Ocean Sciences Meeting, Portland, Oregon, USA, 2/13/2018

Tutorial T002

Ensemble Data Assimilation with the Parallel Data Assimilation Framework

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Special thanks to:

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UND MEERESFORSCHUNG

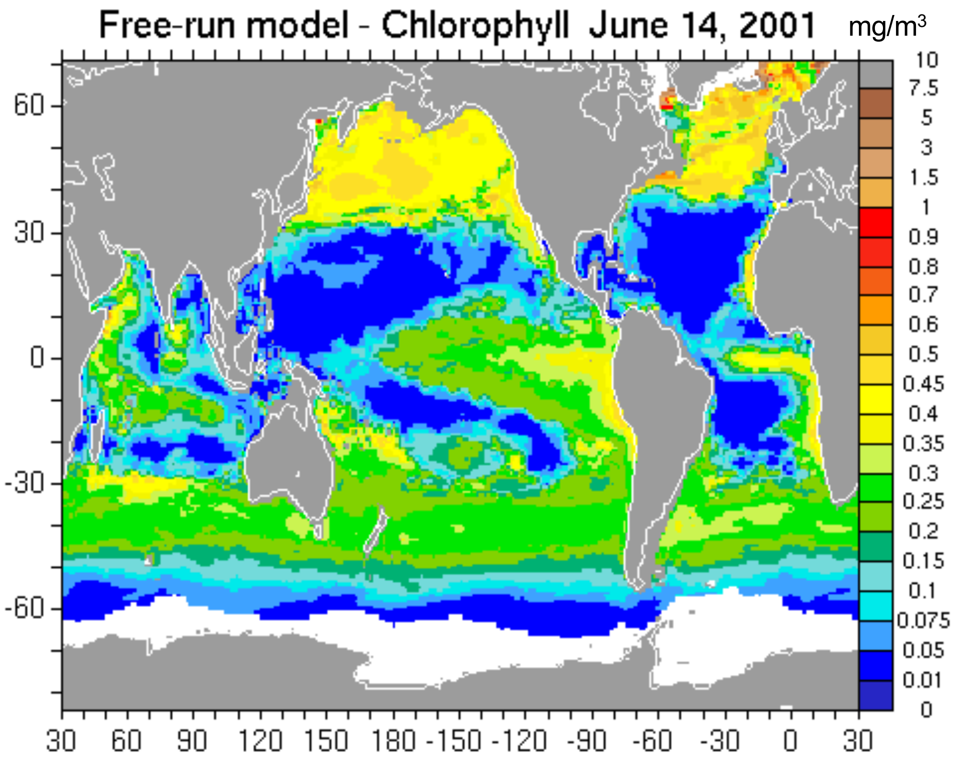
Overview

- Overview of ensemble data assimilation
- Data assimilation software PDAF
  (Parallel Data Assimilation Framework)
- Implementation example MITgcm

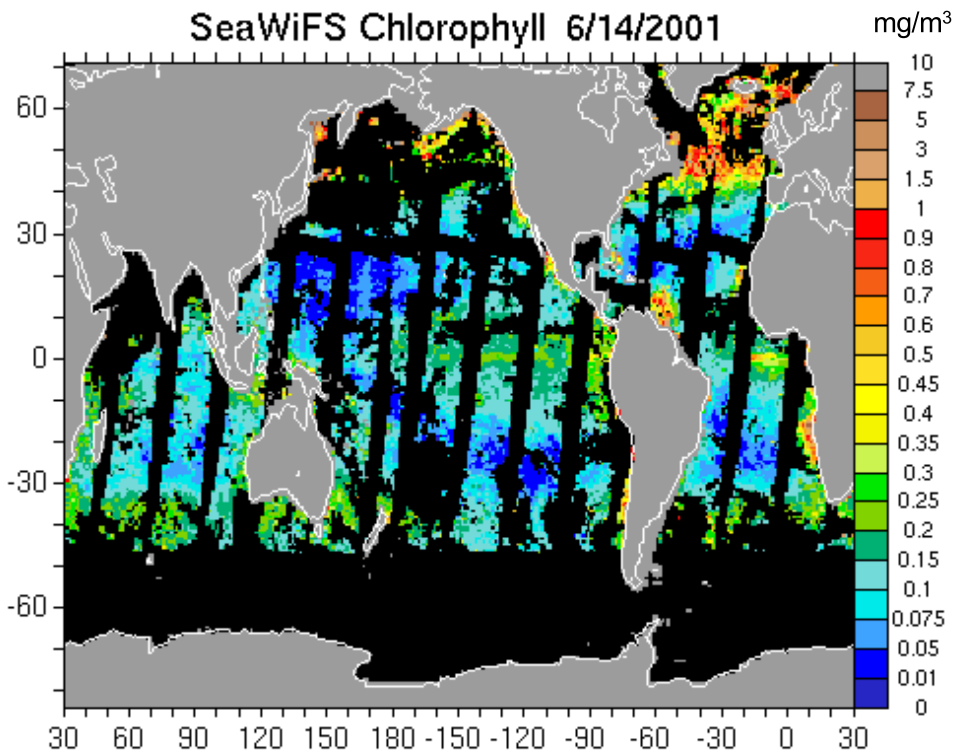
Overview of

Ensemble Data Assimilation

Data Assimilation – Motivation



biogeochemical model



satellite data (1 day)

Data Assimilation

Combine both information source to obtain better estimate of system state

L. Nerger & W.W. Gregg, *J. Marine Syst.* 68 (2007) 237-254

Data Assimilation

Combine model with real data

- Optimal estimation of system state:
  - initial conditions (for weather/ocean forecasts, …)
  - state trajectory (temperature, concentrations, …)
  - parameters (growth of phytoplankton, …)
  - fluxes (heat, primary production, …)
  - boundary conditions and 'forcing' (wind stress, …)
- More advanced: Improvement of model formulation
  - Detect systematic errors (bias)
  - Revise parameterizations based on parameter estimates

