REQUEST FOR A SPECIAL PROJECT 2023–2025

MEMBER STATE: Netherlands

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Other researchers: ~80 researchers from the HIRLAM countries.

Project Title: HIRLAM-C phase 4 (2023-2025) special project

If this is a continuation of an existing project, please state the computer project account assigned previously.	**SP** sehlam___________________	
Starting year: (A project can have a duration of up to 3 years, agreed at the beginning of the project.)	2023	
Would you accept support for 1 year only, if necessary?	YES X☐	NO ☐

Computer resources required for 2023-2025: (To make changes to an existing project please submit an amended version of the original form.)		**2023**	**2024**	**2025**
High Performance Computing Facility	(SBU)	40 MSBU	40 MSBU	40 MSBU
Accumulated data storage (total archive volume)[2]	(GB)	22.000	22.000	22.000

***An electronic copy of this form must be sent via e-mail to**:* *special_projects@ecmwf.int*

Electronic copy of the form sent on (please specify date): 24/6/2022

Continue overleaf

[1] The Principal Investigator will act as contact person for this Special Project and, in particular, will be asked to register the project, provide an annual progress report of the project's activities, etc.

[2] If e.g. you archive x GB in year one and y GB in year two and don't delete anything you need to request x + y GB for the second project year.

Principal Investigator: Jeanette Onvlee

Project Title: HIRLAM-C phase 4 (2023-2025)

Extended abstract

The HIRLAM-C research programme is a cooperation between the national meteorological institutes of Denmark, Estonia, Finland, Iceland, Ireland, Lithuania, Netherlands, Norway, Spain and Sweden. Within HIRLAM-C, research efforts are focussed on the scientific development and implementation of the mesoscale NWP model Harmonie, and its associated ensemble prediction system HarmonEPS, at target horizontal resolutions of 0.15-2.5km. A Harmonie Reference system is being maintained on the ECMWF HPC platform. The emphasis in the requested HIRLAM-C phase 4 Special Project at ECMWF will be primarily on experimentation, evaluation and testing of this Reference System, and its ensemble configuration HarmonEPS. The computational resources from the Special Project will be used mainly to experiment with newly developed model, assimilation, and ensemble generation components, and to integrate them and evaluate their meteorological and technical performance for new Reference releases. As the HIRLAM-C programme has recently been extended to end 2025, the present request is for a Special Project for the period 2023-2025. The main foreseen development and testing activities on data assimilation, atmospheric modeling, surface analysis and modelling, probabilistic forecasting and code aspects in this coming phase are outlined in sections A-E below.

A) Data assimilation developments

A1: Enhanced use of existing high-density observations, and introduction of new observation types

At present, the Harmonie Reference system has been enabled to routinely assimilate a wide range of satellite and ground-based observations, including observations from private weather stations (PWS). In 2023-2025, one aim will be to improve the availability, quality control, and use of these existing data sources. It will be attempted e.g. to better take the footprint of satellite data into account; to improve bias correction procedures; and to make use of cloudy radiances and surface-affected sounder channels. Experience will be gained with the use of machine learning approaches for the development and emulation of observation operators. In addition, work will continue to prepare for the introduction and assessment of new satellite platforms and instruments (in particular MTG and EPS-SG), and wider acquisition, quality control and impact studies for GNSS slant delays, polarimetric radar data, boundary layer lidars and ceilometers. Significant attention will also be devoted to the acquisition, quality control and impact assessment of third party observations: PWS, smart phones, road networks, cars, wind turbines, and urban observation networks.

A2: Development and optimization of flow-dependent assimilation algorithms

A computationally efficient multiple outer-loop Harmonie 4D-Var system has been included in the Reference system, capable of assimilating the same range of observations as 3D-Var. In the coming years, studies aiming to further optimize the meteorological and computational performance of the Harmonie 4D-Var will continue. Experiments will be performed using different time windows and alternative sets of control variables. Studies will be continued to assess and improve 4D-Var' s usefulness in the nowcasting range (see below in A3). Previous work has shown that most of the 4D-Var system can be run in single precision without deterioration of accuracy, but some aspects, e.g. in the minimization, remain to be studied in more detail.

