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Geoscientific Model Development Discussions

Interactive comment on "The ESCAPE project: Energy-efficient Scalable Algorithms for Weather Prediction at Exascale" *by* Andreas Müller et al.

Anonymous Referee #1

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Overall impression

The manuscript under consideration was submitted to GMD as a "development and technical paper". The paper topically spans mathematical formulation, numerical integration techniques, parallelization strategies, language-specific aspects of implementation, hardware-specific optimizations, hardware construction, and operational considerations in the context of both global-circulation and limited-area models.

As the main conclusion from the hereby review, I propose to significantly shorten the article (currently 50-pages and 30 figures) and change its type to a "Review and perspective paper" to match the stated intention of the authors to create "*the flagship publication for the EU project ESCAPE ... introduce the concept of weather & climate*

dwarfs and discuss first results in terms of optimization and performance portability". This path seems to me as much more reasonable than working towards matching the requirements for a "development and technical paper" as defined by GMD guidelines.

The authors aim at: (i) providing a technical report touching upon current-hardware-specific performance measures, (ii) structuring the work as a research paper, and (iii) presenting a project-promoting overview article. These aims are incompatible in my opinion, and trying to achieve all of them at once results in unclear target audience and an apparent lack of a storyline, despite high potential for strong conclusions to be based on the presented results.

Notwithstanding, I do see a point in publishing such a "perspective" paper with the aim of promoting the project results and giving due credit to participating parties. I expect such a shorter "perspective" paper to achieve a higher impact and I encourage the editorial team to offer this option to the authors.

Code availability

The "Code availability" section on page 42 is derisory. The standard that GMD is fostering among the community is to enable readers and reviewers to reproduce results presented in GMD papers. Here, the reader is only given a link to project website where one may not even find a properly defined software license – just a statement that it "permits free of charge use for educational and/or non-commercial research". The final sentence of the referenced website reads: "*If you wish to access any of the implementations, please contact us via the contact form and we will provide further information on the process of obtaining a license*". This stands in clear opposition to the anonymous public access recommendations of GMD. Basing on an educated guess (the most one can anonymously base on given the above), I consider the results presented in the paper as not independently reproducible for reasons including software and hardware availability, as well as lack of availability of the details of the test cases.

As outlined above, a solution would be to move much of the technical details to another publication (a technical report issued by one of the participating institutions – several of those are already cited) and present a "perspective" paper for which GMD does offer an exception in terms of reproducibility level (see https://www.geoscientific-model-development.net/about/manuscript_types.html).

Nevertheless, the code availability section should contain comprehensive information, and clearly inform about the **code** availability, not license availability. Please point to repositories, state precisely the licenses or clearly indicate if the code is not publicly available or its reuse is constrained. In case of lack of public availability, GMD requires to state the reasons for it. Please include information for all the software that was essential in obtaining the presented results, including the participating weather prediction models: IFS, ALARO, COSMO-EULAG as well as the described tools such as GRASS, CLAW and GridTools (the https://github.com/eth-cscs/gridtools repository linked from the GridTools website does not exist as of time of writing this review).

Code availability for hardware-specific tools such as those essential in GPU code development should also be included in the section (see doi:10.1002/2016WR020190 for a recent discussion in the context of hydrological modelling), and in my opinion should also be included in the discussion if a proper "perspective" is to be given. The paper gives an overview of several paths forward in NWP systems development and aims at discussing longer-term strategies. Such discussion calls for mentioning which optimisation strategies are prone to the vendor lock-in threat.

The dwarf nomenclature and technicalities

The authors highlight throughout the paper the concept of separation of concerns in software engineering using the notion of a "dwarf" which the paper introduces in the context of weather and climate models. The reason to introduce a new term is not given. What does the new concept replace (monoliths)? The adopted term is seem-

ingly wrongly attributed (Colella as opposed to Asanović et al.?) and, in my understanding, used in a misleading way. The reason why the 7 dwarfs of Colella, and later the 13 Berkeley dwarfs, the 7 dwarfs of Symbolic Computation, the 13 Parallel Dwarfs (and likely others) were introduced is that the concept they generalize does not easily fit into existing encapsulation nomenclature of: components, frameworks, layers, substystems, libraries, kernels, modules, services, drivers, plug-ins, controllers, etc. Why dynamical core layers, physics modules and numerical libraries are to be renamed? In principle, why not – let us embrace the introduced notion of Weather & Climate Dwarfs, but please do clarify in the paper the reasons to introduce the new nomenclature and clearly differentiate it from existing solutions.

Moreover, among the community, dwarfs are being defined as computation/communication idioms (e.g., OpenDwarfs project) or (design) patterns of high-performance computing (e.g., the mentioned work of Asanović) – is it not misleading to refer to the "components of an Earth system model" borrowing the term that was introduced to define idioms/patterns?

In the conclusions section, the authors note that "*... the entire NWP community has a strong interest in pursuing the creation of dwarfs*". Such community-wide initiatives are, in my opinion, only feasible if backed by interface standardization and "liberation" of the software in question. Please do elaborate on how (technically and legally) the reusability of the envisaged community "dwarfs" is to be assured? Furthermore, the dwarfs' interfaces will determine if the sought after capability of overlapping computations will be feasible.

