Responses to reviewers

Multidimensional method-of-lines transport for atmospheric flows over steep terrain using arbitrary meshes

JCOMP-D-17-00161

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We greatly appreciate the reviewers' detailed comments and questions. The revised manuscript highlights changes with a bold typeface and the text colour corresponds to the section headings below. The revised manuscript also highlights a small number of additional changes **in orange**.

Reviewer #1

This paper presents a multidimensional method-of-lines finite-volume transport scheme, which is second-order accurate and offers high solution quality and robustness under strongly deformed meshes. Among others, the latter is of increasing importance for atmospheric models with complex orography. The proposed scheme is named "cubic-fit", as it fits multidimensional polynomials of up to third-order over an upwind stencil using a least-squares approach. The construction of the polynomials takes into account constraints derived from a linear stability analysis for stencils in regions of highly-deformed computational meshes.

The accuracy and stability of the cubic-fit scheme is studied with a number of well chosen test cases that are relevant to atmospheric models.

In my view, the presented developments definitely warrant publication in JCP. The content of the paper appears of high quality and adheres to the JCP standards. The text is well structured and clearly written. It only needs little improvement as given by the subsequent comments.

I recommend acceptance of the paper subject to minor revisions by the authors.

Comments

1. It is explained in various places that the cubic-fit scheme offers favourable computational efficiency due to the fact that most of the reconstruction depends on the mesh geometry only, and this part can be precomputed. It would be very interesting to see numbers in the paper. It doesn't have to be a comprehensive study, but just to get an impression of the cost, e.g. how does the runtime of the cubic-fit compare to the second-order upwind scheme? Or, if one runs cubic-fit and the upwind scheme such that both produce about the same ℓ_2 error (by using a higher resolution with the upwind scheme), what is then the difference in runtime?

TODO *I think OpenFOAM's linearUpwind implementation would be more efficient if it was expressed as a weighted sum rather than a gradient reconstruction at every time-stage. If I can express linearUpwind as a weighted sum then I can compare the number of multiplies for a given stencil.*

TODO *I also like the idea of comparing computational cost (measured in number of multiplies) for a fixed ℓ_2 error. It would be natural to do this for the 'minimal' resolution measurement that we've already documented for linearUpwind and cubicFit.*

2. As only 2D simulations have been considered in the paper, I wondered how difficult it will be to extend the cubic-fit scheme to 3D? It could useful to provide a short comment about this, just whether complications are anticipated or not. (See also the subsequent comment.)

TODO

- *The stencil construction procedure already applies to two or three dimensions*
- *The definition of candidate polynomials also generalises naturally to three dimensions*
- *Assuming that a 3D mesh comprises prismatic cells arranged in columns then the computational cost in 3D will be three times the computational cost in 2D*

3. Appendix A, p.22: How restrictive is the 1D stability analysis for the multidimensional domains? May this become a more serious issue in 3D configurations?

TODO *We did trade some accuracy on good-quality meshes for stability on certain poor-quality meshes, so the scheme is more damping than it could be. Should we try to analyse this?*

TODO *I'm not sure what to expect regarding stability/accuracy in 3D. Perhaps I should try it. Henry (OpenFOAM) would really like me to get it working in 3D so the code can be pushed upstream.*

4. In various places throughout the paper "icosahedra" is used instead of "icosadedral". I suggest the latter should be used consistently throughout the paper.

Now using the term 'hexagonal-icosahedral mesh' throughout.

5. p.3, end of first paragraph: I suggest to mention here a recent advancement of the finite-volume MPDATA (Kühnlein and Smolarkiewicz, J. Comput. Phys. 2017, `http://dx.doi.org/10.1016/j.jcp.2016.12.054`). Among others, this paper demonstrates applicability of MPDATA for 3D compressible atmospheric dynamics on arbitrary hybrid unstructured meshes.

Thank you, included.

6. p.3, paragraph after Eq. (2b): if there is no specific need, I sugggest to remove "zero-dimensional".

Removed.

7. p.4, last paragraph in Section 2.0: "methods are described next" instead of "methods described next".

Fixed.