Needed for Data Assimilation

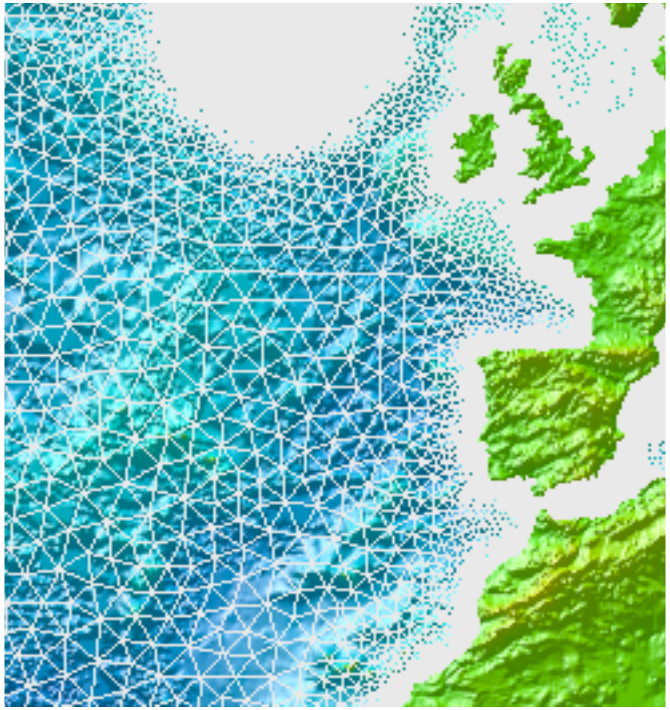
1. Model
   - with some skill
2. Observations
   - with finite errors
   - related to model fields
3. Data assimilation method

Models

Simulate dynamics of ocean

- Numerical formulation of relevant terms
- Discretization with finite resolution in time and space
- "forced" by external sources (atmosphere, river inflows)

- Uncertainties
  - initial model fields
  - external forcing
  - in predictions due to model formulation



Unstructured mesh in North-east Atlantic

Observations

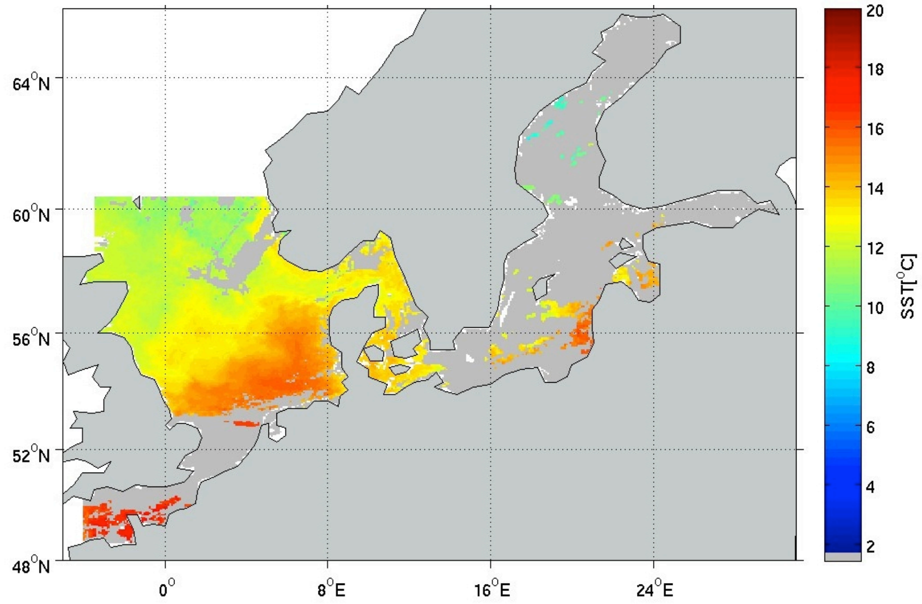
Measure different fields in the Ocean

- Remote sensing
  - E.g. surface temperature, salinity, sea surface height, ocean color, sea ice concentrations & thickness
- In situ
  - Argo, CTD, Gliders, …

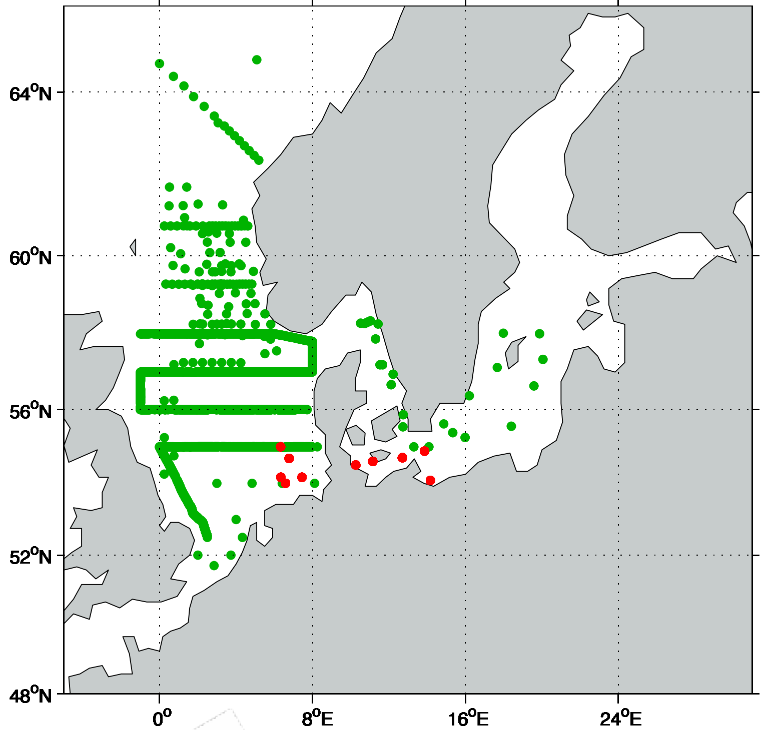
- Data is sparse: some fields, data gaps
- Uncertainties
  - Measurement errors
  - Representation errors:
    Model and data do not represent exactly the same
    (e.g. cause by finite model resolution)

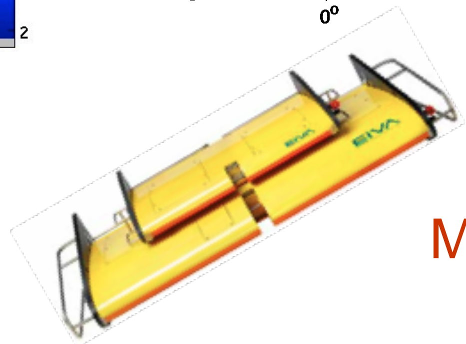
Example: Physical Data in North & Baltic Seas

Satellite surface temperature
(12-hour composite)



