Monitoring Committee Progress Report #5

Numerical Representation of Mountains in Atmospheric Models

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June 2017

1 Introduction

Numerical weather forecast and climate prediction models are using increasingly fine horizontal meshes to resolve small-scale features and make forecasts more accurate. Traditionally, atmospheric models have used uniform latitude-longitude meshes to represent a spherical Earth with terrain-following vertical coordinates to represent Earth's terrain, but these representations become problematic with fine horizontal mesh spacing. First, the cells of latitude-longitude meshes are very small near the Earth's poles, causing a bottleneck in parallel computation (Staniforth and Thuburn, 2012) and placing severe time-step constraints on explicit Eulerian methods. Second, computer storage and computation time increase dramatically when horizontal mesh spacing is reduced uniformly over a latitude-longitude mesh: halving the horizontal mesh spacing results in four times as many cells and simulations require a smaller time-step. Third, fine horizontal meshes resolve small-scale steep slopes that severely distort terrain-following coordinate surfaces, resulting in larger numerical errors (Schär et al., 2002) or even numerical instability (Webster et al., 2003).

In response to these problems, a variety of alternative horizontal and vertical representations have been proposed. Alternative, quasi-uniform meshes avoid small cells near the poles of latitude-longitude meshes (Staniforth and Thuburn, 2012). Some models are already using quasi-uniform meshes: the German ICON model uses an icosahedral mesh (Wan et al., 2013), the Canadian GEM model uses a yin-yang mesh comprising two overlapping sections arranged like a tennis ball (Qaddouri and Lee, 2011), and the UK Met Office are preferring a cubed-sphere mesh for their next-generation Gung-Ho model (Nigel Wood 2017, personal communication). To improve the scalability of computational resources with finer mesh spacing, static mesh refinement and dynamic adaptive mesh techniques create meshes with fewer cells while retaining the numerical accuracy achieved with a uniformly fine mesh (Jablonowski et al., 2009). mprovements have also been made to the vertical representation over steep terrain. Mesh distortions are less severe when terrain-following coordinates are smoothed (Leuenberger et al., 2010; Klemp, 2011), and cut cell meshes are orthogonal everywhere except at the ground.

These alternative meshes alleviate many of the computational and numerical problems that arise due to finer horizontal mesh spacing, but they introduce problems of their own. Unlike latitude-longitude meshes, quasi-uniform meshes have non-zero skewness or non-orthogonality that produces grid imprinting errors and excites computational modes (Weller et al., 2012). Mesh refinement and adaptive mesh techniques also create mesh geometries with non-orthogonalities or hanging nodes (Marras et al., 2016). Cut cell meshes are orthogonal nearly everywhere but the cut cell method creates arbitrarily small cells that impose severe time-step constraints on explicit Eulerian methods (Klein et al., 2009).

This PhD makes three contributions to improve numerical accuracy on arbitrary meshes. First, a new mesh for representing steep terrain avoids the severe distortions associated with terrain-following meshes (Shaw and Weller, 2016) and avoids severe time-step constraints associated with cut cell meshes (Shaw et al., 2017). Second, a new transport scheme is formulated for numerical stability on high-distorted meshes (Shaw et al., 2017). It is second-order convergent on quasi-uniform spherical meshes, terrain-following and cut cell meshes. Third, the Charney–Phillips staggering of variables is generalised for arbitrary meshes and is shown to eliminate the computational mode associated with a Lorenz staggering.

The OpenFOAM computational fluid dynamics library is used throughout the project to enable like-for-like comparisons. Different types of mesh are compared using the same model, and different variable staggerings are compared using variants of a single model. The PhD also contributes two new two-dimensional test cases that are suitable for evaluating dynamical cores. The first test challenges transport schemes near steeply-sloping lower boundaries (Shaw et al., 2017). The second test is designed to excite the Lorenz computational mode. Existing tests that excite the Lorenz computational mode are poorly suited to dynamical core evaluation: the standing waves test by Arakawa and Konor (1996) was designed for a model with no horizontal discretisation, and the radiative heating test by Untch and Hortal (2004) requires a 600-day integration using a three-dimensional spherical Earth. The test that we propose requires a 2-day integration using a two-dimensional Cartesian plane and is based on the test by Arakawa and Konor (1996).