Other remarks

- Optimization is the leitmotif of the paper, and is exemplified with detailed results obtained with current hardware and described in zealous detail (a somehow anecdotal example: replace division by constant with multiplication by the

reciprocal calculated in advance). Yet at the same time, the paper aims at providing "*strategy to evolve weather and climate prediction models to next-generation computing technologies*", exascale is mentioned in the title. Please extend the conclusions section by indicating which of the employed optimizations have the chance to offer "software sustainability" over the years (also in the context of software maintainability tradeoffs), and where, e.g., indirection would be the key to performance (DSLs)?

- There is an abundance of arcane nomenclature in the paper used without introduction and spanning a broad range of domains, e.g.: "*loop fusion optimization*", "*generic reduced Gaussian grid*", "*parallelogram*", "*a perturbative method which determines the (constrained) optical phase*", "*Spherical Harmonics TCo639 test case*", "*baroclinic instability benchmark*", "weighted line Jacobi method", "*V-cycle configuration*", "*major generation and destruction processes, including cloud formation by detrainment from cumulus convection*";
- There is an imbalance in the level of detail of different sections of the paper, e.g. the well-established MPDATA is introduced with an outline touching upon numerical analysis, while the "created" "global shallow-water model named GRASS" is presented with just a reference to a pair of submitted papers; there is a two-page-long introduction to the application of spectral transform methods in NWP, while less than that is devoted to the entire discussion of physics dwarfs; authors do admit that this was intentional (p. 5 last paragraph) for some of the work has not been published elsewhere – this however rather supports publishing it elsewhere than sneaking into an overview paper.
- Some of the tools mentioned target Fortran development (e.g., CLAW DSL) while other cater to a wider set of technologies (e.g., Atlas), this is not mentioned explicitly and the reader is left without a clear statement if the proposed directions of development deviate or not from the Fortran ecosystem;

- The conclusions section contains statements of overly contrasting time horizons: on the one hand, the authors mention "*adding a large number of zero operations*" what is explained in the text to be caused simply by lack of support for a particular feature in the current version of a third-party library; on the other hand, prerequisites and challenges for subkilometer global simulations are mentioned. Please reconsider what are the main project conclusions worth to be listed in the concluding section and abstract.
- That the great majority of referenced works is [co]authored by the manuscript authors amplifies the feeling of some of the methodology, design or vendor choices being given without a proper context on the alternatives:
  - How representative is the chosen set of models (IFS, ALARO, ALADIN and COSMO-EULAG) among the "competition" and how the considered speed-up techniques compare with what has been explored recently (see, e.g., doi:10.1175/BAMS-D-15-00278.1 and references therein)?
  - How the proprietary software and hardware solutions like cuBLAS/cuFFT and NVLink/NVSwitch compare to those provided by other vendors?
  - Overlapping CPU-GPU computation strategy for dynamics/physics has been recently discussed in GMD in context of cloud-resolving simulations (doi:10.5194/gmd-2018-281, e.g. fig. Fig. 1), could the discussion here be supported with references to existing solutions from other domains?
  - mentions of GPU-resident weather forecasting call for citing other recent works (e.g., doi:10.1175/BAMS-D-14-00114.1)
  - What are the alternatives for the used radiation and cloud-physics schemes, are the chosen ones representative of what the community envisages for the mentioned global subkilometer-scale future simulations?
  - Are the CLAW and GridTools DSLs the sole solution available in this context?

- The word “code” is used in a somehow casual way, e.g. “*redesign of the algorithms and codes*”, “*our work on optimising codes*”, “*code used for data assimilation*”, “*models from which the dwarf code originated*”; let me suggest to consider employing more cross-domain notions of implementation, software, etc; similar nomenclature issue: restructure vs. refactor;
- Please remove any mentions of internal labels within the code – this information is unneeded for a research paper audience: “halo_exchange subroutine”, “compute_fluxzdiv”, “this%geom%node2edge_sign”.
- Please limit the use of acronyms/short-forms, and remove those clearly unneeded: PSNC in Fig. 3, EBTI on page 24, GP_dynamics/SP_transforms/SI_solver/RAD in caption of Fig. 5, semi-Lagrange in Fig. 6; Some references are listed with DOI number, some without - please be consistent; FORTRAN/Fortran, TRAP2/Trap2 spelling - please be consistent; Among the affiliations listed, some are given with detailed street addresses, some without - please be consistent.
- The title of the paper reads “*The ESCAPE project: Energy-efficient Scalable Algorithms for Weather Prediction at Exascale*”. Exascale is not discussed or defined and barely mentioned only in the conclusions, while the phrase “weather & climate” is used throughout the paper.
- Statements such as “*ECMWF is world leading in terms of track forecast*”, “*extreme computational capabilities typically required in operational forecast production*”, “*[IFS code] has been continuously optimized over multiple decades*”, “*Feedback from the European and international community at our dissemination workshops and at international conferences has shown that this work was well received*” are, in my opinion, good candidates for removal when shortening the paper – please avoid promotional language and statements which are not falsifiable; another candidates for removal are numerous vague statements: “*most*

speedup seems to be due to avoiding some of the temporary arrays”, “*some more fundamental changes which are more difficult to apply*”, “*whole cycle might employ some form of smoother/solver*”, “*has to be wisely chosen according to the cluster hardware*”, “*we do not know if there will be a clear winner*”, “*The first results of this effort look promising*”.

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