Avalable T and S profiles during July 2008





Scanfish and
CTD profiles

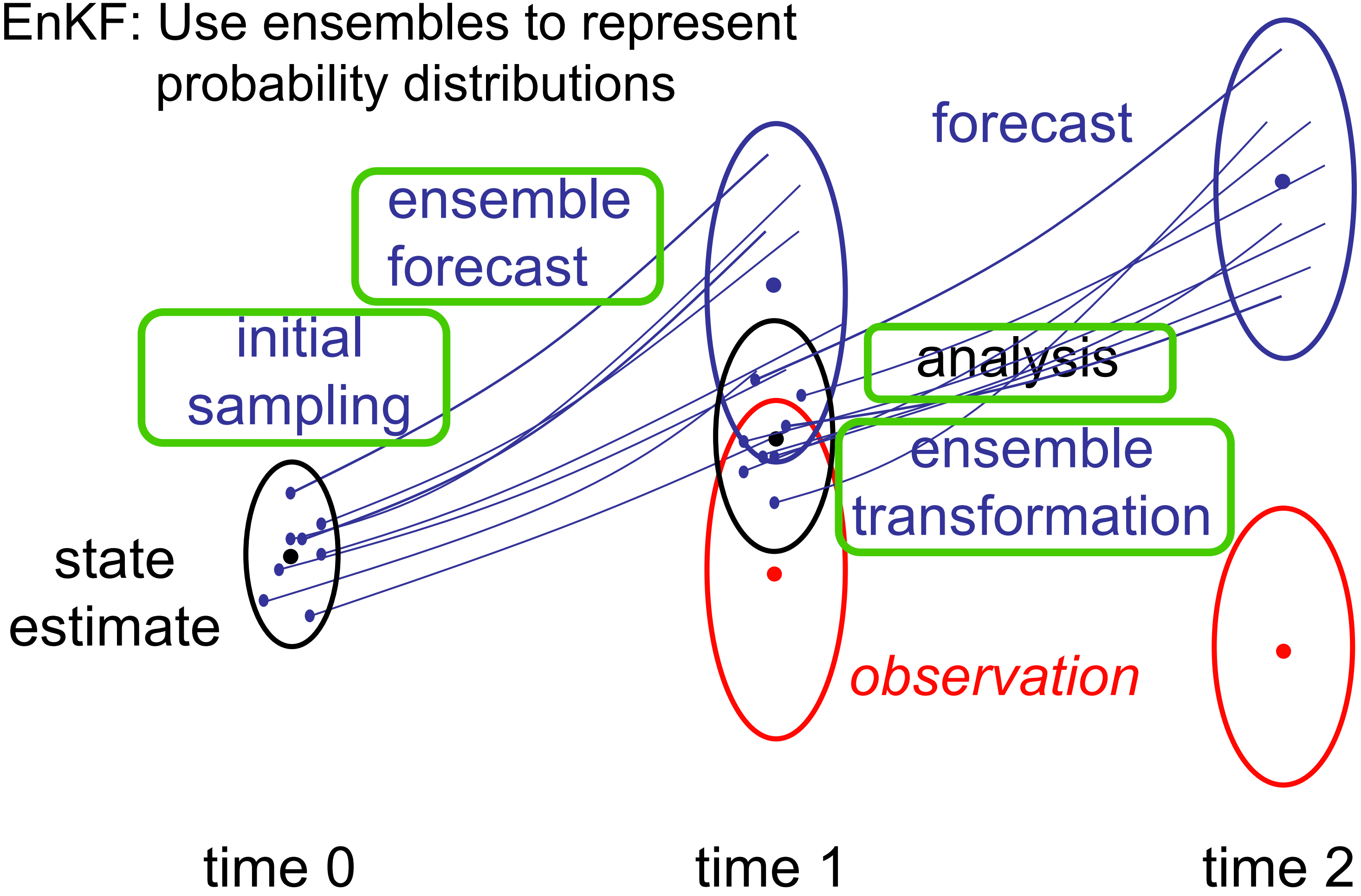
MARNET
stations

Ensemble-based Kalman Filter

First formulated by G. Evensen (EnKF, J. Geophys. Res. 1994)

Kalman filter: express probability distributions by mean and covariance matrix

EnKF: Use ensembles to represent probability distributions

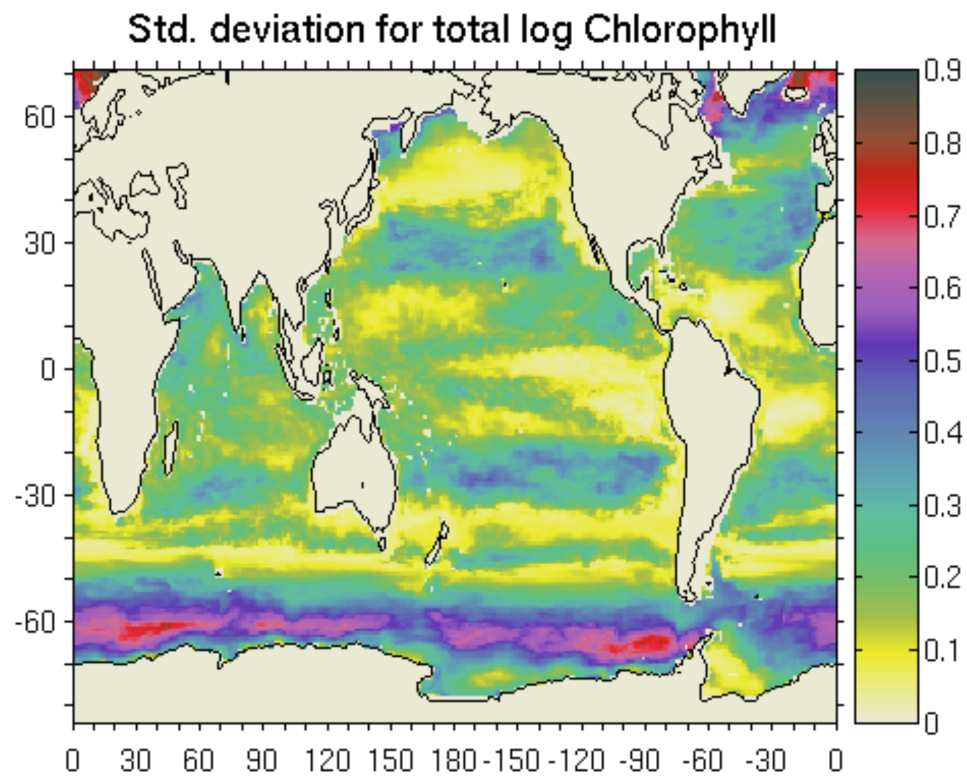


There are many possible choices!

