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

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Overview

How to simplify to apply data assimilation?

- simplify building a data assimilation application

Structure data assimilation application into

- generic part
- case-specific part (model and observations)

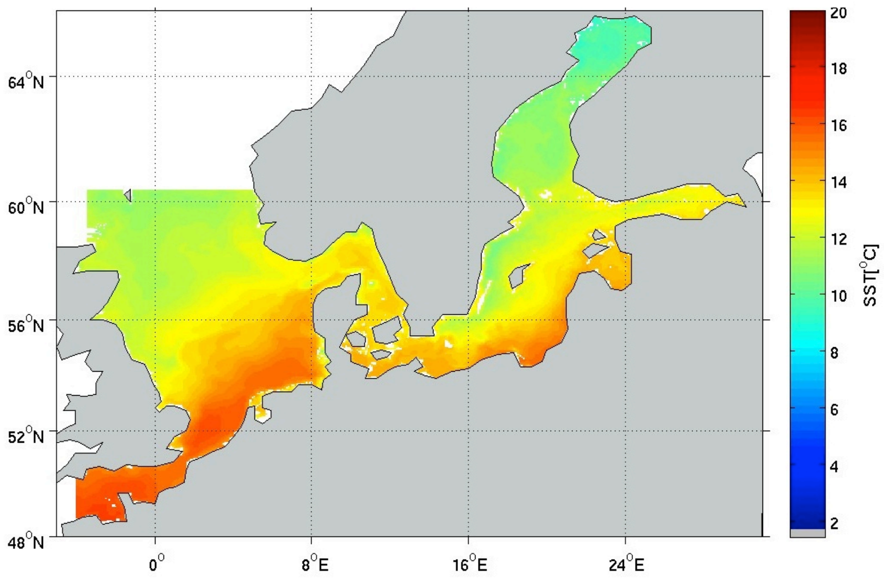
Provide

- software for generic part (e.g. filter methods, incl. methods like localization & inflation)
- code templates and documentation for case-specific part

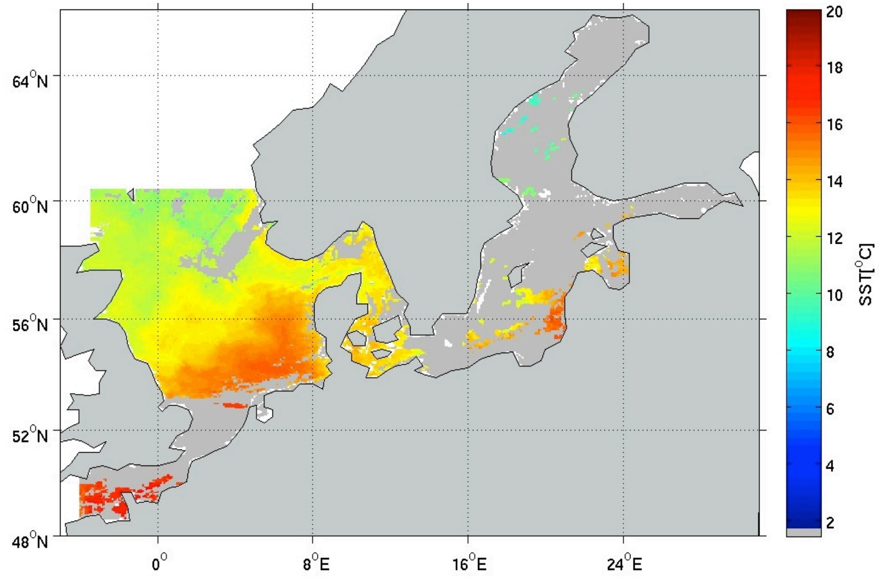
Data Assimilation in Ocean and Ocean-Biogeochemistry

Example: Forecast model for North and Baltic Seas

Model surface temperature



Satellite surface temperature



Focus on ensemble-based assimilation

- Ensemble Kalman filters
- Particle filters

Losa, S.N. et al. *J. Marine Syst.* 105 (2012) 152-162

PDAF: A tool for data assimilation

PDAF Parallel Data Assimilation Framework

PDAF - Parallel Data Assimilation Framework

- a program library for data assimilation
- provide support for ensemble forecasts
- provide fully-implemented filter and smoother algorithms (EnKF, LETKF, LSEIK, LESTKF … easy to add more)
- easily useable with (probably) any numerical model (applied with NEMO, MITgcm, FESOM, HBM, TerrSysMP, …)
- makes good use of supercomputers (Fortran, MPI & OpenMP)
- allows for separate development of model and assimilation algorithms
- first public release in 2004; continued development

