e. the integral of the reconstruction function over the Lagrangian departure cell is computed incrementally one dimension at a time, as in Rancic (1992), Nair and Machenhauer (2002), and Zerroukat et al. (2002). Others have shown that a more fully 2D remapping procedure can also be done, as in Lauritzen et al. (2010), who used the approach in Dukowicz and Kodis (1986) and simplified the 2D remapping procedure by converting the areal integral into a line integral using the Gauss-Green theorem. As long as the integral is exact and there is no gap or overlap between the discrete departure cells, local (and therefore, global) mass conservation is ensured (Lauritzen et al., 2011).

Shape-preserving transport

Related to mass conservation is the desirable property of shape-preservation in tracers. Schemes that ensure shape-preservation prevent new minima and/or maxima from forming in the advected field. In the broader literature, they are sometimes referred as monotonic limiters, essentially non-oscillatory limiters, or positive-definite limiters for those that eliminate negative values. In atmospheric science, shape-preserving filters are often applied in moisture and tracer transport as the minimum and maximum specific concentrations are physically bounded, e.g. the lower end must be
non-negative and the upper end is bounded by the initial maximum value for pure transport cases. Spurious minimum and maximum can be generated through an interpolation or remapping procedure, and the need of shape-preserving limiters is dependent on the advection scheme operators.

Shape-preserving schemes can be applied either \textit{a priori} or \textit{a posteriori}. \textit{A priori} enforcement of the shape-preserving property can be applied for example within the interpolation procedure by constraining the derivative estimates in an interpolation scheme (Rasch and Williamson, 1990b; Bermejo and Staniforth, 1991). \textit{A posteriori} fixers reclaim the initial shape of the field by applying adjustments afterwards. For example, in the shape-preserving fixer described in Williamson et al. (1987), local restoration of moisture at negative specific humidity points can be made by increasing the values to zero there. But to ensure global moisture conservation, specific humidities at the neighbouring grid points are then reduced accordingly. If there is insufficient moisture in the local neighbourhood, then the global moisture field in the domain is reduced by a constant factor to compensate for the moisture restoration at the negative points (and to preserve total moisture content).

In CISL schemes, shape-preserving filters can be applied within the subgrid-cell reconstruction. Since these schemes advect flux-form variables such as moisture mass, care should be taken to only apply the shape-preserving limiter on the specific humidity. Often, new extrema in the moisture mass are physically acceptable, e.g. in a divergent flow where there is convergence/divergence of mass. Nair and Lauritzen (2010) show one way of implementing an \textit{a priori} shape-preserving limiter on only the specific concentration in the subgrid-cell reconstruction of the tracer mass.

\textbf{Consistent transport between air density and tracers}

As mentioned earlier, the maximum time step of an explicit time-stepping scheme with semi-Lagrangian transport is restricted by fast-propagating gravity and acoustic waves, which led to the development of traditional semi-Lagrangian semi-implicit schemes. Following the devising of CISL transport schemes, Machenhauer and Olk (1997) demonstrated for a one-dimensional shallow-water system that their CISL advection scheme, like traditional semi-Lagrangian schemes, can also be implemented with a semi-implicit time-integration scheme. Lauritzen et al. (2006) later derived and extended their discrete CISL continuity equation for a two-dimensional shallow-water system. Similar effort has also been carried out by Zerroukat et al. (2009) using the inherently mass-conserving semi-Lagrangian transport scheme SLICE of Zerroukat et al. (2002).

In existing semi-implicit CISL continuity equations, a divergence term is implicitly coupled to the pressure-gradient terms in the momentum equations. This divergence term will be referred to as the semi-implicit correction to the explicit transport (of air density). Unlike air density however, atmospheric tracers (including moisture) are not physically coupled to the wind field, and their
masses are passively (and explicitly) transported by the advection scheme in the solver. As a result, many models use a different numerical method for tracer transport (e.g. explicit transport) than for solving the continuity equation for air mass (Lauritzen et al., 2011).

If the discrete tracer conservation equation is numerically consistent with the continuity equation, the former should be identical to the continuity equation for a constant tracer mixing ratio of one. As discussed in Lauritzen et al. (2011), air mass and tracer mass may be conserved individually using a mass-conserving transport scheme (enforced either \textit{a priori} or \textit{a posteriori}), but numerical errors due to inconsistent transport schemes may appear when the mixing ratio is diagnosed from the prognostic air and tracer mass variables. These numerical errors will lead to spurious generation or loss of tracer mass, despite using an inherently conserving transport scheme. The need for numerically consistent transport of tracers and air density motivated the first step of developing a semi-implicit CIsL shallow-water equations solver in Lauritzen et al. (2006) in the first place. However, they had found that the use of a mean reference state in the semi-implicit correction term rendered it difficult to ensure numerical consistency in the transport.

1.3 Dissertation contributions

In this dissertation, a new cell-integrated semi-Lagrangian (CISL) semi-implicit nonhydrostatic solver with conservative and consistent transport of air and tracers is presented. The achievements encompassed by this dissertation are fourfold:

1. A fully-compressible nonhydrostatic prototype solver is developed, in anticipation of the effective resolution of current global NWP and climate models extending into the nonhydrostatic regime in the foreseeable future.

2. To ensure conservative transport, a CISL transport scheme is chosen, and the use of this CISL transport scheme in solving the fully-compressible nonhydrostatic atmospheric system is demonstrated for the first time.

3. To ensure consistent transport for all scalars, a new discrete semi-implicit CISL continuity equation is devised.

4. To the best of my knowledge, at the time of writing this dissertation, coupling of a CISL nonhydrostatic atmospheric solver to diabatic effects from a simple cloud microphysics scheme is published for the first time.

The design of the proposed nonhydrostatic solver considers the following. The goal is to further improve the numerical consistency in existing semi-Lagrangian transport methods used for global
NWP and climate modelling purposes. An alternative method in ensuring consistency between air density and scalar transport is devised. Other aspects of the model utilize existing numerical methods, such as the traditional semi-Lagrangian scheme for momentum transport and a conjugate-residual solver as the elliptic solver for the semi-implicit time-integration scheme. As mentioned in the previous section, traditional semi-Lagrangian semi-implicit schemes are widely used in current operational global NWP models, such as the Canadian Global Environmental Multiscale (GEM) model and the ECMWF Integrated Forecasting System (IFS).

To demonstrate that the CISL semi-implicit nonhydrostatic solver is a feasible option for implementation in a more comprehensive NWP model, a two-dimensional $x$-$z$ prototype solver is developed and applied to a suite of idealized test cases. The solver is tested using simplified boundary conditions: periodic in $x$ and rigid top and bottom boundaries. The Arakawa C grid (Arakawa and Lamb, 1977) is used for a more accurate representation of gradient and divergence terms, which have generally been regarded as the dominant terms in fine-scale weather.

To ensure conservative properties for dry air mass, tracer mass, and potential temperature, the continuity equation, tracer mass conservation equation, and the thermodynamic equation are all cast in the flux-form. The approach is based on the Advanced Research Weather Research and Forecasting (WRF-ARW) model (Skamarock and Klemp, 2008), and is also used in the recently developed variable-resolution Model Prediction Across Scales-Atmosphere model (MPAS-A) (Skamarock et al., 2012). All explicit scalar advection is carried out by the conservative semi-Lagrangian transport scheme. A new semi-implicit discretization scheme for the continuity equation is devised and used to maintain numerical consistency among the CISL scalar conservation equations.

### 1.4 Dissertation outline

The model development work is documented as three main stages (in the following three chapters):

1. A two-dimensional shallow-water equations (SWE) solver with conservative and consistent transport (Chapter 2).

   **Overview:** Shallow-water systems are often used as initial testbeds because of their resemblance to the fully-compressible Euler equations. The SWE represent the horizontal dynamics in the three-dimensional hydrostatic primitive equations, i.e. they permit Rossby and inertia-gravity waves, while excluding acoustic waves. The new consistent semi-implicit CISL continuity equation is tested first on the two-dimensional shallow-water equations. The goal is to test that the new SWE solver is stable and accurate for this simplified system. The relative importance of numerical consistency in tracer mass conservation is illustrated using comparisons with the discrete semi-implicit CISL continuity equation presented in Lauritzen et al.
(2006). In addition, this stage validates the coding of the solver components, such as the Lagrangian trajectory computations, Lagrange polynomial interpolation schemes, the elliptic solver, and the marriage of existing conservative semi-Lagrangian transport subroutines to the SWE solver.

2. Extension to a two-dimensional (x-z) nonhydrostatic atmospheric solver with conservative and consistent transport (Chapter 3).

*Overview:* The fully-compressible nonhydrostatic (Euler) equations allow a wide range of atmospheric motions. In addition to gravity waves, compressibility of the atmosphere allows fast acoustic waves to propagate. To test the new solver in these motions, the SWE solver is extended for the two-dimensional vertical-slice nonhydrostatic equations. The nonhydrostatic equations require solving the vertical momentum equation and accounting for buoyancy effects, which may impose a constraint on the numerical stability of the scheme. The semi-implicit nonhydrostatic solver is constructed using an implicit treatment of the fast acoustic waves, the proposed semi-implicit CISL continuity equation, and consistent formulations for all other scalar transport. The goal is to assess this solver in a set of idealized benchmark tests commonly used for nonhydrostatic atmospheric flows. Subgrid-scale latent heat processes, such as evaporation and condensation, are also included in the nonhydrostatic solver using a simple cloud microphysics scheme. The importance of numerical consistency is shown using a 2D idealized convective storm simulation.

3. Extension to a two-dimensional (x-z) nonhydrostatic solver with a transformed vertical coordinate (Chapter 4).

*Overview:* Idealized mountain flows are simulated using the proposed solver. This stage of the development validates that the new CISL nonhydrostatic solver works for more realistic bottom boundary conditions, and demonstrates that only a little modification to the mechanics of the nonhydrostatic solver is required for the change in the vertical coordinate system. The solver is applied for a suite of linear and nonlinear mountain flows, including an orographic cloud formation simulation.

A summary of the dissertation, the broader impact of the effort, and an outline of future research directions for this work to be extended into a more comprehensive weather and climate model are given in the Conclusions (Chapter 5).
Chapter 2

A two-dimensional shallow-water equations solver with conservative and consistent transport

2.1 Introduction

Semi-Lagrangian semi-implicit (SLSI) schemes have been widely used in climate and numerical weather prediction (NWP) models since the pioneering work of Robert (1981) and Robert et al. (1985). The more lenient numerical stability condition in these schemes allows larger time steps and thus increased computational efficiency. Traditional semi-Lagrangian schemes are not inherently mass-conserving due to their use of grid-point interpolation, and the lack of conservation can lead to accumulation of significant solution errors (Rasch and Williamson, 1990a; Machenhauer and Olk, 1997). To address this issue, conservative semi-Lagrangian schemes, also called cell-integrated semi-Lagrangian (CISL) transport schemes (Rancic, 1992; Laprise and Plante, 1995; Machenhauer and Olk, 1997; Zerroukat et al., 2002; Nair and Machenhauer, 2002; Lauritzen et al., 2010), have been developed. Although CISL transport schemes allow for locally (and thus globally) conservative transport of total fluid mass and constituent (i.e. tracer) mass, an issue related to conservation remains when they are applied in fluid flow solvers: the lack of consistency between the numerical representation of the total mass continuity and constituent mass conservation equations (Jöckel et al., 2001; Zhang et al., 2008). The lack of numerical consistency between the two can lead to the unphysical generation or removal of model constituent mass, which can introduce significant errors in applications such as chemical tracer transport (Machenhauer et al., 2009).

Our testbed for developing and testing CISL-based fluid flow solvers are the shallow-water (SW) equations on an $f$-plane:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - f v - g \frac{\partial h}{\partial x} = 0,
\]  

(2.1)
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\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + fu - g' \frac{\partial h}{\partial y} = 0, \tag{2.2}
\]

\[
\frac{\partial h}{\partial t} + \nabla \cdot (hv) = 0, \tag{2.3}
\]

\[
\frac{\partial (hq)}{\partial t} + \nabla \cdot (hqv) = 0 \tag{2.4}
\]

where \(v = (u, v)\) is the horizontal velocity vector, \(f\) is the Coriolis parameter, \(g'\) is the reduced gravity (defined as \(g' = g \Delta \rho / \rho\), where \(g\) is gravitational acceleration, \(\Delta \rho\) is the density difference between the two layers, and \(\rho\) is the mean density), \(h\) is the total fluid depth (a surrogate for total fluid mass), and \(hq\) is the depth portion (mass fraction) of an arbitrary constituent, where \(q\) is its specific concentration. Numerical consistency is satisfied if, for \(q_0 = 1\), the discretization scheme of the constituent equation (2.4) collapses to that for the continuity equation (2.3), also known as free-stream preservation.

The difficulty in maintaining consistency, as will be discussed in more detail, can partly be attributed to the conventional linearization around a constant mean reference state in the semi-implicit form of a CISL continuity equation. To eliminate the reference state, Thuburn (2008) developed a fully-implicit CISL-based scheme for the shallow-water equations that requires solving a nonlinear Helmholtz equation at every time step. The solution of the Helmholtz equation is potentially problematic and expensive (Thuburn et al., 2010). To reduce the dependence of their semi-implicit scheme on a reference state, Thuburn et al. (2010) used an alternative iterative approach to solve the nonlinear system, but it requires multiple calls to a Helmholtz solver per time step, again making the scheme potentially expensive.

In addition to consistency and mass conservation, another desirable property is that the new scheme should be shape-preserving. A shape-preserving scheme ensures that no new unphysical extrema are generated in a field due to the numerical scheme (e.g. Machenhauer et al., 2009). For example, specific concentrations of a passive constituent should not go outside the range of its initial minimum and maximum values. Non-shape-preserving schemes may generate unphysical specific concentrations, such as negative concentration values due to undershooting.

In this paper, using a shallow-water system, we present a new SLSI formulation that uses a CISL scheme for mass conservation and ensures numerical consistency between the total mass and constituent-mass fields. The new scheme is based on the CISL transport scheme called the Conservative Semi-Lagrangian Multi-tracer (CSLAM) transport scheme developed by Lauritzen et al. (2010). Like other typical conservative SLSI solvers, the algorithm requires a single linear Helmholtz equation solution and a single application of CSLAM. To ensure shape-preservation, the scheme is further extended to use existing shape-preserving filters.
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Figure 2.1: (a) Exact departure cell area ($\delta A^*$, dark grey region) and the corresponding arrival grid cell ($\Delta A$, light grey region). (b) Departure cells in CSLAM ($\delta A$) are represented as polygons defined by the departure locations of the arrival grid cell vertices.

The paper is organized as follows. In section 2.2, the conservative semi-Lagrangian scheme CSLAM is described and a discussion of the issue of consistency between total-mass and constituent-mass conservation in its semi-implicit formulation is provided. A new consistent semi-implicit discretization of the CSLAM continuity equation, including the implementation of the shape-preserving schemes, is proposed in section 2.3. Results from four test cases are presented in section 2.4, highlighting the stability and accuracy of the new scheme for linear and highly-nonlinear flows, as well as showing the shape-preserving ability of the scheme. And finally, in section 2.5, a summary of the results and a potential extension of the new scheme are given.

2.2 Mass conservation and consistency in SLSI solvers

2.2.1 CSLAM — a CISL transport scheme

The CSLAM transport scheme is a backward-in-time CISL scheme, where the departure grid cell area $\delta A^*$ is found by tracing the regular arrival grid cell area $\Delta A$ back in time one time-step $\Delta t$ (Fig. 2.1a). The CSLAM discretization scheme for (2.3) is given by

$$h_{\text{exp}}^{n+1} \Delta A = h_{\text{exp}}^n \delta A^*,$$

where the superscript denotes the time level, $h_{\text{exp}}^{n+1}$ is the explicit cell-averaged height solution computed by integrating the height field $h^n$ over $\delta A^*$, which gives departure cell-averaged height value.
\( h^n \). The departure cell area \( \delta A^* \) in CSLAM is found through iterative trajectory computations from the four vertices of an arrival grid cell (unfilled circles in Fig. 2.1b) to their departure points (filled circles in Fig. 2.1b). The departure cell area is then approximated using straight lines as cell edges (dark grey region \( \delta A \) in Fig. 2.1b). To integrate the height field over \( \delta A \), CSLAM implements a remapping algorithm that consists of a piecewise biparabolic subgrid-cell reconstruction of the \( h^n \) field, and then the integration of the reconstruction function over the departure cell area. The area integration in CSLAM is transformed into a series of line integrals using the Gauss-Green theorem, and involves solving for a set of weights that depends only on the departure cell boundary. The use of line integrals greatly enhances the transport scheme’s computational efficiency for multi-tracer transport as the weights can be reused for all tracer species in the model. For full details on the transport scheme, see Lauritzen et al. (2010).

2.2.2 A discrete semi-implicit continuity equation in velocity-divergence form using CSLAM

Lauritzen et al. (2006) (which we will refer to as LKM) developed an SLSI SW equations solver using the explicit CISL transport scheme of Nair and Machenhauer (2002). For the momentum equations (2.1) and (2.2), they used a traditional SLSI discretization [(A.1) and (A.2) in the Appendix but without time-off-centering]. Their momentum equations are then implicitly coupled to a velocity divergence correction term in the continuity equation. In this paper we follow the construction of the SW equations solver described in LKM, but we use CSLAM as the explicit CISL transport scheme. The discrete semi-implicit CISL continuity equation given in LKM [eq.(31) in LKM] is

\[
\begin{align*}
    h^{n+1} &= h_{\text{exp}}^{n+1} - \frac{\Delta t}{2} H_0 \left[ \nabla_{\text{eul}} \cdot \tilde{v}^{n+1} - \nabla_{\text{lag}} \cdot \tilde{v}^{n+1} \right] \\
    &\quad + \frac{\Delta t}{2} H_0 \left[ \nabla_{\text{eul}} \cdot v^n - \nabla_{\text{lag}} \cdot v^n \right] \frac{\delta A^*}{\Delta A},
\end{align*}
\]

(2.6)

where \( h_{\text{exp}}^{n+1} \) is as described above, \( \Delta t \) is the model time step, \( H_0 \) is the constant mean reference height, \( v^{n+1} \) is the velocity field implicitly coupled to the momentum equations, \( \tilde{v}^{n+1} = 2v^n - v^{n-1} \) is the velocity field extrapolated to time-level \( n + 1 \), and \( v^n \) is the velocity field at time-level \( n \). Their semi-implicit correction term [first term in brackets in (2.6)] is the correction to the explicit solution \( h_{\text{exp}}^{n+1} \) from the CSLAM scheme, and the second term in brackets in (2.6) is a predictor-corrector term (where the overbar denotes the departure cell-averaged value). The implicit linear terms are obtained, as in the traditional approach [e.g., Kwizak and Robert (1971); Machenhauer and Olk (1997)], by linearizing the height field around a constant mean reference state, and hence (2.6)
results in a velocity-divergence form. The notations $\nabla_{\text{eul}}$ and $\nabla_{\text{lag}}$ denote discretized divergence operators based on the Eulerian and Lagrangian forms respectively. Using notations in Fig. 2.2, the Eulerian divergence operator is given by

$$\nabla_{\text{eul}} \cdot \mathbf{v} = \frac{1}{\Delta x} (u_r - u_l) + \frac{1}{\Delta y} (v_t - v_b).$$  \hspace{1cm} (2.7)$$

The Lagrangian divergence operator [eq.(25) in LKM] is given by

$$\nabla_{\text{lag}} \cdot \mathbf{v} = \frac{1}{\Delta A} \frac{\Delta A - \delta A}{\Delta t},$$  \hspace{1cm} (2.8)$$

and is computed as the change in cell area in one time step.

The form of the semi-implicit correction term in (2.6) is due to the split-divergence approximation [eq. (26) in LKM]

$$\nabla \cdot \mathbf{v}^{n+1/2} \approx \frac{1}{2} \left[ \nabla \cdot \tilde{\mathbf{v}}^{n+1} + \nabla \cdot \mathbf{v}^{n} \right]$$  \hspace{1cm} (2.9)$$

applied to the linearized divergence term of the semi-implicit continuity equation. The split-divergence approximation is used to evaluate the linear divergence term at the mid-point trajectory (at time-level $n + 1/2$). As explained in Lauritzen et al. (2006), this approximation stems from their trajectory algorithm, where the trajectory is approximated as two segments: (i) from the departure point to the trajectory mid-point (computed iteratively), and (ii) from the mid-point to the arrival grid point (computed using extrapolated winds; see Fig. 1 in LKM). Since the Lagrangian divergence is calculated based on the change of cell area over time, and departure cell areas are computed using the split-trajectory algorithm, the split-approximation can also be applied to the divergence term (Lauritzen et al., 2006).

Ideally, to be consistent, the implicit and the extrapolated divergences would both be solved in a Lagrangian fashion; however, this would lead to a nonlinear elliptic equation instead of a standard Helmholtz equation (Lauritzen, 2005). To retain a linear elliptic equation, Lauritzen et al. (2006) implemented a predictor-corrector approach to correct for the Eulerian discretization of the implicit divergence term, and found that this step was necessary to maintain stability in their model. In our implementation of the LKM solver using CSLAM, we follow the approach of Lauritzen et al. (2006), where the predictor-corrector term [second term in brackets in (2.6)] is evaluated by integrating the departure cell-averaged value over $\delta A^*$. 

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2.2.3 Numerical inconsistency in semi-implicit continuity equations in a velocity-divergence form

Numerical consistency between total mass and constituent mass is difficult to maintain in semi-implicit CISL schemes such as LKM. The prognostic constituent mass variable $h q$ is typically solved explicitly using

$$(h q)_{n+1} = (h q)_{n+1}^{\text{exp}},$$

(2.10)

where $(h q)_{n+1}^{\text{exp}}$ is the CISL explicit solution, $h$ is the shallow-water height (analogous to total air mass in a full model), and $q$ is the specific concentration of an arbitrary constituent. (From here on, the constituent mass will be written without the parentheses for simplicity.) The cell-integrated transport equation in its flux-form helps conserve constituent mass, analogous to the amount of water vapour and other passive tracers in an atmospheric model — an important constraint especially for long simulations. Since the departure cell areas are the same for both total fluid mass and the constituent mass, the weights of the line integrals in CSLAM will need to be computed only once per time step, and represents one of the advantages of this scheme.

If the discrete constituent equation is consistent with the discrete continuity equation, the former should reduce to the latter when $q = 1$, and an initially spatially uniform specific concentration field should remain so. For a divergent flow, however, the semi-implicit correction term in (2.6) may become large enough such that (2.10), in its explicit form, is no longer consistent (Lauritzen et al., 2008).

Alternatively, one can formulate the discrete constituent equation by including similar semi-
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implicit correction and predictor-corrector terms as in (2.6), i.e.

\[ hq_{n+1} = hq_{\text{exp}} + \frac{\Delta t}{2} (HQ)_0 \left[ \nabla_{\text{eul}} \cdot \mathbf{v}^n - \nabla_{\text{lag}} \cdot \mathbf{v}^n \right] \delta A^* \Delta A, \]

where \((HQ)_0\) is a constant mean reference constituent mass, the velocities \(\mathbf{v}^n\) are solutions from the Helmholtz solver, and \(\tilde{v}^n\) and \(v^n\) are the same velocities as in (2.6).

However, (2.11) is only strictly numerically consistent when \(q = Q_0\), where \(Q_0\) is the constant mean reference specific concentration, and that \((HQ)_0\) is the product of \(H_0\) and \(Q_0\). Moreover, the dependence on a constant mean reference constituent mass \((HQ)_0\) may create a source of numerical errors for regions with little constituent mass. For example, in regions where \(hq_{\text{exp}} = 0\), if the flow is highly-divergent such that the terms in square brackets in (2.11) are non-zero, spurious constituent mass will be erroneously generated due to a non-zero constant mean constituent mass. Similarly, in areas where \(hq_{\text{exp}}^n\) is a non-zero constant, spurious deviation from constancy can be generated by the correction terms.

The issue with an inconsistent constant mean reference state for the total fluid mass and constituent mass fields can be resolved with the formulation we present in the next section.

2.3 A consistent and mass-conserving semi-implicit SW solver

Our new scheme ensures numerical consistency between the continuity and constituent equations by formulating the discrete equations, specifically the semi-implicit correction and the predictor-corrector terms, in flux form instead of a velocity-divergence form. The goal is to avoid the use of a constant reference state, such as (2.6). We test this approach for the SW equations, and refer to the model using the flux-form scheme as CSLAM-SW. We formulate the semi-implicit flux-form continuity equation as

\[ h^{n+1} = h_{\text{exp}}^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (h_{\text{exp}}^{n+1} \mathbf{v}^{n+1}) - \nabla_{\text{lag}} \cdot (h_{\text{exp}}^{n+1} \tilde{\mathbf{v}}^{n+1}) \right] \delta A^* \Delta A, \]

and use the explicit CSLAM solution \(h_{\text{exp}}^{n+1}\) as the reference state in the semi-implicit correction term. The shallow-water model CSLAM-SW, like the LKM model, couples the semi-implicit height continuity equation with the traditional semi-Lagrangian momentum equations, as described in the Appendix, and solves the resulting elliptic system with a conjugate-gradient Helmholtz solver.
To ensure consistency, we simply express the constituent equation as

\[
(hq)^{n+1} = hq^{n+1}_{\text{exp}} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (hq^{n+1}_{\text{exp}} v^{n+1}) - \nabla_{\text{lag}} \cdot (hq^{n+1}_{\text{exp}} v^{n+1}) \right] + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (hq^n v^n) - \nabla_{\text{lag}} \cdot (hq^n v^n) \right] \frac{\delta A^*}{\Delta A},
\]

(2.13)

where \(hq^{n+1}_{\text{exp}}\) is the explicit CSLAM update to the constituent mass, the velocities \(v^{n+1}\) in \(\nabla_{\text{eul}} \cdot (hq^{n+1}_{\text{exp}} v^{n+1})\) are from the SLSI solution, and \(hq^n\) and \(v^n\) are the constituent mass and velocity at time-level \(n\) respectively. This scheme also resolves the problem of spurious generation of constituent mass for regions with near-zero specific concentration (as described in the previous section). The specific concentration \(q\) is diagnosed by decoupling the constituent mass using

\[
q^{n+1} = \frac{hq^{n+1}}{h^{n+1}}.
\]

(2.14)

We note that to ensure numerical consistency, we must eliminate machine-roundoff and convergence errors in the Helmholtz solver. In solving for \(hq^{n+1}\), we substitute the solutions of \(v^{n+1}\) derived from the Helmholtz solution \(h^{n+1}\) into (2.13). Prior to diagnosing \(q\) using (2.14), we must correct the solution \(h^{n+1}\) by substituting solutions of \(v^{n+1}\) back into (2.12); otherwise, the values of \(h^{n+1}\) can become inconsistent with \(hq^{n+1}\). The consistent \(h^{n+1}\) solution is then used to solve for \(q\) using (2.14) and in the next time step. To compute \(hq^{n+1}\), we follow Nair and Lauritzen (2010) in separating the subgrid-cell reconstructions for \(h\) and \(q\), and then compute \(hq(x,y)\) using

\[
hq(x,y) = \overline{h} q + \overline{q} (h - \overline{h}),
\]

(2.15)

where \(h = h(x,y)\) and \(q = q(x,y)\) are the reconstruction functions, and \((\overline{h}, \overline{q})\) are cell averages.