Leads to different filter methods

Ensemble Covariance Matrix

- Ensemble represents state estimate and its uncertainty
- uncertainty information (variances + covariances)
- Generated dynamically
  by propagating ensemble of model states



Data Assimilation Software

PDAF

(Parallel Data Assimilation Framework)

PDAF: A tool for data assimilation

PDAF - Parallel Data Assimilation Framework

- a program library for ensemble data assimilation
- provide support for parallel ensemble forecasts
- provide fully-implemented & parallelized filters and smoothers (EnKF, LETKF, NETF, EWPF … easy to add more)
- easily useable with (probably) any numerical model (applied with MITgcm, NEMO, FESOM, HBM, TerrSysMP, …)
- run from laptops to supercomputers (Fortran, MPI & OpenMP)
- first public release in 2004; continued development
- ~280 registered users; community contributions

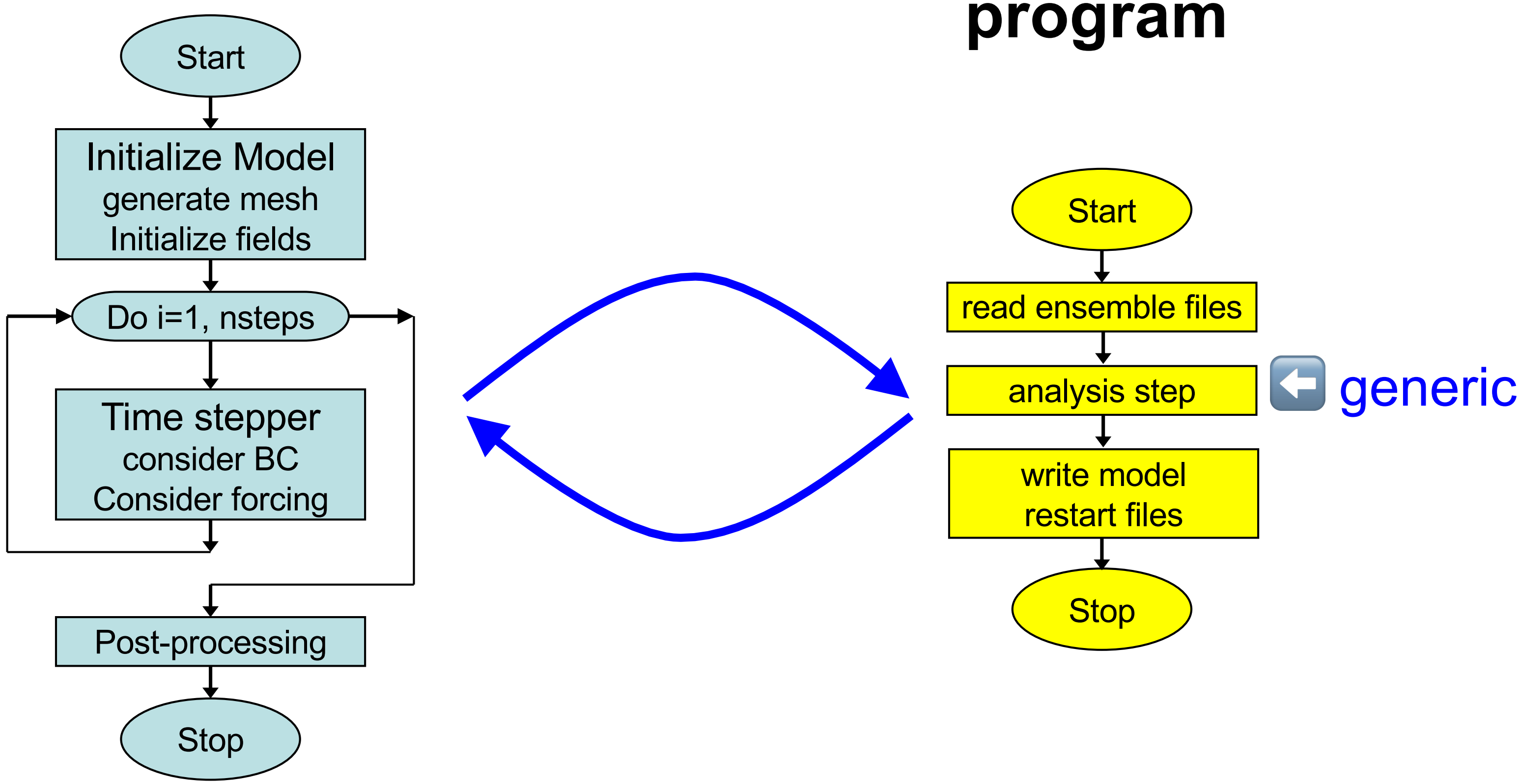
Open source:
Code and documentation available at

