Ensemble Data Assimilation in NEMO using PDAF

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PDAF Parallel Data Assimilation Framework

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PDAF – Parallel Data Assimilation Framework

A unified tool for interdisciplinary data assimilation …

- provide support for parallel ensemble forecasts
- provide assimilation methods (solvers) - fully-implemented & parallelized
- provide tools for observation handling and for diagnostics
- easily useable with (probably) any numerical model
- a program library (PDAF-core) plus additional functions
- run from notebooks to supercomputers (Fortran, MPI & OpenMP)
- ensure separation of concerns (model – DA method – observations – covariances)

Open source:
Code, documentation, and tutorial available at

https://pdaf.awi.de

github.com/PDAF

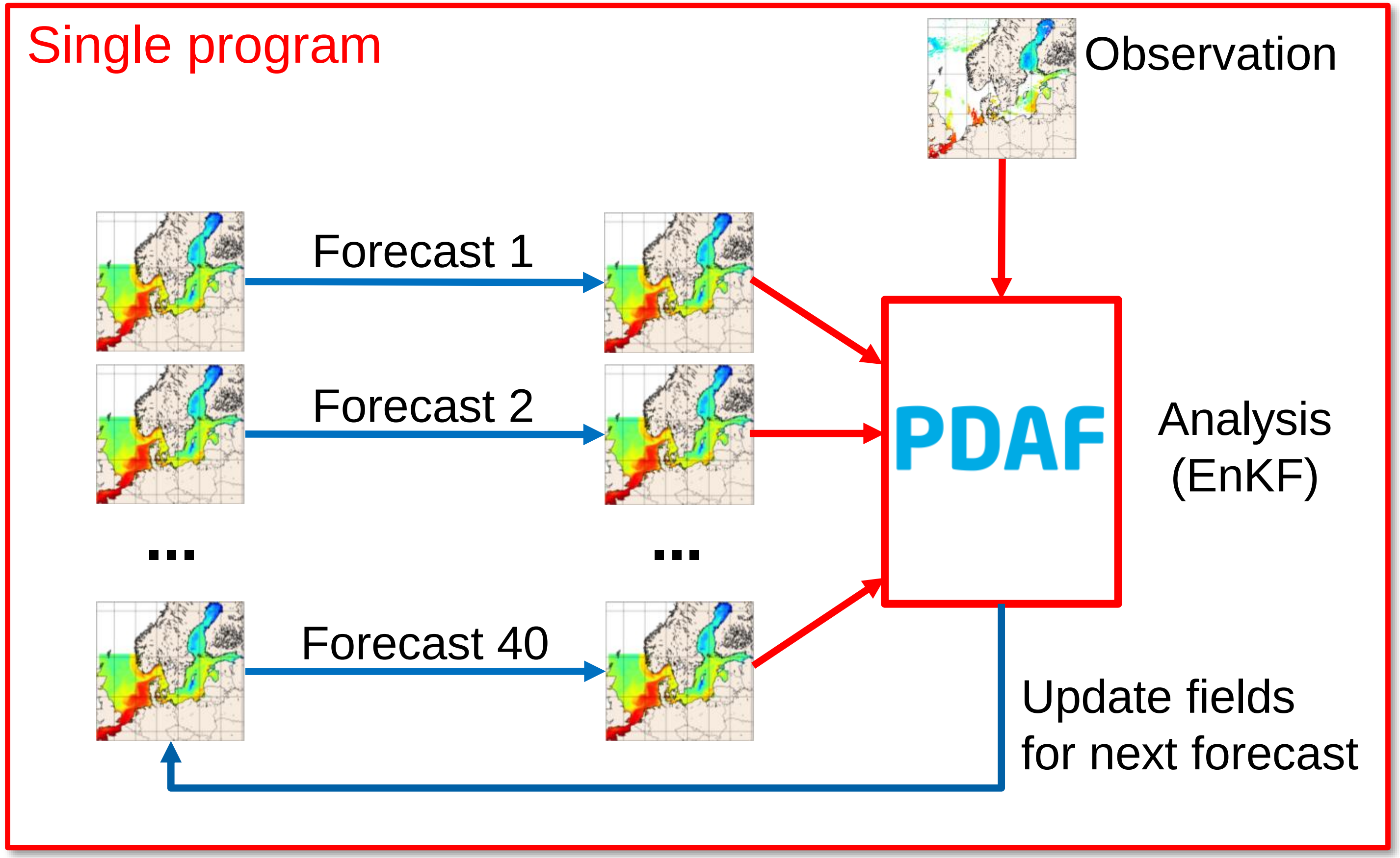
L. Nerger, W. Hiller, Computers & Geosciences 55 (2013) 110-118

Online-Coupling – Assimilation-enabled Model

Couple a model with PDAF

- Modify model to simulate ensemble of model states
- Insert analysis step/solver to be executed at prescribed interval
- Run model as usual, but with more processors and additional options