The new flux-form conservation equations (2.12) and (2.13) involve the computation of an Eulerian flux-divergence and a Lagrangian flux-divergence using extrapolated velocities. Using the mesh described in Fig. 2.2, the discrete Eulerian flux-divergence is given as

\[
\nabla_{\text{eul}} \cdot (hv) = \frac{1}{\Delta x} \left[ (\overline{h} u)_r - (\overline{h} u)_l \right] + \frac{1}{\Delta y} \left[ (\overline{h} v)_t - (\overline{h} v)_b \right],
\]

(2.16)

where \(\Delta x\) and \(\Delta y\) are the grid spacing in the \(x\)- and \(y\)-directions, and each of the fluxes are evaluated as \(\overline{h} u_r, \overline{h} u_l, \overline{h} v_t, \text{ and } \overline{h} v_b\), respectively (see Appendix for operator definitions).

The Lagrangian flux-divergence in (2.13) needs to be consistent with the Lagrangian velocity-divergence (2.8). To derive the new operator, we begin by computing the Lagrangian backward-trajectories of the arrival grid cell vertices given in Fig. 2.2. We define the arrival cell corner points.
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to be at \((\vec{x}_1, \vec{x}_2, \vec{x}_3, \vec{x}_4)\), i.e. \((x_1, y_1)\), \((x_2, y_2)\), \((x_3, y_3)\), \((x_4, y_4)\), and the departure cell corner points as

\[
\vec{x}_{d1} = \vec{x}_1 - \Delta t \cdot (u_c, v_c)_1, \tag{2.17}
\]

\[
\vec{x}_{d2} = \vec{x}_2 - \Delta t \cdot (u_c, v_c)_2, \tag{2.18}
\]

\[
\vec{x}_{d3} = \vec{x}_3 - \Delta t \cdot (u_c, v_c)_3, \tag{2.19}
\]

\[
\vec{x}_{d4} = \vec{x}_4 - \Delta t \cdot (u_c, v_c)_4, \tag{2.20}
\]

where \((u_c, v_c)_i = (\bar{u}^i, \bar{v}^i)_i\) denote the x- and y-velocity components at the \(i^{th}\) vertex, where \(i = 1, 2, 3, 4\).

The area of the departure cell is computed as

\[
\delta A = \frac{1}{2} \left[ \vec{x}_{d21} \times \vec{x}_{d41} + \vec{x}_{d43} \times \vec{x}_{d23} \right], \tag{2.21}
\]

where \(\vec{x}_{d21} = \vec{x}_{d2} - \vec{x}_{d1}\); \(\vec{x}_{d41} = \vec{x}_{d4} - \vec{x}_{d1}\); \(\vec{x}_{d43} = \vec{x}_{d4} - \vec{x}_{d3}\); and \(\vec{x}_{d23} = \vec{x}_{d2} - \vec{x}_{d3}\). We can then rewrite the departure cell area as

\[
\delta A = \Delta x \Delta y - \Delta t \left[ \mathcal{F}_r - \mathcal{F}_l + \mathcal{F}_t - \mathcal{F}_b \right], \tag{2.22}
\]

where

\[
\mathcal{F}_r = \bar{u}^{y}_r \Delta y - (u_c v_c - u_c v_c) \Delta t / 2, \tag{2.23}
\]

\[
\mathcal{F}_l = \bar{u}^{y}_l \Delta y - (u_c v_c - u_c v_c) \Delta t / 2, \tag{2.24}
\]

\[
\mathcal{F}_t = \bar{v}^{x}_t \Delta x - (u_c v_c - u_c v_c) \Delta t / 2, \tag{2.25}
\]

\[
\mathcal{F}_b = \bar{v}^{x}_b \Delta x - (u_c v_c - u_c v_c) \Delta t / 2 \tag{2.26}
\]

(see Appendix for operator definitions).

Using (2.22), the velocity divergence can be written as:

\[
\nabla = \frac{1}{\Delta x \Delta y} \left[ \mathcal{F}_r - \mathcal{F}_l + \mathcal{F}_t - \mathcal{F}_b \right], \tag{2.27}
\]

which is identical to the Lagrangian divergence (2.8). The first flux term in each of \(\mathcal{F}_r, \mathcal{F}_l, \mathcal{F}_t, \) and \(\mathcal{F}_b\) is identical to the Eulerian velocity-divergence using velocities averaged to the cell edges and the remaining terms give the geometric correction for a Lagrangian representation (see Fig. 9 in Lauritzen, 2005). Using this velocity divergence, we now approximate the Lagrangian flux-
divergence term in equation (2.12) as:

$$\nabla_{\text{lag}} \cdot (hv) = \frac{1}{\Delta x \Delta y} \left[ \mathcal{F}_r \tilde{h}_r^x - \mathcal{F}_l \tilde{h}_l^x + \mathcal{F}_i \tilde{h}_i^y + \mathcal{F}_b \tilde{h}_b^y \right]. \quad (2.28)$$

Using (2.16) and (2.28) and replacing $h$ with $hq$, we can further combine each of the terms in brackets of the constituent equation (2.13), which becomes

$$hq_{n+1} = hq_{\text{exp}}^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (hq_{\text{exp}}^{n+1} q_{\text{exp}}^{n+1} v'_{n+1}) \right]$$

$$+ \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (hq^n q^n v^n) \right] \frac{\delta A^*}{\Delta A} , \quad (2.29)$$

where

$$\nabla_{\text{eul}} \cdot (hq^* v') = \frac{1}{\Delta x} \left[ \tilde{h}_r^x q^* v'(u_r - \mathcal{F}_r / \Delta y) - \tilde{h}_l^x q^* v'(u_l - \mathcal{F}_l / \Delta y) \right]$$

$$+ \frac{1}{\Delta y} \left[ \tilde{h}_i^y q^* v'(v_i - \mathcal{F}_i / \Delta x) - \tilde{h}_b^y q^* v'(v_b - \mathcal{F}_b / \Delta x) \right]. \quad (2.30)$$

The corrective velocity $v'$ is defined as the difference between the velocity field used in the Eulerian flux divergence (2.16) and that derived from the Lagrangian flux areas $\mathcal{F}_r$, $\mathcal{F}_l$, $\mathcal{F}_i$, and $\mathcal{F}_b$, divided by the cell face length. The corrective velocity $v'^{n+1}$ in (2.29) is computed using $v^{n+1}$ from the Helmholtz solver and the Lagrangian flux areas based on extrapolated winds divided by the cell face length. The velocity $v^n$ used in the predictor-corrector term in (2.29) is computed using the velocity field $v^n$ at time-level $n$ and the Lagrangian flux areas based on $v^n$, and again divided by the cell face length. Shape-preserving schemes, e.g. the first-order upwind scheme, or higher-order methods such as flux-corrected transport schemes or flux-limiter schemes, can then be applied to the fluxes in (2.29). The first-order upwind scheme is used here, where the upstream values (denoted by the asterisks) $q_{\text{exp}}^{n+1*}$ and $q^{n*}$ at each cell face are determined by the directions of $v^{n+1}$ and $-v^n$ respectively [see e.g., Durran (2010), eq.(5.109)]. The first-order upwind scheme is numerically diffusive (Durran, 2010), but the damping effect on the correction and predictor-corrector terms should be minimal as the corrective velocities $v'^{n+1}$ and $v^n$ are typically very small. To ensure shape-preservation in the explicit CSLAM solution, we implement a simple 2D monotonic filter (Barth and Jespersen, 1989) that searches for new local minima and maxima in the reconstruction function of $q$, and scales the function if these values exceed those in the neighbouring cell.

Testing of the CSLAM-SW model [based on (2.12) for $h$, and (A.1) and (A.2) for the velocity components] revealed an instability related to the averaging of the C-grid velocities to the cell corner.
points in the continuity equation and its interaction with the rotational modes. Following Randall (1994), we can write a generalized discretized dispersion relation for the linearized shallow-water equations as

\[ \omega^3 - \omega (c^2 k_u h + c^2 k_h l_v + f_u f_v) - ic^2 (f_u k_h l_v - f_v k_u l_h) = 0, \]  

(2.31)

where the terms \( f_u \) and \( f_v \) are the discrete Coriolis operators, \( k_u \) and \( l_v \) are the discrete height-gradient operators, \( k_h \) and \( l_h \) are the discrete velocity-divergence operators in the continuity equation (the letter subscripts refer to the equations in which they appear), and \( c^2 = gH \). In the linearized shallow-water dispersion relation for C-grid, the last two terms on the L.H.S. of (2.31), \( f_u k_h l_v \) and \( f_v k_u l_h \), cancel and thus there are no numerical frequencies \( \omega \) with imaginary parts that amplify in time. Although the CSLAM-SW model uses the C-grid, we have found that the discretization of the linearized Lagrangian divergence is equivalent to taking an average of the \( u \) and \( v \) velocities to the corners of the grid cell followed by an averaging back to the cell-faces, i.e. the discretization is equivalent to using a 1-2-1-averaging of the \( u \) velocities in the \( y \)-direction, and of the \( v \) velocities in the \( x \)-direction, at the Eulerian grid cell faces. This averaging leads to non-cancellation of \( f_u k_h l_v \) and \( f_v k_u l_h \), and growing modes. We have found that using the averaging operators \( \overline{f_{xy}^{uv}} \) and \( \overline{f_{yx}^{uy}} \) (see Appendix for operator definitions) on the Coriolis terms in the \( x \)- and \( y \)-momentum equations, respectively, recovers the cancellation and eliminates the unstable mode.

2.4 Test cases

We present four test problems involving divergent flows: a radially-propagating gravity wave (with two different initial perturbations), and two highly-nonlinear barotropically unstable jets [the Bickley and the Gaussian jets from Poulin and Flierl (2003)]. The gravity-wave problem (section 2.4.1) is a simple case to assess the stability and accuracy of the new SLSI solver (CSLAM-SW) with respect to an imposed mean flow speed and the gravity-wave propagation speed. We also use this test case to highlight the issue of numerical inconsistency in the constituent transport scheme of LKM. The nonlinearity of the unstable jet in the second problem is particularly useful in testing the stability limits of the new scheme. The Bickley jet (section 2.4.2) has a moderate gradient in the initial height profile, while the steeper profile in the Gaussian jet (section 2.4.3) drives a more unstable jet. These strong gradients provide a severe test for advection schemes. In addition to those from LKM, solutions from a traditional semi-Lagrangian formulation and an Eulerian formulation (see Appendix) are also presented for comparison. We use the highly-divergent Gaussian jet case to compare the solutions between the shape-preserving CSLAM-SW solver described by (2.29) and the LKM with a shape-preserving explicit transport scheme (section 2.4.4).
2.4.1 A radially-propagating gravity wave

A non-rotating \((f = 0)\) 2D radially-propagating gravity wave is initiated by a circular height perturbation \(h'\) and advected by a mean background flow:

\[
\begin{align*}
  u(x, y, t = 0) &= u_0 = 1.2 \text{ m s}^{-1}, \\
  v(x, y, t = 0) &= v_0 = 0.9 \text{ m s}^{-1}, \\
  h(x, y, t = 0) &= h_0 + h',
\end{align*}
\]

where

\[
h' = \begin{cases} 
  \frac{1}{2} \Delta h \left[ 1 + \cos \left( \frac{\pi r}{10 \text{ km}} \right) \right], & \text{if } r \leq 10 \text{ km}, \\
  0, & \text{otherwise},
\end{cases}
\]

and \(h_0\) is the initial background height, \(\Delta h\) is the magnitude of the initial height perturbation, \(r = \sqrt{(x-x_c)^2 + (y-y_c)^2}\), and \((x_c, y_c)\) is the center of a 200 km \(\times\) 200 km domain. We perform tests for two different initial height perturbations: a linear case with \(\Delta h = 10 \text{ m}\) and \(h_0 = 990 \text{ m}\); and a nonlinear case with \(\Delta h = 500 \text{ m}\) and \(h_0 = 1000 \text{ m}\). A reduced gravitational acceleration of \(g' \approx 0.0204 \text{ m s}^{-2}\) is used, giving an initial gravity wave speed \(c = \sqrt{g'h_0} \approx 4.5 \text{ m s}^{-1}\) for the two cases. The mean advection speed \(\sqrt{u_0^2 + v_0^2} = 1.5 \text{ m s}^{-1}\) is chosen to emulate the speed ratio of the fastest advection of sound waves \((\approx 300 \text{ m s}^{-1})\) in the atmosphere to the speed of the jet stream \((\approx 100 \text{ m s}^{-1})\). The background flow velocities \(u_0 \neq v_0\) are also chosen to ensure that the flow does not align with the mesh.

The model domain consists of 400 \(\times\) 400 grid cells, with a grid spacing of \(\Delta x = \Delta y = 500 \text{ m}\), and is periodic in both \(x\)- and \(y\)-directions. Since there is no analytical solution to the test problem, to evaluate CSLAM-SW, we produce a fine-resolution Eulerian reference solution with a grid spacing of \(\Delta x = \Delta y = 100 \text{ m}\) and a time step of \(\Delta t = 10 \text{ s}\). The center of the gravity wave disturbance in the reference solution is stationary (i.e. \(u_0 = v_0 = 0 \text{ m s}^{-1}\)), and we compare the solutions by translating the gravity wave disturbance in CSLAM-SW to the center of the domain.

In addition to CSLAM-SW, we also run the two initial perturbation cases using LKM, the traditional semi-Lagrangian formulation, and an Eulerian formulation. We use the \(l_2\)-norm of error as the error measure, which for a uniform mesh is

\[
l_2 = \sqrt{\frac{\sum_{i,j} \left[ h(i, j) - h_{\text{ref}}(i, j) \right]^2}{\sum_{i,j} \left[ h_{\text{ref}}(i, j) \right]^2}},
\]

and the results are compared against the reference solution.
where $i, j$ are the grid indices, $h(i,j)$ is the model solution, and $h_{\text{ref}}(i,j)$ is the Eulerian high-resolution reference solution. The $L_2$-norm of error in the height field (at time $T = 1 \times 10^5$ s) for different time step sizes is shown in Fig. 2.3 for all four models. Results from both the linear and nonlinear initial perturbations are plotted. The time truncation error in CSLAM-SW is very comparable to those in the other two semi-Lagrangian models for both cases. Except for the Eulerian model, all model solutions converge as the time step size is reduced to less than $\Delta t = 50$ s. At this point, differences between the errors are mainly due to the spatial discretization schemes (more
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noticeably in the nonlinear case). The Eulerian model and the traditional semi-Lagrangian model have a commonality that they both use a ‘true’ C-grid divergence operator in the continuity equation; whereas as discussed in section 2.3, the CISL computation of divergence in both CSLAM-SW and LKM consists of an extra averaging operator. For this reason, one may see a smaller spatial discretization error in the traditional semi-Lagrangian model and “coarse” Eulerian model when compared to an Eulerian high-resolution reference solution than those in the CISL models, as is the case in Fig. 2.3.

To evaluate the consistency in CSLAM-SW and LKM, a constituent with an initially constant specific concentration distribution ($q_0 = 1$) is initialized in each model. The CSLAM explicit transport scheme conserves constituent mass in both models; however, as discussed in section 2.2.3, when numerical consistency is violated, constancy of the specific concentration is not guaranteed, and generation or removal of constituent mass is possible. The specific concentration is diagnosed by decoupling the constituent mass variable using (2.14). A time step of $\Delta t = 100$ s is used. Fig. 2.4 shows an example of the specific concentration error in LKM at time $T = 1 \times 10^5$ s for both the linear and nonlinear perturbation cases. The error is largest near the leading edge of the gravity wave, where the flow is most divergent and the semi-implicit correction term is non-zero. Fig. 2.5 shows the variation in error with time step size for both the linear and nonlinear perturbations at the same simulation time as in Fig. 2.4. The error measures used are the maximum absolute error, the mean absolute error, and the root-mean-squared error. Errors in the solutions from LKM and CSLAM-SW are shown in solid and dashed lines respectively. Since the inconsistent semi-implicit correction in (2.6) is proportional to $\Delta t$, errors in the scalar field grow with time step size, which can become a major issue for semi-Lagrangian models that take advantage of larger stable time steps. For the nonlinear test, the maximum absolute error from LKM is in the order of $10^{-2}$ to $10^{-1}$, and is significant for constituents like water vapour which has a typical mixing ratio of roughly 0.1% to 3% in air. On the other hand, CSLAM-SW using a consistent formulation is free-stream preserving (up to machine roundoff) for both cases and all time-step sizes tested.

2.4.2 Bickley jet – Ro = 0.1

The stability of CSLAM-SW is further evaluated with two perturbed jets; we begin with the Bickley jet from Poulin and Flierl (2003). The Bickley jet is simulated at the Rossby number, $Ro = U/fL = 0.1$, where $U$ is the flow velocity scale, $f$ is the Coriolis parameter and $L$ is the length scale of the jet width. We choose the Froude number, $Fr = (fL)^2/gH = 0.1$. The jet is characterized by greater heights to the left of the channel and dropping off to smaller heights to the right, geostrophically-balanced by a mean flow velocity down the channel (Fig. 2.6). A height perturbation is superimposed at the initial time, causing wave amplification and eventual breaking of the
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Figure 2.4: Specific concentration error \((q - q_0)\) in LKM for a divergent flow initialized with a constant \(q_0 = 1\) in the (a) linear (\(\Delta h = 10\) m and \(h_0 = 990\) m) and (b) nonlinear (\(\Delta h = 500\) m and \(h_0 = 1000\) m) height perturbation cases. Note the different scales in the plots.
Figure 2.5: Variation of specific concentration error $(q - q_0)$ (maximum absolute error, mean absolute error, and root-mean-squared error) with time step size in LKM (solid line) and CSLAM-SW (dashed line) for the (a) linear height perturbation and (b) nonlinear height perturbation cases.

jet into vortices, and formation of a vortex street along the channel. These vortex streets consist of thin filaments of vorticity with strong horizontal velocity shear, making it a good test because it is challenging for all numerical schemes. A more detailed description of the evolution of these jets can be found in Poulin and Flierl (2003).

The initial geostrophically balanced mean state $(u_0, v_0, \text{and } h_0)$ and height perturbation $h'$ of the Bickley jet is given by:

\begin{align}
    u(x,y,t=0) &= u_0 = 0, \\
    v(x,y,t=0) &= v_0 = -\frac{g'\Delta h}{f\alpha} \text{sech}^2 \left( \frac{x}{a} \right), \\
    h(x,y,t=0) &= h_0 + h',
\end{align}

(2.37) (2.38) (2.39)
Figure 2.6: Initial mean height $h_0$ (top) and velocity $v_0$ (bottom) profiles for the Bickley jet ($\Delta h = 1 \text{ m}, \Delta v = 1 \text{ m s}^{-1}$) and Gaussian jet ($\Delta h = 50 \text{ m}, \Delta v = 56 \text{ m s}^{-1}$).

where

$$h_0 = 100 - \Delta h \tanh \left( \frac{x}{a} \right),$$  \hspace{1cm} (2.40)$$

$$h' = 0.1\Delta h \operatorname{sech}^2 \left( \frac{x}{a} \right) \sin \left( \frac{2\pi y}{Y} - n \right).$$  \hspace{1cm} (2.41)$$

The parameter $\Delta h$ is the maximum amplitude of the height perturbation and depends on $\text{Ro}$, $g'$ is the gravitational acceleration, $a$ is the jet width, $Y$ is the length of the channel, and $n$ is the wavenumber mode of the height perturbation. In our simulations, $L = a = 1 \times 10^5 \text{ m}$, $X$ (width of channel) $= Y = 2 \times 10^6 \text{ m}$, $f = 1 \times 10^{-4} \text{ s}^{-1}$, and $g' = 10 \text{ m s}^{-2}$. For the specified scale of the jet width and a flow with $\text{Fr} = 0.1$, the mean height of $h_0$ is 100 m. The amplitude of the height perturbation $\Delta h = 1 \text{ m}$ is determined by the scale of the initial geostrophically balanced flow speed ($U \sim 1 \text{ m s}^{-1}$) for $\text{Ro} = 0.1$. We choose the most unstable mode of wavenumber $n = 3$ (Poulin and Flierl, 2003) for all of our jet simulations.

Each grid domain has $202 \times 202$ grid cells and a grid spacing of $\Delta x = \Delta y = 9950 \text{ m}$, with solid boundary conditions at $x = -X/2$ and $x = X/2$ and periodic boundary conditions in $y$ where $y \in [-Y/2, Y/2]$. A time step of $\Delta t = 2000 \text{ s}$ was used in all simulations. Based on the initial gravity-wave speed $c \approx 32 \text{ m s}^{-1}$ and initial flow speed $|v| = 1 \text{ m s}^{-1}$, the Courant numbers are $\text{Cr}_{gw} = 6.4$ and $\text{Cr}_{adv} = 0.2$ respectively.
Figure 2.7: Solutions of the Bickley jet at time $T = 5 \times 10^6$ s (after 2500 time steps) for $\text{Ro} = 0.1$, $\text{Fr} = 0.1$ and $\text{Cr}_{\text{adv}} = 0.2$. Plotted are positive (solid line) and negative (dashed line) vorticity between $-1 \times 10^{-5}$ s$^{-1}$ and $1 \times 10^{-5}$ s$^{-1}$ with a contour interval of $5 \times 10^{-7}$ s$^{-1}$. 

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To maintain numerical stability in the Eulerian model, we implemented a second-order explicit diffusion term with a numerical viscosity parameter \( \beta_x = \beta_y = v \Delta t / \Delta x^2 = 0.02 \) (where \( v \) is analogous to the physical viscosity). This value corresponds to the numerical Reynolds number, \( Re = UL/v = 10^2 \), a factor of 10 smaller than that used in the forward-in-time Eulerian model of Poulin and Flierl (2003). Explicit diffusion was not applied to any of the semi-Lagrangian models because the schemes have sufficient inherent damping to maintain numerical stability. For the traditional semi-Lagrangian model, however, we found that time-off-centering in the semi-implicit scheme was needed to maintain stability.

Fig. 2.7 shows the solutions from CSLAM-SW and the three comparison models. Although the exact form of the initial height perturbation was not provided in Poulin and Flierl (2003), we were able to reproduce results very similar to theirs [cf. Fig. 4c of Poulin and Flierl (2003)]. The most noticeable difference among the different model solutions is in the shape and magnitude of the relative vorticity maxima and minima. CSLAM-SW showed very similar vortex shapes to those from LKM and TRAD-SL. The vortices in the Eulerian results are similar to those from the Eulerian model of Poulin and Flierl (2003). The difference between the Eulerian solution and the semi-Lagrangian solutions can be attributed to the inherent damping in the reconstruction step of the CISL schemes and the grid-point interpolation in the traditional semi-Lagrangian scheme.

### 2.4.3 Gaussian jet – Ro = 5.0

The third test case is the Gaussian jet with Ro = 5.0. Similar to the Bickley jet, the Gaussian jet has \( Fr = 0.1 \), and has an initially geostrophically-balanced mean-state with greater heights to the left of the channel and dropping off to smaller heights to the right (Fig. 2.6). The main difference between the two jets is that the Gaussian jet has a slightly steeper height profile at the center of the channel, and therefore, produces a more pronounced nonlinear flow, especially at larger Ro. The initial mean state and height perturbation for the Gaussian jet is given as:

\[
\begin{align*}
    u(x,y,t = 0) &= u_0 = 0, \\
    v(x,y,t = 0) &= v_0 = -\frac{2g'\Delta h}{\sqrt{\pi f}a} \exp(-(x/a)^2), \\
    h(x,y,t = 0) &= h_0 + h',
\end{align*}
\]
where

\[ h_0 = 100 - \Delta h \operatorname{erf}\left(\frac{x}{a}\right), \]  

(2.45)

\[ h' = 0.1\Delta h \left(\frac{2}{\sqrt{\pi}} \exp\left(-\left(x/a\right)^2\right) \sin \left(\frac{2\pi y}{y_L} n\right)\right), \]  

(2.46)

and the notation is as before. All the parameters remain the same, except \( \Delta h = 50 \) m for \( \text{Ro} = 5.0 \), and \( \Delta t = 100 \) s is used. With an initial gravity-wave speed and maximum flow speed of 38 m s\(^{-1}\) and 56 m s\(^{-1}\) respectively, \( \text{Crgw} = 0.4 \) and \( \text{Cradv} = 0.56 \). We note that \( U > c \), i.e. the flow is supercritical. Despite the existence of supersonic waves in the solution, CSLAM-SW is stable even at larger Courant numbers.

As pointed out in Poulin and Flierl (2003), jets in this Rossby regime are highly unstable and of particular interest is the formation of an asymmetric vortex street with triangular cyclones and elliptical anticyclones. As the vortex street is advected towards the deeper water, a strong cut-off cyclone develops due to vortex stretching (adjacent to the main anticyclonic feature). All of our models, including CSLAM-SW, were able to reproduce these features [Fig. 2.8, cf. Fig. 10e of Poulin and Flierl (2003)]. As in the Bickley jet case, we find that CSLAM-SW produced solutions similar to the other two semi-Lagrangian models (LKM and TRAD-SL).

In addition to comparing solutions of CSLAM-SW at time steps allowable by the Eulerian scheme, we also tested the stability of CSLAM-SW at a much larger \( \text{Cradv} = 2.5 \). Figs. 2.9a-c show solutions at various times from the previous CSLAM-SW simulation (\( \text{Cradv} = 0.56 \)), and Figs. 2.9d-f show solutions at each of the corresponding time for \( \text{Cradv} = 2.5 \), using the largest time step allowable by the Lipschitz condition for this flow. The solution from the \( \text{Cradv} = 2.5 \) simulation is almost identical to the solution using \( \text{Cradv} = 0.56 \).

The CSLAM-SW is numerically stable for the highly nonlinear flow in the Gaussian jet and at Courant numbers much greater than unity. To check that consistency and shape-preservation in such a highly divergent flow can be maintained, we repeat the Gaussian jet case using CSLAM-SW and the shape-preserving extensions described in section 2.3.

### 2.4.4 Gaussian jet – Ro = 5.0 with shape-preservation

The shape-preserving CSLAM-SW solver (2.29) is tested using the divergent flow of the Gaussian jet as described in section 2.4.3. We also test the LKM solver with the Barth and Jespersen (1989) filter implemented in the explicit scalar transport scheme of \( h_{q_{\exp}}^{n+1} \). All parameters are as described in section 2.4.3, and a time step of \( \Delta t = 100 \) s is used for results in Figs. 2.10 and 2.11.

To test for numerical consistency in the two solvers, we repeat the consistency test described
Figure 2.8: Solutions of the Gaussian jet for $Ro = 5.0$ and $C_{r_{adv}} = 0.56$ at time $T = 1.8 \times 10^5$ s (after 1800 time steps). Plotted are positive (solid line) and negative (dashed line) vorticity between $-5 \times 10^{-4}$ s$^{-1}$ and $5 \times 10^{-4}$ s$^{-1}$ with a contour interval of $5 \times 10^{-5}$ s$^{-1}$.
Figure 2.9: CSLAM-SW solutions of the Gaussian jet for Ro = 5.0 at three different times (left to right on each row) of the simulation: at time $T = 5 \times 10^4$ s, $1.0 \times 10^5$ s, and $1.4 \times 10^5$ s. (a - c) Solutions using a $C_{adv}$ of 0.56 (same simulation as in Fig. 2.8) (d - f) Solutions using a larger $C_{adv}$ of 2.5. Plotted are positive (solid line) and negative (dashed line) vorticity between $-5 \times 10^{-4}$ s$^{-1}$ and $5 \times 10^{-4}$ s$^{-1}$ with a contour interval of $5 \times 10^{-5}$ s$^{-1}$.

in section 2.4.1 by initializing a constant specific concentration field $q_0 = 1$. The shape-preserving CSLAM-SW solution is able to maintain numerical consistency between $h$ and $hq$ up to machine roundoff for this highly divergent flow and the result is independent of time-step size. As for LKM, despite the shape-preserving transport scheme in the solver, numerical inconsistency is still an issue with a maximum absolute error (defined as the deviation from $q_0 = 1$) of $6.79 \times 10^{-3}$, a mean absolute error of $4.82 \times 10^{-4}$, and a root-mean-squared error of $1.06 \times 10^{-3}$ at time $T = 1.8 \times 10^5$ s (Fig. 2.10), and as in section 2.4.1, the error is a function of the time-step size (not shown).

