PDAF Parallel Data Assimilation Framework

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Efficient Ensemble-Based Data Assimilation for High-Dimensional Models with the Parallel Data Assimilation Framework PDAF

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Motivation

PDAF Parallel Data Assimilation Framework

For efficient application of data assimilation we like to

- simplify the steps to set up a data assimilation system and to apply it
- ensure high computational efficiency
- be able to easily take up new developments in data assimilation
- profit from experience from various data assimilation applications

→ Community data assimilation software allows for this

PDAF: A tool for data assimilation

PDAF Parallel Data Assimilation Framework

PDAF - Parallel Data Assimilation Framework

- a program library for ensemble data assimilation
- provides support for parallel ensemble forecasts
- provides filters and smoothers - fully-implemented & parallelized (EnKF, LETKF, LESTKF, NETF … easy to add more)
- easily useable with (probably) any numerical model
- run from laptops to supercomputers (Fortran, MPI & OpenMP)
- Usable to study assimilation methods and to apply real assimilation
- first public release in 2004; continued development
- ~370 registered users; community contributions

Open source:
Code, documentation, and tutorial available at

http://pdaf.awi.de

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

AWI

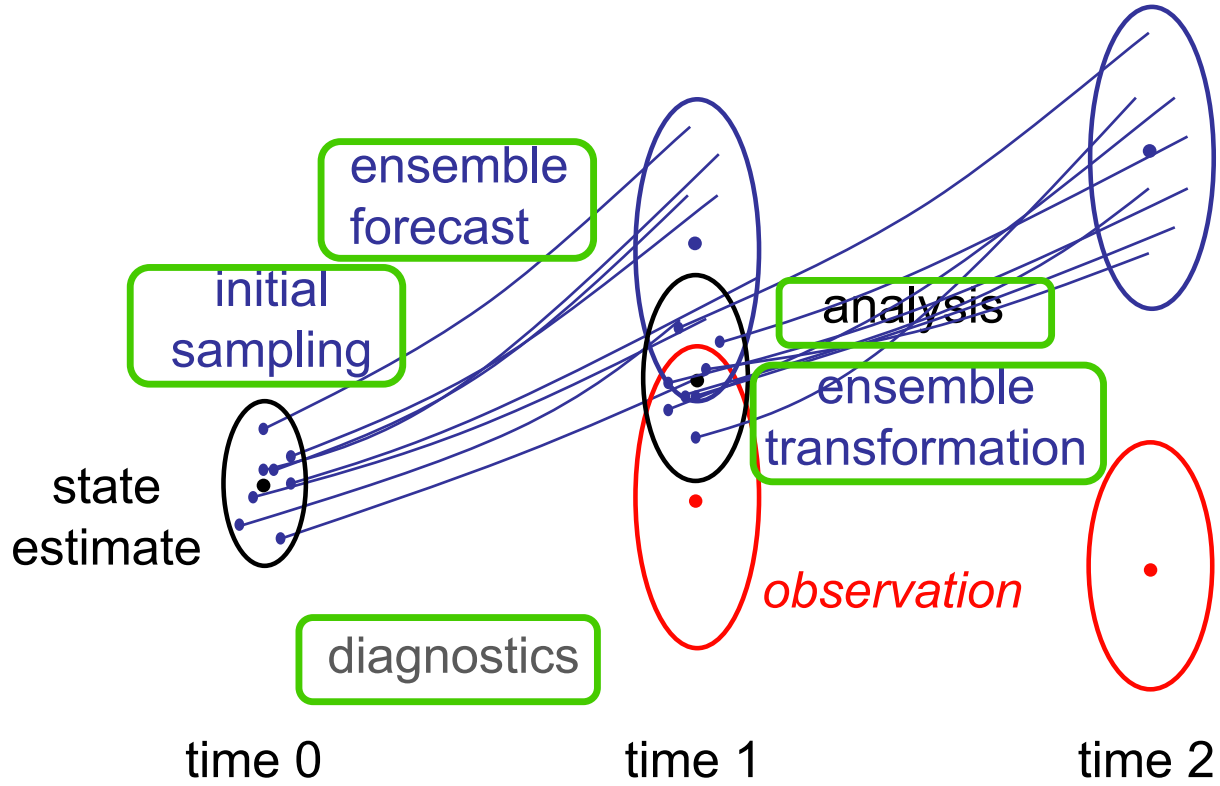
Ensemble Filters

PDAF Parallel Data Assimilation Framework

Ensemble Kalman Filters & Particle Filters

➜ Use ensembles to represent probability distributions (uncertainty)

➜ Use observations to update ensemble



There are many possible choices!