The next step will be to combine the strengths of ensemble and variational approaches in a 3- and 4DEnVar ensemble assimilation system, to the mutual benefit of the model analysis and its probabilistic forecasting ability. A hybrid 3- and 4D EnVar system will be tested for operational use, which will require studies on aspects s uch as finding optimal approaches for localization. It is aimed to integrate all these algorithmic developments, plus several others related to nowcasting (see A3), stepwise into the flexible and modular OOPS code framework.

A3. Development of data assimilation suitable for the nowcasting range

In the coming period, there will a continued focus on moving towards sub-hourly cycling and tackling the challenges for assimilation on those timescales, particularly the issue of model spinup. Technically, sub-hourly cycling has recently been enabled for Harmonie, and experimentation with it has started for 3- and 4D-Var. Deeper diagnostics studies of spinup will be done with various initialization methods and with 4D-Var. Coordinated experiments will be performed for the analysis, intercomparison and combination of various flavours of methods which have been developed earlier with the aim to improve model performance in the first few hours of the forecast:

1) the cloud initialization method (Gregow 2017) in combination with NWC SAF products for a better initialization of cloud characteristics and identification of multi-layer clouds
2) the overlapping windows approach in sub-hourly cycling mode (Yang et al 2017)
3) the field alignment method to deal with displacement errors in the first guess field with respect to radar data (Geijo 2012),
4) the variational constraint method for faster balancing of the model (Geijo and Escriba 2018).

For 4D-Var especially, temporal correlations are an issue to be tackled. For the handling of spatially correlated observations, error modelling approaches will be considered as an alternative to standard thinning or superobbing practices.

B) Atmospheric Forecast model

B1: Studies to reduce systematic model errors for cloud and boundary layer behaviour

The focus in these studies will be on fog, stratiform precipitation and open cell convection, and very stable boundary layer conditions. The main priority is to tackle the overprediction of the extent and depth of fog, particularly over sea. The fog evolution in the model has been shown to be extremely sensitive to the amount and evolution of cloud condensation nuclei (CCN), which the present ICE3 bulk microphysics scheme, with its fixed climatological values for CCN over sea, land and urban areas, is obviously unable to adequately represent. Temporary fixes for this in ICE3 are being investigated, but a more definitive solution will be the use of near-real-time observed aerosol information (see B2) and the new second-moment microphysics scheme LIMA. This combination will be explored in-depth, tuned where needed and compared in performance to the present ICE3 1-moment scheme.

In addition, several ways will be investigated to further improve ICE3 microphysics. ICE3 performance has been shown to be sensitive to the assumed shape parameters of the cloud droplet size distribution. This will be explored further in the context of SPP perturbations for HarmonEPS (see section D). Possible solutions have been prepared for several other shortcomings in the ICE3 microphysics which will need to be tested more thoroughly in the coming years. Hopefully these developments will positively affect the model description of supercooled liquid water, snow and freezing drizzle, open cell convection, and the occurrence and evolution of small-scale showers.

B2: Consistent treatment of the aerosol-cloud-radiation interaction:

Aerosol parametrizations have been developed in the Harmonie radiation and clouds schemes, for a variety of aerosol types (sea salt, hydrophilic black carbon, organic matter, sulphate, nitrate and ammonium) and including aerosol wet deposition. A dataflow has been set up to introduce near-real-time (NRT) aerosol information from CAMS and use this in a consistent manner in the radiation and cloud schemes. A parametrization for the activation of these aerosols, depending on e.g. TKE and vertical velocity is under development. Impact studies for both near-real-time and climatological CAMS aerosol information so far have given mostly positive results.