To compare the shape-preservation ability between CSLAM-SW and LKM, we initialize a specific-concentration distribution that varies only in the $x$-direction and has a sharp gradient that
Chapter 2: A two-dimensional shallow-water equations solver with conservative and consistent transport

Figure 2.10: Specific concentration error \((q - q_0)\) in LKM for the Gaussian jet at time \(T = 1.8 \times 10^5\) s, initialized with a constant \(q_0 = 1\) field.

\[
q(x, y, t = 0) = \begin{cases} 
1.0, & \text{if } -X/2 \leq x < 0, \\
0.1, & \text{if } 0 \leq x < X/2.
\end{cases}
\]  \hspace{1cm} (2.47)

Solutions of \(q\) diagnosed from \(hq\) from the non-shape-preserving CSLAM-SW, LKM with shape-preserving transport, and the shape-preserving CSLAM-SW are presented in Figs. 2.11a-c. The simulation time \(T = 1.8 \times 10^5\) s in the figure corresponds to the vorticity field shown in Fig. 2.8.

For the non-shape-preserving CSLAM-SW solver (Fig. 2.11a), \(q\) reaches an unphysical peak value of 1.233 and an unphysical minimum value of -0.145 (specific concentrations cannot be negative). The LKM solver with shape-preserving transport (Fig. 2.11b) has less severe errors than the non-shape-preserving CSLAM-SW, but loses its shape-preserving ability due to numerical inconsistency. The minimum and maximum \(q\) values are 0.09997 and 1.0063 respectively at time \(T = 1.8 \times 10^5\) s. The overshooting of \(q\) (which may generate spurious constituent mass) appears to be greater in amplitude than the undershooting for this flow. Overshooting occurs mostly within the
strongest anticyclones (negative vorticity centers on the left side of the channel, highlighted in solid black lines in Fig. 2.11b). Using the shape-preserving CSLAM-SW solver (Fig. 2.11c), minimum and maximum values of $q$ are kept within its physical limits (0.1 and 1.0 respectively, up to machine roundoff) and shape-preservation is ensured.

2.5 Conclusion

A conservative and consistent semi-Lagrangian semi-implicit solver is constructed and tested for shallow-water flows (CSLAM-SW). The model uses a new flux-form discretization of the semi-implicit cell-integrated semi-Lagrangian continuity equation that allows a straightforward implementation of a consistent constituent transport scheme. Like typical conservative semi-Lagrangian semi-implicit schemes, the algorithm requires at each time step a single Helmholtz equation solution and a single application of CSLAM.

Specifically, our new discretization uses the flux divergence as opposed to a velocity divergence that requires linearization about a constant mean reference state. For traditional semi-implicit schemes, the dependence on a constant mean reference state makes it difficult to ensure consistency between total fluid mass and constituent mass. When numerical consistency is not maintained, constituent mass conservation can be violated even for solvers that use inherently-conservative transport schemes. More unacceptably, constituent fields may no longer preserve their shapes, e.g. losing constancy or positive-definiteness.

We have shown an example of a traditional discrete cell-integrated semi-Lagrangian semi-implicit continuity equation (LKM), in which inconsistency can generate significant numerical errors in the specific constituent concentration. The inconsistent semi-implicit correction term in LKM causes errors to grow proportionally with time step size and with the nonlinearity of the flow. The ideal radially-propagating gravity wave tests using the LKM solver showed a maximum absolute error in an initially constant specific concentration ($q_0 = 1$) field ranging from an order of $10^{-7}$ to $10^{-3}$ in the linear case, and an order of $10^{-4}$ to $10^{-1}$ in the nonlinear case. The orders of magnitude of these errors are significant relative to the specific concentration of tracers and water vapour in the atmosphere. The consistent formulation in the new CSLAM-SW on the other hand eliminates these errors (up to machine roundoff).

The new flux-form solver (CSLAM-SW) is tested for a range of flows and Courant numbers for the shallow-water system, and is stable and compares well with other existing semi-implicit schemes, including a two-time-level traditional semi-Lagrangian scheme and an Eulerian leap-frog scheme. The Gaussian jet test (the more nonlinear jet of the two presented) showed that CSLAM-SW remains numerically stable when large time steps are used.
We have also identified and eliminated a computational unstable mode in CSLAM-SW and LKM, using the discrete dispersion relation of the linearized shallow-water equations. The numerical instability, associated with the Lagrangian divergence operator on a C-grid, can be eliminated by introducing a new averaging operator on the Coriolis terms in the momentum equations.

Shape-preservation in CSLAM-SW is ensured by applying a 2D shape-preserving filter in the CSLAM transport scheme and the first-order upwind scheme to compute the predictor-corrector and flux-form correction terms. As shown in the Gaussian jet case, without any shape-preserving filter, unphysical negative and unreasonable positive specific concentrations may develop due to undershoots and overshoots. For inconsistent formulations such as that in LKM, the use of a shape-preserving explicit transport scheme cannot guarantee shape-preservation either due to numerical consistency errors. CSLAM-SW, on the other hand, allows for straightforward implementation of existing shape-preserving schemes and filters and ensures shape-preservation (up to machine roundoff).

The initial testing of the semi-implicit formulation in CSLAM-SW shows promising results. We are currently implementing the extension of CSLAM-SW to a 2D (x-z) non-hydrostatic, fully-compressible atmospheric solver. The desirable properties of mass conservation, consistency, and shape-preservation for moisture variables and tracers will likely be important for both short- and long-term meteorological applications.
Figure 2.11: Specific constituent concentration $q$ at time $T = 1.8 \times 10^5$ s. Initial minimum and maximum $q$ are 0.1 and 1.0 respectively. Regions with unphysical overshooting (red) and undershooting (purple) are highlighted.
Chapter 3

Extension to a two-dimensional ($x$-$z$) nonhydrostatic atmospheric solver

3.1 Introduction

Semi-Lagrangian semi-implicit (SLSI) schemes have been widely used in climate and numerical weather prediction (NWP) models since the pioneering work of Robert (1981) and Robert et al. (1985). The more lenient numerical stability condition in these schemes allows larger time steps and thus increased computational efficiency. Traditional semi-Lagrangian schemes are not inherently mass-conserving due to their use of grid-point interpolation, and the lack of conservation can lead to accumulation of significant solution errors (Rasch and Williamson, 1990a; Machenhauer and Olk, 1997). To address this issue, conservative semi-Lagrangian schemes, also called cell-integrated semi-Lagrangian (CISL) transport schemes (Rancic, 1992; Laprise and Plante, 1995; Machenhauer and Olk, 1997; Zerroukat et al., 2002; Nair and Machenhauer, 2002; Lauritzen et al., 2010), have been developed. Although CISL transport schemes, when applied in fluid flow solvers, allow for locally (and thus globally) conservative transport of total fluid mass and constituent (i.e. tracer) mass, a lack of consistency arises between the numerical representation of the total dry air mass conservation, to which we will refer as the continuity equation, and constituent mass conservation equations (Jöckel et al., 2001; Zhang et al., 2008; Wong et al., 2013). Numerical consistency in the flux-form equation for a tracer requires the equation for a constant tracer field to correspond numerically to the mass continuity equation; this consistency ensures that an initially spatially uniform passive tracer field will remain so. The lack of numerical consistency between the two can lead to the unphysical generation or removal of model constituent mass, which can introduce significant errors in applications such as chemical tracer transport (Machenhauer et al., 2009).

Recently, Wong et al. (2013) introduced a new flux-form formulation of the semi-implicit CISL height conservation equation for the shallow-water equations (SWE) solver. They showed that the scheme is accurate and stable even for highly-nonlinear barotropically-unstable jets and large Courant numbers. They also found that the use of a shape-preserving filter in an inconsistent for-
mulation of the continuity equations is ineffective, highlighting the importance of numerical consistency in these models.

In this paper, the flux-form semi-implicit SWE formulation is extended to the fully-compressible two-dimensional (x-z) moist nonhydrostatic equations for the atmosphere. We refer to this new conservative and consistent nonhydrostatic solver as CSLAM-NH. A nonhydrostatic model permits fast-moving internal gravity and acoustic waves. Here, we integrate the terms responsible for the acoustic waves in a semi-implicit manner to allow large time steps while maintaining stability for these waves. As in Wong et al. (2013), our nonhydrostatic solver is based on the Conservative Semi-LAgrangian Multi-tracer (CSLAM) transport scheme, a CISL transport scheme developed by Lauritzen et al. (2010) that has been implemented in NCAR’s High-Order Methods Modeling Environment [HOMME; Erath et al. (2012)].

The semi-implicit CISL nonhydrostatic solver has six main advantages and desirable properties. As we will show, our nonhydrostatic cell-integrated semi-Lagrangian solver is (1) inherently mass-conserving, (2) shape-preserving, and, with the new formulation, (3) has numerically consistent transport. The discretization (4) does not depend on a mean reference state, but maintains the same framework as typical semi-implicit CISL solvers, where (5) a single linear Helmholtz equation is solved and (6) a single application of CSLAM is needed per time step.

The paper is organized as follows. The governing equations of the two-dimensional fully-compressible nonhydrostatic system are first described in section 3.2. We then present the proposed discretization of the governing equations, including a consistent formulation of the moisture conservation equations (section 3.3). The desirable properties of the nonhydrostatic solver are discussed in section 3.4. We test the nonhydrostatic solver with three idealized test cases and compare results with an Eulerian split-explicit time-stepping scheme (section 3.5). A fourth test case on numerical consistency is also presented in section 3.5 to demonstrate the shape-preserving ability of the solver with additional passive tracers. A summary is given in section 3.6.

### 3.2 Governing equations

The model governing equations are the two-dimensional (x-z) moist Euler equations in Cartesian geometry:

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + w \frac{\partial u}{\partial z} = -\frac{\pi}{\rho_m} \gamma R_d \frac{\partial \Theta_m'}{\partial x} + F_u, \tag{3.1}
\]

\[
\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + w \frac{\partial w}{\partial z} = -\frac{\pi}{\rho_m} \gamma R_d \frac{\partial \Theta_m'}{\partial z} + g \rho_m + \frac{g}{\rho_m} \left( \frac{\rho'}{\rho} - \rho_m' \right) + F_w, \tag{3.2}
\]

\[
\frac{\partial \Theta_m}{\partial t} + \nabla \cdot (\Theta_m v) = F_\Theta, \tag{3.3}
\]
Chapter 3: Extension to a two-dimensional ($x$-$z$) nonhydrostatic atmospheric solver

$$\frac{\partial \rho_d}{\partial t} + \nabla \cdot (\rho_d \mathbf{v}) = 0,$$

(3.4)

$$\frac{\partial Q_j}{\partial t} + \nabla \cdot (Q_j \mathbf{v}) = F_{Q_j},$$

(3.5)

$$p = p_0 \left( \frac{R_d \Theta_m}{p_0} \right)^\gamma,$$

(3.6)

where $\pi = (p/p_0)^\kappa$ is the Exner function, $\kappa = R_d/c_p$, $\gamma = c_p/c_v = 1.4$, $R_d = 287$ J kg$^{-1}$ K$^{-1}$, $c_p = 1003$ J kg$^{-1}$ K$^{-1}$, and $g = 9.81$ m s$^{-2}$. Perturbation variables from a time-independent hydrostatically balanced background state are used to reduce numerical errors in the calculations of the pressure gradient terms (Klemp et al., 2007). The hydrostatically balanced background state is defined as $d\bar{p}(z)/dz = -\bar{\rho}_d(z)g$. Perturbation variables are defined as $\Theta_m = \bar{\rho}_d(z)\bar{\theta}(z) + \Theta'_m$, $\pi = \pi' + \pi$, $\rho_d = \bar{\rho}_d(z) + \rho'_d$, and the moist density $\rho_m = \rho_d(1 + q_v + q_c + q_r)$, where $q_v$, $q_c$, and $q_r$ are the mixing ratios for water vapor, cloud, and rainwater, respectively. The $F_{Q_j}$ terms represent diffusion, and any diabatic effects and parameterized physics when moisture is present.

As in Klemp et al. (2007), fluxes are coupled to the dry density $\rho_d$. The flux variables are given as

$$\Theta_m = \rho_d \theta_m \quad \text{and} \quad Q_j = \rho_d q_j,$$

(3.7)

where $\theta_m$ is the modified potential temperature $\theta_m = \theta(1 + a'q_v)$ where $a' \equiv R_v/R_d \simeq 1.61$ and $q_j = (q_v, q_c, q_r)$.

The momentum equations are cast in their advective form, and all other equations, i.e., for density, potential temperature, and moist species, are cast in their conservative flux-form. Pressure is a diagnostic variable given by the equation of state. The governing equations are based on Klemp et al. (2007); the pressure gradient terms in (3.1) and (3.2) have been recast in terms of $\Theta'_m$ using (3.6) to derive the relation

$$\nabla p = \gamma R_d \pi \nabla \Theta_m,$$

(3.8)

and enables us to form an implicit equation for $\Theta'$ (section 3.3). The equations are still exact and no approximations have been applied. The only difference from the governing equations in Klemp et al. (2007) is that their momentum equations are cast in the conservative flux-form, whereas the advective form is used here to facilitate the use of the traditional semi-Lagrangian method.
3.3 A consistent and mass-conserving nonhydrostatic solver

3.3.1 CSLAM — a conservative transport scheme

To ensure mass conservation, we utilize an inherently conservative semi-Lagrangian transport scheme called CSLAM (Lauritzen et al., 2010). The CSLAM transport scheme is a backward-in-time CISL scheme\(^1\), where the departure grid cell area \(\delta A^*\) is found by tracing the regular arrival grid cell area \(\Delta A\) back in time one time-step \(\Delta t\) (Fig. 3.1a). The CSLAM discretization scheme for the lhs of (3.3), (3.4), and (3.5) is given by

\[
\phi_{\text{exp}}^{n+1} \Delta A = \int_{\delta A^*} \phi^n dA = \phi^*_n \delta A^*
\]

where \(\phi = \Theta_m, \rho_d, \text{ or } Q_j\). The superscript denotes the time level, and \(\phi_{\text{exp}}^{n+1}\) is the explicit cell-averaged transport term computed by integrating the field \(\phi^n\) over the departure cell area \(\delta A^*\), which gives the cell-averaged departure value \(\phi^*_n\).

The departure cell area \(\delta A^*\) in CSLAM is found through iterative trajectory computations from the four vertices of an arrival grid cell (unfilled circles in Fig. 3.1b) to their departure points (filled

\(^1\)note that CSLAM may also be cast in flux-form (Harris et al., 2011)
circles in Fig. 3.1b). The departure cell area is then approximated using straight lines as cell edges (dark grey region \( \delta A \) in Fig. 3.1b). To integrate the field \( \phi^n \) over \( \delta A \), CSLAM implements a remapping algorithm that consists of a piecewise quasi-biparabolic subgrid-cell-reconstruction of \( \phi^n \) in the two coordinates as in Nair and Machenhauer (2002) with an additional cross term as described in Jablonowski (2004) that helps smooth subgrid distribution near sharp gradients,

\[
\phi^n(x,z) = \langle \phi^n \rangle + a^x x + b^x \left( \frac{1}{12} - x^2 \right) + a^z z + b^z \left( \frac{1}{12} - z^2 \right) + \frac{1}{2} (c^{xz} + c^{zx}) x z
\]  

(3.10)

where coefficients \( a^x, b^x, a^z, b^z \) of the reconstructed parabolic function in the two coordinates are obtained as in Nair and Machenhauer (2002), and the cross-term coefficients \( c^{xz} \) and \( c^{zx} \) are obtained as in Jablonowski (2004). An average of the two coefficients of the cross term, \( c^{xz} \) and \( c^{zx} \), is taken to avoid a directional bias (Jablonowski, 2004). The cell-average value over the Eulerian grid cell is denoted as \( \langle \phi^n \rangle \).

The integration of the reconstruction function over the departure cell area is then computed. The area integration in CSLAM is transformed into a series of line integrals using the Gauss-Green theorem, and involves solving for a set of weights \( w^{(i,j)} \) that depends only on the departure cell boundary. As described in Lauritzen et al. (2010), the discrete conservative transport scheme for departure cell \( k \) is

\[
\int_{\delta A} \phi^n dA = \sum_{l=1}^{L_k} \sum_{i+j \leq 2} c_j^{(i,j)} w_{kl}^{(i,j)}
\]

(3.11)

where \( c_j^{(0,0)}, c_j^{(1,0)}, c_j^{(0,1)}, c_j^{(2,0)}, c_j^{(0,2)} \) are the coefficients for the constant, \( x, z, x^2 \), and \( z^2 \) terms respectively, \( c_j^{(1,1)} \) is the coefficient for the \( xz \) term in (3.10), and \( l \) is the index for the Eulerian grid cell(s) with which departure cell \( k \) overlaps (of a total of \( L_k \) overlapping Eulerian grid cells). The partitioning of the areal integration into computation of coefficients and weights greatly enhances the transport scheme’s computational efficiency for multi-tracer transport, as the weights can be reused for the remapping of all tracer species in the model. For full details on the basic CSLAM scheme, see Lauritzen et al. (2010); for high-resolution spherical implementations of CSLAM, the reader is referred to the modifications to the scheme documented in Erath et al. (2013). A rigorous assessment of the accuracy of linear transport using CSLAM [for the test case in Lauritzen et al. (2012)] and a comparison of CSLAM to a collection of state-of-the-art transport schemes can be found in Lauritzen et al. (2014).

2higher-order edge approximations have been explored in Ullrich et al. (2012)


\section*{3.3.2 Trajectory algorithm}

To find the departure cell area, we trace the vertices of each arrival grid cell back one time step $\Delta t$ using a trajectory algorithm described in Lauritzen et al. (2006). The trajectory is approximated and split into two segments: departure grid point to trajectory midpoint, and trajectory midpoint to arrival grid point. The split-trajectory approximation facilitates the semi-implicit formulation of the flux-form conservation equation (section 3.3.4).

The displacement in the two linear segments are determined using velocities at time-level $n$ and velocities extrapolated to time-level $n+1$, respectively. The first segment (from the departure point position $r_D^n$ to midpoint trajectory $r_{D/2}^{n+1/2}$) is approximated as

\begin{equation}
    r_{D/2}^{n+1/2} = r_D^n + \frac{\Delta t}{2} v_D^n,
\end{equation}

We iterate (3.12) three times to increase the accuracy of the computation of $v_D^n$. At each iteration, the velocities are interpolated to the estimated departure location using bicubic Lagrange interpolation. The second segment (from midpoint trajectory $r_{D/2}^{n+1/2}$ to the arrival point $r^{n+1}$) is approximated using

\begin{equation}
    r_{D/2}^{n+1/2} = r_D^n - \frac{\Delta t}{2} \tilde{v}^{n+1},
\end{equation}

where $\tilde{v}^{n+1}$ is evaluated at the arrival grid point and denote velocities extrapolated to time-level $n+1$ using a two-time-level extrapolation

\begin{equation}
    \tilde{v}^{n+1} = 2v^n - v^{n-1}.
\end{equation}

To find $r_D^n$, we take the sum of the two half-trajectories [(3.12) and (3.13)].

\begin{equation}
    r_D^n = r_D^n - \frac{\Delta t}{2} (v_D^n + \tilde{v}^{n+1}).
\end{equation}

Higher-order approximations to the trajectory can be made by including an acceleration term as described in McGregor (1993). Tests including an acceleration term (not shown) showed that such a higher-order approximation made little difference to the solutions for this suite of tests.

\section*{3.3.3 Discretization of the momentum equations}

The momentum equations are solved using the traditional semi-Lagrangian semi-implicit method, where material derivatives such as $du/dt = \partial u/\partial t + u\partial u/\partial x + w\partial u/\partial z$ and $dw/dt = \partial w/\partial t +$
\( u \partial w / \partial x + w \partial w / \partial z \) [lhs of (3.1) and (3.2), respectively] are computed using a grid-point interpolation to the departure point. The two-time-level discretizations of the momentum equations are

\[
\begin{align*}
\frac{u^n_{A+1}}{\Delta t} & = \left[ u - \frac{1 - \beta}{2} \left( \frac{\pi}{\rho_m} \right)^x \gamma R_d \delta_x \Theta \right]_D^n + \Delta t (F_u)_D^n, \\
& - \frac{1 + \beta}{2} \left( \frac{\pi^n}{\rho_m^n} \right)^x A \gamma R_d \delta_x \Theta_A^{n+1}, \quad (3.16)
\end{align*}
\]

and

\[
\begin{align*}
\frac{w^n_{A+1}}{\Delta t} & = \left[ w - \frac{1 - \beta}{2} \left( \frac{\pi}{\rho_m} \right)^z \gamma R_d \delta_z \Theta \right]_D^n \\
& + \Delta t \left[ \frac{\pi^n}{\rho_m^n} \left( g \rho_d \frac{\pi^n}{\pi} - g \rho_m^n \right) \delta_z \Theta_A^{n+1/2} \\
& - \frac{1 + \beta}{2} \left( \frac{\pi^n}{\rho_m^n} \right)^z A \gamma R_d \delta_z \Theta_A^{n+1} \\
& + \Delta t (F_w)_D^n, \quad (3.17)
\end{align*}
\]

where the subscripts \( D, D/2 \) and \( A \) denote evaluation at the departure, midpoint trajectory, and arrival grid points, respectively, and the superscripts denote the time level. The spatial operators are defined as

\[
\bar{\bar{\nabla}}^x = \frac{1}{2} \left( \cdot \right)_{i,k} + \left( \cdot \right)_{i+1,k}, \quad (3.18)
\]

\[
\bar{\bar{\nabla}}^z = \frac{1}{2} \left( \cdot \right)_{i,k} + \left( \cdot \right)_{i,k+1}, \quad (3.19)
\]

\[
\delta_x (\cdot) = \frac{\left( \cdot \right)_{i+1,k} - \left( \cdot \right)_{i,k}}{\Delta x}, \quad \text{and} \quad (3.20)
\]

\[
\delta_z (\cdot) = \frac{\left( \cdot \right)_{i,k+1} - \left( \cdot \right)_{i,k}}{\Delta z}. \quad (3.21)
\]

The gradient terms responsible for the fast-moving acoustic waves are solved implicitly with the option of off-centering by setting \( \beta \neq 0 \). Numerical diffusion is represented in \( F_u \) and \( F_w \) in the
form of second-order diffusion with physical viscosity $\nu$,

$$F(\cdot) = \nu \left[ \delta_x^2(\cdot) + \delta_z^2(\cdot) \right]. \quad (3.22)$$

The buoyancy terms in the vertical momentum equation are solved explicitly by extrapolating to time level $n + 1/2$ using

$$\cdot^{n+1/2} = \frac{3}{2} \cdot^n - \frac{1}{2} \cdot^{n-1}, \quad (3.23)$$

and then interpolated to the midpoint trajectory. One way to evaluate the buoyancy term implicitly is to concurrently update the density and pressure perturbation variables ($\rho'_m$ and $\pi'_m$, respectively) at every iteration of $\hat{\Theta}'_m$ in the Helmholtz solver. This implicit treatment of the buoyancy term involves updating the density perturbation using $u^{n+1}$ and $w^{n+1}$ guesses at that iteration, and we have yet to find a feasible way to incorporate this in the Helmholtz solver that ensures convergence at large time steps. The implicit treatment of the buoyancy terms will be the scope of future work.

### 3.3.4 Discretization of the thermodynamic equation

In our nonhydrostatic solver, we form and solve an implicit equation for $\Theta^{n+1}_m$. The implicit equation is formed in two steps. First, we compute the explicit solution of the flux-form thermodynamic equation using the conservative transport scheme CSLAM,

$$\hat{\Theta}^{n+1}_m = \Theta^{n+1\exp}_m + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\Theta^{n}_m v^{n}) - \nabla_{\text{lag}} \cdot (\Theta^{n}_m v^{n}) \right] \frac{\delta A^*}{\Delta A}$$

$$+ \Delta t \left[ F_{\Theta^m_n} \right] \frac{\delta A^*}{\Delta A}, \quad (3.24)$$

where the notation $[\cdot]$ denotes departure cell averages. The first term on the rhs of (3.24), $\Theta^{n+1\exp}_m$, is the explicit CSLAM update. The second term is a predictor-corrector term integrated over the departure cell to account for the discrepancy between the discrete Eulerian and Lagrangian flux divergences in the semi-implicit flux-form correction term. Similarly, in $F_{\Theta_n}$, second-order diffusion (with mixing coefficient given by $\nu$ times the Prandtl number) and the diabatic tendency from the microphysical scheme are evaluated explicitly and integrated over the departure cell area. Since the predictor-corrector and the forcing terms depend only on values at the previous time level, they can be evaluated along with $\Theta^{n+1\exp}_m$ in a single call to CSLAM, giving $\hat{\Theta}^{n+1}_m$. Then, to allow for coupling to the momentum equations, a semi-implicit flux-form correction term is used to form the implicit
equation

\[
\hat{\Theta}^{n+1}_m = \hat{\Theta}^{n+1}_m - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot \left( \hat{\Theta}^{n+1}_m \mathbf{v}^{n+1} \right) - \nabla_{\text{lag}} \cdot \left( \hat{\Theta}^{n+1}_m \mathbf{v}^{n+1} \right) \right],
\]

(3.25)

where \(\hat{\Theta}^{n+1}_m\) is the value of \(\Theta_m\) at the new time level except for a final saturation adjustment that takes place at the end of the time step to correct the diabatic tendency using the microphysics scheme. The new tendency is then carried over to the next time step to be used as an estimate of the diabatic term in (3.24).

The form of the semi-implicit correction term [square-bracketed terms in (3.25)] stems from the split-divergence approximation used in the trajectory computation. The semi-implicit discretization for \(\Theta^{n+1}_m\) is based on the flux-form scheme presented in Wong et al. (2013) for the height equation in their shallow-water equations solver. The flux-form scheme is based on the derivation of a similar semi-implicit discretization for the shallow-water model found in Lauritzen et al. (2006), but the latter scheme uses a time-independent reference state, with which it becomes difficult to ensure numerical consistency and maintain conservative properties (discussed in section 3.4). Instead of using a time-independent reference state, we form the semi-implicit correction term using the explicit solution \(\hat{\Theta}^{n+1}_m\) from (3.24).