What is optimal is part of our research

Different choices in PDAF

3 Components of Assimilation System

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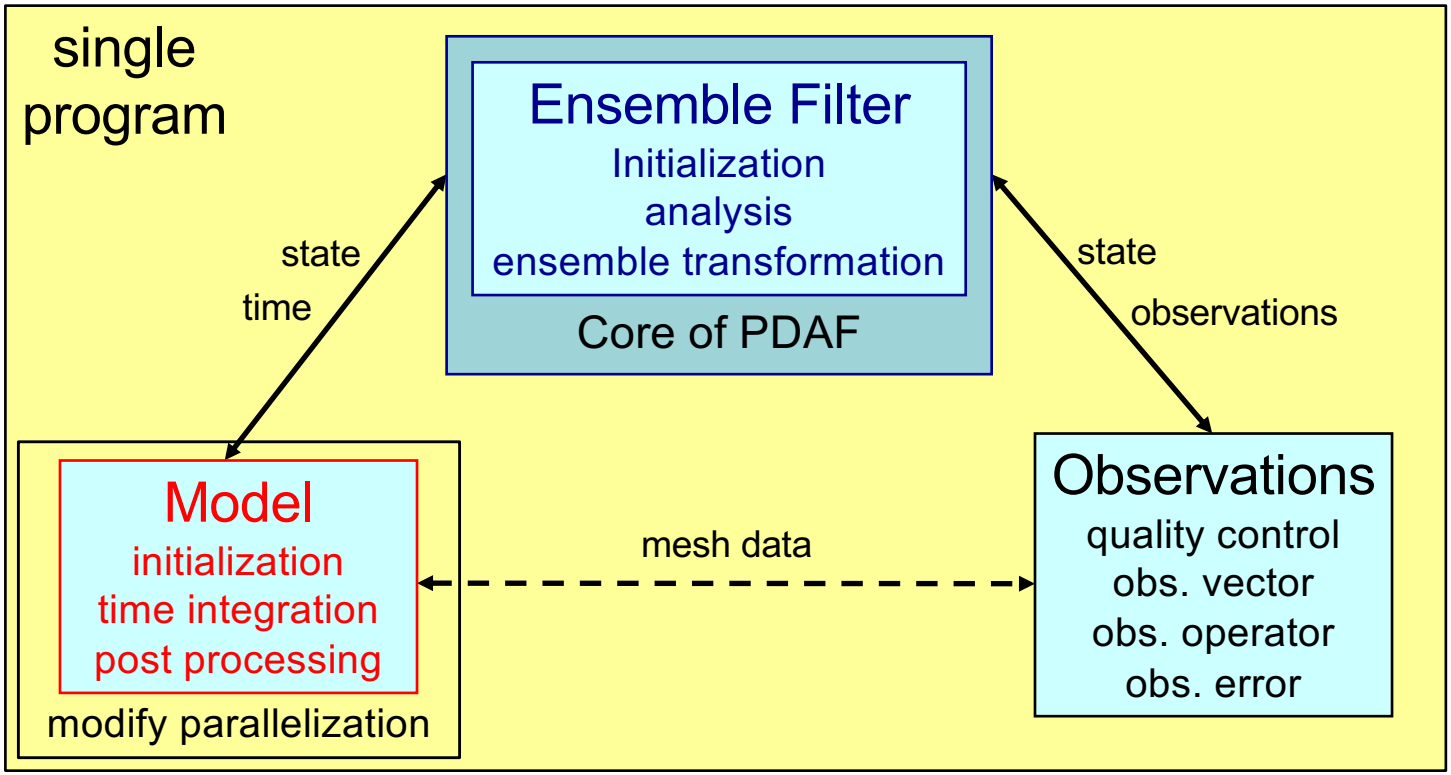

Explicit interface

Indirect exchange (module/common)