8. p.5, first paragraph: Is it "arbitrary meshes" or "arbitrary structured meshes"?

Now using the term 'arbitrary meshes' throughout.

9. p.5, last paragraph of Section 2.1.1.: "dirichlet" should be upper case "Dirichlet".

Fixed.

10. p.7, caption of Fig. 3, last sentence: It is stated that a von Neumann boundary condition is assumed. However, the footnote on p.5 says that Neumann BCs are excluded from the set of stencil boundary faces?

TODO

11. p.9, caption of Fig. 4, first sentence: "A one-dimensional least squares fits" should probably read "One-dimensional least squares fits".

Fixed.

12. p.12, caption of Fig. 6, last but one sentence: "domain is shown" instead of "domain in shown".

Fixed.

13. Section 3: Why are most of the experiments run with maximum CFL numbers < 0.5 or even < 0.4, although the cubic-fit scheme permits a maximum CFL < 1 (Fig. 10)? Is this because the upwind scheme, to which cubic-fit is compared to, is more limited with respect to the time step for the considered test cases?

Lauritzen et al. [1] recommend using a 'typical' Courant number for transport tests on the sphere, and so we follow their recommendation throughout. This is now stated TODO *on page nnn* in the revised manuscript. A maximum Courant number of about 0.4 avoids any accuracy and stability issues caused by time-stepping. A separate series of tests confirm that the stability limit is 1.0, as presented TODO *on page nnn* in the revised manuscript.

14. p. 18, last but one paragraph, last sentence: correct "imprintingin".

Fixed.

Reviewer #2

General remarks

The manuscript presents a new method-of-lines based transport scheme in which fluxes are computed by fitting a multidimensional polynomial over an upwind-biased set of grid cells. The scheme has low computation and memory costs. It is suitable for structured and unstructured grids, and maintains accuracy on strongly distorted grids such as those used in atmospheric models over steep terrain. An idealized analysis suggests how the construction of the polynomial should be constrained to obtain conditional stability of the scheme, and such stability appears to be achieved in practice. I believe the manuscript will be of interest to those developing atmospheric models and to the wider CFD community. I would be happy to recommend publication after the points below are addressed.

Main points

1. It is claimed (in several places) that the scheme requires 'just one vector multiply per face per time step'. Since the two-stage Heun scheme (2) is used, surely the cost must be two vector multiplies per face per time step (or, more generally, one vector multiply per face per *stage*)?

Correct. The term 'time-step' has been replaced with 'time-stage' everywhere this calculation is discussed. TODO *Hilary, is this reasonable terminology? Google suggests it is already used in published literature.*

2. It is claimed in several places that the scheme is stable, but some qualification is appropriate. First, the scheme is *conditionally* stable; the Courant number should not be too large. Then Appendix A gives an analysis deriving constraints on the polynomial reconstruction that should be satisfied for stability. However, the analysis is idealized in various ways: one-dimensional, regular grid, constant v, two- and three-cell stencils, and ignoring the time discretization (also see below). That is fair enough—it might not be possible to generalize the analysis to the full scheme—and it is clearly stated at the end of the Appendix that the constraints are *hypothesized* to apply more generally. However, in section 2.1.4 the language is stronger and suggests that these constraints are definitive: "...stability constraints...", "...must satisfy...", etc.

TODO

3. P14. The calculation of the longest stable timestep *assumes* that the stability limit is given by Co = 1. Given the idealized nature of the analysis in Appendix A, and that most experiments are done with Co $\approx$ 0.4, at least some empirical investigation of the stability limit should be discussed to confirm that it is indeed (exactly or approximately) Co = 1.

TODO *Reviewer one raised similar concerns about the CFL criterion so I've put my response next to their comment for now.*

> 4. The presentation of the analysis in Appendix A is somewhat confusing. It appears to use a time discretization by introducing a time step Δt and an amplification factor A, (and hence a Courant number $v\Delta t/\Delta x$) whereas the analysis is, in fact, continuous in time. It might be clearer to set $\phi(x_j, t) = \hat{\phi}(t)\mathrm{e}^{ijk\Delta x}$ and form an ODE for $\hat{\phi}$, etc. I think the conclusion would be the same.