The semi-implicit correction term is defined as the difference between an Eulerian flux divergence and a Lagrangian flux divergence. On an Arakawa C-grid, these would be defined as

\[
\nabla_{\text{eul}} \cdot (\Theta_m \mathbf{v}) = \frac{1}{\Delta x} \left[ \left( \Theta^x_m \mathbf{v} \right)_r - \left( \Theta^x_m \mathbf{v} \right)_l \right] + \frac{1}{\Delta z} \left[ \left( \Theta^z_m \mathbf{v} \right)_t - \left( \Theta^z_m \mathbf{v} \right)_b \right],
\]

(3.26)

and

\[
\nabla_{\text{lag}} \cdot (\Theta_m \mathbf{v}) = \frac{1}{\Delta x \Delta z} \left[ \Theta^r_m \mathcal{F}_r - \Theta^l_m \mathcal{F}_l \right. \\
\left. + \Theta^t_m \mathcal{F}_t - \Theta^b_m \mathcal{F}_b \right],
\]

(3.27)

respectively, and \(\mathcal{F}(\cdot)\) are Lagrangian flux areas, where the subscripts \(r, l, t, b\) denote the right, left, top, and bottom cell faces of an Eulerian grid cell (Fig. 3.2). We use an exact computation of the Lagrangian flux divergence in an Eulerian manner, where Lagrangian flux areas \(\mathcal{F}(\cdot)\) through each cell face are defined as

\[
\mathcal{F}_r = \mathcal{W}_r^{zz} \Delta z - (u_c w_{c3} - u_c w_{c2}) \Delta t / 2,
\]

(3.28)
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Figure 3.2: Geometric representation of the Lagrangian flux divergence, defined as the flux-area difference between the Eulerian arrival grid cell (solid square) and the departure cell (dashed polygon) in one time step. Velocities associated with the Eulerian grid cell at the cell faces \((u_l, u_r, w_t, w_b)\) and cell vertices \((u_c, w_c)\) for \(i = 1, 2, 3, 4\) are also shown. White arrows indicate the computed trajectories of each departure grid cell vertex.

\[
\mathcal{F}_l = \overline{w_t^{xz}} \Delta z - (u_{c1} w_{c4} - u_{c4} w_{c1}) \Delta t / 2, \tag{3.29}
\]

\[
\mathcal{F}_r = \overline{w_t^{xz}} \Delta x - (u_{c3} w_{c4} - u_{c4} w_{c3}) \Delta t / 2, \tag{3.30}
\]

\[
\mathcal{F}_b = \overline{w_b^{xz}} \Delta x - (u_{c2} w_{c1} - u_{c1} w_{c2}) \Delta t / 2, \tag{3.31}
\]

where the spatial operators are defined as

\[
\overline{\cdot}^{xz} = \frac{1}{4} \left( \cdot \right)_{i-1,k} + 2 \left( \cdot \right)_{i,k} + \left( \cdot \right)_{i+1,k}, \tag{3.32}
\]

\[
\overline{\cdot}^{z} = \frac{1}{4} \left( \cdot \right)_{i,k-1} + 2 \left( \cdot \right)_{i,k} + \left( \cdot \right)_{i,k+1}. \tag{3.33}
\]

The terms proportional to \(\Delta t / 2\) correct for the geometric differences between the Eulerian and Lagrangian flux divergences (shaded areas in Fig. 3.2). [For full details on the derivation of \(\mathcal{F}\) and \(\nabla_{\text{lag}} \cdot (\Theta_m v)\), see Wong et al. (2013)].

Using (3.26) and (3.27), the explicit equation for \(\hat{\Theta}_n^{m+1}\) (3.24) and implicit equation for \(\tilde{\Theta}_n^{m+1}\)
(3.25) can be rewritten as

\[
\hat{\Theta}_m^{n+1} = \Theta_m^{n+1} + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\Theta_m^n v^n) \right] \frac{\delta A^*}{\Delta A} + \Delta t \left[ \frac{F_m^n}{\Theta_m} \right] \frac{\delta A^*}{\Delta A},
\]  

(3.34)

and

\[
\tilde{\Theta}_m^{n+1} = \hat{\Theta}_m^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\hat{\Theta}_m^{n+1} v^{n+1}) \right],
\]  

(3.35)

respectively, where \(v'\) is a corrective velocity and

\[
\nabla_{\text{eul}} \cdot (\Theta_m v') = \frac{1}{\Delta x} \left[ \overline{\Theta}_m^x (u_r - \mathcal{F}_r / \Delta z) - \overline{\Theta}_m^x (u_l - \mathcal{F}_l / \Delta z) \right] + \frac{1}{\Delta z} \left[ \overline{\Theta}_m^z (w_t - \mathcal{F}_t / \Delta x) - \overline{\Theta}_m^z (w_b - \mathcal{F}_b / \Delta x) \right].
\]

(3.36)

### 3.3.5 Helmholtz equation

The Helmholtz equation with variable coefficients for the semi-implicit problem is solved using a conjugate-residual solver. Substitution of the momentum equations (3.16) and (3.17) into (3.35) forms the Helmholtz equation for \(\tilde{\Theta}_m^{n+1}\),

\[
- \left( \frac{\Delta t}{2} \right)^2 \gamma R_d (1 + \beta) \left[ \delta_x (\hat{\Theta}_m^{n+1} \frac{p^n}{\rho_m^x}) \delta_x \tilde{\Theta}_m^{n+1} 
+ \left. \delta_x (\hat{\Theta}_m^{n+1} \frac{p^n}{\rho_m^x}) \delta_\xi \tilde{\Theta}_m^{n+1} \right] + \tilde{\Theta}_m^{n+1} 
= R_\Theta - \frac{\Delta t}{2} (1 + \beta) \left[ \delta_x (\bar{\Theta}_m^{n+1} R_u) + \delta_\xi (\bar{\Theta}_m^{n+1} R_w) \right].
\]

(3.37)

The terms \(R_u\), \(R_w\), and \(R_\Theta\) represent the known terms in (3.16), (3.17), and (3.35). The explicit solution \(\hat{\Theta}_m^{n+1}\) from CSLAM is computed prior to solving (3.37).

Using the explicit solution \(\hat{\Theta}_m^{n+1}\) allows for a straightforward and consistent formulation between the thermodynamic and continuity equations, as long as the reconstruction of \(\Theta_m\) is performed in a consistent manner. To ensure this, in CSLAM we follow Nair and Lauritzen (2010) in separating the subgrid-cell reconstructions for \(\rho_d\) and \(\Theta_m\), and compute the second-order reconstruction function.
\[ \Theta_m(x, z) = \langle \rho_d \rangle \Theta_m(x, z) + \langle \theta_m \rangle \left( \rho_d(x, z) - \langle \rho_d \rangle \right) , \]  

(3.38)

where \( \langle \rho_d \rangle \) and \( \langle \theta_m \rangle \) are Eulerian grid cell values, and \( \rho_d(x, z) \) and \( \theta_m(x, z) \) are reconstruction functions. To check for consistency, we substitute a field of constant \( \theta_m \), i.e. \( \theta_m(x, z) = \langle \theta_m \rangle = 1 \), in (3.38) and see that the rhs of (3.38) properly reduces to \( \rho_d(x, z) \).

In summary, the solution procedure for obtaining solutions for \( \tilde{\Theta}_m^{n+1} \), \( u^{n+1} \), and \( w^{n+1} \), is as follows: (i) obtain solution for \( \tilde{\Theta}_m^{n+1} \) by solving the Helmholtz equation (4.26), (ii) substitute solution for \( \tilde{\Theta}_m^{n+1} \) into (3.16) and (3.17) to obtain solutions for \( u^{n+1} \) and \( w^{n+1} \), respectively, and (iii) recalculate \( \tilde{\Theta}_m^{n+1} \) using \( u^{n+1} \) and \( w^{n+1} \) to eliminate any roundoff errors. This solution procedure is similar to that used in Wong et al. (2013) for the shallow-water equations.

### 3.3.6 Discretization of the continuity equation

We ensure that the flux-form thermodynamic equation is consistent with the continuity equation by using the same numerical scheme, with the inclusion of the semi-implicit correction terms in the continuity equation. Again, we first use CSLAM to obtain the explicit solution \( \tilde{\rho}_d^{n+1} \) in a similar manner as in (3.34),

\[ \tilde{\rho}_d^{n+1} = \rho_{d, \text{exp}}^{n+1} + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot \left( \rho_d^n v^n \right) \right] \frac{\delta A^*}{\Delta A} . \]  

(3.39)

Then, we add the semi-implicit correction term to (3.39) to be consistent with (3.35),

\[ \rho_d^{n+1} = \tilde{\rho}_d^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot \left( \tilde{\rho}_d^{n+1} v^{n+1} \right) \right] . \]  

(3.40)

The new time-level correction term is evaluated by back-substituting the solution of the velocity field \( v^{n+1} \) into \( v^{n+1} \).

### 3.3.7 Discretization of moisture conservation equations

The flux variables of mixing ratios of water vapor \( q_v \), cloud water \( q_c \), and rainwater \( q_r \) are included as prognostic variables in the nonhydrostatic solver. Moist mass conservation equations are integrated using CSLAM. To ensure moisture conservation, numerical consistency between the continuity equation and the moisture conservation equations needs to be ensured. Numerical inconsistency between the continuity equation and other scalar conservation equations can lead to spurious generation or removal of scalar mass, despite using inherently mass-conserving advection...
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A consistent formulation of the moisture conservation equations using the scheme in Wong et al. (2013) for the flux variables \( Q_j = \rho d q_j \) where \( q_j = (q_v, q_c, q_r) \) is

\[
\hat{Q}_j^{n+1} = Q_{j, \text{exp}}^n + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (Q_j^n \mathbf{v}_m^n) \right] \frac{\Delta A^*}{\Delta A} + \Delta t \left[ F_{q_j}^n \right] \frac{\Delta A^*}{\Delta A}, \tag{3.41}
\]

\[
\tilde{Q}_j^{n+1} = \hat{Q}_j^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\hat{Q}_j^{n+1} \mathbf{v}_m^{n+1}) \right] \tag{3.42}
\]

where \( \mathbf{v}_m^n, \mathbf{v}_m^{n+1} \) and the computations for \( \nabla_{\text{eul}} \cdot (\cdot) \) are the same as in (3.40). The explicit CSLAM solution \( \hat{Q}_j^{n+1} \) (3.41) is computed using a consistent reconstruction as in (3.38). \( F_{q_j} \) represents second-order diffusion with a mixing coefficient same as that for \( \Theta_m \), and any diabatic tendencies from the microphysics.

### 3.3.8 Diabatic processes

Microphysical processes are modelled using the simple warm-rain Kessler parameterization, as described in Klemp and Wilhelmson (1978). In the evaluation of the thermodynamic and moisture conservation equations, the diabatic forcing is approximated in \( F_{\Theta_m} \) and \( F_{Q_j} \) [(3.34) and (3.41), respectively] using the most up-to-date values integrated over the departure cell. These values are then removed from the solutions prior to calling the Kessler microphysics scheme. The included microphysical processes are (1) condensation of water vapor into cloud-water, (2) autoconversion by diffusion and collection of cloud-water into rain-water, (3) evaporation of cloud-water and rain, and (4) precipitation of rain which is removed when it reaches the surface. These microphysical processes are computed as a final adjustment at the end of the time step, advancing \( \hat{\Theta}_m^{n+1} \) and \( \hat{Q}_j^{n+1} \) to \( \Theta_m^{n+1} \) and \( Q_j^{n+1} \) in a manner that is consistent with saturation conditions at the new time level.

### 3.3.9 Diagnostic equation of state

Pressure is a diagnostic variable computed using the equation of state (3.6),

\[
p = p_0 \left( \frac{R_d \Theta_m}{p_0} \right)^\gamma \tag{3.43}
\]

where \( p_0 \) is the reference surface pressure set to 100 kPa.
3.3.10 Consistency and shape-preservation

In the CSLAM reconstruction step, we reconstruct $Q_j$ using (3.38) described in section 3.3.5 to ensure consistency. To ensure shape preservation, we follow the two steps as described in Wong et al. (2013). First, we use the simple 2D filter by Barth and Jespersen (1989) that searches for new local minima and maxima in the reconstruction function of a scalar field such as moisture mixing ratio $q_j$, and scales the function if these values exceed those in the neighbouring cell. For chemistry applications, preservation of linear correlations in tracers is important, and it has been found that the limiter preserves linear correlations between tracers, whereas typically linear correlation is only preserved when the limiter is not applied (Lauritzen et al., 2014). Second, to ensure shape-preservation in the flux-divergence terms, we compute the upwind moist species mixing ratio $q^*_j$ by first decoupling $Q_j$ from $\rho_d$. Then, the flux divergences are computed by centering density to each of the cell faces, i.e.

$$\nabla_{\text{eul}} \cdot \rho_d q_j v' = \frac{1}{\Delta x} \left[ (\tilde{\rho}_d q_j^* u')_r - (\tilde{\rho}_d q_j^* u')_l \right] + \frac{1}{\Delta z} \left[ (\tilde{\rho}_d q_j^* w')_t - (\tilde{\rho}_d q_j^* w')_b \right].$$

(3.44)

The upwind $q^*_j$ values are determined using $v'$.

3.4 Desirable properties of CSLAM-NH

The flux-form nonhydrostatic semi-implicit CISL solver CSLAM-NH has six main advantages and desirable properties: (i) inherently mass-conserving using the conservative semi-Lagrangian transport scheme CSLAM, (ii) ensures numerically consistent transport, (iii) independent of a mean reference state, (iv) shape-preserving, and (v) like typical semi-implicit solvers, CSLAM-NH requires solving a single linear Helmholtz equation and (vi) a single application of CSLAM at each time step.

CSLAM-NH uses a formulation of the discretized continuity equation that ensures numerical consistency for a cell-integrated semi-Lagrangian (CISL) solver. In CSLAM-NH, a Helmholtz equation for the potential temperature perturbation is solved. Traditionally, to avoid solving a nonlinear Helmholtz equation, the flux divergence term that is coupled to the momentum equations is...
often first linearized around a mean reference state $\Theta_{m,\text{ref}}$, e.g.,

$$
\Theta_m^{n+1} = \Theta_{m,\text{exp}}^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\Theta_{m,\text{ref}}^{n+1} v^n) \right] + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\Theta_{m,\text{ref}}^n v^n) \right] \frac{\delta A^*}{\Delta A} + \Delta t \left[ F_n^{\phi} \right] \frac{\delta A^*}{\Delta A},
$$

(3.45)

where $\Theta_{m,\text{ref}}$ is a mean reference state that is often time-independent and varies with height. A choice of reference state can be the hydrostatic background state $\rho_d \theta_m$. The scheme (3.45) is a nonhydrostatic extension to the SWE semi-implicit CISL continuity equation in Lauritzen et al. (2006).

To ensure conservation of potential temperature, it is important for the discrete thermodynamic equation to be numerically consistent with the discrete continuity equation. One can include similar semi-implicit correction terms as in (3.45) and discretize the continuity equation as

$$
\rho_d^{n+1} = \rho_{d,\exp}^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\rho_{d,\text{ref}}^{n+1} v^n) \right] + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\rho_{d,\text{ref}}^n v^n) \right] \frac{\delta A^*}{\Delta A}. 
$$

(3.46)

However, note that the above scheme is only strictly consistent with (3.45) for $\Theta_{m,\text{ref}} = \rho_{d,\text{ref}} \theta_m$, which is difficult to achieve as $\theta_m$ is unknown.

Transported material, such as moisture and passive tracers with some mixing ratio $q$, are often solved explicitly using the CISL transport scheme, i.e.,

$$
\phi^{n+1} = \phi_{\exp}^{n+1} + \Delta t \left[ F_n^{\phi} \right] \frac{\delta A^*}{\Delta A},
$$

(3.47)

where $\phi = \rho_d q$ is the scalar mass and $\left[ F_n^{\phi} \right]$ represents diffusion and any diabatic tendency evaluated at time level $n$ over the departure cell. Such explicit schemes would lead to numerical inconsistency between the discrete CISL continuity equation (3.46) and the discrete constituent mass conservation equations such as (3.47). If the discrete conservation equation is consistent with the discrete continuity equation, the former should reduce to the latter when $q$ is a constant, and an initially spatially uniform passive tracer field should remain so. The inconsistent flux-divergence correction term in (3.46) can spuriously generate or remove moisture or tracer mass in the model.

Alternatively, one can formulate the discrete scalar conservation equation in a manner similar
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to (3.46) by including the flux-divergence correction terms,

\[
\phi^{n+1} = \phi^{n+1}_{\text{exp}} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\phi_{\text{ref}} v^{n+1}) \right] + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (\phi_{\text{ref}} v^n) \right] \frac{\delta A^*}{\Delta A} + \Delta t \left[ F_n^{\phi} \right] \frac{\delta A^*}{\Delta A}.
\]

(3.48)

However, similar to the case for \(\Theta_{m,\text{ref}}\), determining an appropriate choice for reference state \(\phi_{\text{ref}}\) is difficult, making a numerically consistent formulation such as (3.48) hard to implement.

The formulations we present for the thermodynamic, density, and moisture conservation equations [(3.35), (3.40), and (3.42), respectively] are all numerically consistent with one another. These consistent formulations are made possible by avoiding the use of a mean reference state. In our formulation, we use the explicit CSLAM solution instead of a mean reference state in the flux-divergence correction terms. This approach eliminates the difficult choice of a mean reference state \(\phi_{\text{ref}}\) for moisture or tracer mass.

Even if an appropriate choice of \(\phi_{\text{ref}}\) can be found, using a time-independent mean reference state in (3.48) can be problematic for regions with little moisture or tracer mass \((\hat{\phi}^{n+1} \ll 1)\). Depending on the magnitude of \(\phi_{\text{ref}}\), the flux divergences are likely nonzero for a divergent flow and can, therefore, generate or remove unphysical mass (Lauritzen et al., 2008). In the nonhydrostatic solver presented here, by computing the flux divergences of the explicit solution \(\hat{\phi}^{n+1}\), the magnitude of the flux divergences are better approximated for regions with little moisture or tracer mass.

As scalar mass conservation is not guaranteed in an inconsistent solver, these solvers also generally do not preserve the shape of scalar fields such as mixing ratios, even when shape-preserving filters are applied to the transport scheme. The implications are that the scalar field may no longer be positive-definite, and new unphysical minima and maxima can occur due to under- and overshooting, respectively. The consistent and shape-preserving transport in the proposed solver ensures that no new (unphysical) minimum and maximum (within machine roundoff) will occur.

### 3.5 Idealized test cases

Two of the three idealized test cases presented, namely a density current simulation and a gravity wave simulation, are commonly used as benchmarks for testing nonhydrostatic solvers. The third idealized test case is a 2D squall line simulation, where the stability of the model is tested with latent heating modeled by a simple warm-rain microphysics scheme. In addition to comparing with available solutions in the literature, comparisons with an Eulerian split-explicit model with 2nd-
order advection [2D version of the solver described in Klemp et al. (2007)] are also presented.

### 3.5.1 Density current

The nonlinear density current test case, described in Straka et al. (1992), is widely used as a benchmark test for nonhydrostatic solvers (e.g., Klemp et al., 2007; Xue et al., 2000). An initial cold temperature perturbation is centered in the domain, and the negatively buoyant cold air descends to the surface and forms symmetric density currents propagating in opposite directions. Straka et al. (1992) provides a well-documented comparison among various compressible and quasi-compressible solvers as well as a high-resolution benchmark solution.

The numerical domain is centered at \( x = 0 \) km, with \(-25.6 \leq x \leq 25.6 \) km and \( 0 \leq z \leq 6.4 \) km. As described in Straka et al. (1992), the initial condition is given by a temperature perturbation \( \Delta T \), where

\[
\Delta T = \begin{cases} 
0.0^\circ C & \text{if } L \geq 1.0 \\
-15.0^\circ C \left[ \cos(\pi L) + 1.0 \right] / 2 & \text{if } L < 1.0,
\end{cases}
\]

where \( L = \sqrt{\left( \frac{x-x_c}{x_r} \right)^2 + \left( \frac{z-z_c}{z_r} \right)^2} \) where \((x_c, z_c) = (0.0, 3.0)\) km is the center of the perturbation, and its width and depth are given by \( x_r = 4.0 \) km and \( z_r = 2.0 \) km. The surface temperature \( \Theta_0 \) is at 300 K in a horizontally homogeneous and neutral environment. A constant physical viscosity of 75 m\(^2\) s\(^{-1}\) is used. The domain is an \( x \)-periodic channel with reflective boundary conditions along the upper and lower boundaries as specified by Straka et al. (1992) that require \( \partial u / \partial z = w = \partial \rho / \partial z = \partial \Theta / \partial z = 0 \).

Following Straka et al. (1992), we simulate the density current test case using grid spacings \( \Delta x = \Delta z = 400, 200, 100, 50, 25 \) m, with Eulerian time step sizes of \( \Delta t = 4, 2, 1, 0.5, \) and 0.25 s, respectively. Figure 3.3 shows the potential temperature perturbation \((\Theta')\) from its mean state from CSLAM-NH and the Eulerian split-explicit scheme with 2nd-order advection at the simulation end time of 15 min using different model resolutions.

The density current is clearly under-resolved using a 400 m-grid spacing, with only the main rotor marginally resolved (7 km \( \leq x \leq 9 \) km). A grid-spacing of 200 m gives a better resolution of the main rotor as well as a second rotor (11 km \( \leq x \leq 12 \) km); however the leading third rotor is still under-resolved. For resolutions finer than \( \Delta x = \Delta z = 100 \) m, all three rotors are well-resolved with the solutions converging and indistinguishable by eye between 50 m and 25 m grid spacings. The differences among the model resolutions agree well with those documented in other nonhydrostatic solvers such as in Straka et al. (1992), Xue et al. (2000), Skamarock and Klemp (2008), and Melvin et al. (2010).

Positions of the density current front (specified to be at \( \Theta' = -1 \) K), the minimum and maximum
\( \Delta x = \Delta z = 400 \text{ m} \)

\( \Delta x = \Delta z = 200 \text{ m} \)

\( \Delta x = \Delta z = 100 \text{ m} \)

\( \Delta x = \Delta z = 50 \text{ m} \)

\( \Delta x = \Delta z = 25 \text{ m} \)

---

**Figure 3.3:** Potential temperature perturbation (K) after 15 min. Contour intervals are every 1 K, starting at 0.5 K. Mean wind \( \overline{U} = 0 \text{ m s}^{-1} \).

The values of \( \theta' \) in the domain, and \( \sum \theta'_\text{sampled} \) for all \( \theta'_\text{sampled} \) and \( \theta'_\text{sampled} > 0 \), and \( \sum \theta'^2_\text{sampled} \) are shown in Table 3.1. We also compare the results with those using SLICE (Table II of Melvin et al. (2010)) and REFC25, the 25 m reference solution in Table IV of Straka et al. (1992). In computing the summation statistics, \( \theta'_\text{sampled} \) from each of the CSLAM-NH runs (except for the 400 m grid-spacing run) are sampled at 200 m resolution. This sampling is done so that we can make a direct comparison with the statistics of REFC25 in Straka et al. (1992) (where they sampled REFC25 at 200 m resolution). Statistics from the 25 m solution agree closely with the nonhydrostatic SLICE model, with a similar slight discrepancy in the density front location when compared to REFC25. Both CSLAM-NH and SLICE are semi-Lagrangian models with inherent dissipation and order of accuracy different from REFC25, an Eulerian compressible solver with 2nd-order advection; these differences could lead to the slight discrepancy in the density front locations. In addition to model differences, like the SLICE model, a different time step size is used to compute the 25 m solution (16 times larger than that used to compute REFC25). At coarser resolutions (400 m and 200 m),
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<table>
<thead>
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<th>Grid size (m)</th>
<th>Time step size (s)</th>
<th>( \theta'_{\text{min}} ) (K)</th>
<th>( \theta'_{\text{max}} ) (K)</th>
<th>Front location (m)</th>
<th>( \sum \theta'_{\text{sampled}} ) (K)</th>
<th>( \sum \theta'_{\text{sampled}} ) (for ( \theta' &gt; 0 )) (K)</th>
<th>( \sum \theta'^2_{\text{sampled}} ) (K²)</th>
</tr>
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Table 3.1: Statistics for the density current simulations at time 15 min using CSLAM-NH at various grid resolutions and time step sizes. Comparison values from the nonhydrostatic x-z solver using SLICE in Melvin et al. (2010) are also presented. REFC25 are values taken from Straka et al. (1992). \( \theta'_{\text{sampled}} \) are solutions sampled at 200 m for comparison with values in Straka et al. (1992).

the minimum \( \theta' \) values are colder than those in SLICE; the front locations therefore also travelled farther out from the centerline. Analytically, the maximum \( \theta' \) should remain zero throughout the simulation, as is the case in the higher resolution runs (50 m and 25 m). The contribution of positive \( \theta' \) values in \( \sum \theta'_{\text{sampled}} \) is also small at these resolutions (in the order of \( 1\times10^{-5} \) K and \( 1\times10^{-8} \) K respectively), increasing up to the order of \( 1\times10^{-1} \) K at 200 m. [Straka et al. (1992) only reported values up to 4 decimal points.]

For the next simulation, mean background wind of \( \overline{U} = 20 \text{ m s}^{-1} \) is applied to the described test case, as is done in Skamarock and Klemp (2008) to examine phase errors. Solutions from CSLAM-NH and the Eulerian split-explicit 2nd-order advection scheme of both the left- and right-moving currents at time 15 min using \( \Delta x = \Delta z = 200, 100, \) and 50 m are shown in Fig. 3.4. Time step sizes are the same as in Fig. 3.3. The solutions from CSLAM-NH in general show proper symmetry about the translating centerline, although very subtle differences between the secondary rotors in the left- and right-moving currents are noticeable at 200 m and 100 m grid spacing. As a comparison, the Eulerian split-explicit 2nd-order advection scheme shows noticeably larger errors in the right-moving current as expected due to the right-moving current moving at a greater speed.
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Figure 3.4: Potential temperature perturbation (K) after 15 min. Contoured as in Fig. 3.3. Solution is translated using a mean wind $U = 20$ m s$^{-1}$.

For this test case, we found that the maximum stable time step size in CSLAM-NH is double of that of the Eulerian scheme. Fig. 3.5 shows solutions for tests where $U = 0$ m s$^{-1}$ at $\Delta x = \Delta z = 100$ m using a time step size of 3 s and 4 s, whereas the maximum stable Eulerian time step size is $\Delta t = 2$ s. The solution using a large time step of 4 s is almost indistinguishable by eye from the 25 m high-resolution solutions (Fig. 3.3). With mean advection ($U = 20$ m s$^{-1}$), the maximum stable time step in CSLAM-NH is 3 s. As we increase the time step size to 4 s, the phase error was large enough to form unphysically steep gradients at the leading edge of the right-moving current, which then caused the violation of the Lipschitz stability condition. The maximum stable time step in the Eulerian model is 1.5 s. Using a time step size of 5 s, instability was observed in the vicinity of the leading edge of the subsiding cold air for both cases with and without the mean wind.

3.5.2 Gravity wave

A second test case of a gravity wave in a periodic channel with solid, free-slip upper- and lower-boundary conditions is used to evaluate the nonhydrostatic solver. The test case is described in Skamarock and Klemp (1994), where they presented results for a Boussinesq atmosphere. The test
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Figure 3.5: Potential temperature perturbation (K) from CSLAM-NH after 15 min for grid spacing \( \Delta x = \Delta z = 100 \text{ m} \) using time step sizes \( \Delta t = 3 \text{ and } 4 \text{ s} \). Mean wind \( \bar{U} = 0 \text{ m s}^{-1} \). The Eulerian split-explicit scheme (not plotted) was numerically unstable for these time steps, as it required \( \Delta t \leq 2 \text{ s} \) for numerical stability of this gravity current. Contoured as in Fig. 3.3.

case is characterized by an initial potential temperature perturbation of amplitude \( \Delta \theta_0 \),

\[
\theta(x, z, t = 0) = \Delta \theta_0 \frac{\sin(\pi z/H)}{1 + (x - x_c)^2/a^2}.
\]  

(3.50)

where \( \Delta \theta_0 = 10^{-2} \text{ K} \), \( a = 5 \text{ km} \) is the half-width of the initial perturbation, \( H = 10 \text{ km} \) is the total depth of the domain, and \( x_c = 0.25L \), where \( L = 300 \text{ km} \) is the length of the domain. The background atmospheric stratification has a constant Brunt-Väisälä frequency \( N = 10^{-2} \text{ s}^{-1} \). For one simulation, no mean wind \( \bar{U} = 0 \) is prescribed. The other simulation uses a mean wind of \( \bar{U} = 20 \text{ m s}^{-1} \), advecting the solution to the right while the two gravity wave modes propagate in opposite directions. Again, the mean advection of the solution accentuates any advective phase speed errors in the scheme. The boundary condition is implemented by linear extrapolating \( u, \Theta, \) and \( \rho \) values into the boundary, consistent with the free-slip boundary conditions, and setting \( w = 0 \).