http://pdaf.awi.de

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

Offline coupling – separate programs

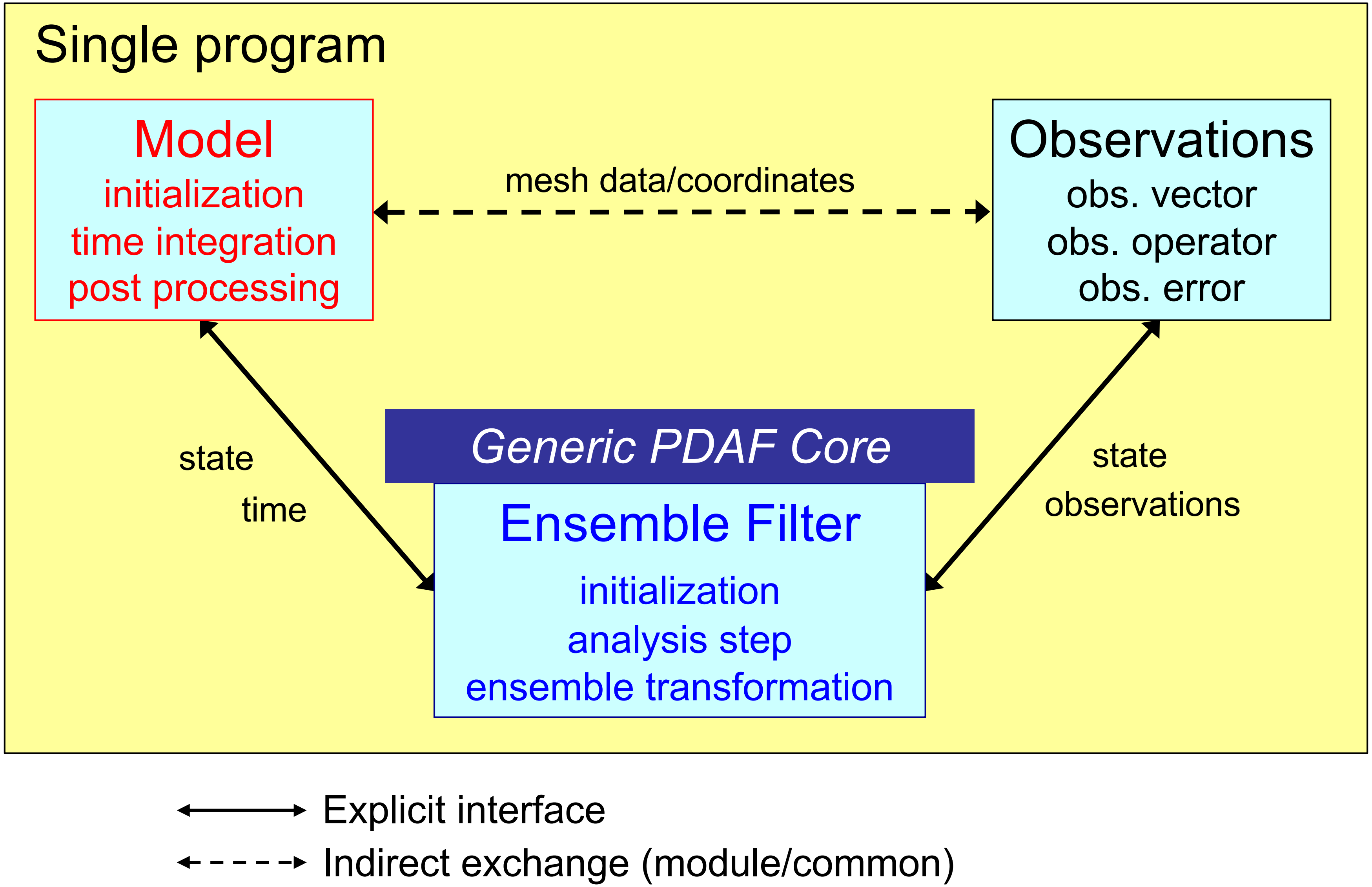
Model | **Assimilation program**



For each ensemble state
- Initialize from restart files
- Integrate
- Write restart files

- Read restart files (ensemble)
- Compute analysis step
- Write new restart files