Open source:
Code and documentation available at

http://pdaf.awi.de

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

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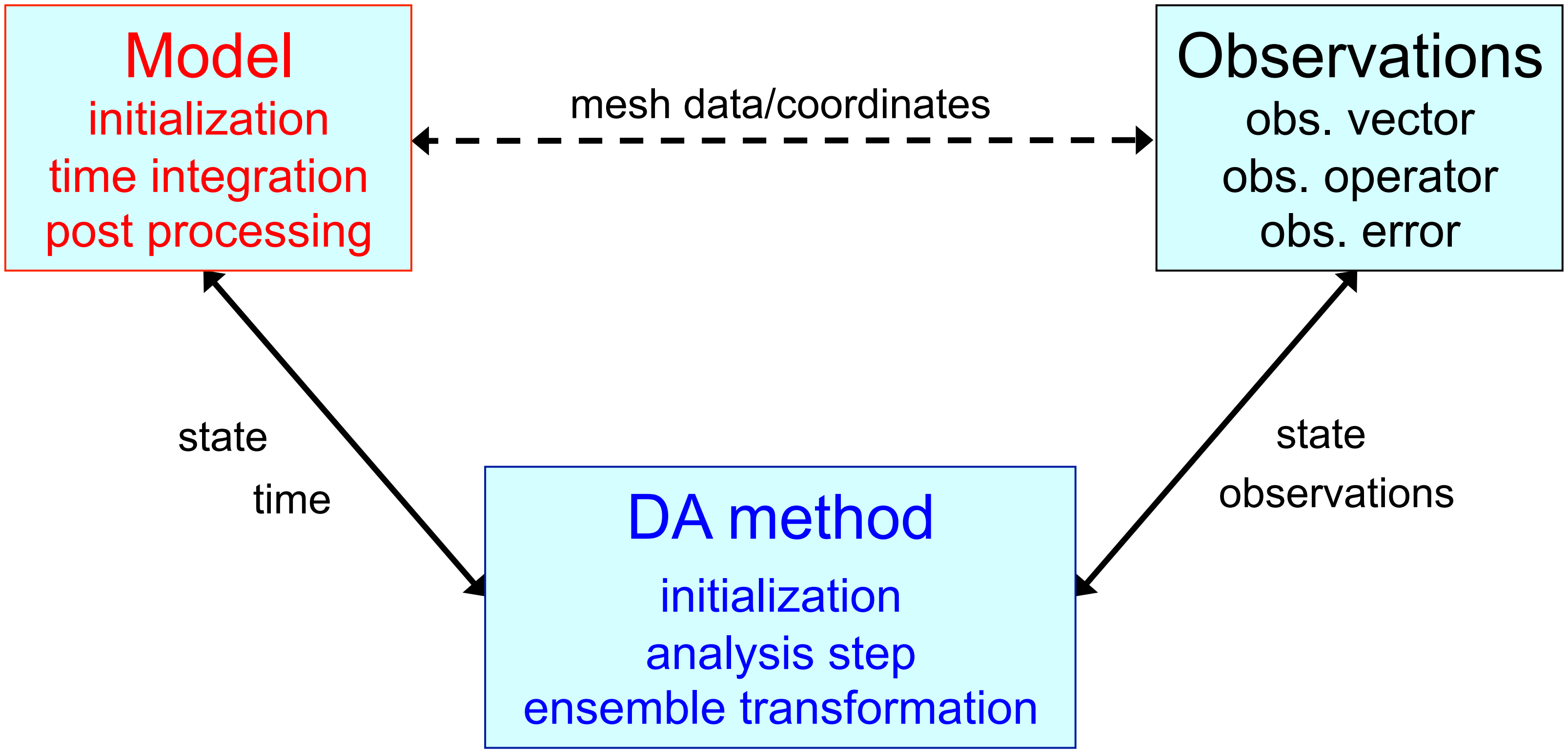
Framework Considerations