We run the gravity wave test case at grid spacings \( \Delta x = \Delta z = 1 \text{ km}, 500 \text{ m}, \) and \( 250 \text{ m} \) using Eulerian time step sizes \( \Delta t = 12 \text{ s}, 6 \text{ s}, \) and \( 3 \text{ s} \), respectively. Solutions from CSLAM-NH at the three resolutions for \( \bar{U} = 0 \) (not shown) are indistinguishable by eye from the 250 m and 500 m solutions for \( \bar{U} = 20 \text{ m s}^{-1} \) in Fig. 3.6 and compare well with those using the WRF-ARW model (solutions using the 5th- and 6th-order advection scheme are available at http://www.mmm.ucar.edu/projects/srnwp_tests/ig_waves/ig_wave.html), with the 2nd-order advection scheme of the same Eulerian split-explicit scheme, and with the SLICE nonhydrostatic vertical model in Melvin.
Figure 3.6: Potential temperature perturbation (K) after 50 min. Contour intervals are every $5 \times 10^{-4}$ K (zero contour line not plotted). Solid lines indicate positive contours and dashed lines indicate negative contours. Solution is translated using a mean wind $\bar{U} = 20$ m s$^{-1}$. Horizontal axis has also been translated with the mean wind so the line of symmetry remains at $x = 0$.

et al. (2010). In Skamarock and Klemp (1994), the solution presented for this nonhydrostatic test case uses a Boussinesq model, where the symmetry of the analytic Boussinesq solution in both $x$ and $z$ is maintained. The density variation in the full Euler equations results in solutions that are asymmetric in $z$, as observed in the CSLAM-NH solutions, the $2^{nd}$-order Eulerian solutions, the $5^{th}$-order Eulerian solutions, as well as the SLICE nonhydrostatic vertical model solutions.

Like in the density current test, we impose a mean advection wind $\bar{U} = 20$ m s$^{-1}$ to examine phase errors. These tests are made at the same grid spacings and time step sizes as in the no mean wind case. The right- and left-moving waves from CSLAM-NH exhibit nearly perfect symme-
try, indicating there is minimal phase error in the solutions. The Eulerian split-explicit 2nd-order advection scheme shows more noticeable phase errors (Fig. 3.6).

Testing of CSLAM-NH using larger time steps in this gravity wave test case reveals a numerical stability condition that is sensitive to the stratification $N$. (We note that CSLAM-NH is unconditionally stable for $N = 0$, i.e. for a near-pure advection case of the initial warm perturbation.) We evaluate the maximum stable CSLAM-NH time step size for the gravity wave case with a mean advection wind speed of $U = 20$ m s$^{-1}$ ($\Delta x = \Delta z = 1$ km) over a range of $N$ (0.01, 0.015, and 0.02 s$^{-1}$). Since the gravity wave phase speed varies with $N$, we increase/decrease the simulation time

---

**Figure 3.7:** Potential temperature perturbation (K) solutions of the gravity wave case using increasingly large CSLAM-NH time steps ($\Delta x = \Delta z = 1$ km) where (a)-(c) $U = 0$ m s$^{-1}$ and (d)-(f) $U = 20$ m s$^{-1}$. Contoured as in Fig. 3.6.
length as appropriate such that the gravity wave solutions are similar to those shown in Fig. 3.6; for example, for $N = 0.015 \, \text{s}^{-1}$, the simulation time is reduced to 2000 s. Test results showed that the maximum stable CSLAM-NH time step sizes are $\Delta t_{\text{max}} = 38, 35, \text{and } 32$ s for $N = 0.01, 0.015,$ and $0.02 \, \text{s}^{-1}$, respectively, whereas in the case of the Eulerian split-explicit scheme, the maximum stable large time steps are found to be $\Delta t = 60, 55, \text{and } 50$ s (with small time step size of 2.4 s), respectively, limited by the stability condition of the advection scheme. The buoyancy terms in the vertical momentum equation are integrated explicitly in CSLAM-NH, and handled implicitly in the Eulerian scheme. When we remove the buoyancy terms from the implicit step and solve them explicitly in the Eulerian model, the time step sizes required to obtain solutions of similar accuracy as those from the vertically implicit model are reduced by 20–35%, and are closer to those found in CSLAM-NH. The devising of an integration scheme that handles the buoyancy terms implicitly in CSLAM-NH will require a robust and stable way of updating the density perturbation in the Helmholtz solver, and this will be addressed in future work.

### 3.5.3 2D (x-z) squall line

We perform a test case of a 2D squall line as described in Weisman and Klemp (1982) to evaluate mass conservation, consistency, and shape-preservation in the nonhydrostatic solver, in addition to testing for any small-scale computational instability in the model due to latent heating.

The numerical domain is centered at $x = 0.0 \, \text{km}$, with $-100 \, \text{km} \leq x \leq 100 \, \text{km}$ and $0 \leq z \leq 20 \, \text{km}$. As in Weisman and Klemp (1982), a conditionally unstable thermodynamic profile is used to initialize the horizontally homogeneous environment. Constant physical horizontal and vertical eddy viscosities of 250 m$^2$ s$^{-1}$ are used. A warm thermal perturbation near the surface is prescribed to initiate convection (Weisman et al., 1988). The initial thermal perturbation has a maximum of $\Delta \theta_0 = 3 \, \text{K}$, centered at $z_c = 1.5 \, \text{km}$ and along the centerline ($x_c = 0$) of the domain, with a horizontal radius $x_r$ of 10 km and a vertical radius $z_r$ of 1.5 km. The shape of the perturbation is a cosine hill given as

$$\theta(x, z, t = 0) = \begin{cases} \Delta \theta_0 \cos^2(\pi L/2), & L < 1.0, \\ 0, & L \geq 1.0, \end{cases}$$

where $L = \sqrt{(x/x_r)^2 + [(z - z_c)/z_r]^2}$.

A weak vertical wind shear within a 2.5 km-layer at the surface is used to promote the growth of the squall line. The initial wind profile is given as

$$u(z, t = 0) = \begin{cases} \frac{u \cdot (z/z_{1s}) - u_s}{u - u_s}, & z < z_{1s}, \\ \frac{u - u_s}{u - u_s}, & z \geq z_{1s}, \end{cases}$$
where $\mathbf{u} = 12 \text{ m s}^{-1}$, $u_s = 10 \text{ m s}^{-1}$, and $z_{ts} = 2.5 \text{ km}$. The environmental potential temperature and relative humidity profiles at the initial time are

$$\bar{\theta}(z, t = 0) = \begin{cases} \theta_0 + (\theta_{tr} - \theta_0)(z/z_{tr})^{\frac{5}{4}}, & z \leq z_{tr}, \\ \theta_{tr} \exp \left[ \frac{g c_p}{\rho_0 T_{tr}} (z - z_{tr}) \right], & z > z_{tr}, \end{cases} \quad (3.53)$$

and

$$RH(z, t = 0) = \begin{cases} 1 - \frac{3}{4}(z/z_{tr})^{\frac{5}{4}}, & z \leq z_{tr}, \\ 0.25, & z > z_{tr}, \end{cases} \quad (3.54)$$

where $\theta_{tr} = 343 \text{ K}$, $z_{tr} = 12.0 \text{ km}$, and $T_{tr} = 213 \text{ K}$ are the potential temperature, geometric height, and actual temperature at the tropopause. The maximum water mixing ratio is capped at $14 \text{ g kg}^{-1}$. The surface potential temperature $\theta_0 = 300 \text{ K}$. The skew-$T$ log-$p$ diagram for this sounding can be found in Fig. 1 of Weisman and Klemp (1982). Numerical simulations (unless otherwise stated) use a grid spacing $\Delta x = \Delta z = 500 \text{ m}$, a time step $\Delta t = 5 \text{ s}$, and a time-off-centering parameter of $\beta = 0.1$ to maintain numerical stability. Like the gravity-wave case, the boundary condition is implemented by linear extrapolating $u, \Theta,$ and $\rho$ values into the boundary and setting $w = 0$, consistent with the free-slip boundary conditions.

A comparison of the squall line development among CSLAM-NH (with shape preservation), the 5th-order split-explicit, and the 2nd-order split-explicit Eulerian models is presented in Fig. 3.8. Instantaneous and accumulated surface precipitation integrated across the model domain are presented in Fig. 3.9; also shown is the rate of condensation over the entire domain. Maximum updraft velocity is shown in Fig. 3.10. The series of updraft velocity peaks highlight the continuous triggering of new convective systems along the advancing front.

All three models (CSLAM-NH, Eulerian 5th-order advection, and Eulerian 2nd-order advection) show similar development of the convective system (Fig. 3.8). At 0.6 h, all three models show an initial downshear orientation of the system due to the ambient wind shear. As the storm continues to develop with the cold pool strengthening behind the system (not shown), convergence and enhanced uplift lead to the storm tilting in a near-upright position ($T = 0.8 \text{ h}$). At 1.3 h, a new cell is triggered near the edge of the cold pool, where uplift of the warm moist air in the boundary layer is enhanced. At 1.7 h, the cold pool is strong enough to generate a circulation such that the system develops an upshear orientation, as described in Rotunno et al. (1988). Comparing to the simulations from the Eulerian 2nd-order model, those from CSLAM-NH show closer resemblance to those from the Eulerian 5th-order model. The better agreement is also evident in the moisture statistics (Fig. 3.9), especially in the accumulated surface precipitation amounts and condensation rate in the domain.
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Figure 3.8: Vertical cross-sections of vertical velocity (color shading in m s$^{-1}$) and solid contour of the convective cloud structure ($q_c = 0.1$ g kg$^{-1}$) at times 0.6, 0.8, 1.3, 1.7 h of the simulation for the 500 m grid-spacing runs with a time step of 5.0 s from (left) CSLAM-NH, (middle) 5th-order split-explicit Eulerian model, and (right) 2nd-order split-explicit Eulerian model.

Focussing on the two models that show more comparable results, the first maximum updraft velocities from CSLAM-NH (34.1 m s$^{-1}$) is slightly greater than that from Eulerian 5th-order advection (31.6 m s$^{-1}$) (Fig. 3.10). CSLAM-NH appears to show a weaker second peak updraft velocity (21.9 m s$^{-1}$) than the Eulerian 5th-order model (28.3 m s$^{-1}$); however, the stronger first peak ($\sim 34$ m s$^{-1}$) and weaker second peak ($\sim 25$ m s$^{-1}$) are also observed in a higher-resolution simulation using the Eulerian 5th-order model at a grid spacing of 250 m and large time step size of 2.5 s (dashed black line in Fig. 3.10). For comparison, maximum updraft from CSLAM-NH at

63
Figure 3.9: Moisture statistics including surface precipitation rate (kg s$^{-1}$), accumulated surface precipitation (kg), and condensation rate (kg s$^{-1}$) from the microphysics using CSLAM-NH, Eulerian 5th-order horizontal advection, and Eulerian 2nd-order horizontal advection at $\Delta x = \Delta z = 500$ m.

$\Delta x = 250$ m and $\Delta t = 2.5$ s (red dashed line in Fig. 3.10) is also shown, and at the higher resolution, the two models agree very well with each other.

The maximum stable time step in the Eulerian split-explicit 5th-order advection scheme is a large time step of 20 s and acoustic time step size of 1.25 s. The maximum CSLAM-NH stable time step is limited to 15 s due to the violation of the Lipschitz stability condition in the vicinity of the updraft when a larger time step is used (the instability occurs when the storm reaches its first maximum vertical updraft, which generates a strong horizontal wind shear between the updraft
and the neighbouring downdraft). In Fig. 3.11, we see at larger time step sizes, maximum updraft velocities remain close to the small time-step solutions.

With the 2D squall-line test case, we examine the shape-preservation properties of CSLAM-NH using the shape-preserving scheme by Barth and Jespersen (1989) in the CSLAM transport scheme and the upwind scheme for the flux-correction terms in the transport equations. An analogous implementation of these schemes for a shallow-water model is described in Wong et al. (2013).

To verify that consistency is achieved, an additional passive tracer with mixing ratio $r$ is introduced into the model. The passive tracer initially has a constant mixing ratio of $r_0 = 1.0 \, \text{g kg}^{-1}$ and we form the discretized conservation equation as in (3.42). The minimum and maximum values of $r$ are maintained at $1.0 \, \text{g kg}^{-1}$ (up to machine roundoff of order $10^{-14}$) throughout the simulation using the consistent formulation in CSLAM-NH.

For a passive tracer that uses an inconsistent discrete conservation equation such as (3.47), unphysical minima and maxima of the passive tracer mixing ratio are generated (Fig. 3.12). At the end of the squall line simulation at 2 h, the minimum and maximum mixing ratios $r$ are 0.986 g kg$^{-1}$ and 1.021 g kg$^{-1}$, respectively (i.e. the error is on the order of 1 part in 100). We note that the shape-preserving limiter described in Barth and Jespersen (1989) was also applied in CSLAM in this test. Due to numerical inconsistency, however, the limiter becomes ineffective agreeing with the results in Wong et al. (2013). This discrepancy from constancy highlights the importance of ensuring numerical consistency to properly maintain conservation of moisture and tracer mass in a
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Figure 3.11: Timing and intensity of the maximum vertical updraft using \(\Delta x = \Delta z = 500\) m at different CSLAM-NH time step sizes (solid lines), as compared to the Eulerian 5th-order horizontal advection vertical velocity (dashed lines). (Only first hour is plotted.)

3.6 Summary

A new cell-integrated semi-Lagrangian (CISL) nonhydrostatic atmospheric solver, CSLAM-NH, for the moist Euler equations is introduced in this paper. The two-dimensional \((x-z)\) Cartesian nonhydrostatic solver uses a CISL transport scheme, CSLAM, for conservative transport. It also incorporates a new approach to ensure numerical consistency among the CISL continuity equation and the conservation equations for potential temperature, moisture species, and passive tracers. A semi-implicit time integration scheme is used to stably handle the fast-moving acoustic waves in the compressible system.

Based on a recently tested shallow-water equations solver, the extended nonhydrostatic atmospheric solver presented here, CSLAM-NH, possesses a number of features ideal for weather and climate modelling purposes. The solver:

1. is inherently mass-conserving through the use of a conservative transport scheme CSLAM,
2. ensures numerical consistency between the continuity equation and other scalar mass conservation equations (the lack of which may lead to violation of scalar mass conservation),
3. does not depend on a mean reference state,
Figure 3.12: Mixing ratio errors (g kg$^{-1}$) due to numerical inconsistency associated with (3.47). The passive tracer is initialized with a uniform mixing ratio field of 1.0 g kg$^{-1}$. The consistent formulation in CSLAM-NH (which does not use (3.47)) ensures mixing ratio constancy of the same passive tracer up to machine roundoff of order $10^{-14}$ (not shown).

4. can be easily implemented with existing shape-preserving filters to ensure shape-preservation of scalar fields,

5. requires a single linear Helmholtz equation solution (as in typical semi-implicit solvers) per time step [for an explicit treatment of the gravity wave terms]$^3$, and

6. requires a single application of CSLAM per time step.

Here, we tested the nonhydrostatic extension for three idealized test cases: a density current, a gravity wave, and a squall line. To represent microphysical processes in the squall line test, the Kessler warm-rain microphysics parameterization scheme is coupled to the dynamics. The 2D solver currently does not admit flow in the y-direction, and therefore, Coriolis terms are neglected; however, the tests we present allow for sufficient testing of typical meteorological flows. Results compare well with other existing Eulerian (such as WRF-ARW) and nonhydrostatic CISL solvers

$^3$not in manuscript
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(such as the nonhydrostatic SLICE model). In the density current and gravity wave tests, we see that CSLAM-NH allows for stable time steps two times larger than that in an Eulerian model. In the highly-nonhydrostatic flow of the squall line test case, the maximum stable time step size is of similar magnitude as the Eulerian split-explicit model. The strong wind shear across the storm updraft imposes a time step limit in CSLAM-NH due to the Lipschitz stability condition (violation of which leads to the crossing of trajectories).

Plans to extend the nonhydrostatic solver to include orographic influences are also underway. This work involves transformation of the nonhydrostatic equations into a terrain-following height coordinate. In traditional semi-Lagrangian semi-implicit solvers, flow over topography has been found to trigger spurious resonances and time off-centering in the implicit scheme has been found to eliminate these noises. Thus far, without orography, we have found that our nonhydrostatic solver only requires time off-centering (β = 0.1) in the squall line case to maintain numerical stability. The nonhydrostatic solver with orography will allow us to test the conservative and consistent transport and stability of the new semi-implicit CISL discretization under the influence of a terrain-following coordinate.
Chapter 4

Extension to a two-dimensional (x-z) nonhydrostatic solver with transformed vertical coordinates

4.1 Introduction

Semi-Lagrangian semi-implicit (SLSI) schemes have been widely used in climate and numerical weather prediction (NWP) models since the pioneering work of Robert (1981) and Robert et al. (1985). The fully compressible nonhydrostatic equations permit fast-moving waves which limit the model time step size. The combination of a semi-Lagrangian advection scheme with semi-implicit treatment of these waves allows for larger stable time steps, and therefore, increased computational efficiency. Conservative semi-Lagrangian advection schemes, also known as cell-integrated semi-Lagrangian (CISL) transport schemes, are finite-volume methods that inherently conserve mass by tracking individual grid cells each time step (Rancic, 1992; Laprise and Plante, 1995; Machenhauer and Olk, 1997; Zerroukat et al., 2002; Nair and Machenhauer, 2002; Lauritzen et al., 2010). CISL transport schemes allow for locally (and thus globally) conservative transport of total fluid mass (such as dry air in the atmosphere) and constituent (i.e., moisture and tracer) mass.

However, some CISL schemes lack consistency between the numerical representation of the total dry air mass conservation, which we will refer to as the continuity equation, and constituent mass conservation equations (Jöckel et al., 2001; Zhang et al., 2008; Wong et al., 2013). Numerical consistency in the discrete tracer conservation equation requires the equation for a constant tracer field to correspond numerically to the discrete mass continuity equation; this consistency ensures that an initially spatially uniform passive tracer field will remain so.

To allow for large advection time steps, Lauritzen et al. (2010) developed a CISL transport scheme called the CSLAM (‘Conservative Semi-LAgrangian Multi-tracer’) transport scheme. The CSLAM scheme has recently been implemented in the National Center for Atmospheric Research
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(NCAR) High-Order Methods Modeling Environment (HOMME) and was found to be an efficient and highly scalable transport scheme for atmospheric tracers (Erath et al., 2012). To ensure consistent numerical representations of the continuity equation and other scalar conservation equations, Wong et al. (2014) proposed a new discretization of the semi-implicit CISL continuity equation using CSLAM. They showed that the new formulation can be straightforwardly extended to the scalar conservation equations in a fully consistent manner. Wong et al. (2013) also showed that any discrepancy between the numerical schemes can lead to spurious generation or removal of scalar mass. We refer to this nonhydrostatic atmospheric solver with conservative and consistent transport as CSLAM-NH.

Idealized 2D benchmark test cases for a density current, gravity wave, as well as a squall line, using CSLAM-NH have been performed in Wong et al. (2014). These test cases used flat bottom boundary conditions for simplicity. In the real atmosphere, the bottom fluid boundary is often not flat. Mountains act as a stationary forcing and generate horizontally and vertically propagating internal gravity waves in the atmosphere. Under certain atmospheric conditions they can also induce highly nonlinear flows such as wave amplification and breaking. Numerical simulations of these mountain waves have been extensively studied by many (e.g. Klemp and Lilly, 1978; Peltier and Clark, 1982; Durran and Klemp, 1983; Durran, 1986) and several of these cases have become benchmark tests in model development and intercomparison studies (e.g. Pinty et al., 1995; Bonaventura, 2000; Xue et al., 2000; Doyle et al., 2000; Melvin et al., 2010). To further develop CSLAM-NH as a viable nonhydrostatic atmospheric solver, we have incorporated orography into the model and have conducted a suite of these mountain-wave cases documented in the literature. The test suite includes linear hydrostatic and nonhydrostatic dry mountain waves, a highly nonlinear dry mountain wave with amplification and overturning of the waves, and a moist mountain flow with cloud and rain formation.

The paper is organized as follows. A model description of CSLAM-NH is given in section 4.2. In section 4.3, simulations from the suite of idealized mountain wave tests are presented. Finally, a summary is given in section 4.4.

4.2 Model description

4.2.1 Governing equations

The major modification to the model prognostic equations described in Wong et al. (2014) is the transformation of the vertical coordinate from geometric height to a terrain-following height coordinate. In addition to this modification, we have also included the treatment of the gravity-wave
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terms in the implicit solver. The previous version of CSLAM-NH solves the buoyancy terms in the vertical momentum equation explicitly using a two time-level extrapolation scheme. For a gravity-wave test originally proposed in Skamarock and Klemp (1994), the time-step limit was found to be restricted by the explicit treatment of these buoyancy terms (Wong et al., 2014). To circumvent this time-step restriction, an iterative approach is used to include these terms in the implicit solve. We will focus on the description of these two modifications and provide a basic description of the solver [readers are referred to Wong et al. (2014) for a more detailed description].

A height-based coordinate is used to avoid the complication of a time-varying vertical coordinate system, as is the case with mass (pressure) coordinates. The use of terrain-following coordinates substantially simplifies the bottom boundary condition when topography is present. For cell-integrated semi-Lagrangian advection, in a geometric height coordinate, approximated departure cell boundaries may intersect the orography and create more complex cell configurations (e.g., more cell edges/vertices, which complicate the subgrid-cell reconstruction). On a computational grid defined by terrain-following vertical coordinates, however, the lowest cell boundaries will always remain at the surface.

Following Gal-Chen and Somerville (1975), the 2D terrain-following height coordinate \( \zeta \) is expressed using the linear transformation

\[
\zeta = z - \frac{h(x)}{z_t - h(x)},
\]

where \( z(x, \zeta) \) is the physical height, \( h(x) \) is the terrain profile, and \( z_t \) is the height of the model top [with the bottom defined as \( z = h(x) \)].

The 2D governing equations expressed in \((x, \zeta)\)-coordinates are:

\[
\begin{align*}
\frac{\partial u}{\partial t} + \left(u \frac{\partial u}{\partial x}\right)_\zeta + \omega \frac{\partial u}{\partial \zeta} &= -\frac{1}{\rho_m} \gamma R_d \pi \left[ \frac{\partial \Theta_m'}{\partial x} + \frac{\partial (\zeta, \Theta_m')}{\partial \zeta} \right] + F_u, \\
\frac{\partial w}{\partial t} + \left(u \frac{\partial w}{\partial x}\right)_\zeta + \omega \frac{\partial w}{\partial \zeta} &= -\frac{1}{\rho_m} \gamma R_d \pi \frac{\partial (\zeta, \Theta_m')}{\partial \zeta} - g \tilde{\rho}_d \pi' + g \tilde{\rho}_m' \right] + F_w,
\end{align*}
\]

\[
\frac{\partial \Theta_m}{\partial t} + (\nabla \cdot \mathbf{v}) \Theta_m)_\zeta = F_\Theta, \\
\frac{\partial \tilde{\rho}_d}{\partial t} + (\nabla \cdot \mathbf{v}) \tilde{\rho}_d)_\zeta = 0, \\
\frac{\partial Q_j}{\partial t} + (\nabla \cdot \mathbf{v} Q_j)_\zeta = F_{Q_j},
\]

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p = p_0 \left( \frac{R_d \Theta_m}{p_0} \right) \gamma, \quad (4.7)

where \( \mathbf{v} = (u, w) \) is the horizontal and vertical wind components, \( \pi = (p/p_0)^\kappa \) is the Exner function, \( p_0 = 100 \text{ kPa} \) is the reference pressure, \( R_d = 287 \text{ J kg}^{-1} \text{ K}^{-1} \) is the gas constant for dry air, \( c_p = 1003 \text{ J kg}^{-1} \text{ K}^{-1} \) is the specific heat for dry air at constant pressure, \( c_v = 717 \text{ J kg}^{-1} \text{ K}^{-1} \) is the specific heat of dry air at constant volume, and the ratios \( \kappa = R_d/c_p \approx 0.286 \) and \( \gamma = c_p/c_v \approx 1.4 \). Perturbation variables from a time-independent hydrostatically balanced background state are used to reduce numerical errors in the calculations of the pressure-gradient terms (Klemp et al., 2007). The hydrostatically balanced background state is defined as \( d \bar{\rho}/dz = -\bar{\rho}g \). Flux-form variables are coupled to a scaled dry density adjusted to the transformed coordinate, \( \bar{\rho}_d = \rho_d/\zeta_c \), i.e. \( \Theta_m = \bar{\rho}_d \theta_m \) and \( Q_j = \bar{\rho}_d q_j \). The notations \( (\cdot)_\zeta \) refer to the spatial derivatives of \( \zeta \). Perturbation variables (primed) are defined via \( \Theta_m = \bar{\rho}_d(z) \tilde{\Theta}(z) + \Theta_m, \pi = \bar{\pi} + \pi', \rho_d = \bar{\rho}_d(z) + \rho'_d \), and the moist density \( \bar{\rho}_m = \bar{\rho}_d(1 + q_v + q_c + q_r) \), where \( q_v, q_c, \) and \( q_r \) are the mixing ratios for water vapor, cloud, and rainwater, respectively. The modified potential temperature \( \theta_m \) is defined as \( \theta_m = \theta(1 + d'/q_v) \) where \( d' \equiv R_v/R_d \approx 1.61 \).

Notations \( (\cdot)_\zeta \) denote evaluation at constant \( \zeta \), and \( (\nabla \cdot \mathbf{v})_\zeta = \delta_v(ub) + \delta_\zeta(ab) \) for any scalar variable \( b \). The variable \( \omega = d\zeta/dt \) is the vertical motion perpendicular to the coordinate surface. For simplicity, we assume a non-rotating atmosphere. The terms \( F_u \) and \( F_w \) represent diffusion, and \( F_\theta \) and \( F_Q \) represent diffusion as well as any diabatic source terms from parameterized physics.

The governing equations used in CSLAM-NH include the advective form of the momentum equations [(4.2), (4.3)] so that we can use a traditional semi-Lagrangian discretization. The flux-form advection for potential temperature, density, and moisture/passive scalar variables [(4.4), (4.5), (4.6), respectively] are solved using the conservative semi-Lagrangian scheme CSLAM. Pressure is a diagnostic variable given by the equation of state (4.7). Following Klemp et al. (2007), the pressure-gradient terms are written in terms of potential temperature. The recasting allows for coupling of the implicit pressure-gradient terms with the flux divergence term in the potential temperature equation. The compressible nonhydrostatic equation set is still exact and no approximations have been applied.

### 4.2.2 CSLAM — a cell-integrated semi-Lagrangian transport scheme

When advection terms are evaluated using an Eulerian scheme, the model time step sizes are restricted by the well-known Courant stability condition. To allow for larger advective time steps, the nonhydrostatic solver uses a cell-integrated semi-Lagrangian (CISL) transport scheme called the CSLAM (Conservative Semi-LAgrangian Multi-tracer) transport scheme developed by Lauritzen et al. (2010). This inherently conservative (both locally and globally) transport scheme is used to
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(a) Non-self-intersecting departure cell (b) Self-intersecting departure cell

Figure 4.1: Discrete departure cells in CSLAM-NH are approximated using straight edges (shaded in grey). The departure cell vertices (black circles) are computed using backward-in-time trajectories (arrows) from the vertices (white circles) of the Eulerian arrival grid cell (white box). The CSLAM transport scheme is stable as long as the discrete departure grid cells are (a) non-self-intersecting, and becomes problematic if (b) the departure cell self-intersects since the scheme is no longer mass-conserving.

solve the continuity and potential temperature equations, and for transport of any moist species or other tracers.