- EnOI and 3D-Var also possible:
  - Evolve single model state
  - Prescribe ensemble perturbations or covariance



Initialize ensemble

Ensemble forecast

Analysis step in between time steps

NEMO-PDAF Online Coupling

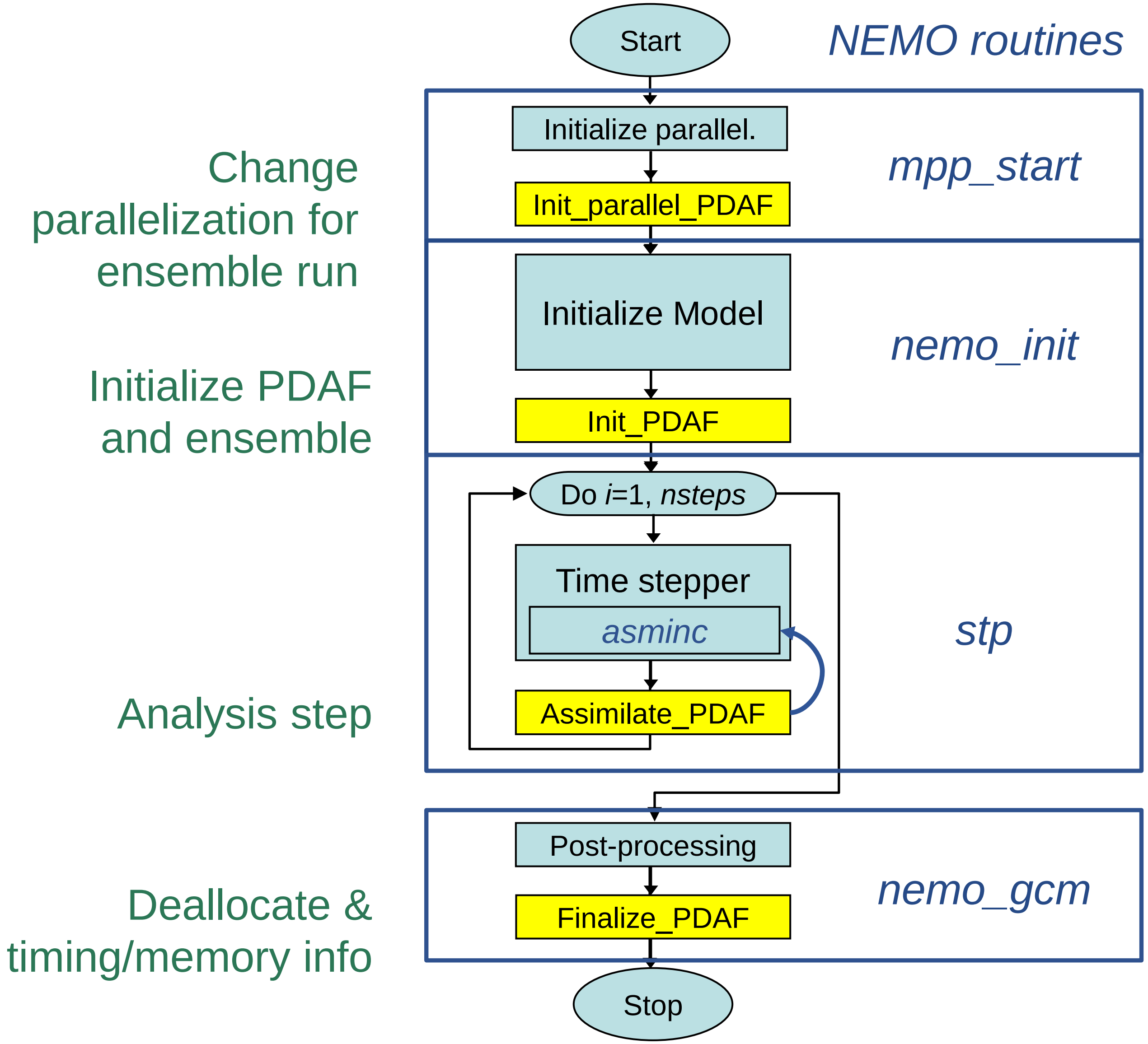
Model code | DA code

PDAF Parallel Data Assimilation Framework

Augment NEMO with DA functionality

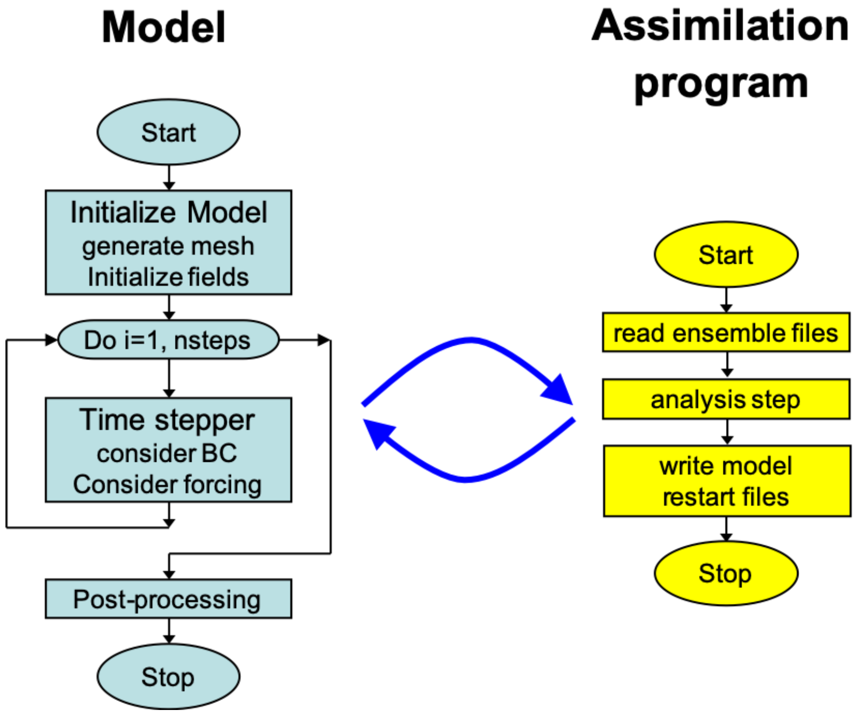
- Insert 4 subroutine calls
- Modify parallelization for ensemble mode
- Transfer data between model and PDAF in memory
- Adapt NEMO's ASM module:
  PDAF provides increments in memory
- No changes to XIOS, but to file_def*.xml

- Very efficient & highly scalable
- Direct access to model grid and fields through Fortran modules
- File output kept to minimum
- No model restarts for cycled assimilation



NEMO-PDAF Offline Coupling

Offline



Currently used by CMEMS Baltic-MFC with NEMO-4

- Separate programs for model and DA
  - no modification of model code (unless e.g. model error is to be applied)