3 components of an assimilation system

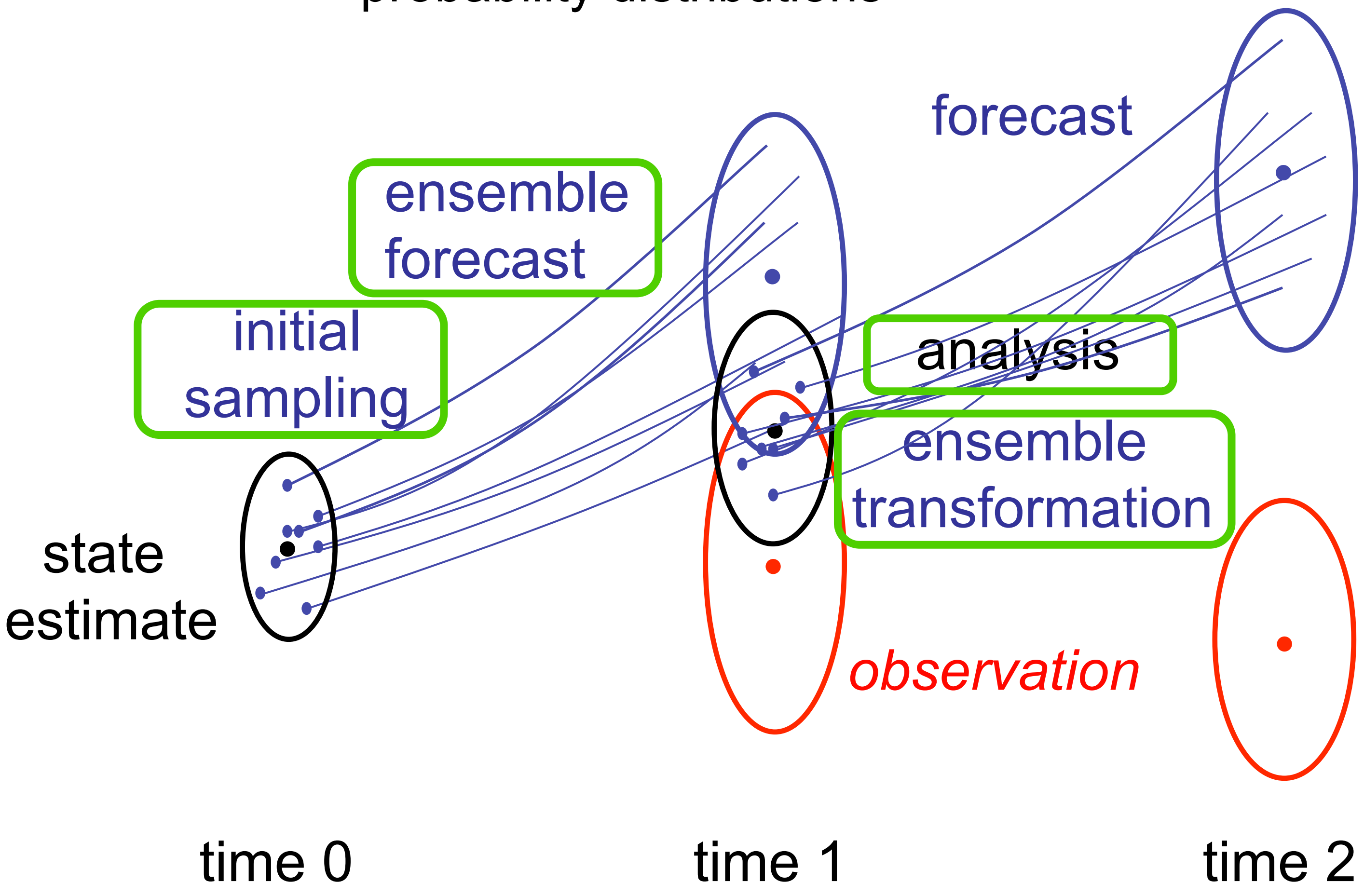


Nerger, L., Hiller, W. Software for Ensemble-based DA Systems – Implementation and Scalability. Computers and Geosciences 55 (2013) 110-118