TODO *I'll try this*

> 5. Might it be possible to include the time discretization (2) in the stability analysis? It would be interesting to know if the weak instability of (2) (noted on p3) affects the constraints (57), (58), (63).

TODO *I'll try this*

> 6. The Courant number as defined by (4) would appear to vanish for a non-divergent flow. A more natural definition might be to sum only over outflow faces (and remove the factor 1/2). For non-divergent flow that would be equivalent to replacing $\mathbf{u} \cdot \mathbf{S}_f$ by $|\mathbf{u} \cdot \mathbf{S}_f|$ in (4).

Equation (4) should use the absolute value $|\mathbf{u} \cdot \mathbf{S}_f|$. This is how the Courant number is calculated in OpenFOAM[1]. Equation (4) has been corrected in the revised manuscript.

> 7. Section 3.2 and Table 1: what resolution is used?

Added a sentence near the beginning of section 3.2. The mesh spacing is the same as Schär et al. [2] with $\Delta x = 1000$ m and $\Delta z = 500$ m.

Minor points

> 8. It would be interesting to know if there was some rationale for the choice of the polynomial (5) and the stencil discussed in section 2.1.1. Given that the scheme is second order convergent, might it be possible to use a lower degree polynomial and smaller stencil?

TODO *want higher order in the direction of flow, hence cubic in x. upwind-biasing is for stability (citation? leonard?)*
A previous version of cubicFit was in the dynamical core developed by Weller and Shahrokhi [3] in order to correctly simulation Schär mountain waves [2]. They found that smaller stencils and lower degree polynomials produced incorrect results, although comparisons between advection schemes were not presented in the paper.

> 9. The first two paragraphs on p2 refer to quadrilateral meshes. It seems the discussion has slipped into the 2D vertical slice case without explicitly saying so.

The term 'quadrilateral' has been removed from these paragraphs since it is sufficient to say that the methods modify regular meshes. These meshes may be rectilinear for a limited area domain or curvilinear for a global domain.

> 10. P2, 5th paragraph. Perhaps mention that dimensionally-split schemes are only possible when the grid permits it (e.g. not a hexagonal grid).

The revised manuscript explains these limitations, "**Dimensionally-split schemes have only been used with quadrilateral meshes where dimensions are inherently separable. Special treatment is required at the corners of cubed-sphere panels where local coordinates differ [4, 5]. For similar reasons, dimensionally-split schemes have only be used with terrain-following coordinate transforms and not cut cells.**"

[1] `https://github.com/OpenFOAM/OpenFOAM-dev/blob/master/src/finiteVolume/cfdTools/incompressible/CourantNo.H#L39`

11. P9, last sentence of section 2.1. Should w_d be m_d?

TODO Yes, fixed.

12. The discussion of previous work is generally very good. On p2 is it worth mentioning the SLICE scheme of Zerroukat and co-authors? In the first paragraph of section 3.3, credit for the hexagonal-icosahedral mesh should probably be given to Heikes and Randall.

The revised manuscript now mentions the three-dimensional semi-Lagrangian finite volume scheme, SLICE-3D [6].

In addition to citing Thuburn et al. [7], the manuscript now cites the original Heikes and Randall articles [8, 9] on which the hexagonal-icosahedral mesh generator is based.

13. Some brief comments on how the approach extends to three dimensions would be appropriate.

TODO *Reviewer one also asked us to comment on an extension to 3D. I've responded to their request for now.*

Typos, etc

14. Introduction, second sentence: 'modification of the lower boundary' is an odd way to think of it.

Reworded to say, "the mesh is necessarily distorted **next to** the lower boundary".

15. P2, 5 lines from the bottom: '...non-simply connected domains...'. I found this phrase confusing.

The revised manuscript includes an explanation that is more intuitive and describes the example illustrated by Lauritzen et al. [10].

16. P3 line 17: 'cubic, upwind-biased stencil'. Surely it is the polynomial that is cubic, rather than the stencil?

Yes, reworded to say, "the scheme fits **a multidimensional cubic polynomial over an upwind-biased stencil**".

