"Vertically nested LES for high-resolution simulation of the surface layer in PALM (version 5.0)" by Huq *et al.*.

Manuscript:	GMD-2018-287
Title:	Vertically nested LES for high-resolution simulation of the surface layer in PALM (version 5.0)
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Recommendation

Major revisions (but not very major)

Evaluation of Referee:

	Excellent	Good	Fair	Poor
Scientific significance	x			
Scientific quality:		x		
Scientific reproducibility		x		
Presentation quality		x		

General

- The paper describes a modification of the PALM large-eddy simulation code that enables vertical grid nesting in the layer adjacent to the Earth's surface. The resulting increase in resolution in the surface layer improves the representation of turbulence (since a smaller fraction of the turbulent motion has to be represented by the subgrid parameterization). With this technique, it becomes feasible to study turbulence in the surface layer while still resolving the full atmospheric boundary layer above it.
- The employed method builds on existing and established methods. The main contribution of the paper is that it describes the implementation of vertical nesting for a code that is publically available.
- The paper is well written and in general well structured.

However, I do have some comments:

a. I miss a thorough discussion on how the subgrid fluxes are handled at the interface between the course grid domain and the fine grid domain. I could imagine that the subgrid fluxes at the boundary between CG and FG would need to be interpolated. Or continuity of the subgrid fluxes at that interface could be ensured by the subgrid models on either side of the interface. However, I so not see how the subgrid flux between CG and FG are handled in a conserving way: what leaves the CG should enter the FG and the other way around.

b. The validation of the results of the nested simulation (characteristics of turbulent fields) is rather superficial (fluxed and variances, no spectral analysis or higher order moments; also little consideration for subgrid contributions).

c. The analysis of the timing of the simulations (scaling, overhead, net gain etc.) is limited.

d. The application of boundary conditions to the nested grid is insufficiently clearly described:
   - Is the Dirichlet condition for horizontal wind components and scalars applied to a point

just above the fine grid domain, of to the highest point just inside the fine grid?

- The equations given for the interpolation algorithm lack explanation.

e. The structure of the introduction could be improved. After the overview of the history of LES, I would expect a clear definition of the problem (we need high resolution where it matters: close to the surface (and in the entrainment zone), an overview of how people have solved this until now, what is that we still not know/can/have?, and how are you going to solve it. Also the structure of section 2 could be improved to more clearly separate the different aspects of the new model.

Below I will provide detailed comments

Note: in the comments below, the comment is preceded by the page number-line number.

Detailed comments

1. 2-27: You immediately make the jump to grid-nesting. However, the main point is that you need increased resolution. And if you cannot afford to increase the resolution in the entire domain, you want to do it locally. *One* way of doing that is by grid-nesting. But there are other ways: if one does not insist to stick to a structured grid, local grid refinement (without nesting) is feasible. This grid refinement can even be made dependent on the flow itself (see van Hooft *et al.*, 2018). So: grid-nesting is just one of the ways to locally increase resolution.
2. 3-7 to 16: here you explain why vertical nesting is needed. But you started that argument already in line 2-28 to 30. Please restructure your argumentation (either move 3-7 to 16 to the point where you introduce vertical nesting (and then talk about horizontal nesting to show what we know from that), or first introduce horizontal nesting and then make the step to vertical nesting (or ignore horizontal nesting altogether, since vertical nesting is in itself not new, just your implementation in PALM is new).
3. 3-17: it seems that Clark and Hall (1991) deals with horizontal nesting. To what extant is it still relevant for this paper?
4. 3-23: '...superior when the waves ...': doe you mean 'when' or 'if'? And what happens if/when the waves are not well resolved? In what way is this relevant for the present paper on the simulation of turbulence?
5. 3-28: '.... both the resolved and SGS fluxes...': does this also hold for the finite difference code used here? In what way would/does it increase coding complexity?
6. 4-17: please explain the variables used in the equations. In particular the notation for resolved variables and subgrid variables is important. Furthermore, I assume you include the tendency equation for potential temperature because the potential temperature plays a role in the SGS-TKE equation and in the momentum equation. But then you should also include the moisture tendency in order to be able to determine the tendency of the virtual potential temperature (which then also should be used in the buoyancy terms). Finally, the heat flux that appears in equation (4) is the subgrid heat flux: (1) apparently you denote subgrid variations by a single prime and the filtering operation by an overbar and (2) in the model the subgrid heat flux is parameterized using a gradient hypothesis (also the next term, the transport term, is parameterized).
7. 4-20: 'guarantees a stable': how does the choice of the time integration method guarantee a stable solution. The magnitude of the time step would still play a role (and it does, as later on you invoke the CFL criterion). So why mention stability here?
8. 4-23: I assume that you refer the *vertical* zero pressure gradient here.
9. 5-9: apart from updating the ghostpoint, there is also global communication needed in the

Poisson solver. This involves way more communication than the ghostpoint update.