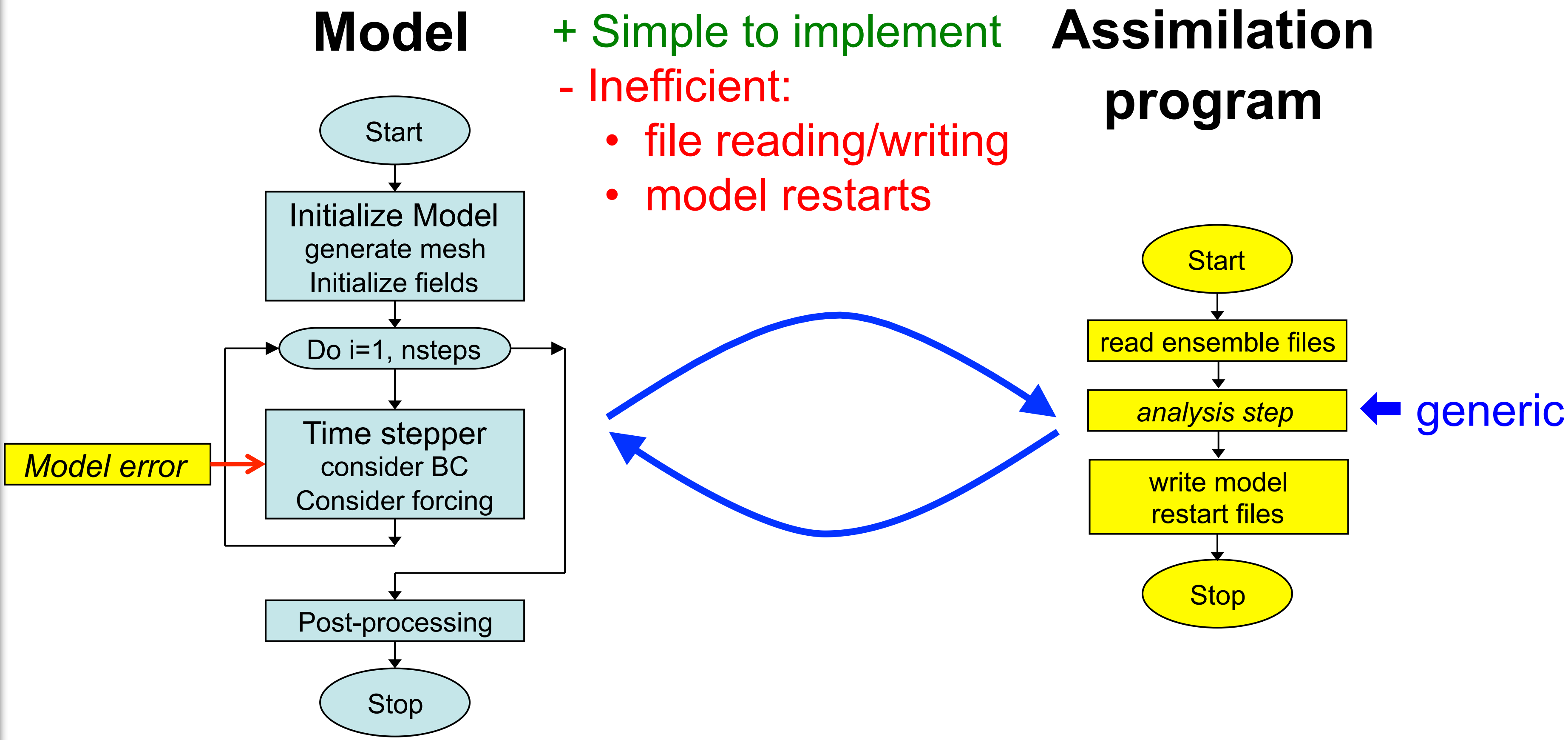
Ensemble-based Kalman Filter

Kalman filter: express probability distributions by mean and covariance matrix

EnKF (Evensen, 1994): Use ensembles to represent probability distributions



Offline coupling – separate programs

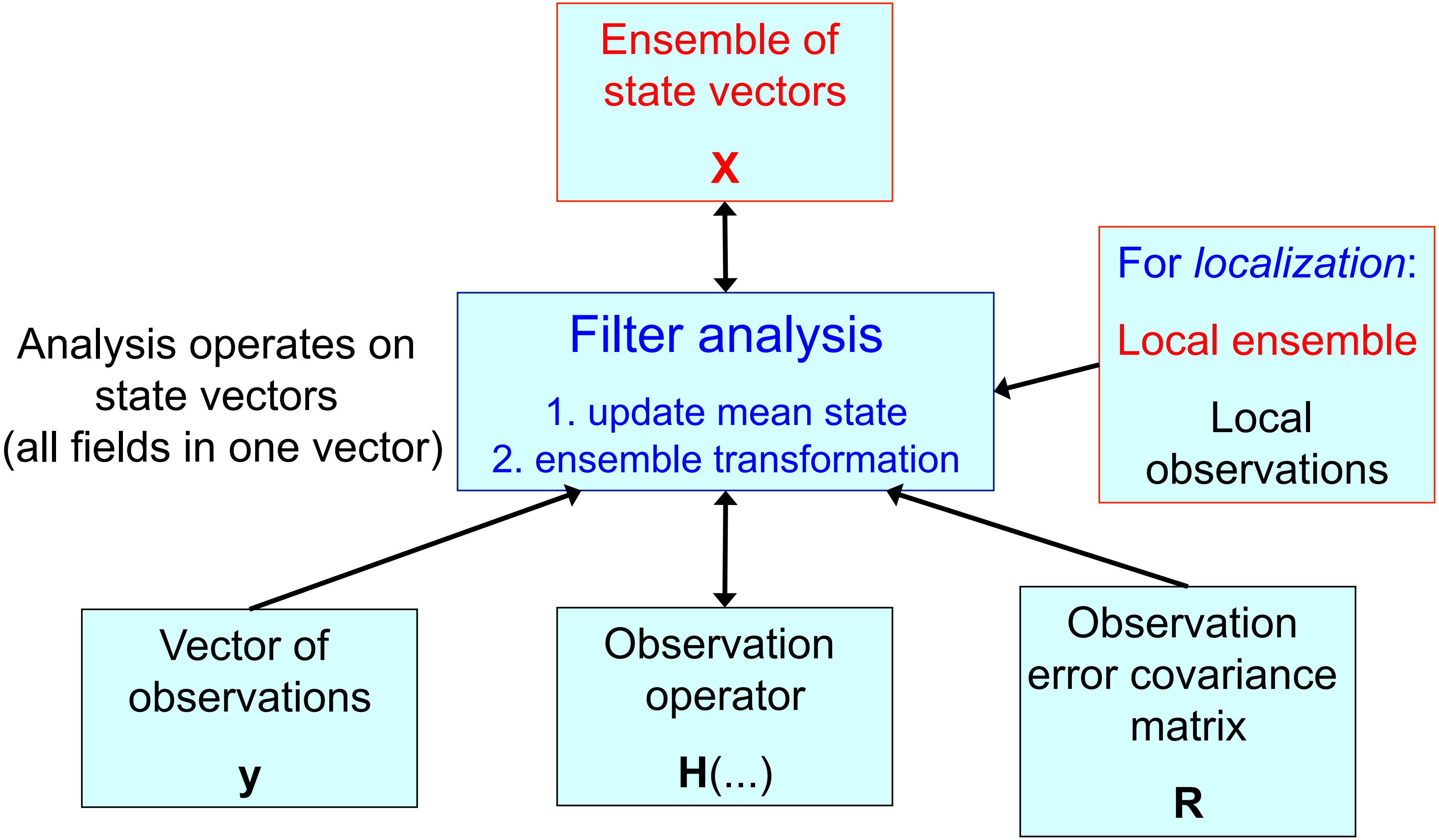


For each ensemble state

- Initialize from restart files
- Integrate
- Write restart files