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

Augmenting a Model for Data Assimilation

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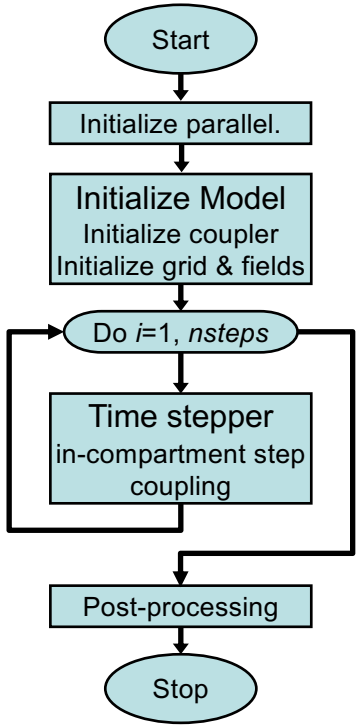
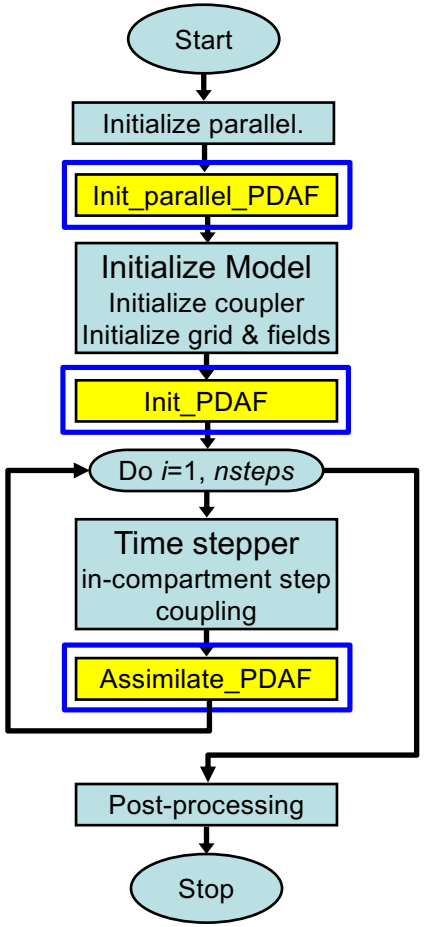
Model

single or multiple executables

coupler might be separate program





Extension for data assimilation

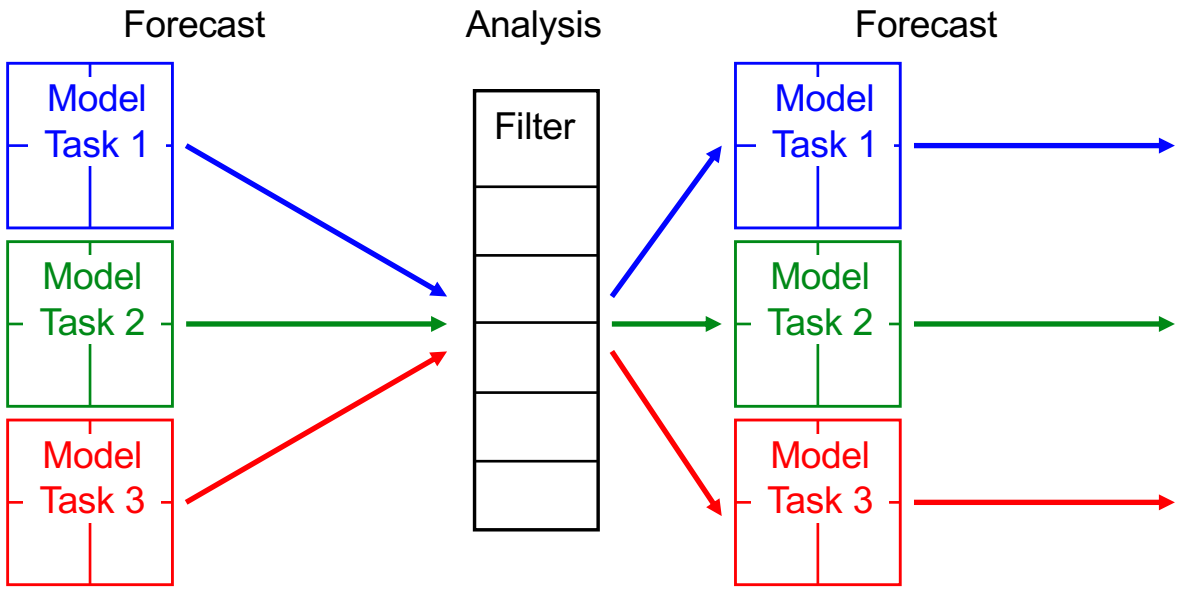
plus:
Possible model-specific adaption

e.g. in NEMO: treat leap-frog time stepping

revised parallelization enables ensemble forecast

2-level Parallelism

PDAF Parallel Data Assimilation Framework



1. Multiple concurrent model tasks
2. Each model task can be parallelized

- Analysis step is also parallelized
- Configured by "*MPI Communicators*"