Online Coupling

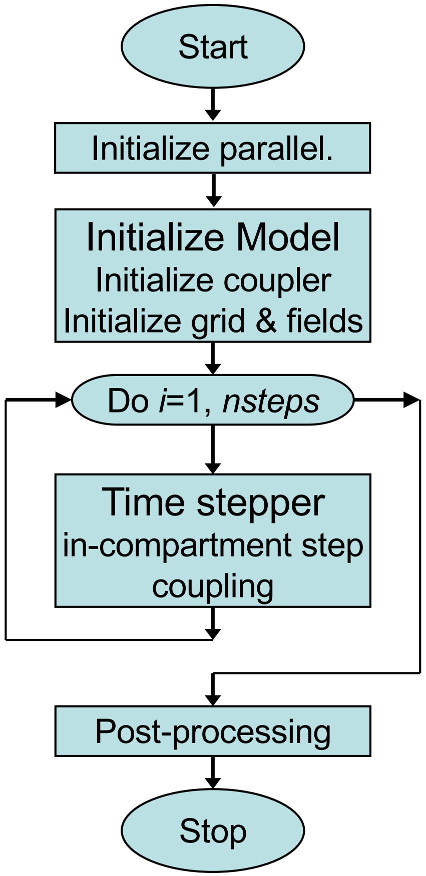


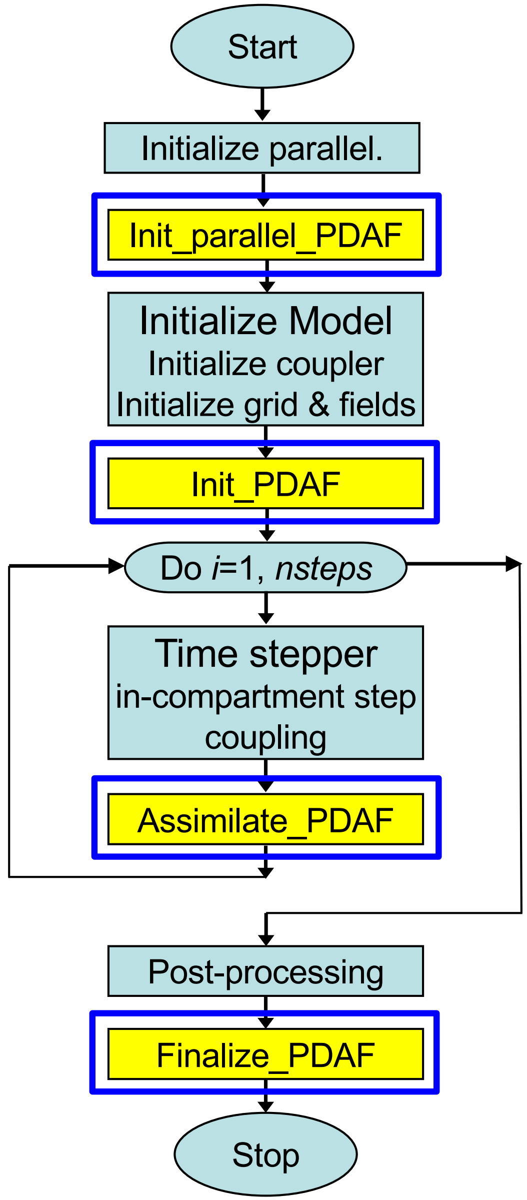
Extending a Model for Data Assimilation

Model

single or multiple executables

coupler might be separate program





Extension for data assimilation

plus:
Possible model-specific adaption

for MITgcm:
adapt name of STDOUT files for ensemble

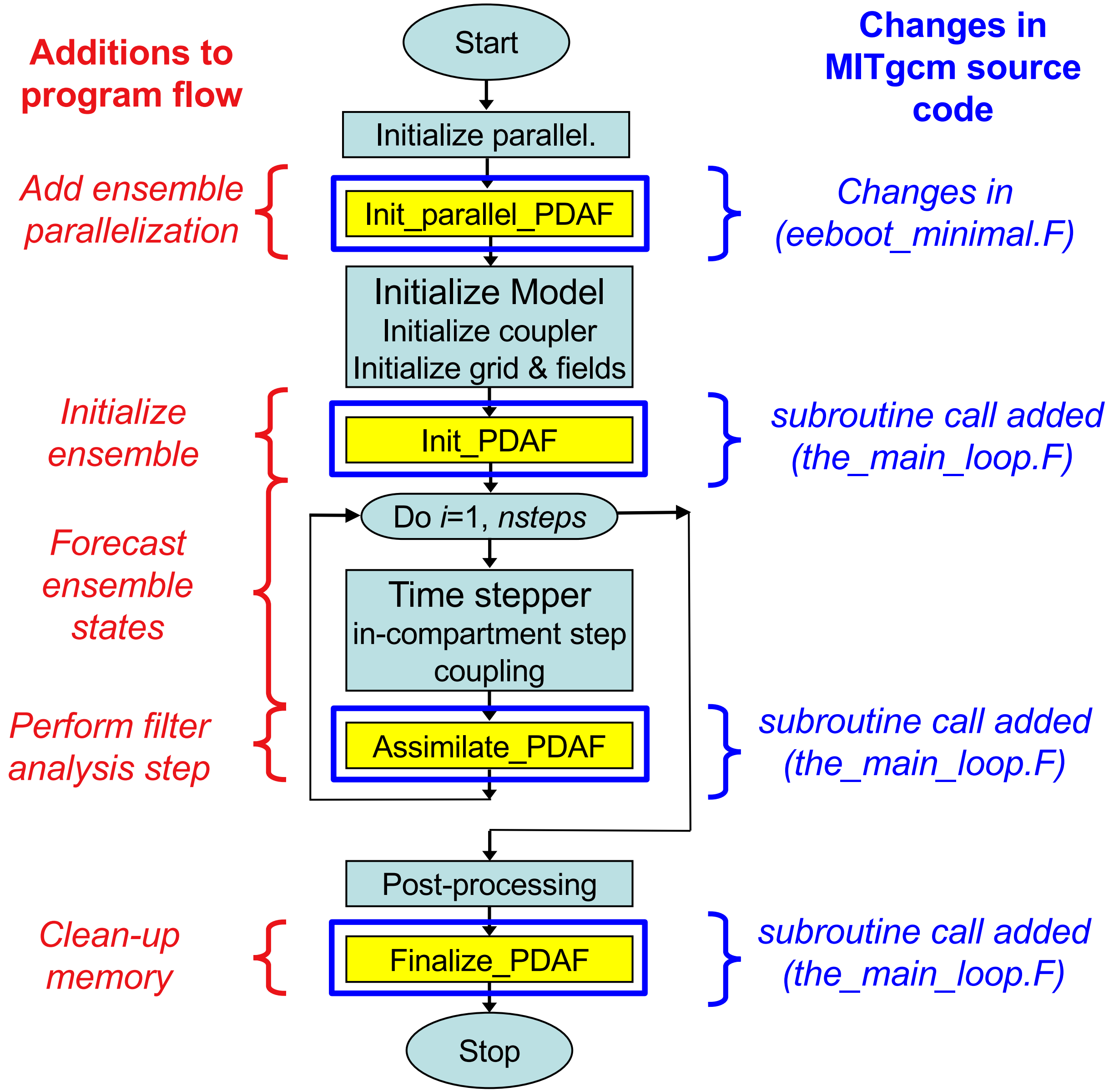
revised parallelization enables ensemble forecast

Implementing Ensemble DA

Example of MITgcm

MITgcm extension for Data Assimilation

PDAF Parallel Data Assimilation Framework



- All changes included in MITgcm repository version
- PDAF interface routines activated by preprocessor setting -DUSE_PDAF

For convenience:

- *eeboot_minimal*: also change the index of STDOUT file
- *the_main_loop*: timers for PDAF calls

PDAF model binding routines

Interface routines

- `init_parallel_pdaf, init_pdaf, assimilate_pdaf, finalize_pdaf`

Call-back routines

- Set number of time steps between analysis steps
- Observation handling
- Write model fields into PDAF's state vector and back into model fields

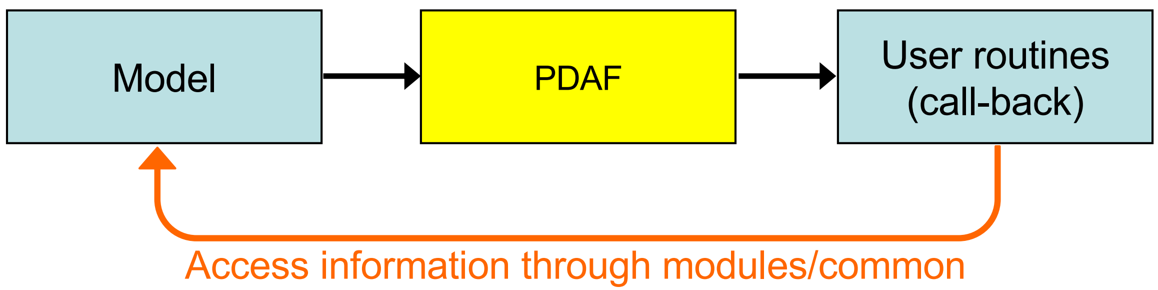
PDAF release includes set of model binding routines for MITgcm

- ➢ for a simple test case
- ➢ just download and adapt for your needs

PDAF interface structure

PDAF Parallel Data Assimilation Framework

- Interface routines call PDAF-core routines
- PDAF-core routines call case-specific routines provided by user (included in model binding set)
- User-supplied call-back routines for elementary operations:
  - field transformations between model and filter
  - observation-related operations
- User supplied routines can be implemented as routines of the model (for MITgcm: Fortran-77 fixed-form source code)