2 A stable transport scheme for atmospheric flows over steep slopes

We submitted a manuscript to the Journal of Computational Physics in February 2017 documenting the finite volume transport scheme, "cubicFit". The final article (Shaw et al., 2017) was made available in April 2017 after one round of minor corrections. The cubicFit scheme is largely insensitive to mesh distortions and maintains second-order convergence on highly distorted meshes. Idealised tests demonstrate that the cubicFit scheme is more stable and more accurate than a standard multidimensional linear upwind scheme.

Having presented our work at PDEs on the Sphere in April Hans Johansen, a researcher from the computational research group at Lawrence Berkley National Lab, told me that his group have developed a high-order finite volume scheme for solving Poisson's equation on cut cell meshes (Devendran et al., 2015). Hans is keen to help me apply these techniques to the cubicFit transport scheme in order to achieve convergence higher than second-order. If time permits, I hope to collaborate with Hans to take this work further.

3 Generalisating the Charney–Phillips staggering for arbitrary meshes

The Charney–Phillips vertical staggering of variables (Charney and Phillips, 1953) is suitable for structured meshes with cells stacked in columns. This staggering has been adopted by several operational models (Davies et al., 2005; Yang et al., 2007; Girard et al., 2014) because it avoids the computational mode that is associated with the Lorenz vertical staggering (Arakawa and Konor, 1996). The generalisation of the Lorenz staggering for unstructured or arbitrarily-structured meshes is straightforward (Weller and Shahrokhi, 2014) but this is not true for the Charney–Phillips staggering.

On a finite volume mesh, variables are ordinarily placed at cell centres or cell faces. In the Charney–Phillips staggering, the thermodynamic variable is placed at only those cell faces that lie on vertical coordinate surfaces, and vertically-oriented faces have no thermodynamic information. This arrangement is unsuitable for arbitrarily-structured finite volume meshes because faces can have any orientation.

Work is on schedule to develop a generalisation of the Charney–Phillips staggering of variables. The prognostic thermodynamic variable b_f is stored at all cell faces such that $b_f = \theta_f \hat{\mathbf{g}} \cdot \hat{\mathbf{n}}_f$ where f is a face, θ_f is the potential temperature, $\hat{\mathbf{g}}$ is the unit vector of gravitational acceleration and $\hat{\mathbf{n}}_f$ is the unit vector that is outward normal to the face. This arrangement is illustrated in figure 1.

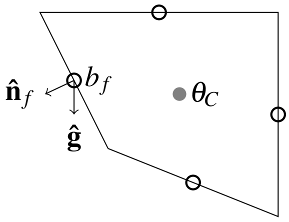


Figure 1: A quadrilateral cell with the prognostic thermodynamic variable b_f stored at face centres marked by open circles. b_f is calculated from the potential temperature θ_f such that $b_f = \theta_f \hat{\mathbf{g}} \cdot \hat{\mathbf{n}}_f$ where $\hat{\mathbf{n}}_f$ is the unit vector outward normal to face f, and $\hat{\mathbf{g}}$ is the unit vector of gravitational acceleration. The potential temperature at the cell centre, θ_C, is reconstructed from surrounding values of b_f using equation (2).

To outline the discretisation, let us consider its application to a Cartesian mesh with no diagonal faces. First, potential temperature is transported in advective form,

$$\theta_f^{n+1} = \theta_f^{\ell} - \Delta t \mathbf{U}_f \cdot (\nabla_c \theta_f)_F \tag{1}$$

where θ_f^{n+1} is the value of θ_f at the new time-step, θ_f^{ℓ} is the lagged value from the previous solver iteration, $\mathbf{U}_f$ is the wind, $(\cdot)_F$ denotes an interpolation from cell centres to faces, and ∇_c denotes a cell centre gradient (Weller and Shahrokhi, 2014). Next, b_f is calculated such that $b_f = \theta_f \hat{\mathbf{g}} \cdot \hat{\mathbf{n}}_f$. On a Cartesian mesh, b_f is zero for entirely vertical faces and $b_f = \theta_f$ for entirely horizontal faces.