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

Ensemble filter analysis step



Filter analysis implementation

Operate on state vectors

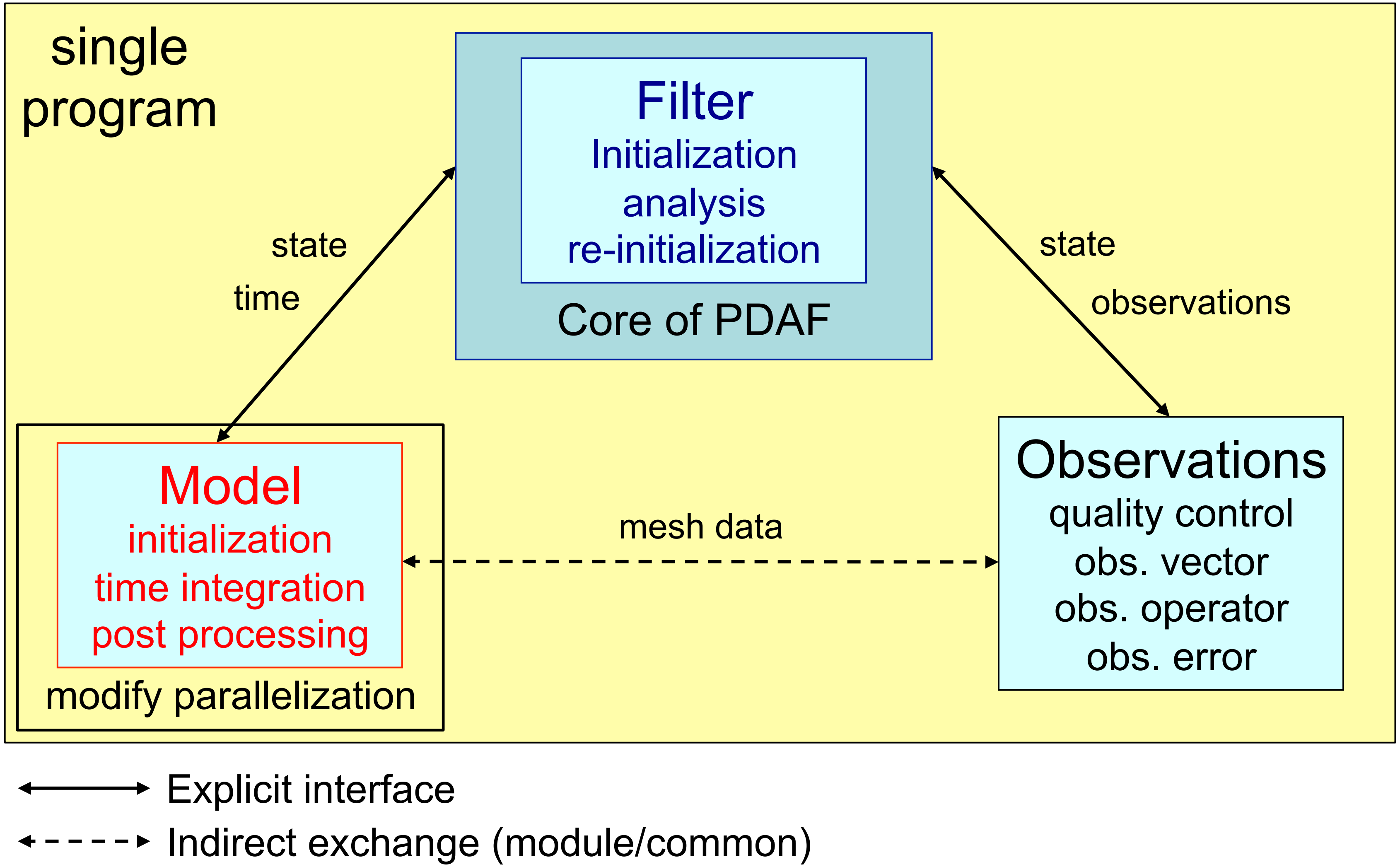
- Filter doesn't know about 'fields'
- Computationally most efficient
- Call-back routines for
  - Transfer between model fields and state vector
  - Observation-related operations
  - Localization operations