The stability criterion for the CSLAM transport scheme is limited by the trajectory approximations of the grid-cell vertices. To ensure stability in traditional semi-Lagrangian schemes, the Lipschitz stability condition requires that, in 1D, no trajectories in the space-time domain should intersect one another (Smolarkiewicz and Pudykiewicz, 1992). In the CSLAM scheme, the stability condition is slightly different in that the trajectories of neighbouring vertices may cross, as long as the discrete departure cells remain non-self-intersecting. In all test cases presented here, linear trajectories as described in Wong et al. (2014) are assumed. Figure 4.1a shows a discrete arrival grid cell (white box) originating from a non-self-intersecting discrete departure cell (grey box) with straight edges that are computed using the approximated displacement over one time step (arrows). As long as the departure cells remain non-self-intersecting, the scheme is stable and ensures global mass conservation. In Fig. 4.1b, a more distorted flow causes the departure cell edges to intersect. This ‘twisting’ of the departure cell causes adjacent departure cells to overlap. In such a case, the scheme is no longer mass-conserving and becomes unstable. The stability and accuracy of the
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CSLAM scheme in highly deformed flows may be improved by using higher-order trajectory approximations and/or higher-order approximations of departure cell boundaries. One such example is to use the parabolic (curved) departure cell edges that account for acceleration in the trajectory approximations developed by Ullrich et al. (2012). In the present study, we did not test any geometrical definitions other than quadrilateral departure cells, but the option could be explored in the future.

4.2.3 Discretized momentum equations

The momentum equations are solved in a traditional semi-Lagrangian semi-implicit manner, where the total derivatives \( \frac{du}{dt} \) and \( \frac{dw}{dt} \) are computed using a grid-point interpolation to the departure point. Bicubic Lagrange interpolation is used for all departure point evaluations. The two time-level discretizations of the momentum equations are

\[
\begin{align*}
\frac{u^{n+1}}{A} &= \frac{u^n}{D} + \Delta t (F_u)^n_D \\
&\quad - \frac{\Delta t}{2} \left\{ \frac{\gamma R}{\rho_m} \pi^x \left[ (\delta_x \Theta_m') \zeta + \delta_{\zeta} (\zeta_x \Theta_m') \right] \right\}^D_n \\
&\quad - \frac{\Delta t}{2} \left\{ \frac{\gamma R}{\rho_m} \pi^x \left[ (\delta_x \Theta_m') \zeta + \delta_{\zeta} (\zeta_x \Theta_m') \right] \right\}^A_{n+1},
\end{align*}
\]

(4.8)

and

\[
\begin{align*}
(1 + \mu \Delta t) \frac{w^{n+1}}{A} &= \frac{w^n}{D} + \Delta t (F_w)^n_D \\
&\quad - \frac{\Delta t}{2} \left\{ \frac{\gamma R}{\rho_m} \pi^z \left[ \delta_{\zeta} (\zeta_x \Theta_m') \right] - \frac{1}{\rho_m} \left[ \frac{g \tilde{\rho}_d \pi'}{\overline{\pi}} - g \tilde{\rho}_m' \right] \right\}^D_n \\
&\quad - \frac{\Delta t}{2} \left\{ \frac{\gamma R}{\rho_m} \pi^z \left[ \delta_{\zeta} (\zeta_x \Theta_m') \right] \right\}^A_{n+1} - \frac{1}{\rho_m} \left[ \frac{g \tilde{\rho}_d \pi'}{\overline{\pi}} - g \tilde{\rho}_m' \right] \right\}^A_{n+1},
\end{align*}
\]

(4.9)

where subscripts \( D \) and \( A \) denote evaluation at the departure and arrival grid points, respectively, and superscripts denote the time level. To reduce gravity wave reflection at the upper boundary, a Rayleigh damping term \(-\mu w\) is added to the vertical momentum equation, where the damping coefficient \( \mu \) is a function of height \( z \) and applied in the top layers of the domain. The spatial averaging operators are defined as

\[
\overline{\cdot} = \frac{1}{2} \left( \cdot \right)_{i,k} + \left( \cdot \right)_{i+1,k}, \quad \text{and}
\]

(4.10)
(\cdot)^{\xi} = \frac{1}{2} \left((\cdot)_{i,k} + (\cdot)_{i,k+1}\right), \quad (4.11)

and gradient operators as

\[ \delta_x(\cdot) = \frac{(\cdot)_{i+1,k} - (\cdot)_{i,k}}{\Delta x}, \quad \text{and} \]

\[ \delta_\xi(\cdot) = \frac{(\cdot)_{i,k+1} - (\cdot)_{i,k}}{\Delta \xi}. \quad (4.13) \]

The prognostic variable for vertical motion perpendicular to the terrain-following vertical coordinate \( \zeta \) is

\[ \omega^{n+1} = \zeta_x u^{n+1} + \zeta_w^{n+1}. \quad (4.14) \]

We use the following notations to combine the known rhs terms in the momentum equations:

\[ R_U \equiv u_D^n + \Delta t (F_u)_D^n - \frac{\Delta t}{2} \left\{ \gamma R_d \frac{\pi'}{\rho_m} \left[ \delta_x (\Theta'_m) \zeta + \delta_\xi (\zeta_x \Theta'_m \zeta) \right] \right\}_D^n, \quad (4.15) \]

\[ R_W \equiv w_D^n + \Delta t (F_w)_D^n - \frac{\Delta t}{2} \left\{ \gamma R_d \frac{\pi'}{\rho_m} \left[ \delta_\xi (\zeta_x \Theta'_m) \right] - \frac{1}{\rho_m} \left[ \frac{\pi'}{\pi} - g \tilde{\rho}'_m \right] \right\}_D^n, \quad (4.16) \]

the implicit pressure-gradient terms:

\[ PG_U = -\frac{\Delta t}{2} \left\{ \gamma R_d \frac{\pi'}{\rho_m} \left[ (\delta_x \Theta'_m) \zeta + \delta_\xi (\zeta_x \Theta'_m \zeta) \right]^{n+1} \right\}_A, \quad (4.17) \]

\[ PG_W = -\frac{\Delta t}{2} \left\{ \gamma R_d \frac{\pi'}{\rho_m} \left[ \delta_\xi (\zeta_x \Theta'_m) \right]^{n+1} \right\}_A, \quad (4.18) \]

and the implicit half of the buoyancy term:

\[ B_W = \frac{\Delta t}{2} \frac{1}{\rho_m} \left[ \frac{\pi'}{\pi} - g \tilde{\rho}'_m \right]^{n+1} \zeta. \quad (4.19) \]
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The subscripts in the notations denote the momentum equations to which the terms belong. Using (4.8), (4.9), and the notations above, the vertical momentum equation can be rewritten as:

\[
\omega^{n+1} = \frac{z}{R_\Omega} (1 + \mu \Delta t)^{-1} (R_W + B_W) + \frac{z}{R_\Omega} PG_U + \frac{z}{R_\Omega} (1 + \mu \Delta t)^{-1} PG_W. \tag{4.20}
\]

The notation \( R_\Omega \) is used here to represent all the known terms plus the implicit buoyancy term (4.19).

Often, off-centering of the time-averaged terms is needed in semi-Lagrangian semi-implicit time-stepping schemes to help eliminate computational noise, especially when orographic forcing is present and at large Courant numbers (e.g., Rivest et al., 1994). In CSLAM-NH, no off-centering was needed to attain the numerical stability in the solver for the test cases presented here.

### 4.2.4 Conservative and consistent flux-form equations

As noted by Lauritzen et al. (2006) and demonstrated in Wong et al. (2013) and Wong et al. (2014), when a numerical scheme different from the one used to evaluate the continuity equation is used to transport scalar variables, conservation of scalar mass will no longer be guaranteed, despite the use of a conservative transport scheme. The problem of numerical consistency in cell-integrated semi-Lagrangian schemes is resolved through the use of a new flux-form CISL continuity equation introduced in Wong et al. (2013) for the shallow-water equations and tested for a 2D nonhydrostatic atmosphere without topography (Wong et al., 2014). The new flux-form CISL continuity equation allows for a straightforward implementation of a CISL scalar transport scheme that ensures numerical consistency. Here, we further test the proposed formulation based on the CSLAM transport scheme for 2D idealized cases over mountains.

The potential temperature, continuity, and scalar-mass conservation equations are all solved consistently using the same numerical scheme presented in Wong et al. (2014):

\[
\hat{\Theta}_m^{n+1} = \Theta_{m,exp}^{n+1} + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (v^{n+1} \hat{\Theta}_m) \frac{\delta A^*}{\Delta A} \right] + \Delta t F_{\Theta_m} \frac{\delta A^*}{\Delta A}, \tag{4.21}
\]

and

\[
\tilde{\Theta}_m^{n+1} = \hat{\Theta}_m^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (v^{n+1} \hat{\Theta}_m^{n+1}) \right]. \tag{4.22}
\]

The flux divergence in terms of a corrective velocity \( v' \) in the semi-implicit correction term is
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defined as:

$$\nabla_{\text{eul}} \cdot (\Theta_m v) = \frac{1}{\Delta x} \left[ \Theta_m^x (u_r - \mathcal{F}_r / \Delta \zeta) - \Theta_m^x (u_l - \mathcal{F}_l / \Delta \zeta) \right]$$

$$+ \frac{1}{\Delta \zeta} \left[ \Theta_m^\zeta (\omega_b - \mathcal{F} / \Delta x) - \Theta_m^\zeta (\omega_b - \mathcal{F} / \Delta x) \right],$$

(4.23)

where \( \mathcal{F} = \mathcal{F}(u, \omega) \) are Lagrangian flux areas, computed as in Wong et al. (2014). The velocities \( u_r, u_l, \omega_b, \) and \( \omega_b \) are staggered velocities at the cell faces (Arakawa C grid).

In the semi-implicit flux-form equation, instead of linearizing around a mean reference state, we utilize \( \hat{\Theta}_m^{n+1} \) using the CSLAM transport scheme to ensure consistency of the semi-implicit correction term among all the scalar flux-form equations. Included in this CSLAM computation are all the terms to be integrated over the departure cell: the explicit conservative CSLAM solution (\( \Theta_m^{n+1, \exp} \)), a predictor-corrector term (the flux divergence term at time level \( n \)), explicit diffusion, and diabatic tendency (the latter two are combined in \( F_{\Theta_m} \)). The diabatic tendencies are approximated using values at the previous time level. The resulting approximation \( \hat{\Theta}_m^{n+1} \) (4.21) is then used in (4.22). The solution from (4.22) is the solution from the dynamics, and prior to any adjustment to saturation by a moist microphysics scheme.

Consistent formulations of the continuity equation and scalar mass conservation equations are straightforwardly discretized as:

$$\hat{\phi}^{n+1} = \phi^{n+1}_{\exp} + \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (v^n \hat{\phi}^n) \right] \frac{\delta A^*}{\Delta A}$$

$$+ \Delta t P_{\phi}^n \frac{\delta A^*}{\Delta A},$$

(4.24)

and

$$\tilde{\phi}^{n+1} = \hat{\phi}^{n+1} - \frac{\Delta t}{2} \left[ \nabla_{\text{eul}} \cdot (v^{n+1} \hat{\phi}^{n+1}) \right],$$

(4.25)

where \( \phi = \tilde{\rho}_d \) or \( Q_j \). Similar to (4.21), (4.24) combines the advected quantities in the explicit solution using the CSLAM scheme, the predictor-corrector flux divergence term, diffusion, and diabatic tendencies from the previous time level. The solution of the velocities at the new time level are used to compute the flux divergence in (4.25).
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4.2.5 Helmholtz equation

By eliminating $v^{n+1}$ in the potential temperature equation (4.22) using the horizontal and vertical momentum equations, we form the Helmholtz equation:

$$\tilde{\Theta}^{n+1} + \frac{\Delta t}{2} \left\{ \delta_x \left( PG_U \tilde{\Theta}_m^{n+1} \right) + \delta_\zeta \left[ (\xi U_{GZ})_m^{n+1} + \xi (1 + \mu \Delta t)^{-1} PG_W \tilde{\Theta}_m^{n+1} \right] \right\} =$$

$$\hat{\Theta}_m^{n+1} - \frac{\Delta t}{2} \left[ \delta_x \left( R_U \tilde{\Theta}_m^{n+1} \right) + \delta_\zeta \left( R_\Omega \tilde{\Theta}_m^{n+1} \right) \right], \quad (4.26)$$

where $PG_U$ and $PG_W$ are, as defined earlier, the implicit pressure-gradient terms expressed as functions of $\tilde{\Theta}_m^{n+1}$. All the terms on the rhs of (4.26) are pre-computed at the beginning of each time step, and the implicit buoyancy term in $R_\Omega$ is updated at each iteration of the Helmholtz equation solver (described next).

4.2.6 Iterative centered-implicit time-stepping scheme

The compressible Euler equations permit fast horizontally- and vertically-propagating acoustic and gravity waves. To alleviate the time-step limit due to acoustic waves, in the previous version of CSLAM-NH (Wong et al., 2014), an implicit time-stepping scheme was used to solve the pressure-gradient and mass-divergence terms. The remaining buoyancy terms were evaluated explicitly using a two time-level extrapolation scheme. The semi-implicit time integration scheme allowed the use of time steps much larger than those allowed in a classical explicit scheme, which would otherwise have been restricted by the speed of sound. The buoyancy terms responsible for gravity waves, however, imposed a restriction to the maximum stable time step.

Instead of evaluating the gravity wave terms explicitly using time extrapolation, we use an iterative approach for a more accurate and implicit treatment of these terms. The solution procedure can be summarized in two main components as follows. First, the departure cell areas are approximated using backward trajectories from the arrival grid cell vertices. The forcing terms ($R_U$, $R_\Omega$) and the explicit departure cell-averaged potential temperature, $\tilde{\Theta}_m^{n+1}$ [using (4.21)] are evaluated and form the RHS of the Helmholtz equation (4.26). The implicit buoyancy term $B_W$ in $R_\Omega$ is evaluated at time level $n$ as an initial estimate. The explicit departure cell-averaged density $\hat{\rho}_d^{n+1}$ [using (4.24)] is also pre-computed. The second component involves solving the linear Helmholtz equation for $\tilde{\Theta}_m^{n+1}$; here we use a conjugate gradient residual solver (Skamarock et al., 1997). The solution $\tilde{\Theta}_m^{n+1}$ is then back-substituted into the momentum equations (4.8) and (4.20) to get $u^{n+1}$ and $\omega^{n+1}$, respectively. Finally, the implicit buoyancy term $B_W$ in $R_\Omega$ is updated using (i) $\hat{\rho}_d^{n+1}$ by evaluating (4.25) and (ii) $\pi^{n+1}$ directly from $\tilde{\Theta}_m^{n+1}$ using the equation of state $\pi \equiv (R_\Omega \tilde{\Theta}_m/p_0) R/c_v$. At the end of the second component, the trajectories and forcing terms (first component of the procedure) are
recomputed using the latest solution of $u^{n+1}$ and $\omega^{n+1}$.

Depending on the test case, two to four iterations of each component are performed. For the nonlinear flow tests, iterating more than twice did not further improve the maximum stable time step size. For the linear cases, the maximum time step can be further increased by performing more iterations (iterating more than four times does not further improve stability). At each iteration, the Helmholtz solver converges progressively faster (since the latest estimate of $\tilde\Theta_{m}^{n+1}$ is used as the starting point). The iterative scheme is used for advancing the dry dynamics; after which, tracers are advected using (4.25) and the moist physics are called (once at each time step).

The use of an iterative centered-implicit scheme is found to substantially increase the stable time step size in CSLAM-NH at the expense of solving the Helmholtz equation more than once per time step. To demonstrate this behaviour, we conduct the gravity-wave test originally proposed in Skamarock and Klemp (1994), using CSLAM-NH as was done in Wong et al. (2014) with a grid spacing of $\Delta x = \Delta z = 1$ km and an imposed mean wind $\bar{U} = 20$ m s$^{-1}$. Wong et al. (2014) used an explicit treatment of the buoyancy terms and found that the maximum stable time step was restricted to $\Delta t = 38$ s [at a nominal advective Courant number (Cr) of 0.76]. In the current version of the iterative centered-implicit CSLAM-NH, we have found that for the same simulation, the maximum stable time step increased to 100 s, roughly by a factor of 2.6 (Cr = 2). For comparison, the maximum stable time step for an Eulerian split-explicit third-order Runge-Kutta time stepping scheme was 60 s (Cr = 1.2) (Wong et al., 2014).

Similar iterative approaches were found to improve numerical stability in other semi-Lagrangian solvers. In the Canadian Global Environmental Multiscale (GEM) model, Côté et al. (1998) discretized the governing equations in a fully implicit manner and used an iterative procedure to avoid solving a nonlinear Helmholtz equation. This procedure is also implemented in Melvin et al. (2010) for the vertical-slice nonhydrostatic solver using the ‘Semi-Lagrangian Inherently Conserving and Efficient’ (SLICE) transport scheme. An alternative predictor-corrector (thus, also iterative) approach was tested in the European Centre for Medium-Range Weather Forecasts (ECMWF) Integrated Forecast System (IFS) model by Cullen (2001). In that study, a positive improvement in accuracy was noticeable only when the advective velocities, in addition to the buoyancy terms, were iterated. Using an idealized analysis of acoustic modes in a 1D nonhydrostatic vertical column, Cordero et al. (2005) demonstrated the impact of using time-extrapolated and -interpolated trajectory computations on the numerical stability of a semi-Lagrangian centered-semi-implicit scheme. When extrapolation and large time steps were used for the trajectories, the vertical structure of the acoustic modes were found to be distorted (with spurious zeros forming with time). The time interpolation scheme on the other hand was found to be stable in all cases. The idealized analysis by Cordero et al. (2005) supports the findings in Cullen (2001) and the method used in Côté et al.
(1998), with a recommendation for time-interpolated trajectory computations (e.g. by repeating the first component of the CSLAM-NH solution procedure).

The disadvantage of this approach is that the linear Helmholtz equation for potential temperature $\Theta_m$ is solved a number of times with the buoyancy terms updated at the end of each iteration. However, the increased stability will allow a larger time step to be used and can help offset the added computational expense of solving the dry dynamics (calculated once at each time step). After the dry dynamics, the solver then advects passive tracers (once at each time step). With a larger time-step size, the total number of times tracers are advected during the entire simulation is reduced. Therefore, the overall execution time spent on scalar transport is also reduced. This reduction may have a significant impact on computational time, especially when the number of tracers used in chemistry applications is large.

### 4.2.7 Boundary conditions

Periodic-in-$x$ and free-slip top and bottom boundary conditions are applied in all our tests. The vertical velocities at the top and bottom boundaries are set to $\omega = 0$, and ensures no normal flux through them. The boundary conditions are implemented by extrapolating $\Theta_m$, $\rho_d$, and $\mu$ into the boundary.

### 4.2.8 Implicit Rayleigh damping

To prevent the reflection of vertically-propagating gravity waves along the rigid model top, a damping term, $-\mu w$, is added in the vertical momentum equation based on the scheme proposed in Klemp et al. (2008) and implemented in Melvin et al. (2010). The damping profile $\mu(z)$ proposed by Klemp and Lilly (1978) is used:

$$
\mu(z) = \begin{cases} 
\mu_{max} \sin^2 \left( \frac{\pi}{2} \frac{z - z_d}{z_t - z_d} \right) & \text{if } z > z_d, \\
0 & \text{if } z \leq z_d.
\end{cases}
$$

The profile is characterized by a gradual increase of viscosity with height, which is desirable to prevent any reflections that would otherwise occur from a sharp increase in viscosity. The damping layer starts from a user-specified height $z_d$ and extends to the top of the domain $z_t$. The values of $\mu_{max}$ are specified for each test case. Klemp et al. (2008) analyzed the reflection properties of this implicit Rayleigh damping layer. The scheme they proposed is slightly different from the one applied here; in particular, they proposed implementing the damping term as an adjustment step. The adjustment step approach includes an extra damping term that resembles vertical diffusion, in addition to the effect of a damping term $-\mu w$ added directly in the vertical momentum equation.
For smaller (nonhydrostatic) horizontal scales, however, the effect of the damping term dominates and there is little difference between the two approaches. Klemp et al. (2008) also provided some guidance in selecting a suitable $\mu_{\text{max}}$ value based on the reflection properties of the scheme. Based on their experimentation, smaller damping coefficients $\mu_{\text{max}}$ should be used for smaller dominant horizontal wavelengths.

### 4.3 Idealized test cases: results

#### 4.3.1 Linear mountain waves over bell-shaped mountain

To test the response of the nonhydrostatic solver to orographic forcing, two adiabatic linear mountain-wave simulations are conducted first. Both cases assume a simple hill profile $h(x)$ of a witch-of-Agnesi curve, defined as

$$h(x) = \frac{h_m a^2}{x^2 + a^2}, \quad (4.28)$$

with a small amplitude $h_m = 1$ m but different half-widths, $a$. Gravity waves generated by flow moving over a wide hill under conditions where $U/Na \ll 1$ are approximately hydrostatic and are vertically propagating (Smith, 1979). We simulate flow with a constant upstream wind speed $U = 20$ m s$^{-1}$, in an atmosphere initially in hydrostatic balance and isothermal at $T = 250$ K (equivalent to a stratification of $N^2 \approx 3.83 \times 10^{-4}$ s$^{-2}$, where $N^2 = g^2/c_p T$ for an isothermal atmosphere). The mountain half-width is set at $a = 10$ km to give $U/Na = 0.1$, such that nonhydrostatic effects are small for this broad low hill. The analytical steady-state solution of vertical velocity using the linear theory and fast-Fourier transform algorithm described in Smith (1980) is plotted for this flow in Fig. 4.2. The physical domain is 120 km wide and 25 km deep. The simulation is run for a nondimensional time $Ut/a = 30$ (equivalent to $t = 15000$ s) to ensure the solution has reached steady state. The numerical domain has dimensions $120 \times 100$ ($\Delta x = 1$ km and $\Delta z = 250$ m). A Rayleigh damping layer ($\mu_{\text{max}} = 0.1$ s$^{-1}$) is implemented in the top 10 km of the domain (approximately 1.5 times the vertical wavelength, $\lambda_z = 2\pi U/N = 6.4$ km).

Results from simulations using a small Courant number $Cr = 0.2$ and large $Cr = 1.5$ are shown in Fig. 4.3. An upstream tilt of the phase lines is observed, corresponding to energy originating from the ground (the mountain) and propagating upwards. As expected, the amplitude of the vertical velocity also increases with height ($\propto \rho^{-1/2}$), corresponding to the effect of wave amplification due to decreasing density at higher altitudes. The slight downstream tilt of the wave pattern with height is due to weak nonhydrostatic influences and is also observed in other nonhydrostatic models for the same test case (e.g. Melvin et al., 2010). The modelled vertical velocities of Fig. 4.3 compare very well with the exact linear solution shown in Fig. 4.2.
Figure 4.2: Analytical steady-state solution for the linear hydrostatic mountain waves obtained following Smith (1980).

Figure 4.3: CSLAM-NH simulation of a linear hydrostatic wave \( (U/Na \approx 0.1) \) for a low wide mountain showing vertical velocity \( w \) (in m s\(^{-1}\)) after \( T = 15000 \) s using (top) \( \Delta t = 10 \) s (Cr = 0.2) and (bottom) \( \Delta t = 75 \) s (Cr = 1.5). Contour interval is \( 5 \times 10^{-4} \) m s\(^{-1}\). Mean wind is from left to right.

For a narrow mountain \( (\bar{U}/Na \approx 1) \), the mountain waves are strongly nonhydrostatic. These waves are highly dispersive, with shorter horizontal scales propagating farther downstream with height, and scales less than \( 2\pi \bar{U}/N \) becoming evanescent. To simulate such a flow, the half-width \( a \) of the mountain is reduced to 1 km, and the initial background state has a constant stratification of \( N^2 = 1 \times 10^{-4} \) s\(^{-2}\). The impinging flow has an upstream wind speed of \( U = 10 \) m s\(^{-1}\) \( (\bar{U}/Na = 1) \). The analytical steady-state solution of vertical velocity obtained following Smith (1980) is plotted for this flow in Fig. 4.4. The domain is 144 km wide and 25 km deep. The numerical domain has dimensions \( 360 \times 100 \) grid cells (\( \Delta x = 400 \) m and \( \Delta z = 250 \) m). Even though the mountain is only
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Figure 4.4: Analytical steady-state solution for the linear nonhydrostatic mountain waves obtained following Smith (1980).

Figure 4.5: CSLAM-NH simulation of a linear nonhydrostatic wave \( (U/Na = 1) \) for a narrow mountain showing vertical velocity \( w \) (in m s\(^{-1}\)) after \( T = 9000 \) s using (top) \( \Delta t = 5 \) s (Cr = 0.125) and (bottom) \( \Delta t = 60 \) s (Cr=1.5). Contour interval is \( 6 \times 10^{-4} \) m s\(^{-1}\). Mean wind is from left to right.

marginally resolved at this model resolution, the configuration is kept for comparison purposes with Melvin et al. (2010). The Rayleigh damping layer is applied to the top 13 km of the domain (twice the length of \( \lambda_z \)) with \( \mu_{\text{max}} = 0.05 \) s\(^{-1}\).

Results from CSLAM-NH are shown in Fig. 4.5 for two different time step sizes (Cr = 0.125 and Cr = 1.5). As expected, far downstream of the mountain, the solutions exhibit a more pronounced (relative to the linear hydrostatic case of Figs. 4.3 and 4.2) downstream tilt of the phase due to the nonhydrostatic component of the waves, and the waves also decay with height (note: only part of the domain is shown in the figure). This solution also compares well with the analytical solution
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shown in Fig. 4.4.

4.3.2 Downslope windstorm

To test the nonhydrostatic solver in a highly nonlinear flow, a simulation of the famous downslope windstorm that occurred on 11 January 1972 in Boulder, Colorado (Lilly, 1978) is conducted. Strong surface winds, gusting to 55 m s$^{-1}$, were observed in Boulder, Colorado on that day. The windstorm has been a long-standing case for theory development and numerical model verification, e.g., Klemp and Lilly (1978); Peltier and Clark (1979); Durran (1986). More recently, Doyle et al. (2000) carried out a model intercomparison study of 11 different high-resolution models to assess their ability in numerically simulating the wave breaking process of this windstorm. Prior to Doyle et al. (2000), smoothed soundings were used to initialize the models; here, we use the same 12 UTC 11 January 1972 Grand Junction, Colorado sounding as in Doyle et al. (2000), where they showed that a more realistic simulation of the windstorm was generated.

The numerical set-up is based on Doyle et al. (2000). The mountain half-width is 10 km with a height of 2 km. The domain is 240 km wide and 25 km deep. The numerical domain dimensions are 240 $\times$ 125 grid cells ($\Delta x = 1$ km and $\Delta z = 200$ m). The time step sizes used in Doyle et al. (2000) ranged from 1 s to 12 s [the largest time step size of 12 s was run using the Durran and Klemp (1983) model that uses a time-splitting scheme with a small time step of 3 s]. To compare the results with these models, a similar time step size of 10 s is used in CSLAM-NH. A Rayleigh damping layer ($\mu_{\text{max}} = 0.05$ s$^{-1}$) is applied only in the top 7 km of the domain (18 $\leq z \leq$ 25 km) to prevent the damping of the physically significant wave breaking in the lower stratosphere. A fourth-order horizontal smoothing filter is applied with a coefficient $K_D = 1 \times 10^9$ m$^4$ s$^{-1}$, which smooths out any small-scale variations and helps maintain numerical stability in the model. Unlike most of the models in that study, no turbulence parameterization or any other explicit diffusion was used; turbulent dissipation is solely dependent on the hyperviscosity applied and any inherent numerical dissipation associated with the model discretization.

In the results presented within Doyle et al. (2000), all models produced significant strengthening of the winds on the lee of the mountain and wave breaking in the upper troposphere and stratosphere at time 3 h. Despite using identical initial conditions, however, significant differences were found among the model results due to differences in the model formulations (e.g. spatial and temporal discretizations, type of explicit diffusion used), as well as the nonlinearity of the flow.