Where potential temperature is required at the cell centre, it is reconstructed from bordering faces,

$$\theta_C = \hat{\mathbf{g}} \cdot \left(\sum_{f \in c} \hat{\mathbf{n}}_f \mathbf{S}_f \right)^{-1} \cdot \sum_{f \in c} \mathbf{S}_f b_f \tag{2}$$

where θ_C is the reconstructed potential temperature, $f \in c$ denotes the faces f bordering cell c, and $\mathbf{S}_f$ is the vector with magnitude equal to the face area and an outward normal direction. On a Cartesian mesh, θ_C is simply a linear interpolation from the face values immediately above and below the cell centre.

Finally, θ_f is recalculated from b_f and θ_C,

$$\theta_f = |\hat{\mathbf{g}} \cdot \hat{\mathbf{n}}_f \theta_f| + (1 - |\hat{\mathbf{g}} \cdot \hat{\mathbf{n}}|)\,(\theta_C)_F\,. \tag{3}$$

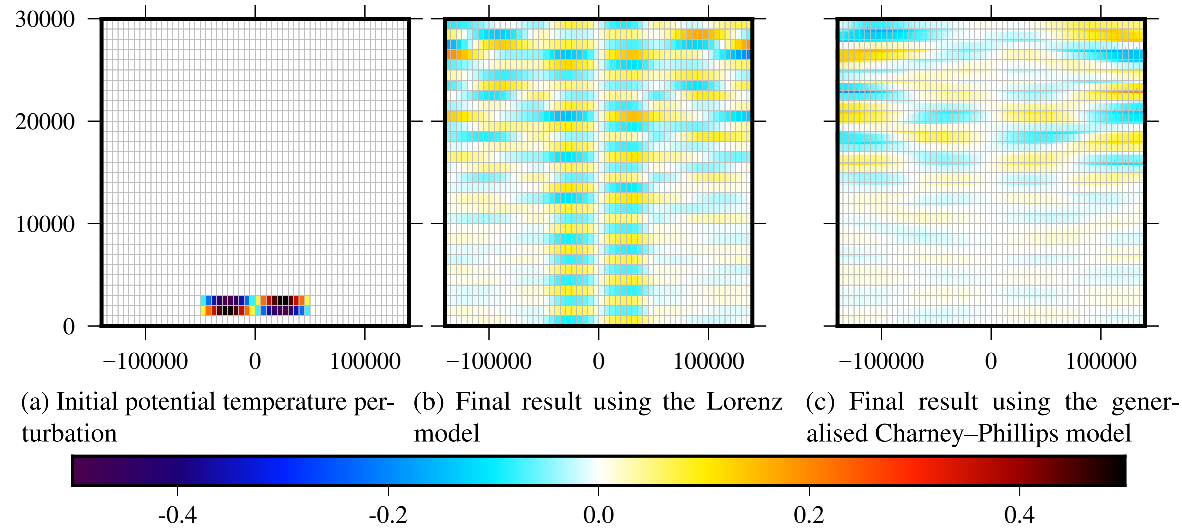
This ensures that values of θ_f on vertical faces is calculated from nearby b_f values and is not retained across time-steps. We have created a new variant of the nonhydrostatic model by Weller and Shahrokhi (2014) that implements this generalised Charney–Phillips formulation.

We have also created a new two-dimensional vertical slice test case that we use to compare the Lorenz and generalised Charney–Phillips model variants. The new test case is based on the standing waves test by Arakawa and Konor (1996), which was designed for a vertically discrete model with no horizontal discretisation. Grid-scale potential temperature perturbations are added to an isothermal atmosphere in hydrostatic balance (figure 2a). The details of the test configuration have yet to be finalised.

After a two day integration, preliminary results using the Lorenz model show a spurious grid-scale oscillation occupying the entire depth of the domain, having propagated upwards from the position of the initial perturbation (figure 2b). This grid-scale error indicates that the Lorenz computational mode has been excited. No such error is found with the generalised Charney–Phillips model (figure 2c).