10. 5-10: regarding the structure of the rest of section 2: I would suggest to restructure this section as follows:
    2.2 Model structure
    2.2.1 Grid configuration (now 2.2, up to line 5-29)
    2.2.2 Nesting algorithm
    2.3 Translation between grids (line 5-9 until7-4)
    2.3.1 Anterpolation
    2.3.2 Interpolation
    2.4 Parallel inter grid communication
    (after 2.2.2 it is clear where and why anterpolation and interpolation are needed).
11. 5-30: only the vertical velocity really has a boundary *at* the top of the FG. For the other velocity components and scalars it is unclear whether the boundary condition (interpolation from CG) is applied to a ghost point (just above the FG) or to the first point just below the boundary of the FG.
12. 5-32: what is the 'logical' direction? If figure 1 would be upgraded (see below), this 'logical' linear interpolation would probably become clear.
13. Figure 1: the current figure is not very informative. I would suggest to replace it by a figure in which you show a few CG cells as well as the FG cells within one or two of them (preferably with a grid ratio of 3, not more). Then clearly show how the interpolation of vertical velocities, as well as horizontal velocities and scalars works (in order to support the interpretation of equations (5) as well as the notion that the velocities are interpolated in a 'logical' direction. The connection to equations (5) could also clarify the meaning of the various indices (lowercase and uppercase).
14. Please completely rework the equations and add explanations:
    - Make clear that the first equation is the actual interpolation, and all the other equations just define the various parameters occurring therein.
    - In which coordinate direction does *i* vary: only in the *x*-direction, or also in other directions. Or are we actually looking at a 2D or 3D stencil of which only one dimension is shown?
    - The capital indices *I, J,* and *K* are counting through the entire domain, I assume. But how about the lower case indices: do they start counting at 1 (or zero) within each CG cell, or do they also count globally?
    - In the 2nd-4th equations you introduce H_k. What is the value of the index *k*. Or does the repeated index imply summation? If so, what is the range of values that *k* can take: 1, 2 and 3 because of the dimensionality, or 1, 2, ... n_x because of the number of FG cells in a CG cell?
15. 6 - equation (6): what is the range of values for *i, j* and *k* ? Is there a mapping that gives the global *i,j,k* values for a given *I,J,K* or, are these local *i,j,k* values, running as 1, 2, ... n_x ?
16. 7 - equation (7): idem
17. 8-7 and 11: please keep the discussion on the solution of the Poisson equation in one place. What is the value of the pressure gradient that is imposed as a Neumann boundary condition? If it is zero, reflections could occur, but if you use something non-zero: how do you determine the value of this gradient? Is it derived from the CG pressure field?
18. 8-12 and 13: please clarify how the value of the imposed pressure gradient is determined/chosen.
19. 8-31: '... the higher number of PE available in the FG.': this is stated as if the reader already knows that there are more PEs in the FG (although for any grid ratio above 2 it is indeed logical that the number of FG PEs is larger than the number of CG PEs). But in addition, it

is unclear to me why the higher number of FG PEs would be relevant for the FG-to-CG communication.

20. 9-2 'should be kept lower': please explain the logic of this statement. I assume that the idea is that you want to reduce the total amount of idle CPU time on the FG PEs (*N* cores x wait time), which can be achieved by under-utilization of the (only) *M* cores running CG (better waste time on a few CG cores than on many FG cores). In order to know how this plays out in practice, you should show in your results the amount of time spent in the various steps in a RK substep: which fraction (and absolute time) of a time step is devoted to which substep in figure 2, and how much of this time is wasted time.
21. 9-12 'Dirichlet condition': to which values are the velocities set: zero for vertical wind and geostrophic for horizontal?
22. 9-13: what is the imposed temperature gradient at the surface?
23. 9-15 and 16: is the wind profile interpolated *linearly* from zero at the surface to geostrophic at the top? Does this out-of-balance initialization lead to an inertial oscillation?
24. Table 1: what is the boundary condition for wind? MOST with an imposed roughness length (what is the value) or an imposed stress?
25. Table 2:
    - please add the number of time steps needed to complete this simulation (in that way the reader can easily determine the time spent per gridpoint per time step.
    - For the reader it would also helpful to include the number of grid points per PE and the CPU time per grid point (but both numbers *can* be derived from the available data, so the reader could do it for themselves).
    - the number of cores devoted to CG and FG respectively is not motivated. Whereas later on you advise to assign to a CG PE 40-80% of the number of grid points that is assigned to a FG PE, here you use a fraction of 16%.
    - it is unclear to what extent the PE's are saturated in terms of memory usage: could this problem be run on even a smaller number of processors to improve performance?
    - Please include information on the time (absolute and/or as a fraction) that is used waiting for input from CG to FG or the other way around. This would be helpful to determine the optimal division of labor between CG PEs and FG PEs (in terms of grid points per node).
26. 10-2: what initial perturbation is applied to get turbulence started? How did you verify that after 9000 s the flow was in equilibrium?
27. 11-5: part of the ingredients for the scaling variables are in fact imposed boundary conditions (the surface heat flux), whereas indeed another part (the surface shear stress) results from the flow (and hence need to be derived from one of the simulation results (assuming that a roughness length is prescribed).
28. 11-6 and 8: surface heat flux in the expression for w^*: overbar is missing and this is not a turbulent flux (so do not use a covariance flux).
29. 11-8: although it will not change the lines in the graph, normalizing the temperature with the surface value is very illogical. Please plot the temperature with some reference value (e.g. the surface value) subtracted and normalized with θ^*.
30. 12-1: what would/could be the mechanism that makes that the higher resolution in the surface layer would affect the variance profile well above the FG domain?
31. 12-3: please use the same scaling variable for all velocity components! If not, the different variances (which together constitute the turbulent kinetic energy) cannot be compared. Furthermore, the given flow is close to free convection, so using the friction velocity as a scaling variable does not make sense.
32. 12-5: you refer to an overshoot in the *v* variance. The *u* variance shows an overshoot as well.