The CSLAM-NH results at 3 h are presented in Fig. 4.6. The wave breaking regions in CSLAM-NH can be identified as the adiabatic (well-mixed) regions (Fig. 4.6a) and highly turbulent areas (Richardson number, $R_i < 0.25$) (Fig. 4.6c, where to be consistent with Doyle et al. (2000), the Richardson number $\text{sgn}(R_i)|R_i|^{0.5}$ is plotted). The Richardson number used in Fig. 4.6c is the bulk
Figure 4.6: CSLAM-NH simulation for the 1972 Boulder windstorm case (a) potential temperature $\theta$ (K) (with contour interval of 8 K), (b) horizontal velocity $U$ (m s$^{-1}$) (with contour interval of 8 m s$^{-1}$), and (c) Richardson number $\text{sgn}(R_i)|R_i|^{0.5}$ ($-5 \leq R_i \leq 1$ are plotted with contour interval of 0.5, following Doyle et al. (2000); grey contour shows negative values) at $T=3$ h using a time step $\Delta t = 10$ s.
Richardson number (dry),

\[ R_i = \frac{g/\theta(\Delta\theta/\Delta z)}{\left(\Delta u/\Delta z\right)^2}. \] (4.29)

For locally statically stable air \((R_i > 0)\), the critical Richardson number at which wind shear is strong enough to sustain turbulence and overcome the damping by negative buoyancy is 0.25. The wave breaking regions appear to be in the vicinity of \(12 \leq z \leq 16 \text{ km}\) and \(17 \leq z \leq 20 \text{ km}\), comparable to the results in the intercomparison study. An initial critical level at \(z = 21 \text{ km}\) (where \(U = 0\)) is also found to be damping in the CSLAM-NH model simulation, and traps the vertically-propagating gravity waves. The damping effect is evident in the smooth isentropes and lack of turbulence (large \(R_i\), not contoured) above that height.

The lateral position of the hydraulic jumps at time 3 h varied among the models given in Doyle et al. (2000), with several occurring over the leeslope and others farther downstream. The associated maximum leeslope winds from the 11 models were found to range from 43 m s\(^{-1}\) to 86 m s\(^{-1}\). In CSLAM-NH, the hydraulic jump feature is found on the leeslope, and the simulated maximum downslope wind speed at the surface (lowest model level) is located at 10.5 km downstream from the mountain crest at 56.6 m s\(^{-1}\) (Fig. 4.6b). Flow features aloft such as the flow reversal at \(5 \leq z \leq 10 \text{ km}\) that were present in many of the models in Doyle et al. (2000), is also present in the CSLAM-NH results. This weakening of the winds above the hydraulic jump was also observed in the aircraft flight data analysis (see, e.g., Fig. 2b in Doyle et al., 2000).

The hyperviscosity coefficients used by the models in the model intercomparison study ranged from \(1.1 \times 10^8\) to \(5.0 \times 10^9\) m\(^4\) s\(^{-1}\). Time series of simulated maximum downslope wind speeds using different diffusion coefficients in CSLAM-NH are given in Fig. 4.7. Results from varying the horizontal smoothing coefficient from \(1.5 \times 10^8\) to \(1 \times 10^9\) m\(^4\) s\(^{-1}\) show slight variation in the simulated maximum downslope wind speed, with values at time 3 h ranging from 53.1 m s\(^{-1}\) to 56.6 m s\(^{-1}\). The impact of using different magnitudes of horizontal smoothing is apparent once the waves begin to break, giving a maximum range of predicted downslope wind speeds of approximately 12 m s\(^{-1}\). The general trend of the downslope windstorm development, however, is similar with maximum surface winds of the simulation occurring at around 3 h, with weakening thereafter due to the limited horizontal extent of the domain and periodic lateral boundaries.

The maximum stable time step in CSLAM-NH for this wave breaking case is 20 s (when \(K_D = 5.0 \times 10^9\) m\(^4\) s\(^{-1}\) is applied). With a time step larger than 20 s, the errors of the linear trajectory approximations become large enough that the departure cells self-intersect as illustrated in Fig. 4.8. In this case, the flow is characterized by a strong horizontal shear of the vertical wind speeds as well as large vertical Courant number, \(C_{rz} \approx 3\) (not shown). Higher-order cell-edge approximations have been explored by Ullrich et al. (2012), and may help alleviate the time step limit by increasing the
accuracy of the area integration. Overall, CSLAM-NH is able to generate comparable results to the other models, and at a maximum time step size that is roughly double of those used in Doyle et al. (2000).

### 4.3.3 Moist flow over a mountain in a nearly neutral environment

The nonhydrostatic solver is tested for another nonlinear flow, but in this case, we also include the effects from moist processes. A simulation of saturated flow over a mountain in an initially nearly neutral environment is conducted. This test case also demonstrates the ability of the solver in producing realistic orographic precipitation. The simulation is based on the test cases presented in Miglietta and Rotunno (2005). Moisture in the atmosphere is an important factor in modifying flow over topography. Durran and Klemp (1983) studied the influence of moisture on mountain waves using numerical simulations. In both a linear mountain-wave test and a downslope-windstorm test, they found that the inclusion of upstream moisture can greatly reduce the amplitude of these waves relative to their dry analogs. As the mountain enhances lifting of the moist flow over the windward side, condensation commonly occurs, leading to clouds and precipitation. The downstream evaporation of these clouds and precipitation can reduce the static stability at these altitudes, and the air can become desaturated on the lee side of the mountain due to rainout processes and diabatic warming in the descent.

For a nearly neutral flow, Miglietta and Rotunno (2005) simulated the transition of saturated air upstream to unsaturated air downstream due to diabatic warming in the downward motion on the lee. The inverse Froude number $N_m h_m / U$ is near zero, indicating that the resistance due to gravity
Figure 4.8: A self-intersecting departure cell (highlighted in red with vertices marked by black circles) in CSLAM-NH when a large time step size of 25 s is used for the strongly sheared flow in the 1972 Boulder downslope windstorm case. Black circles indicate departure grid cell vertices, and white circles the Eulerian arrival grid cell vertices. Arrows symbolize the computed backward-in-time trajectories. Trajectories and the arrival grid cell associated with the self-intersecting departure cell are highlighted in red.

is minimal and the flow can freely translate over the mountain.

To include moisture effects when determining local static stability, Lalas and Einaudi (1974), and later verified by Durran and Klemp (1982), derived an expression for the moist Brunt-Väisälä frequency:

\[
N_m^2 = g \Gamma \left( \frac{d \ln \theta}{dz} + \frac{L_v}{c_p T} \frac{dq_s}{dz} \right) - \frac{g}{1 + q_w} \frac{dq_w}{dz},
\]

where \( T \) is the absolute temperature, \( q_s \) is the saturated water vapour mixing ratio, \( q_w \) is the total water mixing ratio, and

\[
\Gamma = \frac{1 + \frac{L_v}{c_p T} \frac{\partial q_s}{\partial \ln \theta} \bigg|_{\pi}}{1 + \frac{L_v}{c_p T} \frac{\partial q_v}{\partial \ln \theta} \bigg|_{\pi}},
\]

is the ratio of the moist to dry adiabatic lapse rates. (All other variables are as defined previously.)
A few more specifics regarding the generation of the moist neutral sounding that supplements the derivation presented in Miglietta and Rotunno (2005) are given. Following the procedure in Miglietta and Rotunno (2005), to generate the initial sounding of a specific $N_m$, a first-order ordinary differential equation is solved. To create the initial nearly neutral sounding, the first-order ordinary differential equation for potential temperature is solved iteratively based on a specified surface temperature ($15^\circ{}C$) and reference pressure ($p_0 = 100$ kPa). To be consistent with Miglietta and Rotunno (2005), the Wexler’s formula for saturated vapour pressure (in mb) is used:

$$e_s(T) = 6.11 \exp \left( \frac{17.67(T - 273.15K)}{T - 29.65K} \right).$$  \hspace{1cm} (4.32)

The definition for $q_s = e_s(p - e_s)$, where $e = R_d/R_v$ is used to derive $\partial q_s/\partial \ln \theta|_\pi$ in (4.31). First, differentiating $q_s$ with respect to $\ln \theta$ at constant $\pi$ gives

$$\frac{\partial q_s}{\partial \ln \theta} \bigg|_\pi = \frac{q_s}{e_s} \frac{p}{p - e_s} \frac{\partial e_s}{\partial \ln \theta} \bigg|_\pi,$$  \hspace{1cm} (4.33)

and differentiating (4.32) (using $T = \pi \theta$) with respect to $\ln \theta$ at constant $\pi$ gives the expression

$$\frac{\partial e_s}{\partial \ln \theta} \bigg|_\pi = e_s T \frac{17.67(243.15)}{(T - 29.65)^2}.$$  \hspace{1cm} (4.34)

To find $\theta(z)$ for a specific $N_m$, (4.30) must be iterated to convergence ($10^{-12}$) at each pressure level (or height) since $q_s = q_s(\pi, \theta)$ and $\Gamma$ are also functions of the unknown. To get the pressure at each height, the hydrostatic equation is used:

$$\frac{\pi_{j+1} - \pi_j}{\Delta z} = - \frac{g}{c_p} \frac{1 + q_w}{\bar{T}_m}.$$  \hspace{1cm} (4.35)

For each model level $j$, the discrete form of the ODE solving for $\theta$ at height $z$ is

$$\ln \theta_{j+1} + \frac{L_w}{c_p T} (q_{s,j+1} - q_{s,j}) - (q_{w,j+1} - q_{w,j}) \left( \frac{1}{(1 + q_w)\Gamma} \right)^z = \ln \theta_j + \frac{N^2 m}{g\Gamma} (z_{j+1} - z_j).$$  \hspace{1cm} (4.36)

[Note: Miglietta and Rotunno (2005) expresses this equation in terms of $(T, p)$]. Other aspects of the Kessler microphysics scheme also require modification. Following Miglietta and Rotunno (2005), no autoconversion from cloud water to rain is permitted in the first five hours to allow for initial adjustment of the flow to the impulsive introduction of terrain. For a consistent definition of
$q_s$ throughout the model, the production of cloud water due to saturation is also modified:

$$\frac{dq_s}{dt} = \frac{q_v - q_s}{1 + \frac{L_v}{c_p}(\frac{dq_v}{dT})|_p},$$

(4.37)

where, based on the Wexler’s equation for $e_s$:

$$\frac{\partial q_s}{\partial T}|_p = \frac{q_s p}{p - e_s (T - 29.65)^2}.$$  

(4.38)

Miglietta and Rotunno (2005) used a small $N_m^2 = 3 \times 10^{-6}$ s$^{-2}$ to represent a nearly neutral troposphere due to the limitations of the single machine precision accuracy of their model. They found that using any smaller $N_m$ led to solutions that were apparently convectively unstable. The CSLAM-NH solver has machine double precision accuracy, so for this moist neutral flow case, an initial $N_m = 0$ in the troposphere is applied. Simulations using a range of ‘small’ $N_m^2 \sim 10^{-11}$ in the initialization step show solutions similar to applying $N_m = 0$ and resemble those in Miglietta and Rotunno (2005) more than using their $N_m^2 = 3 \times 10^{-6}$ s$^{-2}$. An initial $N_m^2 = 4.84 \times 10^{-4}$ s$^{-2}$ is used for the isothermal stratosphere.

Two mountain cases with different heights, $h_m = 700$ m and 2 km, were chosen from Miglietta and Rotunno (2005) for their distinct differences in orographic distribution of moisture. Both test cases are run using the Witch-of-Agnesi curve with a half-width of 10 km. The same numerical domain that is 800 km wide and 20 km deep is used, and the grid dimensions are $400 \times 80$ grid cells ($\Delta x = 2$ km and $\Delta z = 250$ m). In both cases, a mean wind $\overline{U} = 10$ m s$^{-1}$ is applied. The atmosphere is initially saturated ($q_v \equiv q_s$) with constant cloud-water mixing ratio $q_c = 0.05$ g kg$^{-1}$ set everywhere in the domain to prevent the atmosphere from becoming subsaturated due to the impulsive introduction of the mountain at initial time. The Rayleigh damping layer ($\mu_{\text{max}} = 0.1$ s$^{-1}$) is applied in the top 5 km of the domain. Second-order filters in the horizontal and vertical directions are applied with coefficients 3000 and 3 m$^2$ s$^{-1}$, respectively. The Prandtl number is 3. This configuration is the same as that in Miglietta and Rotunno (2005).

Both cases suggest a desaturation of the air downstream of the mountain with time. Miglietta and Rotunno (2005) noticed in their simulations that for intermediate mountain heights (500 m $\leq h_m \leq 1500$ m) the unsaturated region downstream of the hill unexpectedly extends upstream as well. A later study by Keller et al. (2012) showed that this upstream extent of the subsaturated air is due to local adiabatic descent and warming caused by a transient upstream-propagating gravity wave, a fundamental feature of a two-layer two-dimensional atmosphere with topography introduced impulsively. The purpose of performing the test case as prescribed in Miglietta and Rotunno
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(2005) with a mountain 700 m high is to ensure that CSLAM-NH can generate comparable results to models used in the literature, such as that in Miglietta and Rotunno (2005) who used the Weather and Research Forecasting (WRF) model v1.3.

Fig. 4.9 shows the solution from CSLAM-NH [c.f. Fig. 5d of Miglietta and Rotunno (2005)] using a time step size of 20 s. The white region indicates subsaturated air, as described previously. Although the upstream region of the subsaturated air in Miglietta and Rotunno (2005) extends farther upstream \((x = -100 \text{ km})\) than that found using CSLAM-NH, the solution from CSLAM-NH compares very well with that obtained in Miglietta and Rotunno (2005). The maximum stable CSLAM-NH time step size is 50 s with two iterations of both components in the iterative centered-implicit scheme.

Fig. 4.10a shows the CSLAM-NH cloud-water mixing ratio at time 5 h 10 mins (10 mins after autoconversion of rain is permitted) of a simulation using \(\Delta t = 20 \text{ s}\) for the large-amplitude mountain \((h_m = 2 \text{ km})\) case [c.f. black contours in Fig. 8a in Miglietta and Rotunno (2005)]. Similar to the results presented in Miglietta and Rotunno (2005), no upstream region of the subsaturated air is found. In addition, the formation of convective cells due to the reduction of local static stability downstream of the mountain is also detected in the CSLAM-NH simulation. The instability is found to be primarily associated with a hydraulic jump feature downwind. Fig. 4.10b shows the rainwater
mixing ratio for the same simulation time as in Fig. 4.10a.

Compared to the results in Miglietta and Rotunno (2005), CSLAM-NH indicates more rain spillover to the lee of the mountain (c.f. grey contours in Fig. 8a in Miglietta and Rotunno (2005)). Simulation of our case using an Eulerian split-explicit model similar to the one used in Miglietta and Rotunno (2005) shows virtually the same distributions of cloud- and rainwater as in the CSLAM-NH simulation (Fig. 4.10). The similarity of the CSLAM-NH solution to that of the second Eulerian model seems to suggest that the discrepancy is not specific to CSLAM-NH and may be related to certain aspects of the initialization procedure. Miglietta and Rotunno (2005) suggested that their simulations were sensitive to small changes to $N_m \approx 0$. If there is a slight discrepancy between the value of $N_m$ specified in the initialization than that used in Miglietta and Rotunno (2005), the flow dynamics may be altered. In this situation, the greater amount of waterloading to the lee of the mountain could imply a lower effective terrain height ($N_m h_m / U$), i.e. lower stability and/or stronger winds, such that the advection of the hydrometeors happens at a faster time scale than the fallout of precipitation.

Figure 4.10: (a) CSLAM-NH cloud-water mixing ratio $q_c$ (g kg$^{-1}$) at time 5 h 10 mins from an initially saturated nearly neutral flow (with an initial $q_c = 0.05$ g kg$^{-1}$) over a 2 km mountain. White region above ground indicates subsaturated air ($q_c = 0$ g kg$^{-1}$) (b) CSLAM-NH rain-water mixing ratio $q_r$ (g kg$^{-1}$) at the same simulation time.
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4.3.4 Computational performance (This section is not in the manuscript.)

The computational expense associated with the iterative centered-implicit scheme in CSLAM-NH is examined. The iterative scheme allows a larger CSLAM-NH time-step size, at the expense of solving the Helmholtz equation more than once. Taking a larger time step increases computational efficiency by requiring fewer time steps; however, it may also slow down the convergence rate in the Helmholtz solver. The moist neutral flow described in section 4.3.3 has the greatest complexity of topographical and latent heating effects and will be used to examine some of the computational aspects in CSLAM-NH.

To examine whether the larger time steps allowable by the iterative scheme actually save computational time, simulations using CSLAM-NH are made for a range of time-step sizes allowable by the iterative solution procedure. Fig. 4.11 shows the computational times required for each time-step size as compared to using $\Delta t = 20$ s (which is the time-step size used in section 4.3.3). Without using the iterative centered-implicit scheme, the maximum stable time-step size is 5 s. The smaller time step required a total computational time roughly 23% more (dashed line in Fig. 4.11) than that in section 4.3.3. The solid line shows the computational times using two iterations for time-step sizes between 10 and 50 s.

Using the iterative scheme to double the time-step size to $\Delta t = 10$ s increases the computational time by 9% as compared to not using the iterative scheme. The added computational expense stems from the iterations and the slower convergence in the Helmholtz solver. Comparing to $\Delta t = 20$ s, the time step is reduced by half. However, a reduction of time-step size by half does not double the computational time, which indicates that some components of the solver are running more efficiently at smaller time steps, such as the elliptic solver attaining faster convergence.

When the time-step size is increased to 30 s, an improvement in the solver efficiency is observed. The larger time-step size is able to reduce the computational time by 13%. When the time-step size is increased further to $\Delta t = 40$ s, the computational time is reduced by another 4%, and by another 3% when increased to $\Delta t = 50$ s. The negative impact of the slower Helmholtz solver convergence rate on the model performance is evident at the larger time-step sizes. Although there is still improvement in the net efficiency when using large time steps, the benefit is greatly hindered by the elliptic solver. In comparison to the non-iterative stable time-step size, the iterative scheme improves the overall efficiency by about 43%. In the iterative scheme, the need to recompute the trajectories (briefly discussed in section 4.2.6) was found to help stabilize CSLAM-NH in the numerical experiments. The stability properties of the trajectory recomputations in CSLAM-NH may be worth further investigation.

The distribution of the computational expense of the current CSLAM-NH solver can be sep-
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Figure 4.11: Computational times for the moist neutral flow over a 2 km mountain using different CSLAM-NH time-step sizes ($\Delta t$). Times are normalized to that using $\Delta t = 20$ s for comparison purposes. The solid line indicates computational times using the iterative centered-implicit scheme. Dashed line indicates using the non-iterative CSLAM-NH with $\Delta t = 5$ s.

The computational expense is heavily skewed towards the elliptic solver. The total computational time for the moist neutral flow case using a time-step size of 50 s (372 time steps) is distributed as follows. (Note: the following discussion accounts for 99.7% of the total computational time, while the neglected 0.3% is from the initialization procedure and a limited number of I/O processes.) The computational expense is dominated by the solution procedure of the dry dynamics (96.5%) and in particular, by the elliptic solver, which accounts for 86.1% of the total computational time. The physics component is defined as the components unrelated to the dry dynamics, i.e. all tracer transport processes and subgrid-scale physics, such as the microphysics parameterization scheme. In CSLAM-NH, this component accounts for the remaining 3.2% of the total computational time.

In the current development of CSLAM-NH, the conjugate-residual method in Skamarock et al. (1997) is used to solve the Helmholtz equation that arises from the semi-implicit time-stepping scheme. The conjugate-residual solver is flexible and allows the Helmholtz equation to have a variable coefficient structure. However, without a good preconditioner, the scheme has a slow convergence rate. A possible way of improving the efficiency of the Helmholtz solver in CSLAM-NH is by relaxing the stopping criterion. Analogous to the results found in Smolarkiewicz et al. (1997) for the anelastic equations, Skamarock et al. (1997) noted that for elastic systems (such as that in CSLAM-NH), the stopping criteria in conjugate residual solvers need not converge to machine pre-
cision, which is the current implementation in CSLAM-NH. Rather, the stopping criterion can be determined through a more physical justification of a small change in the divergence solution relative to the mean flow. An examination of whether CSLAM-NH model behaviour changes with more relaxed levels of convergence will help determine if the stopping criterion can be eased off to improve efficiency. In CSLAM-NH, each call to the Helmholtz solver in the iterative centered-implicit scheme may also require a different level of convergence.

Other elliptic solvers that could be explored to increase the efficiency include the use of preconditioners in residual solvers (Thomas et al., 1997) and the multigrid method (Fulton et al., 1986; Buckeridge, 2010). In a multi-processor environment, an efficient parallelizable geometric multigrid solver has recently been explored by Müller and Scheichl (2014). The authors demonstrated that comparing to other elliptic solvers (algebraic multigrid methods and preconditioned conjugate residual solvers), the geometric multigrid method is roughly 5 to 10 times faster. The use of such a solver can likely help improve the efficiency of CSLAM-NH by an order of magnitude and for it to become on a par with that of the Eulerian solver, closing the gap between the two computational times needed when the elliptic solve dominates the run time in CSLAM-NH (e.g., Fig. 4.12a). As the purpose of this dissertation is to develop a nonhydrostatic semi-implicit cell-integrated semi-Lagrangian solver, and not Helmholtz solvers (as these are an entire field in itself), the development of efficient Helmholtz solvers is not explored here. However, when CSLAM-NH is to be implemented in a more comprehensive weather and climate model, advances in the field such as those in Müller and Scheichl (2014) can be considered.

Passive tracers are not physically coupled to the dry dynamics, but are passively advected using the solution of the flow at the end of each dry dynamics step. Using a single processor, the introduction of more passive tracers, in addition to the existing moisture species (water vapour, cloudwater, and rainwater), therefore should increase the computational time in a linear fashion. Shown in Fig. 4.12a are the CPU times for CSLAM-NH ($\Delta t = 50$ s) and an Eulerian solver. This Eulerian solver is the same as the second comparison Eulerian solver described in section 4.3.3 and is run with the same number of tracers with $\Delta t = 20$ s (and a small time step $\Delta \tau = 2$ s). As expected, the times increase linearly with each additional tracer. The maximum number of 16 passive tracers is limited by the available memory on the workstation.

As mentioned earlier, for a small number of tracers, the computational time in CSLAM-NH is dominated by the elliptic solver. As the number of tracers in the model increases, the computational expense shifts towards expenses related to the tracer transport scheme. In each call to the CSLAM-NH tracer transport (advection) subroutine, computations using the explicit CSLAM transport scheme and of the corrective fluxes for the “semi-implicit correction term” are made. The computations of the corrective fluxes increases the computational expense by about 26% per time
Figure 4.12: Comparison of the computational times using CSLAM-NH and an Eulerian split-explicit solver. (a) CPU times (in seconds) for the two solvers for a range of tracer counts. (b) Projected computational times using best linear fits. (c) Ratio of CPU times of CSLAM-NH to the Eulerian solver.

Because the total required computational time is almost directly proportional to the number of tracers, one can approximate the time required ($T$) for a number of tracers ($\#_{\text{tracers}}$) using the following best linear fits:

\[
T_{\text{CSLAM-NH}} = 10.017 \cdot \#_{\text{tracers}} + 1497.75 \quad (r^2 = 0.9895),
\]

\[
T_{\text{Eulerian}} = 5.060 \cdot \#_{\text{tracers}} + 132.63 \quad (r^2 = 0.9987).
\]

The best linear fits are plotted as dashed lines in Fig. 4.12b. The $y$-intercept represents the computational base time of the respective solver (mostly dependent on the dry dynamics; in CSLAM-NH, mostly on the Helmholtz solver), and the slope indicates the cost associated with advecting additional tracers. For this case (i.e., the test flow and the corresponding maximum stable time-step size), the cost of the cell-integrated transport scheme in CSLAM-NH is roughly double of that in
the Eulerian solver (estimated using the ratio of the two slopes). The cost of the tracer transport schemes can also be visualized by projecting the computational time for a very large number of tracers, at which point, tracer advection dominates the computational expense. For example, Fig. 4.12c shows that, when projected for 800 tracers, the ratio of the two solvers’ computational times approaches two.

For the current version of CSLAM-NH to be competitive with the Eulerian split-explicit solver for a large number of tracers, the maximum CSLAM-NH stable time-step size (based on this moist neutral flow case) will need to be roughly five times of that of the Eulerian solver. To demonstrate this, the Eulerian time step is reduced to $\Delta t = 10$ s. The linear relationship between CPU time and number of tracers for the Eulerian solver [as in (4.39) and (4.40)] is

$$T_{\text{Eulerian}} = 10.653 \cdot \#\text{tracers} + 218.41 \quad (r^2 = 0.9977).$$  

(4.41)

For the nonlinear test cases, the maximum stable CSLAM-NH time-step size is found to be limited by self-intersecting departure cells (as in Fig. 4.8). Application of artificial dissipation in these regions may help prevent the occurrence of these departure cells, and increase the stability of CSLAM-NH.

The results in this section indicate that the cost effectiveness of scalar transport in CSLAM-NH is limited in a single-processor setting. The Eulerian split-explicit solver uses small time steps to handle fast-moving acoustic waves and a Runge-Kutta 3rd-order time-integration scheme, that requires solving the dry dynamics three times. Despite having to transport passive scalars three times in the Runge-Kutta time-stepping scheme, the Eulerian solver is still more efficient. The scalar transport code in CSLAM-NH is likely under-optimized in minor aspects. For example, for subgrid-cell reconstruction purposes, ghost cells are filled at each time step in the advection subroutine in CSLAM-NH. The Eulerian solver does not include filling of any ghost cells (whereas in a limited area model, the lateral boundary conditions will likely require some ghost cell specifications).

The performance of CSLAM-NH will likely compare very differently on multiple processors, based on the results related to the recent effort of Erath et al. (2012). The authors implemented and optimized the CSLAM transport scheme to run in HOMME, one of the dynamical core options in CAM (see the introduction of this chapter for definitions of the acronyms). CAM with the dynamical core HOMME is collectively referred as ‘CAM-SE’ [since HOMME uses a spectral element (SE) method] (Dennis et al., 2012). Comparing to the existing CAM-SE tracer transport scheme, which is a three-stage second-order Runge-Kutta time-stepping scheme, the CSLAM transport scheme can use a larger time step and requires only one call to CSLAM per time step (as opposed to three calls in the existing scheme). The computational performance of using the CSLAM transport scheme was
found to be much more efficient and more scalable than the CAM-SE advection scheme. The authors found that the CSLAM scheme was able to outperform the existing scheme, not because of fewer floating-point operations, but largely because the CAM-SE advection scheme required much more (approximately ten times) communication time than CSLAM when a large number of processors are used. Therefore, in a parallel environment and for a large number of tracers, CSLAM-NH may still have an advantage over an Eulerian solver that uses a multi-stage Runge-Kutta time-stepping transport scheme.

Finally, another factor related to the computational efficiency in the solvers is the number of times the physics parameterization schemes are called. In both solvers, a straightforward time-splitting approach is used to couple the dynamics to the physics (in this case, to the cloud microphysics subroutine). The time-splitting approach is defined as the sequential calling of the dynamics and physics, so that the solution from the dry dynamics is used as input to the physical parameterization schemes. In both solvers, the microphysics scheme is called once at each time step. Because larger time steps are used in CSLAM-NH, fewer calls are made to the microphysics scheme, which help reduce the computational expense.