For forecast

- Transfer data from state vector to model fields

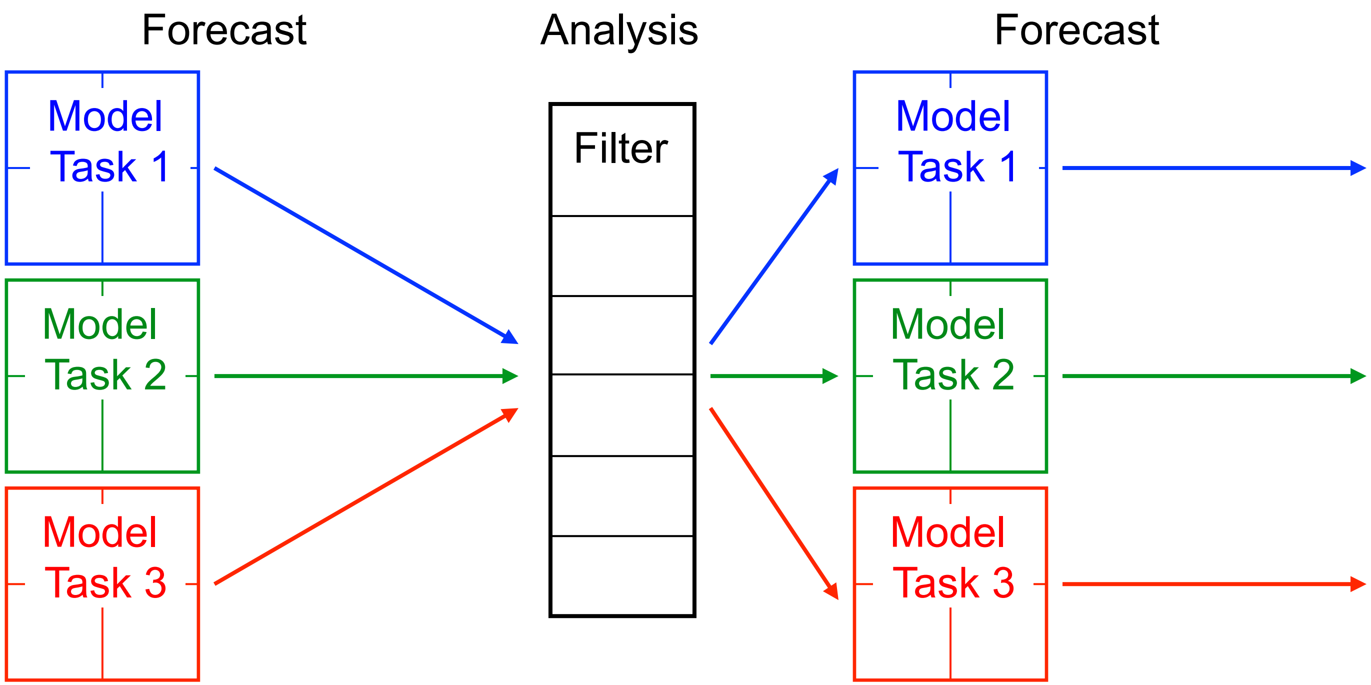
Logical separation of assimilation system

PDAF Parallel Data Assimilation Framework



Nerger, L., Hiller, W. (2013). Software for Ensemble-based DA Systems – Implementation and Scalability. Computers and Geosciences. 55: 110-118