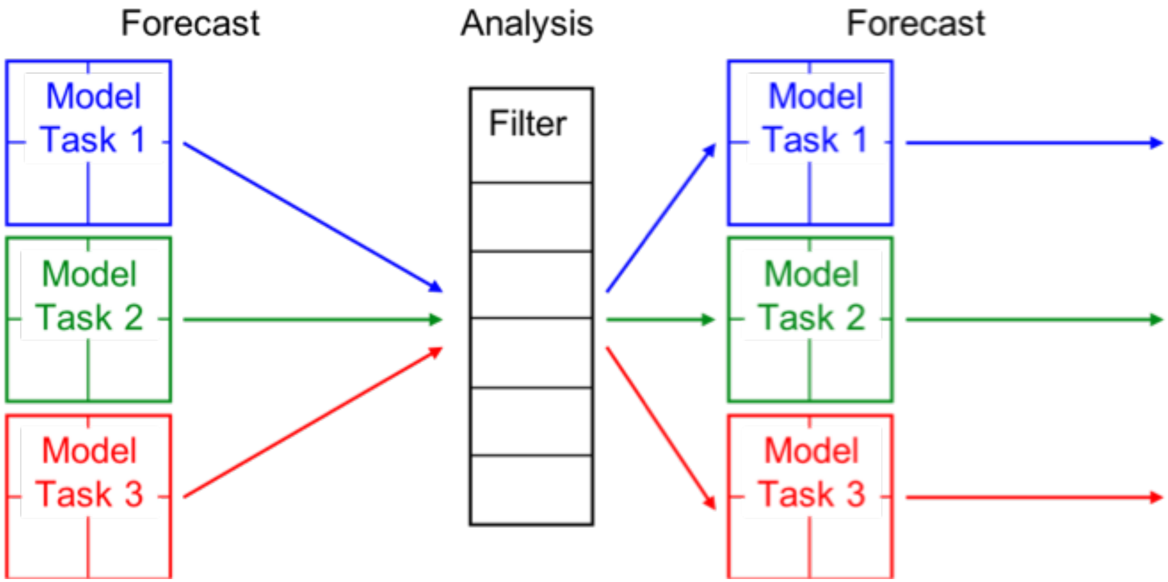
Init_parallel_PDAF

Parallelization of Assimilation Program

We use MPI (Message Passing Interface)

- It's the standard for highly scaling parallelization
- MITgcm uses MPI (like most large-scale models)

Change of parallelization is fully implemented for MITgcm!



Init_PDAF

Initialization of Assimilation

Set parameters, for example

- select filter
- set ensemble size

Calls `PDAF_init`

- initialization routine of framework
- provide parameters according to interface
- provide MPI communicators
- provide name of routine for ensemble initialization

Ensemble initialization routine – called by PDAF_init

- a "call-back routine"
- defined interface: provides ensemble array for initialization
- user-defined initialization

Simple Subroutine Interfaces

Example: ensemble initialization

```
SUBROUTINE init_ens_pdaf(filtertype, dim, dim_ens, state,
matrU, ens, flag)

  IMPLICIT NONE

! ARGUMENTS:
  INTEGER, INTENT(in) :: filtertype ! Type of filter
  INTEGER, INTENT(in) :: dim        ! Size of state vector
  INTEGER, INTENT(in) :: dim_ens    ! Size of ensemble
  REAL, INTENT(out) :: ens(dim, dim_ens) ! state ensemble
  INTEGER, INTENT(inout) :: flag    ! PDAF status flag
```

Task to be implemented:

- Fill ens with ensemble of initial model states

Assimilate_PDAF

Ensemble Forecast and Analysis Steps

calls `PDAF_assimilate`

- checks whether ensemble integration reached time for analysis step

- **If false:**
  - return to model and continue integration
- **If true:**
  - Write forecast fields into state vectors (call-back routine)
  - Compute analysis step of chosen filter
  - Set length of next forecast phase (call-back routine)
  - Write state vectors into model field arrays (call-back routine)

Finalize_PDAF

Clean-up of Data Assimilation Program

Clean-up at end of program

- Display timing and memory information for PDAF
- Deallocate arrays inside PDAF

Calls to

`PDAF_print_info`	(memory and timing info)
`PDAF_deallocate`	(deallocate arrays)

Fully implemented for MITgcm!

Filter analysis implementation

Operate on state vectors

- ➢ Write all model fields into a 1-dimensional vector
- Filter doesn't know about 'fields'
- Computationally most efficient
- Call-back routines for
  - Transfer between model fields and state vector
  - Observation-related operations
  - Localization operations