- Flexible to run
  - each model task can be run separately
- Needs frequent model restarts and file output
  - overhead by model restarts
  - overhead by file writing & reading

Assimilation program

- mostly same routines as for online-coupling
- differences
  - reading restart and writing increment files
  - get information on model grid from files (at central point in code)
  - compression of state vector to wet grid points

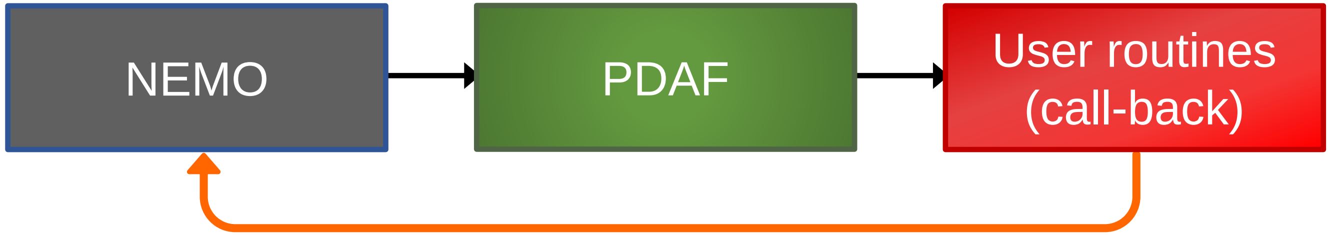
Model code | DA code

PDAF interface structure

- **Model-sided Interface:** Defined calls to PDAF routines
  (called by driver program for offline coupling)
- **Case-related Interface:**
  User-supplied call-back routines for elementary operations:
  - transfers between model fields and ensemble of state vectors
  - observation-related operations
- User-supplied routines can be implemented as routines of the model and can share data with it (low abstraction level)