In the coming years, it is intended to introduce the ECRAD radiation and 2-moment LIMA microphysics schemes as options into this workflow. First ECRAD and LIMA will be assessed individually and their settings optimized where needed. Next, intercomparisons will be done against their predecessors and options will be considered to enhance their computational efficiency through emulation by machine learning. For LIMA, machine learning will also be considered for the optimization of values for sensitive parameters.

B3: Preparing the model for use on hectometer scales

Studies performed in the 500-1000m resolution range have demonstrated the potential of these Harmonie configurations to capture small-scale (extreme) meteorological features realistically. In the coming years, we will explore the use of Harmonie at even finer scales, down to ~150m grid scale. At such scales, the limits of applicability of the physics parametrizations for turbulence and shallow convection should be taken into account and the use of 3D physics formulations must be considered. Several approaches for (quasi-)3D formulations for turbulence will be investigated in steep and flat terrain. Options will be explored for gradually shutting down the shallow convection parametrization towards finer scales. It is aimed to model 3D cloud shading effects on radiation with the combined use of ECRAD and its SPARTACUS solver and machine learning. Hectometric models may require a much-reduced time step to keep the model dynamics stable; however, it is not obvious that such short time steps would also be required, or desirable, for the full model physics. For this reason, and to keep the increased computational costs of the quasi-3D physics schemes within bounds, we will investigate the use of process-dependent time-stepping and grid resolution, and of emulation by machine learning methods, in the first instance for the radiation scheme but later also for other parametrizations. Model performance will be compared with that of LES models, field studies and high-resolution observation networks. In regions with steep orography, the effects of sub-grid orographic parametrizations for radiation and momentum at hectometric resolutions will be assessed in depth. In view of the expected limited predictability on these scales, several options for introducing fully stochastic physics schemes for turbulence and microphysics will be investigated. In urban areas, existing but still unexplored options of the TEB urban surface module will be studied. A workflow will be developed for creating appropriately detailed physiographic information for an accurate description of the surface (see C2).

The aim is to eventually develop data assimilation and ensemble setups for these hectometer scale models as well, at least down to 500m resolution. It will therefore be investigated which (nowcasting) data assimilation setups and which observation types are most suitable to initialize the frequently run hectometer scale models. For high-resolution ensembles, the so-called overlapping window technique developed by Yang et al. (2017) will be explored. In all these studies, it will be considered what will be the optimal way to spend available computational resources, seeking the best balance between horizontal and vertical resolution, domain size, ensemble size and model complexity.

C) Surface analysis and modelling

<u>C1: Enhanced use of satellite surface observations with more advanced surface assimilation</u>

To enable the assimilation of a wide range of relevant remote sensing surface observations, a new surface assimilation framework has been constructed consisting of a set of Simplified Extended Kalman Filters (SEKFs) for soil, snow, lake and sea ice assimilation, and an alternative treatment of horizontal spatialization (called pysurfex/gridpp). Pre-operational testing of this setup in combination with more advanced surface model components is ongoing (see also C2). After operationalization of this new surface assimilation and modelling setup, the aim is to progressively introduce and exploit a variety of remote sensing observations: ASCAT, SMOS, MODIS, CryoClim, Sentinel and SAF products for soil moisture, LAI, surface temperature, lake water temperature and ice fraction assimilation, sea ice and snow cover and depth. Preparatory work to implement and assess the potential of these observations and retrievals is already far advanced.

Several lines will be pursued with the goal to move towards strongly coupled atmospheric-surface assimilation. In the short term, experiments will be done e.g. with adding an additional layer of "screen level values" to the 3D-Var control vector in the OOPS framework. Another option to be explored is to make the results of land surface DA available to atmospheric assimilation via running Surfex offline for 1 time step. After the introduction of the SEKF soil and snow assimilation, it is intended to move stepwise towards a more advanced ensemble Kalman filter (EnKF) setup which can be used as a basis for a strongly coupled atmosphere-surface data assimilation system and the assimilation of satellite surface radiances. An initial EnKF setup has been prepared, which is running with AMSR2 and SMOS radiance observations. Also particle filter solutions will be investigated.