17. P3 below (2): 'stable ... with some upwinding'. Presumably some qualification is required (with sufficient upwinding)?

Reworded to say "with **sufficient upwinding**" as suggested.

18. P5 footnote: could be made

Fixed.

19. P14 5 lines from the bottom: cubic should be cubicFit?

Fixed.

20. P18 2 lines from the bottom: imprinting in

Fixed.

Reviewer #3

The author describes a standard finite volume algorithm for solving the advection equation on unstructured grids. Using a method of lines the spatial discretization consists in computing face values of a cell centered given function by high order polynomial point wise approximation in contrast to a more common area wise procedure. The proposed algorithm has three phases, choose of two upwind dominated stencils for each face, determination of a subset of candidate polynomials with at most order three, weighting of the individual contributions in a least squares approximation to increase stability with respect to the advection equation.

The stencil choice starts with the determination of opposing faces in the upwind cell with respect to to the destination face, and adding further cells in a two step procedure. The candidate polynomials with at most order three are all polynomials where the corresponding least squares problem has full rank. For the third step the candidate polynomials are ordered with respect to the number of unknowns and and larger minimal singular value in case of polynomials with the same number. In the second step following the first ordering a weighting sequence is tested until a stability criterion is fulfilled which can finally end in a simple upwind scheme.

The paper is well written and illustrates all steps by intuitive examples. The new test example for the two-dimensional example with the boundary following velocity field enriches the number of problems for testing numerical advection schemes.

Comments and questions

1. Can you comment on the stencil for triangular grids. In case of a slightly perturbed triangular grid with equilateral triangles the stencil changes in comparison the unperturbed case.

We haven't explored triangular meshes in this paper, and more work would be needed to evaluate the suitability of stencils and stability criteria on these meshes. We would not expect the stencil topology to change for triangles that are slightly perturbed from equilateral because such triangles will always have two opposing faces as given by equations (6) and (8).

2. Why do you prefer the point wise approximation?

A point-wise approximation is computationally cheaper than a swept-area approach which must enforce integral constraints on the polynomial reconstruction.

TODO *There is existing CFD literature that uses point-wise polynomial least squares reconstructions [11, 12]. They call this a 'top-down' approach: "we work with* pointwise *values of the conserved variables, associated to the cell-centroids". This is unlike the traditional 'bottom-up' finite volume approach. This approach uses a cell-average, discontinous conserved field and a polynomial reconstruction of a piecewise continuous flow field from the a piecewise constant flow field representation.*

TODO *What is Cueto-Felgueroso's motivation for choosing it? Would we expect weighting by cell volume to have any advantages? My monitoring committee asked this a long time ago. Certainly it would not ensure numerical stability.*

3. The singular value test should be relative to the largest singular value.

TODO *We should try this. Does it change the coefficients for any tests? The ratio of largest and smallest condition numbers gives the condition number of the matrix (citation?)*

4. The weighting can degrade the condition number of the least squares problem.

We restrict multipliers to be at most 1024 so that the matrix equation does not become ill-conditioned. TODO *I could measure this, see above comment, too*

5. Is there a smoothing of hexagonal-icosahedral mesh after refinement.

The hexagonal-icosahedral mesh is not smoothed but iteratively refined. The revised manuscript includes citations for this procedure [8, 9].

> Can you comment on the projection to the tangent plane for the spherical test example. Note that projection to another grid can change the interpolation/approximation essentially, like the transformation of a boundary following grid in physical space to a Cartesian grid in computational space. Why is the interpolation/approximation not done in 3 dimensional physical space.

The tangent-plane projection has been used in existing method-of-lines transport schemes [13, 14]. TODO *Using a projection means we can a two-dimensional polynomial. Skamarock and friends mention that results are insensitive to the various details of the tangent-plane approximation. I'm not sure what the details are? They mention that [15] found little sensitivity to various approaches, too.*

TODO *Hilary mentioned at least one other possible projection other than tangent-plane which preserves great-circle distances. We also discussed the implications for avoiding a projection altogether and including a third dimension in the polynomial reconstruction. What was the outcome of this discussion?*

References

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