Minimal changes to NEMO

PDAF Parallel Data Assimilation Framework

Add to *mynode* (lin_mpp.F90) just before init of myrank

```
#ifdef key_USE_PDAF
   CALL init_parallel_pdaf(0, 1, mpi_comm_opa)
#endif
```

Add to *nemo_init* (nemogcm.F90) at end of routine

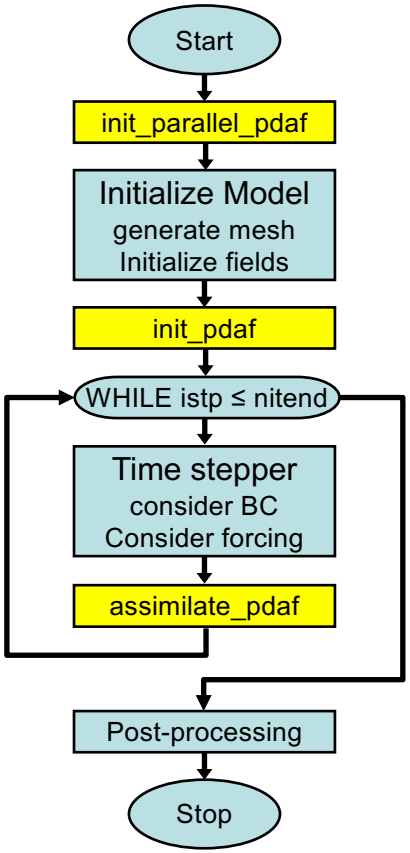
```
#ifdef key_USE_PDAF
   CALL init_pdaf()
```

Add to *stp* (step.F90) at end of routine

```
#ifdef key_USE_PDAF
   CALL assimilate_pdaf()
```

Modify *dyn_nxt* (dynnxt.F90) – for Euler time step

```
#ifdef key_USE_PDAF
   IF((neuler==0 .AND. kt==nit000) .OR. assimilate)
#else
```



For MITgcm: calls included in MITgcm release version.
PDAF provides the model-binding routines

Why Online coupling? Efficiency

PDAF Parallel Data Assimilation Framework

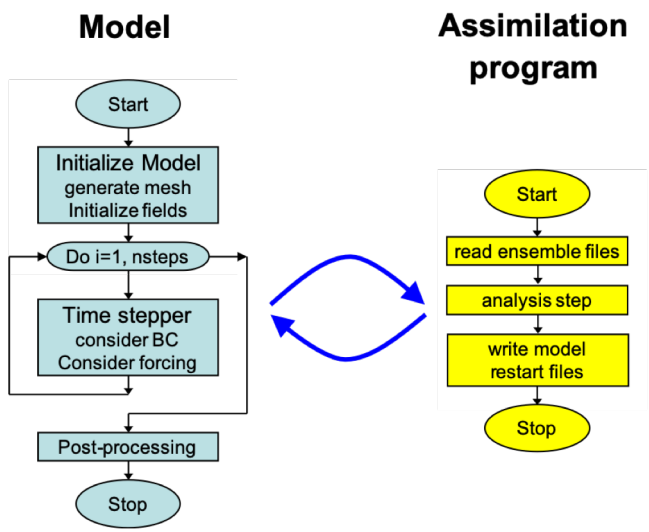
Offline-coupling is simple to implement but can be very inefficient

Example:
Timing from atmosphere-ocean coupled model (AWI-CM) with daily analysis step:

Model startup:	95 s	overhead
Integrate 1 day:	28 s	
Model postprocessing:	14 s	
Analysis step:	1 s	