<u>C2: Introduction of more advanced surface model descriptions</u>

After careful assessment in the past few years, it is aimed to replace the present set of relatively simple surface schemes in Harmonie by a combination of more sophisticated ones: the many-layer soil and snow schemes (ISBA-DIF, ES), the new sea scheme ECUME6, the MEB snow-over-forest scheme, an extension of the Flake lake model with ice and snow over ice parametrizations, enhancements to the SICE sea ice model, a sub-grid scale orographic parametrization for radiation, and a wind farm parametrization. Testing of this combined set of modules, together with the new SEKF surface assimilation scheme, has started and will extend into 2023.

Following this big upgrade of the surface model, studies will be performed with new, still unexplored options within Surfex, such as prognostic LAI from the A-gs vegetation scheme and non-standard options in the TEB town scheme. A roughness sublayer formulation has been implemented; its potential for providing a more realistic description of surface fluxes for very heterogeneous surfaces will be explored. Several Harmonie/Surfex setups have been created with a coupling to 1D and 3D ocean models (GOTM, NEMO), wave models (WaveWatch3, WAM) and hydrological models (TRIP), using OASIS couplers. The performance of these coupled systems will be assessed more deeply.

One important activity will be the development of a workflow by which a surface physiography which is sufficiently detailed for use in hectometer-scale NWP models can be created for European domains and updated when needed. The idea is to start from a set of existing land cover databases and thematic maps of O(10m) resolution for the European area, which are regularly updated within Copernicus. Machine learning will then be used to "translate" this aggregation of maps to a higher resolution version of ECOCLIMAP-SG, with the same labelling (set of land cover types, water bodies and urban local climate zones).

D) Probabilistic forecasting

The main focus in the developments of HarmonEPS in the coming years will be the representation of model uncertainty. The SPP scheme for perturbing model parameters (Frogner et al. 2022) will be pre-operationally tested, further extended and refined. Sensitivity studies will be carried out to identify relevant new parameters from existing physics parametrizations (e.g. particle size distributions in the microphysics), the many-layer surface schemes (see C2) and the dynamics (e.g. the SLHD scheme) and from new schemes (e.g. LIMA, ECRAD, aerosol formulations in radiation and microphysics). Experiments will be continued to assess the impact of alternative parameter pdf distributions (uniform and shifted uniform vs the default lognormal distribution). Other aspects to be studied will be the sensitivity to applying different scales in the perturbation patterns for different parameters, and the best way of handling correlated parameters. Ways will be sought to reduce the computational cost of SPP, e.g. by calling the perturbation pattern less frequently.

Studies will be continued to determine the optimum temporal and spatial scales for perturbations of surface fields. New surface fields to perturb will be investigated, such as snow depth, sea ice extent and stomatal resistance.

Sensitivity studies of the existing EDA and hybrid 3D-EnVar setups (Frogner et al. 2019) for generating initial condition perturbations will continue. The aim is to assess and optimize these configurations both for ensemble and data assimilation performance. These studies will involve aspects like the optimal ensemble size, spatial scale-dependent localization lengths, use of full or hybrid EnVar, and spinup issues. Intercomparisons between EDA, (hybrid) EnVar, 3D-Var and 4D-Var will be carried out. In preparation for the move to sub-km horizontal resolutions, the present overlapping windows approach (Yang et al. 2017) will be extended to, and assessed on, these scales.

Aspects of HarmonEPS setups which will need to be re-assessed when moving to higher model resolutions, such as the optimal balance between the number of ensemble members, model horizontal and vertical resolution, and domain size. Also, the best balance between different types of perturbations is something to be investigated further.

Reduction of the computational costs of the ensemble is an important aim, e.g. through the option of running perturbed ensemble members in single precision (which will be tested soon), or the use of machine learning to emulate large ensembles with deep learning techniques (longer-term research).