4 Future research

I have completed tasks up to May 2017 according to the schedule set out in monitoring committee report #4 and we are making good progress generalising Charney–Phillips. My supervisors and I are keen to



(a) Initial potential temperature perturbation (b) Final result using the Lorenz model (c) Final result using the generalised Charney–Phillips model

Figure 2: Potential temperature perturbations from the isothermal state in the two-dimensional standing waves test case. Initially, grid-scale perturbations with a maximum amplitude of $\pm 0.5\,\mathrm{K}$ are added in the centre of the domain near the ground. These perturbations generate gravity waves that spread through the domain. A spurious grid-scale oscillation indicates that the Lorenz computational mode is excited using the Lorenz model. No such error is present using the generalised Charney–Phillips model. Only the central part of the domain is shown with cell edges marked by grey lines. Axes are in units of metres.

develop this work into a third article to be submitted to the Quarterly Journal of the Royal Meteorological Society, and I believe a third publication will benefit a future academic career.

With the agreement of the monitoring committee, I would like to apply for a six-month extension for the completion of my PhD. This extension application is based on a number of grounds. First, as of May 2017, I have spent a total of five months addressing reviewer comments: designing new mesh generation techniques, performing new experiments and revising manuscripts (Appendix C). Second, I expect to spend about two months writing a third journal article. Third, my second article supercedes parts of my first article. As such, a one-to-one mapping between articles and thesis chapters in all instances, and reorganisation, new prose and new figures will be required for the thesis. Finally, I have completed two masters modules, one of which was assessed.

Timeline of future work

A thesis plan is presented in Appendix A. I intend to interleave the writing of my thesis with technical work on generalised Charney–Phillips. Chapters 5 and 6 will be written following the third journal article.

August 2017 Complete technical work for the generalised Charney–Phillips staggering (chapter 5): improve non-orthogonal treatment of the thermodynamic discretisation, create refined meshes, and obtain accurate results comparable to those obtained with the Lorenz model.

September 2017 Attend SciCADE conference. Complete chapter 4, documenting and assessing the flux-form cubicFit transport scheme.

October 2017 Complete chapters 2 and 3, a review of existing methodologies and a description of the slanted cell method.

February 2018 Develop a new advective-form transport scheme for chapter 6.

April 2018 Submit a manuscript to the Quarterly Journal of the Royal Meteorological Society on the advection scheme and dynamical core for the generalised Charney–Phillips staggering.

May 2018 Complete chapters 5 and 6 on the generalisation of Charney–Phillips.

June 2018 Complete chapter 1, introduction.

July 2018 Submit thesis.

5 Personal development

Since the last monitoring committee meeting in November 2016 I have been invited to speak at the RMetS south-east meeting at the University of Reading, and at a numerical methods workshop at Imperial College. I am helping to organise the NERC student conference, lead by students from NERC DTPs in London, and I have applied to present at SciCADE, a conference on scientific computation and differential equations.

I am now considering my options for future employment, and I am keen to continue research in numerical methods, either applied to weather and climate modelling or other disciplines. Hilary has kindly introduced me to a number of colleagues in UK institutions and I am following up with those who may have positions opening soon.

I am also interested other academic roles that promote good practices in reproducible science and research software engineering. I have applied for a 10-month Mozilla science fellowship that supports researchers wanting to promote open science within their institution. The international programme selects four fellows each year, with this year's fellows being chosen in June 2017. Mozilla allow fellows to spend 20% of their time on their own research and so, should I be chosen, I would need to work on my PhD part-time and postpone the completion date for 8 months.

If I cannot find a suitable academic job I am considering computational fluid dynamics positions and software engineering positions elsewhere. I submitted an application in May to the UK Met Office who have several software engineering vacancies.

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Appendix A: Thesis plan

The progress on each section is recorded here. I have provided a citation where a section is documented in an article but has not yet been included in the thesis. I also note where technical and mathematic work is still in development and documentation has yet to be written.