Restarting this model is ~3.5 times more expensive than integrating 1 day

→ avoid this for data assimilation

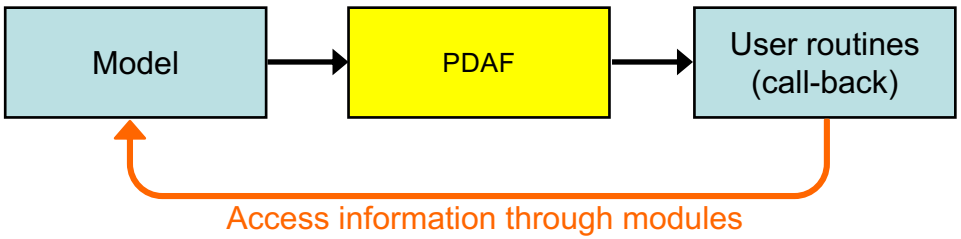


Offline-coupled assimilation
=
Separate programs
Data transfers through files

PDAF interface structure

PDAF Parallel Data Assimilation Framework

- Defined calls to PDAF routines and to call-back routines
- Model und observation specific operations:
  elementary subroutines implemented in model context
- User-supplied call-back routines for elementary operations:
  - transfers between model fields and ensemble of state vectors
  - observation-related operations (observation operator, …)
  - filter pre/post-step to analyze ensemble
- User supplied routines can be implemented
  as routines of the model (e.g. share common blocks or modules)



PDAF: User-friendliness

PDAF Parallel Data Assimilation Framework

Assumption: Users know their model

➜ let users implement assimilation system in model context

For users, model is not just a forward operator

➜ let users augment their model for data assimilation

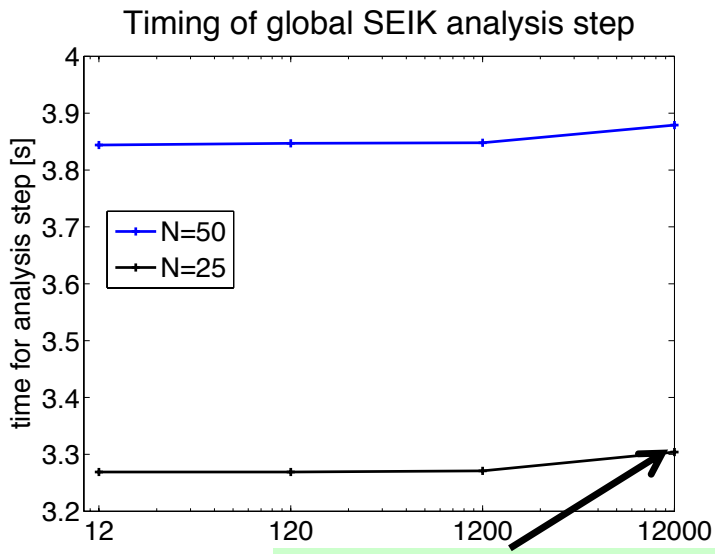
Keep simple things simple:

- Define subroutine interfaces to separate model and assimilation based on arrays
- No object-oriented programming
  (most models don't use it; most model developers don't know it; not many objects would be involved)
- Users directly implement observation-specific routines
  (no indirect description of e.g. observation layout)
- Users run their model as without data assimilation, but with additional options

PDAF Capability: Very big test case

PDAF Parallel Data Assimilation Framework

- Simulate a “model”
- Choose an ensemble
  - state vector per processor: 10^7
  - observations per processor: $2 \cdot 10^5$
  - Ensemble size: 25
  - 2GB memory per processor core
- Apply analysis step for different processor numbers
  - 12 – 120 – 1200 – 12000



State dimension: 1.2e11

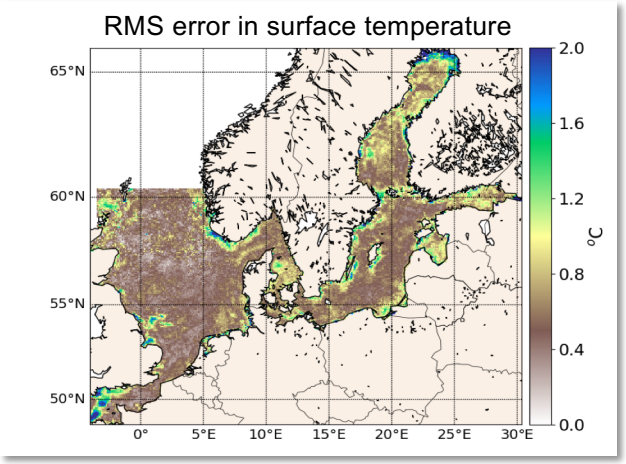
Observation dimension: 2.4e9

- Very small increase in analysis time (~1%) (Ideal would be constant time)
- Didn’t try to run a real ensemble of largest state size (no model yet)