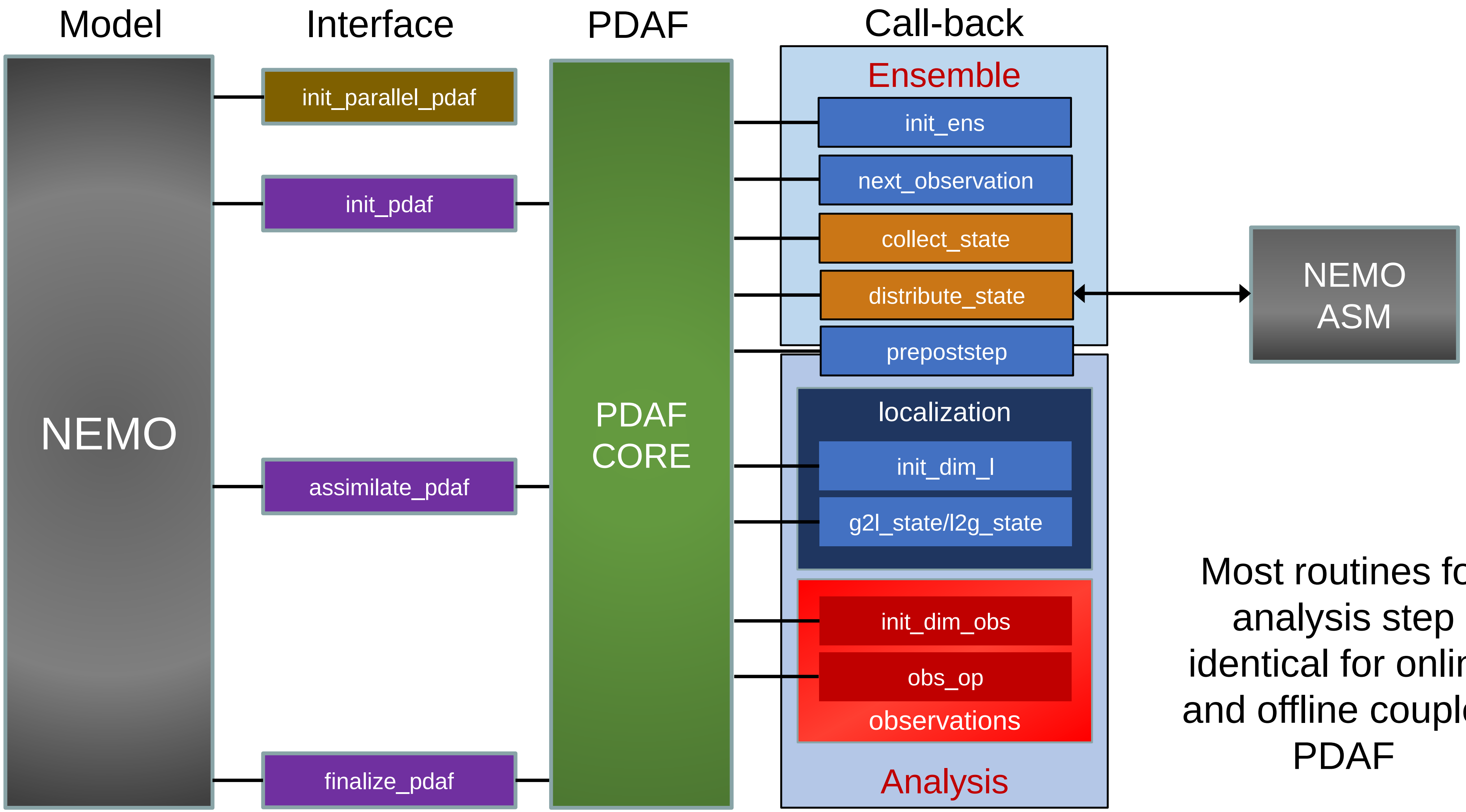
PDAF is model agnostic

model specific code only in user-supplied routines



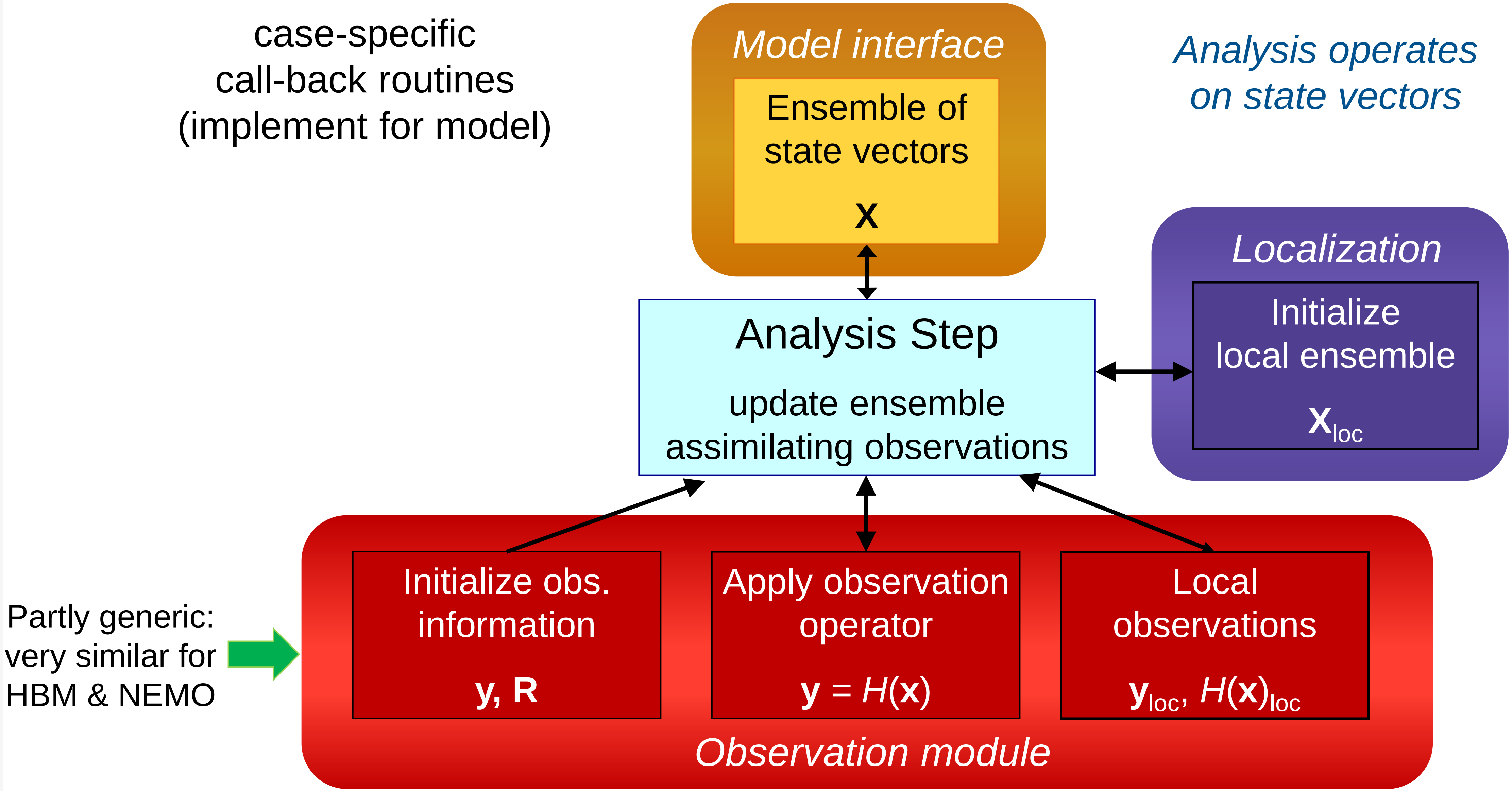
Online: Access model information through modules / static variables
offline: initialize model information from files

PDAF Calling Structure



Most routines for analysis step identical for online and offline coupled PDAF

Implementing the Ensemble Filter Analysis Step



case-specific
call-back routines
(implement for model)

Model interface

Ensemble of state vectors

$\mathbf{X}$

Analysis operates on state vectors

Localization

Initialize local ensemble

$\mathbf{X}_{\mathrm{loc}}$

Analysis Step

update ensemble assimilating observations

Partly generic: very similar for HBM & NEMO

Initialize obs. information

$\mathbf{y}, \mathbf{R}$

Apply observation operator

$\mathbf{y} = H(\mathbf{x})$

Local observations

$\mathbf{y}_{\mathrm{loc}}, H(\mathbf{x})_{\mathrm{loc}}$

Observation module

Adaptions to ASMINC

- Settings for asminc provided by PDAF user code
    - Ensure consistency between PDAF and ASM

- Adaptions for cycled DA
    - Adapt IAU weights array for repeated application
    - Direct initialization option performed in PDAF user code
    - PDAF user-code initializes bkginc and bgk fields
    - Divergence damping routine in user code for repeated application