E) Code efficiency, portability and scalability

<u>E1: Preparation of model code for use on alternative (hybrid) architectures</u>

To prepare the Harmonie code for efficient use on alternative architectures, HIRLAM is following the ECMWF/ACCORD strategy of "separation of concerns". The first step is to refactor the forecast model Fortran code, in preparation for step 2, which is the near-automated code adaptation to permit effective use of GPU's and other (hybrid) architectures. The refactoring of Harmonie will be done along the lines of a prototype refactored code which has been made for Arome-France, starting in the second half of 2022. After the Fortran code refactoring, which should be concluded early 2023, the second step is to use hardware-optimized external libraries and code transformation tools to create hardware-specific code (largely automatically) for use on alternative HPC platforms.

A containerized version of the full Harmonie model and the single column model MUSC have been developed to facilitate porting of the model to, and cooperation with, university partners and HPC providers. Smaller code kernels (e.g. for individual parametrizations) will be created to facilitate a faster localization of technical problems in computational efficiency on new platforms.

<u>E2: Code efficiency improvements and monitoring:</u>

Investigations into the use of single vs. double precision have shown that most Harmonie components can be "safely" run in single precision, yielding ~40% reduction run time reductions. Some components still remain to be investigated in this respect, in particular the minimization in 4D-Var. Activities to adapt scientific algorithms towards greater computational efficiency and/or scalability will include e.g. the development of EnVar data assimilation techniques (which are faster and more scalable than 3- or 4D-Var); the use of overlapping windows and non-linear spectral grids in sub-km resolution nowcasting ensembles; and the study of non-spectral Helmholtz solvers and multi-grid approaches. Machine learning will be increasingly explored for emulating physics-based algorithms, for both 1D physics and (quasi)3D physics on hectometer scale resolutions. Open source tools for computational performance assessment developed by the Barcelona Supercomputing Center will be implemented in the Harmonie testbed at ECMWF and applied regularly there in the testing of new major components and model cycles.

Duration of the project and estimated resource requirements:
The duration of the HIRLAM-C programme has been prolonged until 31-12-2025. The present request is for special project resources in the last three years (1-1-2023 until 31-12-2025) of HIRLAM-C.

For testing and tuning of the deterministic Harmonie 4D-Var system at ECMWF at 2.5km horizontal resolution and 90 vertical levels over the DMI domain, runtime costs amount to ~20000 HPCF units per experiment day. The estimated needs for the testing of the deterministic Reference system are:

- pre-release technical tests: 12 months in total
- parallel validation: 12 months total
- pre-operational impact and sensitivity tests evaluating individual components: 12 months
- debugging, problem detection and fixing activities: 12 months
- real time trunk suite, 12 months in total

So in total roughly 60 months or 60 * 30 * 20000 units = 36 million HPCF units are estimated to be required per year for testing and experimentation with the deterministic Harmonie Reference System at ECMWF in the coming years.

To test HarmonEPS, an ensemble of 10 members is run over the MetCoop domain with one forecast per day running to +36h, and three +6 forecasts per day to keep the cycling. This requires ~120 000 HPCF units per day. Typically, updates are tested for 3 weeks in summer and 3 weeks in winter, so 42 days per update. With 2 tests for each perturbation type per year (initial, LBCs, surface, model and structural) we end up with: 120 000 HPCF units * 42 days * 10 experiments = 50.4 million HPCF units per year.

In total therefore, the testing of the Harmonie and HarmonEPS configurations require ~ 86 million HPCF units per year. A considerable fraction of these total requirements will be covered through explicit contributions from member states to a dedicated Hirlam SBU pool supplementing the special project resources, which is formed through direct billing to the member state HPCF quotas. For the Hirlam-C phase 4 special project, we apply for 2023-2025 for 40 million HPCF units/year, and a data storage of 22,000 GB, most of latter on temporal storage (ECTMP).

References:

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