I assume that the profiles shown are based on the resolved variances only. In that case, we should keep in mind that in the CG domain a larger proportion of the TKE is contained in the subgrid scales. Could this explain the jump? Please include an analysis of the difference in SGS-TKE between the two domains at the top of the FG (of course there is the difficulty of separating the SGS TKE into the three components, but at least quasi-quantitatively such an analysis could shed light on these jumps/overshoots.

33. 12-7: how would the anterpolation influence the vertical velocity variance in the FG domain. Please explain the/a mechanism. Or is it a result of the fact that the upper boundary conditions for pressure at the top of the FG is not well-defined?
34. 13 figure 6: the variance profiles give some information on the quality/realism of the simulated turbulence. One analysis that is missing (related to the point made above regarding the overshoot) is whether the increased resolved TKE is the amount that would be expected based on the increased resolution (and hence reduced reliance on the subgrid model). To properly analyse that one would need turbulent spectra to see how much kinetic energy is contained in the additionally resolved scales.
    Additionally, spectral analysis (preferably with 2D spectra) would help to show to what extent the extra resolved turbulence has the expected turbulent characteristics (increased variance is nice, but does not need to be additional turbulence, it could also be increased noise).
35. 13-1: The heat flux profile is not the prime quantity at all! For a quasi-stationary convective boundary layer with imposed surface flux the heat flux profile is the most boring part of the simulation. Provided that the entrainment flux is represented well, the flux profile is by definition linear, varying between the imposed surface flux (so no surprises there) and the entrainment flux (which, admittedly, needs to be represented correctly by the simulation: still some freedom there). This linear flux profile is completely independent of the quality and resolution of the simulation. The only freedom there is is which part of that flux is carried by the resolved scales and which part is carried by the subgrid model. Hence the perfect correspondence between all simulations (full FG, full CG, nested CG and nested FG). Hence, please do not use the heat flux profile as a measure of the quality of the simulation.
36. 14-4: '...we increase the resolution further': do you mean to increase the grid ratio, the size of the FG region, or the overall resolution of the CG domain?
37. 14-9: 'in terms of communication time': do you only look at communication time because that is the most restricting, or because you are only interested in that (in this context)? And why should the number of domains be equal in x and y direction: please explain the logic of this (and does it also hold if the length of the domain is different in x and y direction?
38. 15-1 to 5: why is the setup of these simulations (in terms of the total number of points and ratio of number of grid points between CG cells and FG cells) so different from the original runs? Are the performance results still relevant to understand those first runs? If so, why? Please give the setup of these runs in a table similar to table 2 (not 'number of grid points is *around...*').
39. 15- Figure 8:
    - on a log-log scale everything looks nice. Please give a more informative representation. E.g. use the strong scaling efficiency, which will vary between 1 and somewhere below 1 (for your data, using the left-most simulation as a reference, the efficiency goes down to about 90% for the right-most. But the question is, what would have been the CPU time for the smallest possible number of processors on which this case could have been run (memory-wise).
    - In addition, find a more informative way to quantify the waiting time overhead.