Assimilating Phytoplankton Carbon in NEMO-FABM-MEDUSA

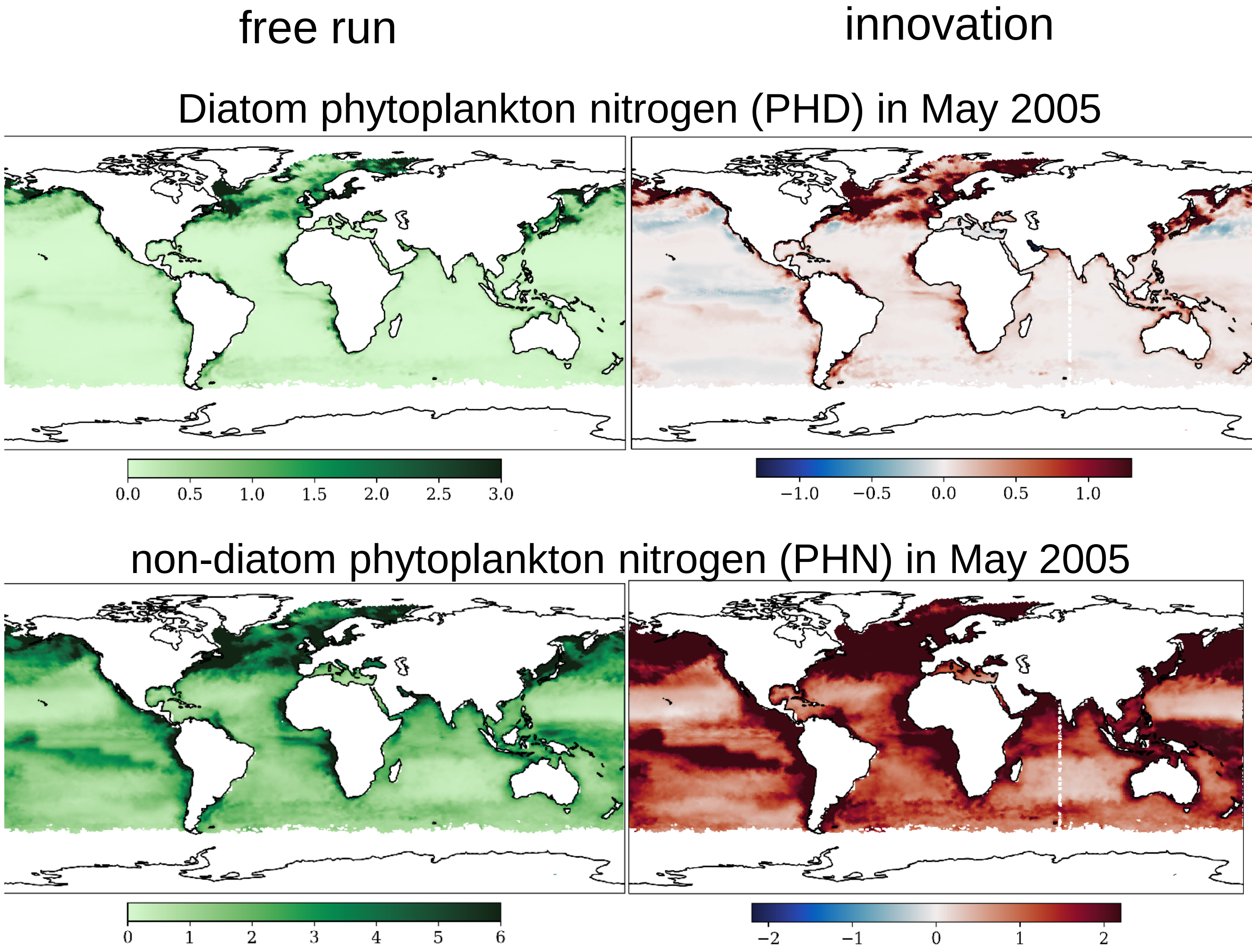
Model setup

- ORCA1 grid
- Year: 2005
- Base currency: nitrogen

Observations

- phytoplankton carbon products from BICEP project
- gridded product with a resolution of 9 km
- superobbing around 0.5°
- conversion from carbon to nitrogen based on a fixed C:N ratio specified by the model