2-level Parallelism

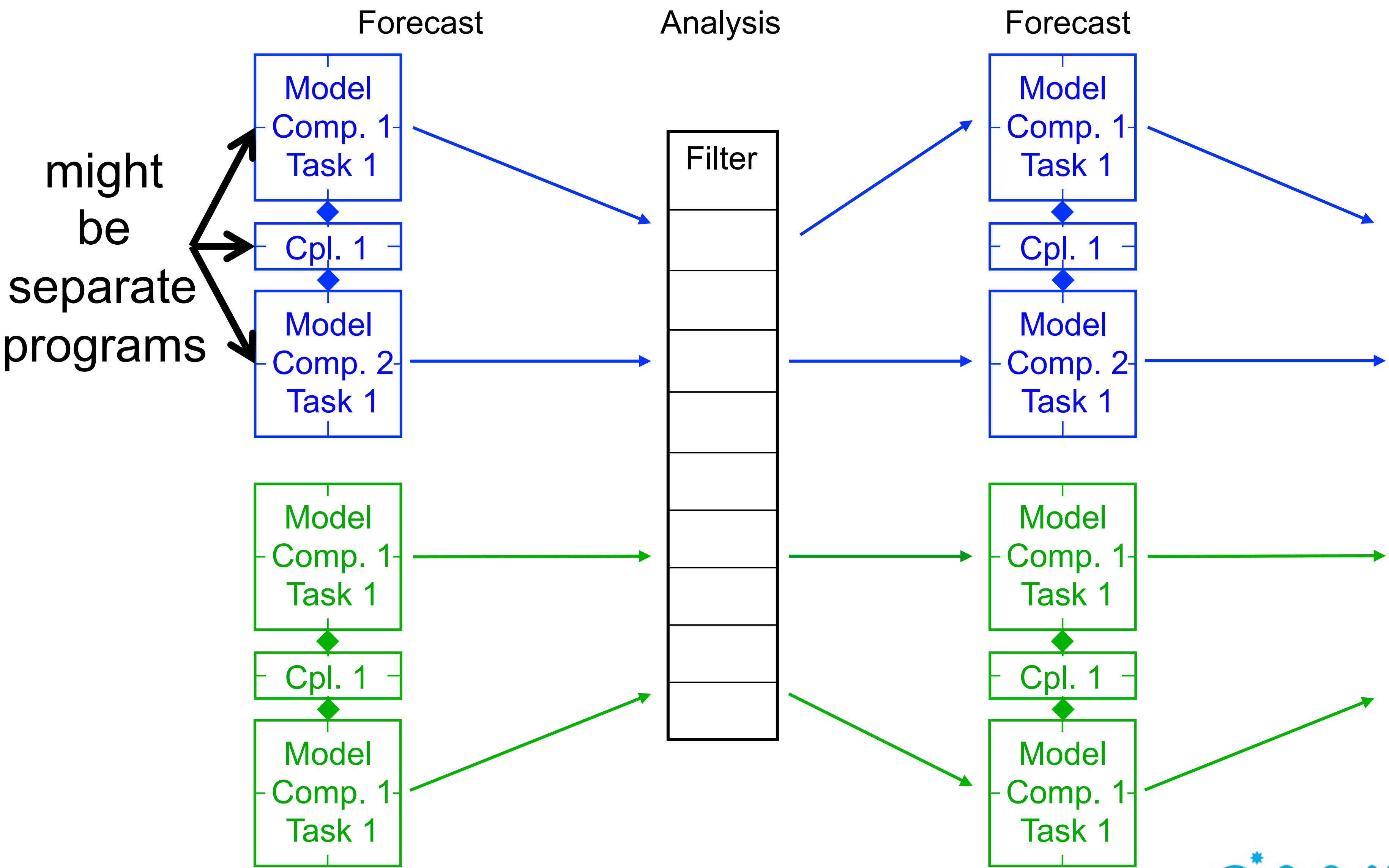


1. Multiple concurrent model tasks
2. Each model task can be parallelized

- Analysis step is also parallelized

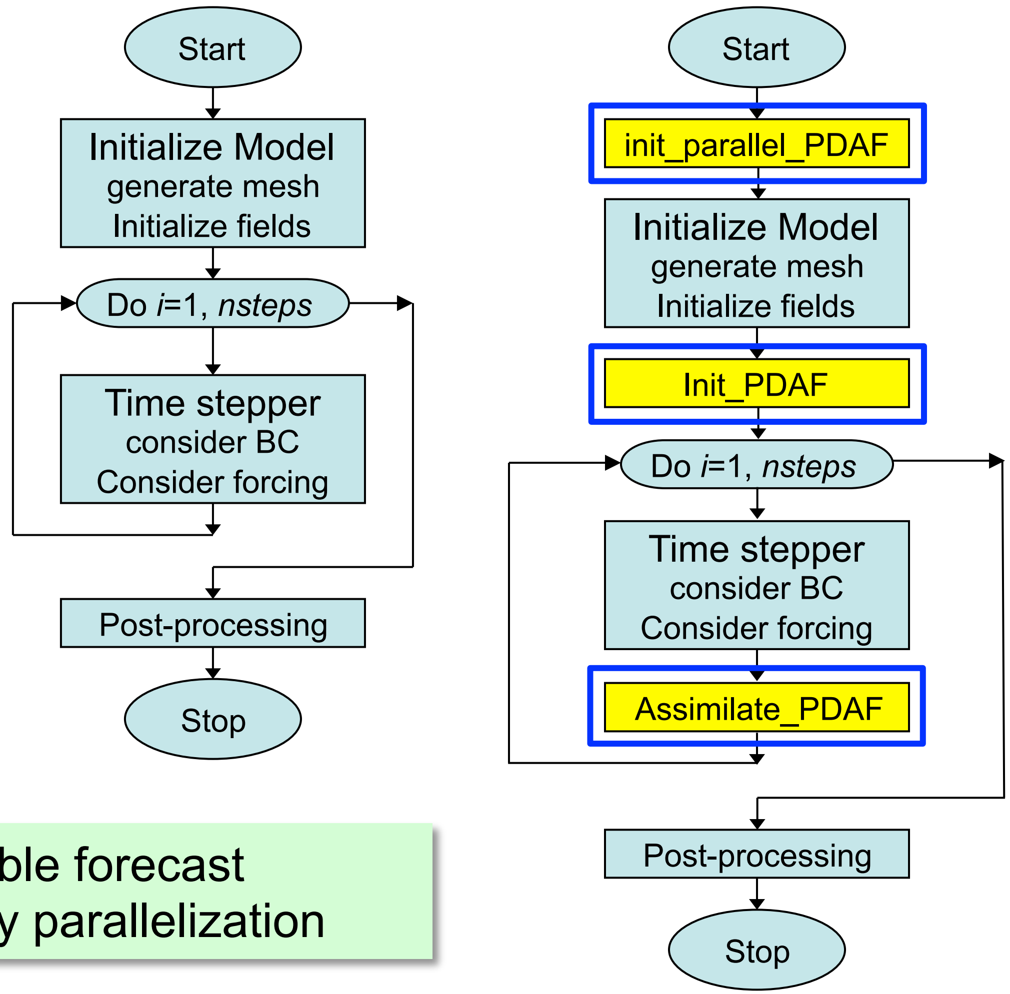
- Configured by "*MPI Communicators*"