1. Introduction

Not started	This project is motivated by the need for alternative horizontal and vertical representations of Earth's atmosphere in the proximity to mountainous terrain

2. Existing methodologies

Shaw and Weller (2016)	Introduce existing types of mesh: terrain-following layers and cut cells
Shaw and Weller (2016)	Describe the nonhydrostatic model for arbitrary meshes with Lorenz staggering
Not started	Describe Lorenz and Charney–Phillips staggerings for structured quadrilateral meshes

3. A new mesh for representing the atmosphere above terrain

The slanted cell mesh improves pressure gradient accuracy and avoids severe time-step constraints.

Shaw and Weller (2016); Shaw et al. (2017)	Describe the new slanted cell method
Shaw and Weller (2016), revision needed	A two-dimensional test of a quiescent atmosphere above steep slopes, comparing terrain-following, cut cell and slanted cell meshes using the standard linear upwind scheme

4. A stable transport scheme for atmospheric flows over steep slopes

The cubicFit transport scheme is stable and accurate over steep slopes with arbitrary, distorted meshes.

Shaw et al. (2017)	Document the cubicFit transport scheme
	Test results comparing a standard linear upwind scheme and the cubicFit transport scheme:
Shaw et al. (2017)	• transport test over steep slopes on terrain-following, cut cell and slanted cell meshes
Shaw et al. (2017)	• deformational transport tests on a spherical Earth

5. Generalising the Charney–Phillips staggering for arbitrary meshes

The Charney–Phillips staggering avoids the Lorenz computational mode, but it has only been formulated for structured quadrilateral meshes. A generalised formulation will be suitable for arbitrary meshes. In this chapter, rectangular meshes with different refinement methods will be used, without any sloping terrain.

In development	Describe the generalised Charney–Phillips formulation
In development	Describe the simple advective-form transport scheme
In development	Document the necessary changes to the nonhydrostatic model
	Document the new two-dimensional standing waves test case and compare results:
Not started	• a uniform mesh, and meshes with non-conformal block refinement and conformal refinement (with diagonal faces)
In development	• Lorenz and Charney–Phillips model variants to demonstrate the presence and absence of the Lorenz computational mode respectively

6. A dynamical core for atmospheric flows over terrain represented by arbitrary meshes

The final chapter brings together the three aspects of the project: the slanted cell mesh, the cubicFit transport scheme, and the generalised Charney–Phillips formulation.

Not started	Document a new advective-form transport scheme, based on the flux-form cubicFit scheme, for potential temperature on the generalised Charney–Phillips staggering
Not started	Compare accuracy with the simple transport scheme used in chapter 5, assessed using the tracer transport test from (Shaw et al., 2017)
	Evaluate the transport scheme using the Schär et al. (2002) gravity waves test. Results should be compared between
Not started	• terrain-following, cut cell and slanted cell meshes
Not started	• the two advective-form transport schemes
Not started	• Lorenz and Charney–Phillips model variants

Appendix B: Training record

Mathematics modules

Spring 2017	M5A47	Finite elements: numerical analysis and implementation	unassessed, partially completed
Spring 2016	MA3NAT	Numerical Analysis II	unassessed
Spring 2015	MAMNSP	Numerical Solution of Partial Differential Equations	78%

RRDP modules

23 June 2017	Graduate school conference
3 May 2017	Effective CVs
28 Feb 2017	Getting your first post-doc position
9 Nov 2016	Open Access and research data management
24 Mar 2016	Voice coaching: looking after your voice
26–27 Jan 2016	Preparing to teach (introduction, marking & feedback, leading small groups)
2 Dec 2015	An essential guide to critical academic writing
17 Nov 2015	Understanding the UK higher education context
19 May 2015	How to avoid plagiarism
10 Mar 2015	How to write a literature review
19 Feb 2015	How to write a paper

External courses

June 2016	Dynamical core intercomparison project summer school, NCAR
13 May 2016	Peer review: the nuts and bolts, Sense about Science
June 2015	Advanced numerical methods for Earth-system modelling, ECMWF