→ Biased non-diatom phytoplankton nitrogen


free run

innovation

Diatom phytoplankton nitrogen (PHD) in May 2005

non-diatom phytoplankton nitrogen (PHN) in May 2005

National Centre for Earth Observation
NATURAL ENVIRONMENT RESEARCH COUNCIL

University of Reading

PML Plymouth Marine Laboratory

Assimilating Phytoplankton Carbon in NEMO-FABM-MEDUSA

DA setup

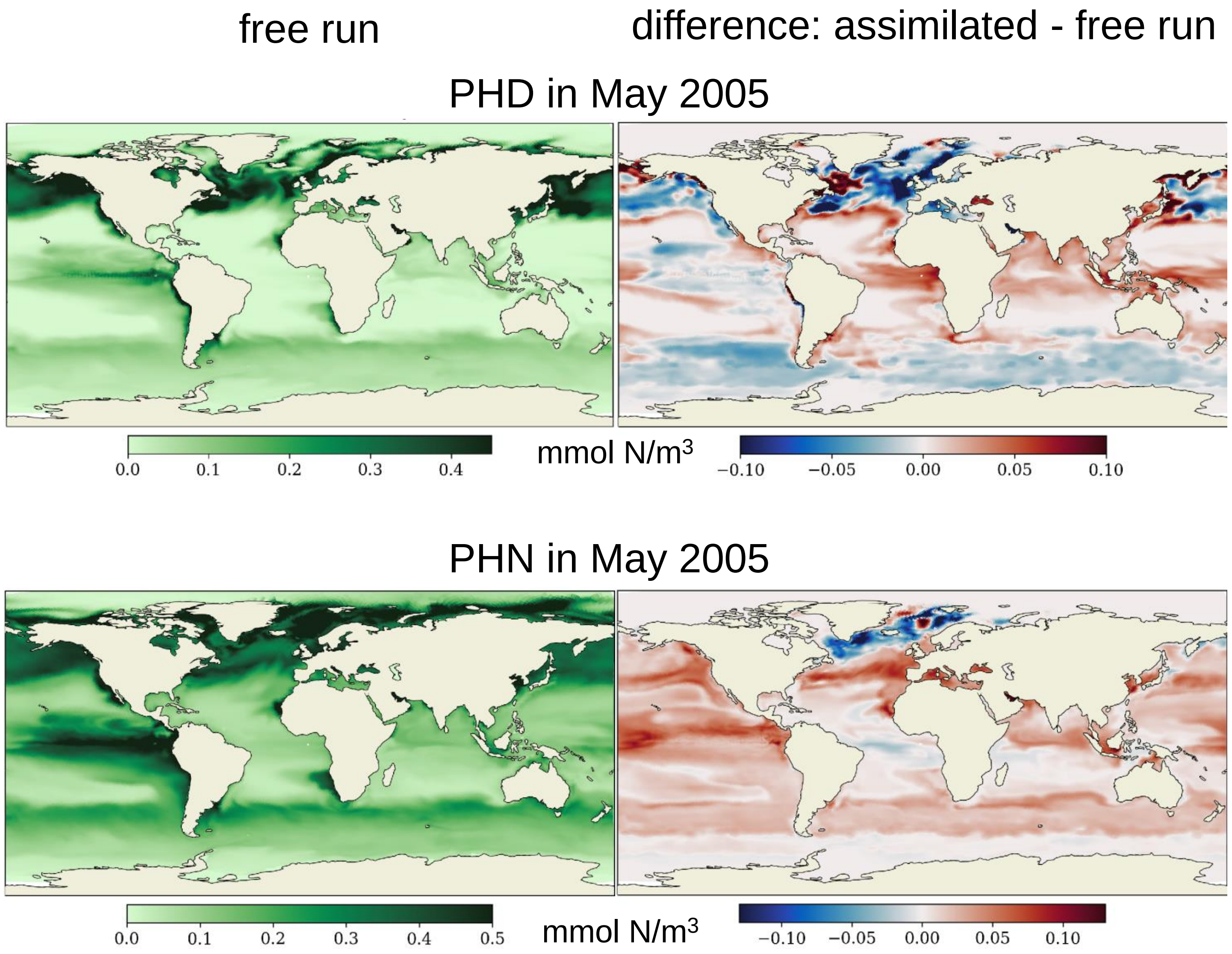
- Kalman filter: LESTKF
- Localisation radius: 200 km
- Forgetting factor: 0.95
- Ensemble size: 30

Technicalities

- No. PEs for ensemble models: 5400
- No. XIOS servers: 480
- Runtime for one-year: ~9 hrs
- Slower than individual ensemble run
- Potential Bottleneck:
  - I/O: switching to multiple file output in the hope for faster I/O

State vector

- Diatom phytoplankton nitrogen (PHD)
- non-diatom phytoplankton nitrogen (PHN)
- Dimension of the state vector: 1.45×10^7