4.4 Summary

A nonhydrostatic atmospheric solver (CSLAM-NH) that uses a new discrete formulation of the semi-implicit continuity equation for cell-integrated semi-Lagrangian transport schemes is further tested for flows over idealized orography. Here, the solver using the Conservative Semi-LAgrangian Multi-tracer (CSLAM) transport scheme is tested against various idealized mountain-wave cases and exhibits accurate and stable behaviour under the influence of a terrain-following height coordinate. An implicit Rayleigh damping layer is also implemented in this extended version of CSLAM-NH to help prevent unphysical reflection of vertically-propagating gravity waves at the model top.

The new discrete semi-implicit continuity equation used in CSLAM-NH allows for a straightforward implementation of consistent flux-form equations for scalars in the model. This aspect of the model is important in ensuring inherent mass conservation of these scalars, such as moisture and chemical species, and may prove to be important in longer NWP and climate simulations. The time integration of both the gravity and acoustic waves are handled implicitly in the solver using an iterative centered-implicit scheme. The iterative scheme allows for larger maximum stable time step sizes at the expense of solving the linear Helmholtz problem in the dynamics more than once. As the same time step size is used for tracer transport in CSLAM-NH, these larger time steps will consequently reduce the number of tracer advection steps per simulation, which may help compensate for the added expense. Moreover, at each time step, the solution procedure for the dry dynamics
is carried out only once, and then followed by the transport of any tracers in the solver. In large climate and chemistry models, the computational cost associated with the parameterized physics and the transport of the many (order of $10^2$) tracer species is likely to outweigh that associated with the dynamics. The computational ‘burden’ of tracer transport makes the selection of a multi-tracer efficient transport scheme, such as the CSLAM transport scheme, important.

Three idealized test cases available from the literature were used to verify the stability and accuracy of the proposed solver over topography. Simulations of linear hydrostatic and nonhydrostatic mountain waves compared well with numerical solutions from the literature. The simulation of a highly nonlinear wave-breaking case of the 11 January 1972 Boulder windstorm highlighted the ability of the solver to handle highly-sheared flow at large time steps. Due to the strong nonlinearity of the flow, the simulations from the models used in the intercomparison study of Doyle et al. (2000) varied in their fine-scale features. Although there is limited predictability of the precision of these features, all models, including CSLAM-NH (the simulation of which is presented here), showed similar main features of the windstorm, such as the locations of the wave breaking regions and hydraulic jump downstream of the mountain. Finally, moist nearly neutral orographic flows based on Miglietta and Rotunno (2005) are tested. Two mountain profiles were used: a lower 700-m tall mountain and a much higher 2 km mountain. For the lower mountain case, CSLAM-NH shows comparable results with those in Miglietta and Rotunno (2005), including downstream and upstream regions of subsaturated air. For the higher mountain case, there is more rain spillover to the leeside of the mountain as compared to the results presented in Miglietta and Rotunno (2005). However, similar solutions are found using another comparison Eulerian split-explicit model, which suggests that certain aspects (e.g., initialization) of the model other than model formulation may be causing the discrepancy, and that the discrepancy is not specific to CSLAM-NH.

In its current state of development, CSLAM-NH is a two-dimensional prototypical nonhydrostatic atmospheric solver in Cartesian geometry that has shown promising potential for weather and climate applications. Attractive features of this solver include the consistent formulation of the semi-implicit cell-integrated semi-Lagrangian continuity and scalar conservation equations, in conjunction with the inherently conservative multi-tracer CSLAM transport scheme. Further development work (e.g. implementation of three-dimensional CSLAM transport, extension of the scheme to a sphere) remains for the solver to be implemented as a dynamical core in a full NWP and climate model.
Chapter 5

Conclusion

5.1 Summary of contributions

In this dissertation, an alternative cell-integrated semi-Lagrangian (CISL) semi-implicit nonhydrostatic solver for the atmosphere is presented. Existing CISL semi-implicit solvers either do not use consistent numerical schemes in transporting air and tracer mass and require iterations to improve consistency between the discrete equations (Thuburn et al., 2010), or solve a nonlinear Helmholtz equation, as proposed by Thuburn (2008).

A novel, easy-to-implement flux-form semi-implicit time-stepping scheme for CISL solvers is proposed here. This scheme features a new discrete semi-implicit continuity equation that can be straightforwardly extended to other constituent-conservation equations. The approach works by eliminating the dependence on a mean reference state. The implicit system still forms a linear Helmholtz equation that can be solved using existing elliptic solvers. The proposed solver is tested in two dimensions using nine idealized test cases. Most of these cases are used by other model developers as benchmark tests for dynamical cores in atmospheric models. Results from these test cases show that the new nonhydrostatic solver produces comparable results, and shows potential for further development and implementation in a more comprehensive weather model.

The development of the two-dimensional nonhydrostatic prototype solver for the atmosphere can be summarized as follows.

- The initial testbed for the prototype solver is the shallow-water equations (SWE) system. Chapter 2 provides a detailed description of the proposed discrete semi-implicit height equation. The SWE solver utilizes the conservative semi-Lagrangian transport scheme CSLAM to ensure local mass conservation. The SWE solver, named CSLAM-SW (after the transport scheme), uses a new semi-implicit formulation to ensure that air mass and tracer constituents are transported in a consistent manner. CSLAM-SW is shown to be stable and accurate at a Courant number of 2.5 for a highly nonlinear barotropic jet. Results from a different solver with inconsistent transport schemes showed that numerical errors in the passive advection of
the specific concentration of a constituent grows with time step size and nonlinearity of the flow. Moreover, the application of shape-preserving schemes to the tracer mixing ratio becomes ineffective. Using CSLAM-SW, these errors are successfully eliminated (reduced to machine roundoff).

- Nonhydrostatic modelling using the CSLAM transport scheme and a semi-implicit time integration scheme is performed for the first time (Chapter 3). The proposed discrete semi-implicit height equation for the SWE solver in Chapter 2 is extended and tested for the two-dimensional nonhydrostatic moist Euler equations in the vertical plane. The nonhydrostatic solver is coupled to an existing microphysics scheme to represent subgrid-scale diabatic effects due to phase changes. CSLAM-NH solutions for a density-current test case and gravity-wave test compare well with those presented in the literature. The gravity-wave test highlights the need to integrate the buoyancy terms in the vertical momentum equation in an implicit manner (addressed in Chapter 4). A third idealized test case of a 2D squall line shows comparable results to an existing Eulerian nonhydrostatic solver [similar to the one used in the Weather Research and Forecasting Advanced Research and Weather (WRF-ARW) model]. The mixing ratio error induced by the lack of numerical consistency at the end of a two-hour squall line simulation is shown to be on the order of 1 part in 100.

- Test cases with the inclusion of topography are presented in Chapter 4. The test cases presented in this chapter include linear mountain waves, a nonlinear downslope windstorm, and orographic cloud formation. Results from CSLAM-NH for the linear mountain waves and the nonlinear downslope windstorm are comparable to those found in the literature. In the downslope windstorm case, the maximum vertical Courant number was approximately three, before CSLAM-NH eventually becomes unstable due to self-intersecting departure cells. These self-intersecting cells appear in regions with strong wind gradient, such as in the wave breaking region in the downslope windstorm simulation. In one of the moist orographic flow cases, the spatial distribution of rain differs from that presented in the literature, but a second Eulerian solver shows virtually the same results as CSLAM-NH. This second set of results indicates that factors other than the solver component may be in play, e.g., sensitivity to the initial moist static stability.

In summary, the nonhydrostatic solver CSLAM-NH possesses the following desirable features:

1. It inherently conserves mass using the ‘Conservative Semi-LAgrangian Multi-tracer’ (CSLAM) transport scheme.
2. It consistently transports scalar variables using a new semi-implicit formulation of the continuity equation.

3. It does not depend on a mean reference state.

4. It prevents spurious generation/removal of tracer mass through the use of shape-preserving filters.

5. It requires an elliptic solver that resembles those in traditional semi-Lagrangian semi-implicit solvers.

6. It requires a single call to the conservative semi-Lagrangian transport scheme at each time step for each tracer.

5.2 Impact on the broader community

There is growing research interest in the influence of trace gases and aerosol concentrations on the atmosphere. Trace gases, such as carbon dioxide, methane, and ozone, make up only a very small portion of atmospheric constituents. However, their limited concentrations can still have significant contributions to the radiation budget in the atmosphere, as some are highly radiatively-absorbing species (Petty, 2006). Other aerosols such as dust particles and sea spray can be advected by the jet stream and be carried far from their source locations. These aerosols, aside from having a direct impact on the radiation budget, also have an indirect effect through cloud microphysical processes. Dust particles and sea spray can serve as cloud condensation nuclei or ice nuclei, and enhance precipitation formation. For example, Creamean et al. (2013), through winter observations from a field campaign called Calwater in the Sierra Nevada region, showed that the long-range transport of dust and biological aerosols from Asia and the Sahara desert likely contributed to the positive feedback mechanism in orographic precipitation formation in the region.

The impact of these aerosols and trace gases on the global radiation and water budget is often studied through atmospheric chemistry and global climate models (GCMs). The representation of physical and chemical processes related to these trace gases in current GCMs and atmospheric chemistry models is becoming more sophisticated. The number of prognostic aerosols and chemical species in current comprehensive atmospheric models far exceeds the number of scalars (roughly 10) required by the model dynamics alone. For example, in the fully-coupled online chemistry model in the Weather Research and Forecasting – Chemistry model (WRF-CHEM) (Grell et al., 2005), the basic configuration involves 39 basic prognostic chemical species, 34 aerosols, and about 10 other variables associated with organic aerosols. (An online chemistry model has the advantage of allowing a feedback mechanism for the aerosol radiative impact back to the meteorological...
model.) In the chemistry version of NCAR’s Community Atmospheric Model (CAM), the number of prognostic tracers is on the order of 100.

Cloud microphysical schemes in NWP models are also becoming more sophisticated. Cloud microphysical schemes are explicit representations of cloud processes in a model (as opposed to implicit representations using convective parameterizations). In bulk microphysical schemes, hydrometeor interactions are represented by pre-defined (typically empirical) functional relations for the particle-size distribution. The simplest microphysical scheme only predicts hydrometeor mixing ratios (these are referred to as single-moment schemes), and only predicts for warm-rain species such as cloud and rain droplets. More advanced microphysical schemes now typically include six classes of hydrometeors, with the addition of ice, snow, graupel, and hail. In double-moment schemes, the concentrations are also predicted to help give a better estimate of particle size distributions (Stensrud, 2007). The total number of prognostic variables then increases from two to 12. The growing demand for representation of these tracers and cloud processes in our models calls for more accurate and efficient solvers.

Another desirable property when modelling multiple tracers is the ability to maintain relative tracer concentration ratios of long-lived chemical tracers. The inability to preserve the functional relations among tracers can be interpreted as erroneous numerical mixing of these tracers (Lauritzen et al., 2011). The relationships among tracers can be linear or nonlinear. Only fully Lagrangian transport schemes (such as those used in direct numerical simulations) are likely able to handle both, whereas Eulerian and semi-Lagrangian schemes should ideally preserve linear relations. Recall that shape-preservation is a desirable property in the case of tracer transport. Ovtchinnikov and Easter (2009) identified a problem when monotonocity constraints are applied in the transport of individual tracers. The shape-preserving filters studied were found to be nonlinear algorithms that could not preserve relative tracer concentrations. By transporting three inter-related aerosol and cloud particles in an idealized cloud simulation, they found that the percentage error in the (supposedly constant) total sum of the three mixing ratios can reach 30%. Based on the same notion, inconsistent transport can also lead to the destruction of the (ideally conserved) total mixing ratios of inter-related tracers. Testing of functional relation preservation in CSLAM-NH is outside the scope of the dissertation. However, the shape-preserving filter described in Barth and Jespersen (1989) and implemented in the CSLAM component of this solver has been shown to preserve tracer relations fairly well in a recent comparison study of transport schemes by Lauritzen et al. (2014).

Recent testing using the CSLAM transport scheme for advection of tracers in CAM showed that

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1The Community Atmosphere Model (CAM) is developed at the National Center for Atmospheric Research (NCAR) for the weather and climate research communities. CAM is the atmospheric component of the broader Community Earth System Model (CESM) [one of the participating climate models used in the Intergovernmental Panel on Climate Change report (AR5)].
the transport scheme is computationally efficient and highly scalable in a parallelized environment (Erath et al., 2012). The adaptability of CSLAM for a large number of tracers is shown through their simulations with up to 800 tracers. However, the numerical scheme used to solve the air density continuity equation is not consistent with that for the tracer continuity equation. The continuity equation in Erath et al. (2012) is solved using the spectral element dynamical core (HOMME). The issue of numerical consistency therefore remains. The method proposed in this dissertation can be used to provide consistent transport and ensure tracer mass conservation in the model.

5.3 Further work

Several aspects of the CSLAM-NH dynamical solver developed in this work will warrant more research if it is to be deployed in a more comprehensive weather and climate model. The main topics include (i) dimensionality, (ii) potential ways to enhance CSLAM-NH stability, and (iii) cost-effectiveness in a parallelized environment.

5.3.1 Dimensionality

At its current state of development, CSLAM-NH remains a two-dimensional prototype solver in the vertical plane. Despite being a two-dimensional solver, the idealized test cases chosen in this dissertation are representative of typical meteorological flows. The governing nonhydrostatic equations permit vertical acceleration; the solver demonstrates that it is able to accurately and stably handle strong vertical motion. The nonhydrostatic prototype solver in the vertical plane (Chapters 3 and 4) is, therefore, a logical step forward from a shallow-water model (Chapter 2), in the development of a full atmospheric solver. Alas, the world is not flat; the atmosphere is three-dimensional (or four, including temporal evolution) and the solver will need to include this third spatial dimension. The dimensionality of CSLAM-NH is limited by the inherently conservative transport scheme. To extend a transport scheme to three dimensions, various paths are given in Lauritzen et al. (2011) (their Chapter 8), and a brief description is given here.

The first option is a very rigorous approach of extending the CSLAM transport scheme to carry out three-dimensional remapping. The fully semi-Lagrangian version of the CSLAM transport scheme was developed as a two-dimensional transport scheme. Thus far, the CSLAM transport in the vertical plane tested here is a straightforward implementation of the existing infrastructure using a terrain-following vertical coordinate. The work required to extend the transport scheme to three dimensions will require new reconstruction and remapping methods. In two dimensions, the transport scheme requires a 2D reconstruction function and a remapping scheme that relies on knowledge of the departure cell boundary. In three dimensions, using a similar notion of applying
the Gauss-Green theorem will require some surface integral of the departure cell (assuming planar and quadrilateral faces in three dimensions, the cell will be a hexahedron). The surface integral can be approximated as the sum of the area integral over each face, which can each be decomposed into separate line integrals as is done in the 2D version of CSLAM. Creation of the search algorithm for the cell boundaries (i.e., each face’s boundaries) in three dimensions will be a challenging task. Garimella et al. (2007) has, however, demonstrated that such a remapping algorithm works in Cartesian geometry using piecewise linear reconstruction functions.

The second option is to employ a Lagrangian vertical coordinate as is done in several fully semi-Lagrangian solvers, and originally proposed by Lin (2004). The use of a Lagrangian vertical coordinate assumes that transport is done along a horizontal surface that moves with the flow. This assumption eliminates the vertical advection terms in the discretized equations of motion, and the remaining horizontal advection is calculated by the two-dimensional CSLAM transport scheme. For the hydrostatic approximation, as is used in Lin (2004), the vertical coordinate (pressure) position of each model level can be determined using the hydrostatic equation, with the model top specified at a fixed pressure. The distribution of the prognostic variables in the Lagrangian column will become less resolved in regions that are more vertically divergent. Periodic remapping from the vertical Lagrangian column back to an Eulerian reference grid is therefore needed. For a nonhydrostatic solver that uses a terrain-following height coordinate, the vertical position can be determined using the prognostic contravariant vertical velocity. In nonhydrostatic flows, vertical remapping will need to be performed more frequently than for hydrostatic flows because strong vertical accelerations will likely lead to more deformed flows. The advantage of this approach over the fully three-dimensional CSLAM transport is that this implementation would require very little modification to the method proposed in this dissertation.

The third option is a ‘cascade approach’, similar to those employed in Nair et al. (2002) and Zerroukat et al. (2002). The cascade approach is similar to using a Lagrangian vertical coordinate where remapping is not done in a fully three-dimensional manner. In Nair et al. (2002) and Zerroukat et al. (2002), sequential application of one-dimensional conservative remapping along each coordinate is performed to achieve conservative remapping in two- to three-dimensions. The cascade approach utilizes an intermediate grid as a “stepping stone” for remapping along each coordinate from the Eulerian grid to the Lagrangian grid. In CSLAM-NH, one could apply two-dimensional remapping onto an intermediate grid in $x$-$z$, and then apply one-dimensional conservative remapping in the $y$-direction from the intermediate grid to the Lagrangian grid (or intermediate grid in $x$-$y$ space, and then, in the $z$-direction). As mentioned in Lauritzen (2007), directional biases may occur in splitting schemes, but can be reduced by alternating the sequence of splitting (directions) every time-step and/or using smaller (such as halved) time-steps per sweep to reduce the errors. A comparative study
5.3.2 Enhancement of CSLAM-NH stability

Model time steps are limited by two main factors: accuracy and stability. The main advantage of using semi-Lagrangian schemes is their larger stable time steps, such that accuracy becomes the only limiting factor when choosing time step sizes. In other words, the model time step size is chosen to acquire an accurate representation of the physical phenomena of interest.

For the more complex and nonlinear test cases presented, the stable CSLAM-NH time steps are often limited by self-intersecting departure cells in CSLAM, which is a stability issue. An important criterion for any numerical scheme is its robustness in terms of numerical stability, and this criterion is especially important when model output is used as a part of an operational forecasting system. In an operational forecast model, tuning of various diffusion options often allows enhanced numerical stability by damping unwanted waves. In the current test cases, minimal explicit diffusion is used in CSLAM-NH.

Possible improvements to the stability of CSLAM-NH are described next. As mentioned in Chapter 4, higher-order departure cell-edge approximations may help alleviate the time step limit. The recommendation stems from the work of Ullrich et al. (2012). They introduced quadratic fits (as opposed to straight line approximations) of the cell edges and showed that using quadratic-fit cell boundaries led to more accurate transport of a tracer in a strongly nonlinear sheared flow. On the contrary, tracing back more points along the cell edge and connecting them with line segments showed less of an improvement. In addition to using curved cell edges, they also used a fourth-order Runge-Kutta trajectory algorithm to find the departure point of each cell vertex. Their approach was implemented for a simplified flux-form version of the CSLAM transport scheme, but the method can also be used in the fully semi-Lagrangian version of CSLAM (as used here).

Explicit diffusion is often used in numerical weather prediction models to control spurious noise and to enhance the stability of a numerical scheme. The introduction of dissipation mechanisms in CSLAM-NH to control the appearance of these self-intersecting departure cells might also be explored. For example, in the downslope windstorm case, unlike 90% of the models in Doyle et al. (2000), CSLAM-NH did not use a turbulence parameterization scheme. Self-intersection of departure cells is mostly due to strong wind gradients, which often generate turbulence in the real atmosphere (analogous to the Lipschitz stability condition), and some parameterization of turbulence will likely help increase the stability of CSLAM-NH.

In the case of the detection of a self-intersecting departure cell, the two problematic cell vertices can be swapped to “untwist” the self-intersecting departure cell (Lauritzen, 2013, personal commu-
nication). Like other filters, the application of such a “smoother” will need to be carefully examined to determine its damping effect. The application will likely be analogous to applying diffusion to smooth out local regions with strong wind gradients. When such an algorithm is used, it may be necessary to apply a correction to the velocities of the associated grid points to maintain consistency between the trajectory computations and the divergence terms.

5.3.3 Cost-effectiveness in a parallel environment

As shown in Chapter 4, the efficiency of the current prototype solver can be further improved. Computational expenses in CSLAM-NH are dominated by the elliptic solver. The elliptic equation in CSLAM-NH is constructed to be similar to those in traditional semi-Lagrangian semi-implicit solvers. Recently, Müller and Scheichl (2014) performed a comprehensive comparison of a range of algorithms typically used to solve the Helmholtz equation and tested the elliptic solvers in a parallel environment with up to 65536 cores, in anticipation of global semi-Lagrangian semi-implicit solvers being applied for high-resolution simulations. The authors tested and optimized five algorithms, which include two variants of algebraic multigrid solvers, two variants of preconditioned conjugate-gradient solvers, and a geometric multigrid solver. The authors performed a series of weak scaling assumption tests using all five algorithms and strong scaling tests with the geometric multigrid solver.

In the weak scaling tests, the number of grid cells \(2^{19}\) per processor remained unchanged. The problem size was then increased (effectively doubling the resolution of each subsequent test). The number of processors was also increased until all 65536 cores were in use. The time step size was decreased accordingly so that the Courant number of the problem stayed the same. The authors found that three of the five tested solvers showed generally good weak scalability, with the geometric multigrid solver performing the best. The latter took only 0.14 to 0.17 s per iteration, and six iterations to converge, using a total time of 0.86 to 1.06 s. Compared to the other four methods, the elliptic solve of their geometric multigrid method is roughly 5 to 10 times faster.

The elliptic solver in operational traditional semi-Lagrangian semi-implicit NWP models is likely optimized for operational use. Since the Helmholtz equation in CSLAM-NH is formulated to be similar to those used in these traditional solvers, existing optimized techniques can be applied. Newer developments, such as those described above from Müller and Scheichl (2014), are also applicable when updating and optimizing the Helmholtz solver in CSLAM-NH to more modern techniques.

As mentioned in section 5.2, the CSLAM transport scheme has been implemented in the CAM-SE model for tracer advection. Erath et al. (2012) re-designed the CSLAM scheme to work efficiently in a parallel environment by minimizing the amount of inter-processor communication,
which was mostly needed in the subgrid-cell reconstruction calculations. They found that the computational time needed to advect a second tracer was only 1/23 of the time needed for advecting the first, valid up to 1014 processors. With more processors (tested for up to 4056 processors) and a large number of tracers, the communication time limits the scalability slightly. In the latter case, the computational time needed to advect a second tracer was 1/14 of the time for the first tracer.

5.4 Summary

Cell-integrated semi-Lagrangian transport schemes are relatively recent developments within the field of atmospheric solvers. Traditional semi-Lagrangian transport schemes are much more widely used in operational forecasting. At the time of writing this dissertation, many operational NWP centres are aware of the benefits of using an inherently conservative semi-Lagrangian transport scheme, and therefore, have developed and/or implemented some version of a cell-integrated semi-Lagrangian solver. However, these solvers have only been applied in research mode, and the development of CSLAM-NH in this dissertation fits into this category. Currently, very few operational global models are nonhydrostatic, but this will likely change: current global model horizontal resolution is already approaching 25 km.

As research interest in the impact of trace gases and aerosols continues to grow, accurate tracer transport will become more important. Not only may the neglect of numerically consistent transport lead to spurious generation and removal of tracer mass, but also shape-preservation may no longer be ensured. CSLAM-NH uses a consistent and conservative transport scheme for all scalars. Consistent transport schemes will likely be important in ensuring other (stricter) properties such as functional relation preservation of long-lived chemical constituents.

The consistent semi-implicit continuity equation formulation has only been tested in CSLAM-NH thus far. The implementation of the consistent formulation in other CISL solvers will determine the generalizability of this scheme.
Bibliography


Appendix A

Supporting Materials

A.1 Numerical schemes for comparison

A.1.1 A two-time-level traditional semi-Lagrangian semi-implicit model

A traditional grid-point semi-implicit semi-Lagrangian model on a staggered C-grid is constructed for comparison purposes. The scheme uses a forward-in-time off-centering parameter $\beta$ for numerical stability purposes. The discretized system is given by

$$u^{n+1}_A = \Delta t \left( \frac{1 + \beta}{2} \right) \left[ f v^{xy} - g' \delta_x h \right]_{A}^{n+1} + R_u^n,$$

(A.1)

$$v^{n+1}_A = \Delta t \left( \frac{1 + \beta}{2} \right) \left[ - f u^{xy} - g' \delta_y h \right]_{A}^{n+1} + R_v^n,$$

(A.2)

$$h^{n+1}_A = -\Delta t \left( \frac{1 + \beta}{2} \right) H_0 \left( \delta_u + \delta_y \right)_{A}^{n+1} + R_h^n + R_h^{n+1/2},$$

(A.3)

where

$$R_u^n = u^n_d + \Delta t \left( \frac{1 - \beta}{2} \right) \left[ f v^{xy} - g' \delta_x h \right]_{d}^{n},$$

(A.4)

$$R_v^n = v^n_d + \Delta t \left( \frac{1 - \beta}{2} \right) \left[ - f u^{xy} - g' \delta_y h \right]_{d}^{n},$$

(A.5)

$$R_h^n = h^n_d - \Delta t \left( \frac{1 - \beta}{2} \right) H_0 \left( \delta_u + \delta_y \right)_{d}^{n},$$

(A.6)

$$R_h^{n+1/2} = -\Delta t \left( h' \delta_u + h' \delta_y \right)_{d/2}^{n+1/2},$$

(A.7)

and $h' = h - H_0$. The operators are defined as

$$\delta_x \phi = \frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x}; \quad \delta_y \phi = \frac{\phi_{i,j} - \phi_{i,j-1}}{\Delta y},$$

(A.8)
\[ \bar{\phi} = \frac{1}{2}(\phi_{i,j} + \phi_{i+1,j}), \quad \text{(A.9)} \]

\[ \bar{\phi}_x = \bar{\phi}_y = \bar{\phi}_z = \frac{1}{4}(\phi_{i,j} + \phi_{i,j+1} + \phi_{i+1,j} + \phi_{i+1,j+1}). \quad \text{(A.10)} \]

The \( R^n \) terms define the known terms that are evaluated at time level \( n \) and interpolated to the departure point. The \( R^{n+\frac{1}{2}} \) term is the nonlinear term evaluated by extrapolating values from time level \( n \) and \( n-1 \) to time level \( n + \frac{1}{2} \), and interpolated to the estimated mid-point trajectory. The time-off-centering parameter \( \beta \) is set to 0.1 for all runs.

### A.1.2 An Eulerian leap-frog semi-implicit advective model

The Eulerian C-grid staggering model uses the semi-implicit leap-frog time-stepping scheme and momentum equations in the advective form. The model has an Asselin time-filter and a time-off-centering parameter (\( \beta = 0.1 \)) to eliminate spurious oscillations. Numerical viscosity is also applied for certain test cases (see section 4b). Using the same notations as for the traditional semi-Lagrangian model, the discretized system is given by

\[ u^{n+1} = \Delta t \left( 1 + \beta \right) \left( f \bar{v}_x - g \delta_x h \right)^{n+1} + R_u, \quad \text{(A.11)} \]

\[ v^{n+1} = \Delta t \left( 1 + \beta \right) \left( - f \bar{v}_y - g \delta_y h \right)^{n+1} + R_v, \quad \text{(A.12)} \]

\[ h^{n+1} = - \Delta t \left( 1 + \beta \right) H_0 \left( \delta_x u + \delta_y v \right)^{n+1} + R_h, \quad \text{(A.13)} \]

where

\[ R_u = u^{n-1} - 2\Delta t \left( u \delta_x u + v \delta_y u \right)^n + \Delta t \left( 1 - \beta \right) \left( f \bar{v}_x - g \delta_x h \right)^{n-1}, \quad \text{(A.14)} \]

\[ R_v = v^{n-1} - 2\Delta t \left( u \delta_x v + v \delta_y v \right)^n + \Delta t \left( 1 - \beta \right) \left( - f \bar{v}_y - g \delta_y h \right)^{n-1}, \quad \text{(A.15)} \]

\[ R_h = h^{n-1} - \Delta t \left( 1 - \beta \right) H_0 \left( \delta_x u + \delta_y v \right)^{n-1} - 2\Delta t \left( h' \delta_x u + h' \delta_y v \right)^{n+\frac{1}{2}}. \quad \text{(A.16)} \]