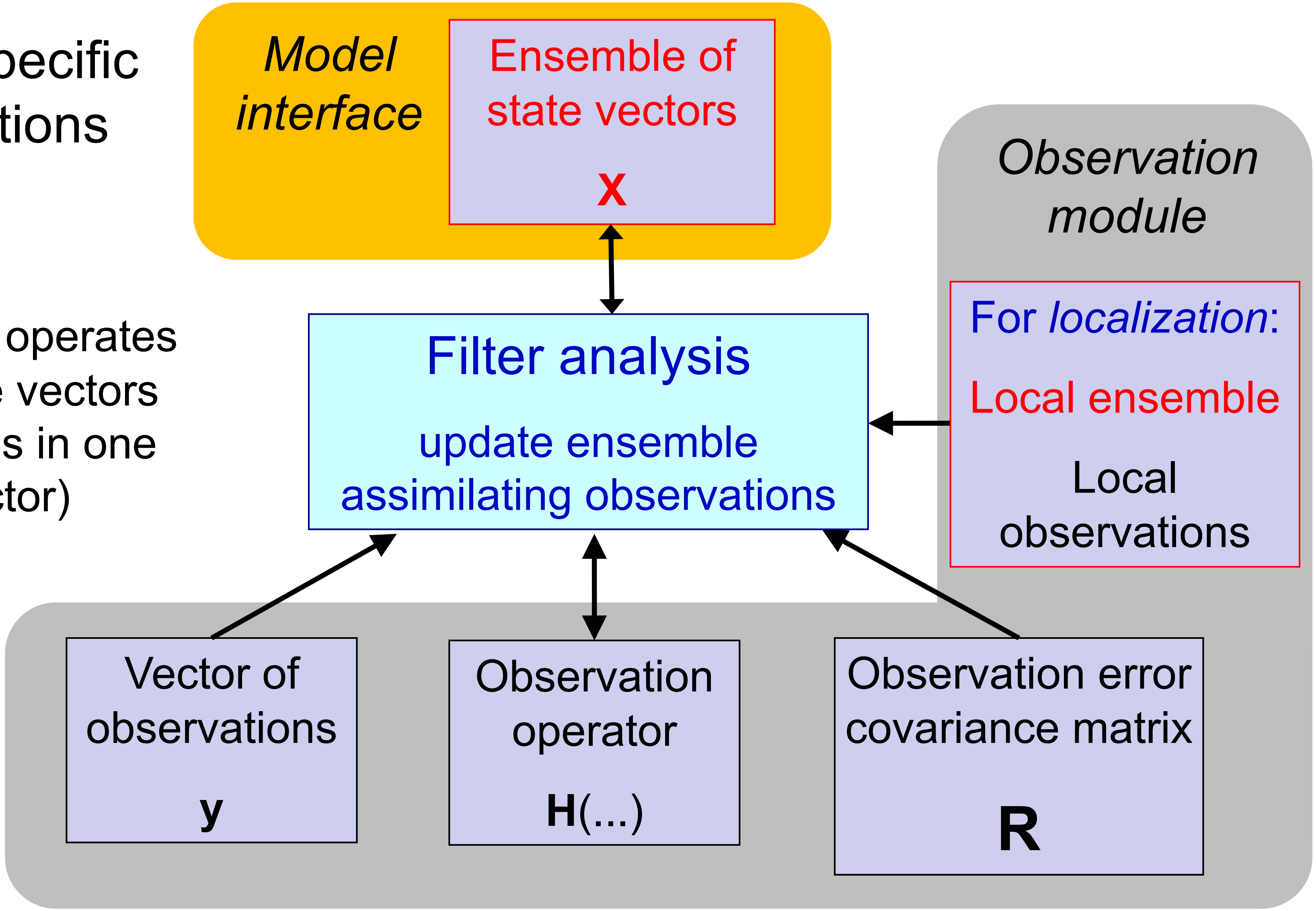
For forecast

- Transfer data from state vector to model fields

Ensemble Filter Analysis Step

case-specific operations

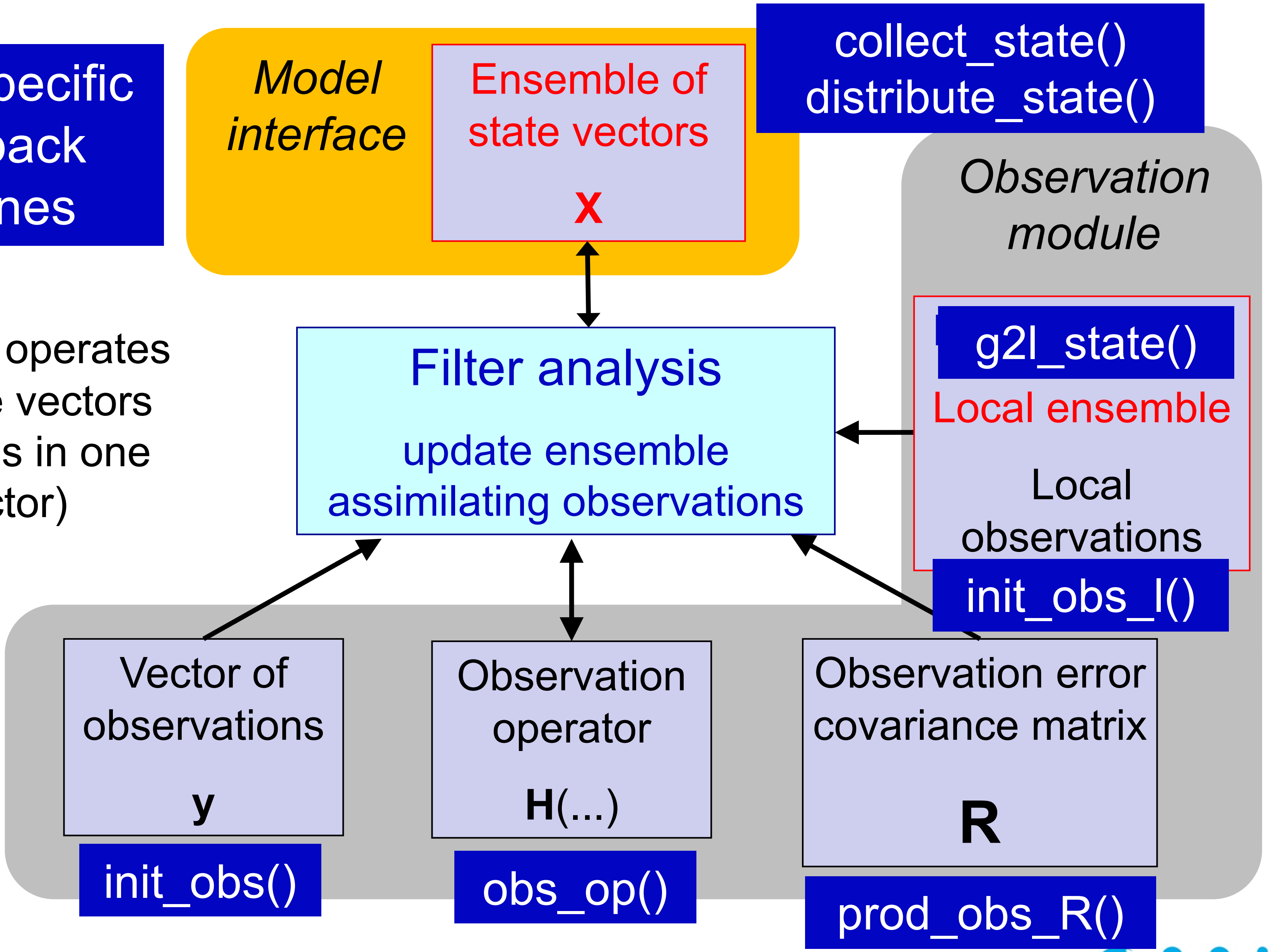
Analysis operates on state vectors (all fields in one vector)



Ensemble Filter Analysis Step

case-specific call-back routines

Analysis operates on state vectors (all fields in one vector)



Summary

Ensemble Data Assimilation with PDAF

- augment program for ensemble data assimilation
- assimilation methods provided by PDAF
- model-binding routines required
  - provided for MITgcm for test case
  - easy to code yourself
- PDAF is available as free open-source

Thank you!

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http://pdaf.awi.de

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