free run

difference: assimilated - free run

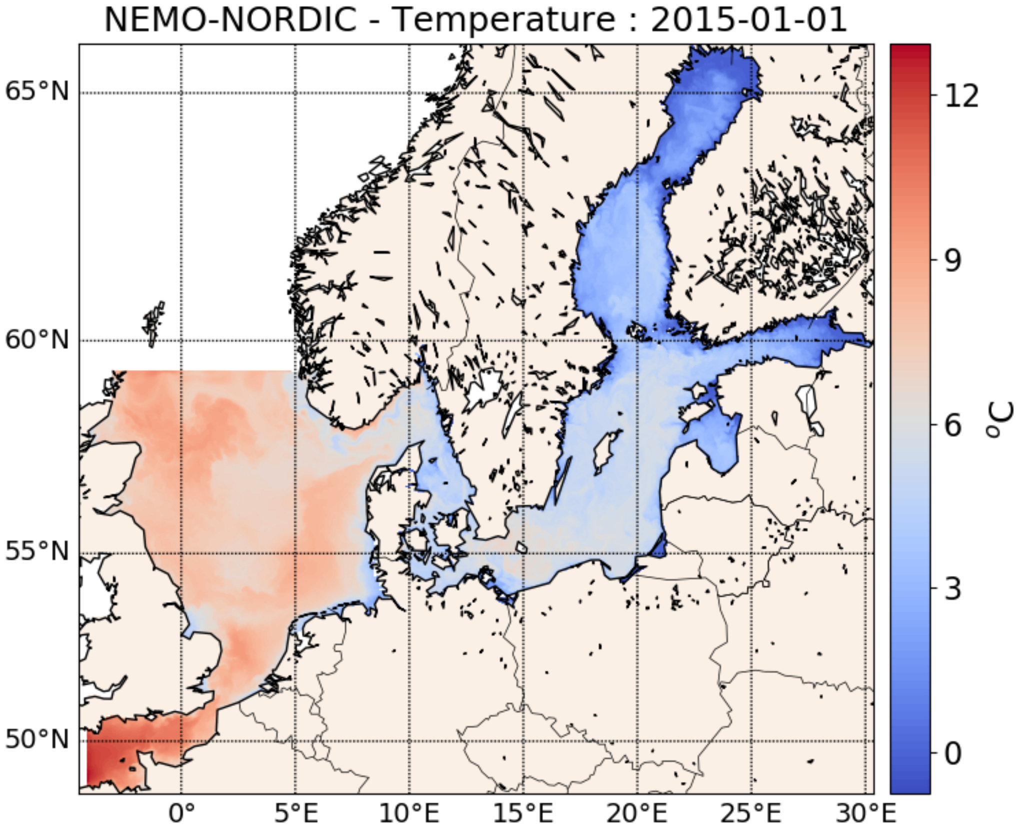
PHD in May 2005

PHN in May 2005

Assimilating SST and Chlorophyll in NEMO-ERGOM

- Model setup
  - NEMO-NORDIC + ERGOM biogeochemistry
  - 1 nm resolution (ca. 1.8km); 56 layers
  - time step 90 sec
- DA setup
  - Kalman filter: LESTKF
  - Ensemble size: 30
- Observations
  - SST and chlorophyll from CMEMS
- State
  - 5 physics variables
  - 16 ERGOM prognostic variables + 4 diagnostic variables
  - state dimension: $704 \cdot 10^6$ (at analysis $153 \cdot 10^6$)
- Compute requirements:
  - each NEMO-ERGOM task: 186 cores (+6 for XIOS)
  - run times: forecasts ~45 minutes per 24h
    analysis 0.5 minutes
    file writing 3 minutes (2x state, 1x variance)

Results to be presented in my talk tomorrow



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Some Challenges

- Initial run problems
  - Program got stuck when integration started
    (apparently in reading of forcing and boundary data)
- Needed to
  - Convert all input files to NetCDF4
  - Transition from Intel MPI to OpenMPI 4
    (issue of combination of XIOS/MPI/parallel NetCDF)
  - Use distributed restart file instead of global ones

PDAF package: DA Algorithms and Models

PDAF originated from comparison studies of different filters

Ensemble Filters and smoothers - *global and localized*

- EnKF (Evensen, 1994, perturbed obs.)
- (L)ETKF (Bishop et al., 2001/Hunt et al. 2007)
- (L)ESTKF (Nerger et al., 2012)
- (L)NETF (Toedter & Ahrens, 2015)
- Particle filter
- Hybrid LETKF-LNETF
- *EnOI mode*

Model bindings

- MITgcm
- AWI-CM / FESOM

Toy models (full implementations with PDAF)

- Lorenz-96 / Lorenz-63
- Lorenz-2005 models II and III

User routines not yet coded for NEMO

3D-Var schemes
(incremental with control variable transformation)

- 3D-Var with parameterized covar.
- 3D Ensemble Var
- Hybrid 3D-Var

Community:

- pyPDAF (Python-coded models)
- TerrSysMP-PDAF

In progress

- SCHISM/ESMF (VIMS)
- GOTM/FABM “EAT” (BB ApS)

Summary – NEMO-PDAF

- Coupled NEMO and PDAF for (ensemble) data assimilation
  - state vector can include ocean physics / sea ice / BGC …
  - easy addition of observation types
  - supports cycled DA without model restarts
  - utilize NEMO’s ASM-module: IAU and direct initialization
  - Currently for NEMO 4.0.x – NEMO 4.2 in progress

- Code will be made open source

PDAF is open source:
Code, documentation, and tutorial available at

https://pdaf.awi.de

github.com/PDAF

References

- https://pdaf.awi.de (The website also provides a list of studies using PDAF)
- https://github.com/PDAF
- Nerger, L., Hiller, W. (2013). Software for Ensemble-based Data Assimilation Systems - Implementation Strategies and Scalability. Computers and Geosciences, 55, 110-118. doi:10.1016/j.cageo.2012.03.026
- Nerger, L., Hiller, W., Schröter, J.(2005). PDAF - The Parallel Data Assimilation Framework: Experiences with Kalman Filtering, Use of high performance computing in meteorology : proceedings of the Eleventh ECMWF Workshop on the Use of High Performance Computing in Meteorology, Reading, UK, 25 - 29 October 2004 / Eds.: Walter Zwieflhofer; George Mozdzynski, Singapore: World Scientific, 63-83. doi:10.1142/9789812701831_0006
- Nerger, L., Tang, Q., Mu, L. (2020). Efficient ensemble data assimilation for coupled models with the Parallel Data Assimilation Framework: Example of AWI-CM. Geoscientific Model Development, 13, 4305–4321, doi:10.5194/gmd-13-4305-2020