PDAF Application Examples

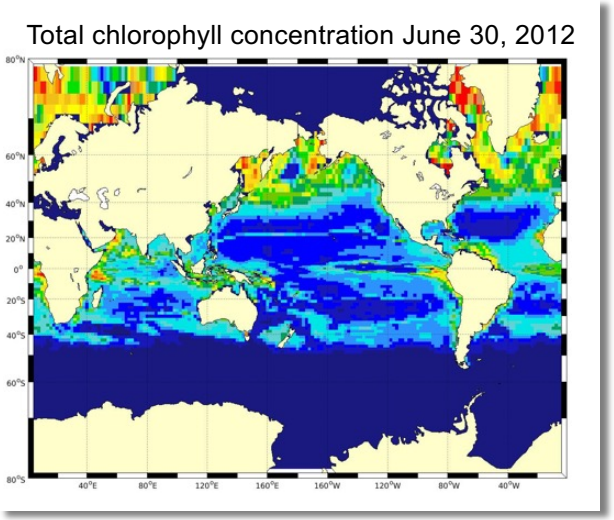
PDAF Parallel Data Assimilation Framework

HBM: Coastal assimilation of SST, in situ and ocean color data (S. Losa, M. Goodliff)

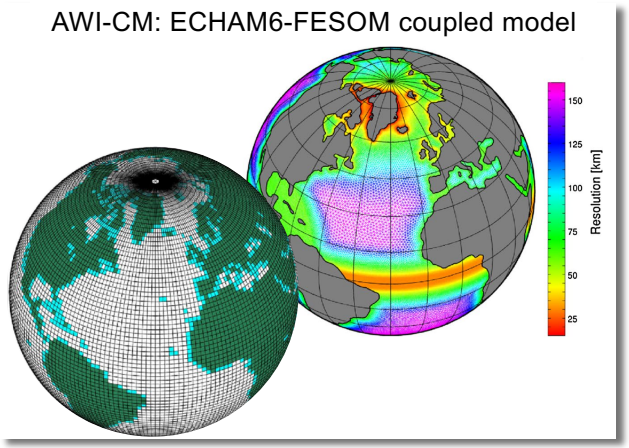


MITgcm-REcoM: global ocean color assimilation (Himansu Pradhan)

→ Talk tomorrow



AWI-CM: coupled atmos.-ocean assimilation (project ESM, Qi Tang)



+ external applications & users, like

- MITgcm sea-ice assim (NMEFC Beijing)
- Geodynamo (IPGP Paris, A. Fournier)
- TerrSysMP-PDAF (hydrology, FZ Juelich)
- CMEMS Baltic-MFC (DMI/BSH/SMHI)
- CFSv2 (J. Liu, IAP-CAS Beijing)
- NEMO (U. Reading , P. J. van Leeuwen)

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Current algorithms in PDAF

PDAF Parallel Data Assimilation Framework

PDAF originated from comparison studies of different filters

Filters and smoothers

- EnKF (Evensen, 1994 + perturbed obs.)
- (L)ETKF (Bishop et al., 2001)
- SEIK filter (Pham et al., 1998)
- ESTKF (Nerger et al., 2012)
- NETF (Toedter & Ahrens, 2015)

Not yet released:
- serial EnSRF
- particle filter
- EWPF
- Generate synthetic observations (V1.14)

All methods include

- global and localized versions
- smoothers

Model binding

- MITgcm

Not yet released:
- NEMO

Toy model

- Lorenz-96

Summary

PDAF Parallel Data Assimilation Framework

- PDAF: Software framework
  simplifies building data assimilation systems
- Efficient online assimilation coupling
  with minimal changes to model code
- Setup of data assimilation with coupled model
  1. Configuration of parallelization
  2. Implementation of user call-back routines
     - for interfacing with model code and
     - observation handling

Open source:
Code, documentation, and tutorial available at

http://pdaf.awi.de

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References

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- http://pdaf.awi.de
- Nerger, L., Hiller, W. *Software for Ensemble-based DA Systems – Implementation and Scalability*. Computers and Geosciences 55 (2013) 110-118
- Nerger, L., Hiller, W., Schröter, J.(2005). *PDAF - The Parallel Data Assimilation Framework: Experiences with Kalman Filtering*, Proceedings of the Eleventh ECMWF Workshop on the Use of High Performance Computing in Meteorology, Reading, UK, 25 - 29 October 2004, pp. 63-83.

Thank you !

AWI