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40. 16-9: 'large scale forcing .... compatible': do you refer to the large scale forcing in terms of pressure gradient/geostrophic wind? Or another large scale forcing? Why would it, or would it not, be compatible. Please clarify.
41. 16-12: 'accuracy': for accuracy in what sense (interpolation errors, truncation errors, turbulence statistics, stability, ...) should the grid ratio be not too large?
42. 16-14: 'first five grid points are unreliable': for which variables does this hold, in which aspect are the grid points unreliable (I assume you mean '*the results* at the first five grid points vertically displaced from the surface'): turbulence characteristics, mean profiles, noise, ...? Do you have a reference for this bold statement?
43. 16-16: I would like to see a quantitative motivation for this 40-80%.

Very detailed comments

1. 2-14: 'possible, by the time' → 'possible. By the time'
2. 2-18: 'supercomputers': also the people before Kröniger et al. used supercomputers. So remove 'with the help of supercomputers'.
3. 2-19: remove 'speeds'
4. 2-21: 'higher detail': 'higher' than what/when/who?
5. 2-28: 'Nesting has been applied...': because the previous sentence talks about vertical nesting, the reader may think that this sentence gives examples of that. But then at the end it turns out to talk about *horizontal* nesting. Please rephrase.
6. 3-3/4: 'techniques *are* ..... but often *uses* ...': 'uses' should be 'use' (plural)
7. 3-18: '... CG, there ...' → '... CG, and there ...'
8. 3-24: make explicit that the 'two different approaches' only refer to the 'anterpolation' mentioned in the sentence before. Furthermore, nothing is said –explicitly- about the 'pressure deficit correction' ("there are two types of cars: blue cars")
9. 4-9: 'additional equation': additional to what? The SGS-TKE equation *is* in the Deardorff method, so it is *not* additional to his work.
10. 4-11: 'The prognostic ...': move this sentence to below the equations (only after having presented the equations you need to talk about their discretisation).
11. 5-17: 'the grids' → 'grids' (this occurs in multiple places, please check.
12. 5-18: please explain here already that uppercase symbols refer to CG and lowercase symbols to FG.
13. 6-1: 'similar interpolation': in which way is it similar, and which way is it different?
14. 6-5: 'scalars' → 'CG scalars'
15. 6-5: 'The scalars .... corresponding FG scalars (eq. 6)'. How much more are you saying than 'An average is an average'. If you want to state more, please make that clear and explicit.
16. 7-6: 'We implement....'. Well, that does not really come as a surprise: you gave that away already (see my suggestions for an alternative structure for section 2).
17. 8-7: '... is also updated...'. What else is updated? You mean the pressure? And is the vertical velocity updated throughout the FG, or are you only referring to the vertical velocity at the CG-FG interface?
18. 8-20: '...process. Whereas....' → '...process, whereas....'
19. 8-20: 'exchange' → 'exchange*d*'
20. 8-23: 'local PE's 2D processor co-ordinate': in what way is the PE different from the processor? → 'local 2D processor (or PE) coordinate'
21. 9-11: 'is set to' → 'has'
22. 10, Tables 1 and 2: please format the tables properly as tables should be formatted (including column headings and a consistent demarcation of rows and columns)

Table 1: please note that the surface heat flux is not a turbulent flux (there is no vertical velocity (variation) *at* the surface. Furthermore, even if you would like to denote it as a turbulent flux, please add an overbar.

23. 11, figure 4: the lower panel is –vertically- not exactly to scale with the area indicated with the dashed line in the upper panel.
24. 11-2: ‘flux profiles’ → ‘fluxes’
25. 11-3: the given expressions are not fluxes, but products of resolved deviations: please include an averaging operator to make it a flux.
26. 11-13: ‘at the boundary layer height’ → ‘at the top of the boundary layer’
27. 12-1: ‘An one-way’ → ‘A one-way’
28. 12-5: ‘variance seen’ → ‘variance can be seen’.
29. 14-5: ‘Simulations with O(1) ...’: are you referring to that resolution for a full domain, or only for the FG part of a nested simulation? In fact, it is unclear where you are heading with lines 14-2 to 14-6.
30. 14-13: ‘new nested simulation’: new relative to? I assume that you mean new relative to the runs described in tables 1 and 2. These new simulations were made for the performance test only?
31. 16-4: ‘Poisson equation’ → ‘the Poisson equation’
32. 16-7: ‘FFT’ → ‘an FFT’
33. 16-28: ‘energy conserving methods’: I have not seen that term earlier in the paper. Where was this discussed before? Or are you referring to the anterpolation of SGS TKE? In that case, please be a bit more explicit.
34. ‘... optimized for performance’: how were they optimized, where can I read about that optimziation?

References

van Hooft, J.A., Popinet, S., van Heerwaarden, C.C. et al. (2018). Towards Adaptive Grids for Atmospheric Boundary-Layer Simulations. *Boundary-Layer Meteorol* **167**: 421-443. https://doi.org/10.1007/s10546-018-0335-9