Conferences and workshops

September 2017	Applicant	International conference on scientific computation and differential equations, University of Bath
August 2017	Co-organiser	NERC student conference (working title)
July 2017	Speaker	UK Met Office GungHo network meeting, University of Exeter
June 2017	Participant	Docker containers for reproducible research, University of Cambridge
April 2017	Speaker	PDEs on the Sphere, École normale supérieure, Paris
March 2017	Attendee	Open in practice: inspirations, strategies and methods for open research, University of Reading
March 2017	Participant	Effective quadratures workshop, University of Cambridge
February 2017	Invited speaker	Numerical methods for geophysical fluid dynamics, Imperial College London
January 2017	Attendee	Research software management, sharing and sustainability, British Library
December 2016	Invited speaker	South-East local centre meeting, Royal Meteorological Society
October 2016	Speaker	Numerical and computational methods for simulation of all-scale geophysical flows, ECMWF
November 2015	Attendee	GungHo workshop on next generation weather and climate prediction, UK Met Office
June 2015	Attendee	Hoskins@70
June 2015	Poster	SCENARIO DTP conference
March 2015	Speaker	Galerkin methods with applications in weather and climate forecasting, ICMS

Teaching

Oct 2016	Teaching assistant	MTMW11 fluid dynamics
Oct 2015	Teaching assistant	MTMG02 atmospheric physics
Sep 2015	Teaching assistant	NCAS summer school
Sep 2014	Course teacher	MPE python and linux short course

Visits and collaborations

July 2016	Organised visit from Simon Clark, stratospheric PhD researcher and YouTube vlogger
Summer 2016	Worked with Hilary's MSc student, Christiana Skea, studying variable timestepping for ODEs
June 2016	Visited NCAR, hosted by Ram Nair
2015 – 2017	Coauthoring an article about dimensionally-split and multidimensional transport schemes, written with Hilary, her former student Yumeng Chen, and Stephen Pring at the UK Met Office

Outreach

17 Mar 2017	"The advection process: simulating wind on computers", Social Metwork blog article
14 Jul 2015	Schools physicist of the year awards
14 Jun 2015	East Reading festival
15 Feb 2015	Brighton science festival

Presentations

19 Jun 2017	HHH group	Quantifying uncertainty with effective sub-sampling (working title)
30 Mar 2017	Mesoscale group	Modern advection schemes for weather and climate models (working title)
17 Nov 2016	Comp. Atmos. Dyn. group	A review of atmospheric transport schemes
9 Nov 2016	PhD group	Replicable computational atmospheric science
31 Oct 2016	HHH group	Advection over steep slopes
22 Sep 2016	PhD poster session	Improving numerical accuracy over steep slopes
23 Mar 2016	Quo Vadis	Numerical representation of orography in dynamical cores (honourable mention)
17 Feb 2016	PhD group	Multidimensional advection schemes for arbitrary meshes
9 Feb 2016	Mesoscale group	Curl-free pressure gradients for accurate modelling of cold air pools
19 Oct 2015	HHH group	Improving modelled mountain flows with alternative representations of terrain
27 Apr 2015	HHH group	A like-for-like comparison between terrain following and cut cell grids
21 Apr 2015	PhD group	Discrete vector calculus on Arakawa C grids
12 Feb 2015	UK Met Office	Poster presentation for Met Office Academic Partnership
18 Jan 2015	PhD group	Python and linux tips
17 Dec 2014	MPECDT jamboree	Poster presentation for Mathematics for Planet Earth Centre for Doctoral Training jamboree
12 Sep 2014	Lunchtime seminar	Gain control of your documents and code: hands-on with revision control and build automation

Appendix C: Publication milestones

10 Jun 2015	First MWR manuscript submitted
19 Aug 2015	Major revisions required to MWR manuscript
29 Oct 2015	Second MWR manuscript submitted
9 Dec 2015	Major revisions required to MWR manuscript
5 Feb 2016	Third MWR manuscript submitted
2 Feb 2017	First JCP manuscript submitted
13 Mar 2017	Minor revisions required to JCP manuscript
21 Apr 2017	Second JCP manuscript submitted