2 compartment system – strongly coupled DA



Extending a Model for Data Assimilation

Model



Extension for data assimilation

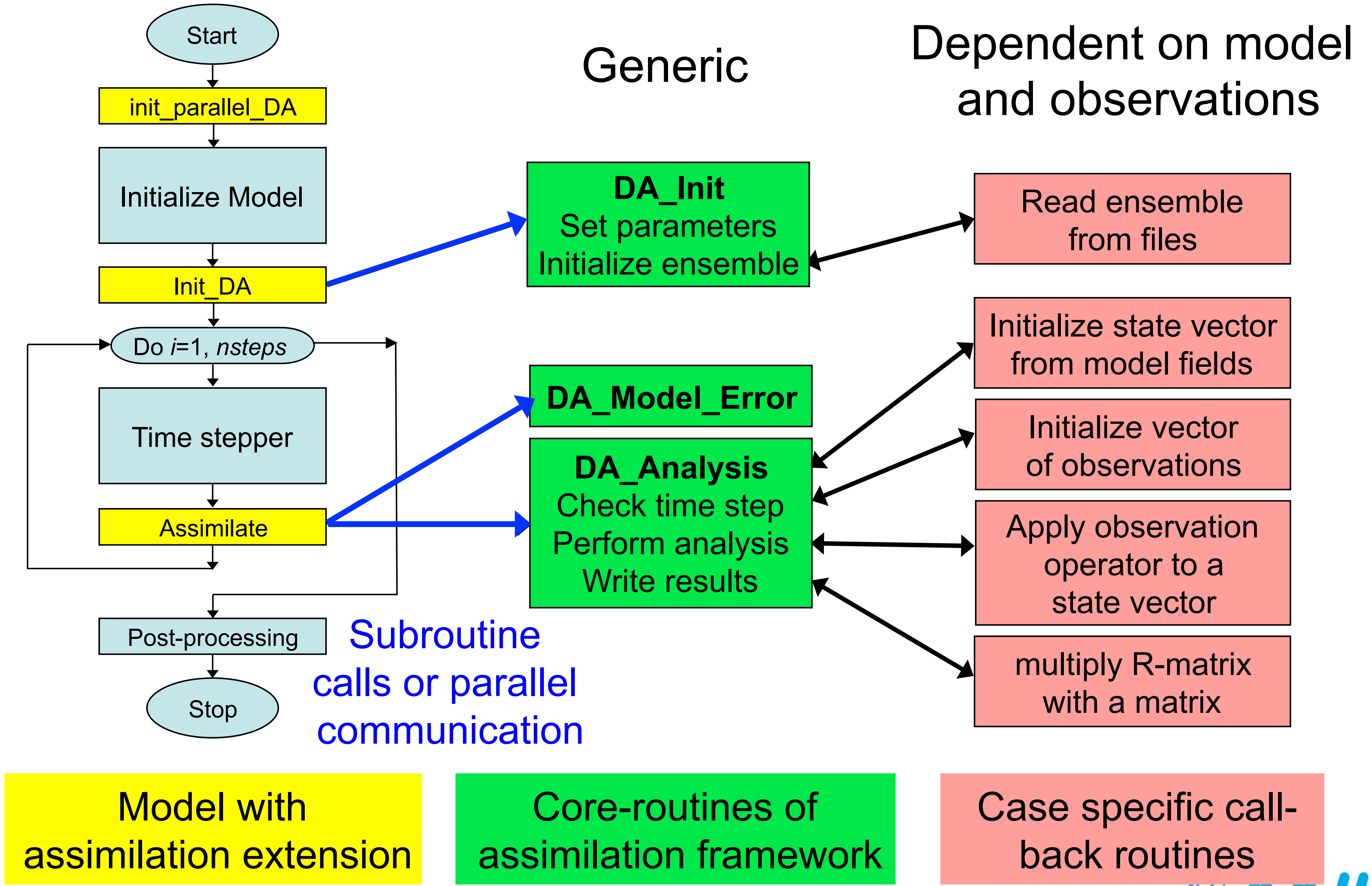
plus:
Possible model-specific adaption.

e.g. Euler time step after assimilation (NEMO model)

ensemble forecast
enabled by parallelization

also possible for coupled models
with several executables

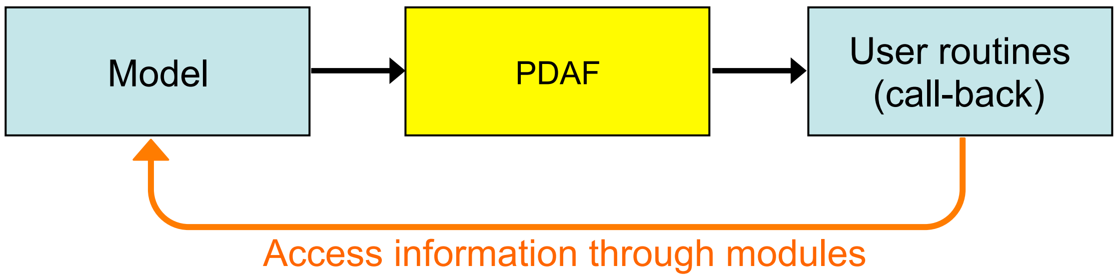
Framework solution with generic filter implementation



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
  - 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)



Current algorithms in PDAF

PDAF Parallel Data Assimilation Framework

PDAF originated from comparison studies of different filters

Filters

- EnKF (Evensen, 1994 + perturbed obs.)
- ETKF (Bishop et al., 2001)
- SEIK filter (Pham et al., 1998)
- SEEK filter (Pham et al., 1998)
- ESTKF (Nerger et al., 2012)

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Not yet released:

- serial EnSRF
- particle filter
- EWPF
- NETF

- LETKF (Hunt et al., 2007)
- LSEIK filter (Nerger et al., 2006)
- LESTKF (Nerger et al., 2012)

Localized filters

Smoothers for

- ETKF/LETKF
- ESTKF/LESTKF
- EnKF

Global and local smoothers

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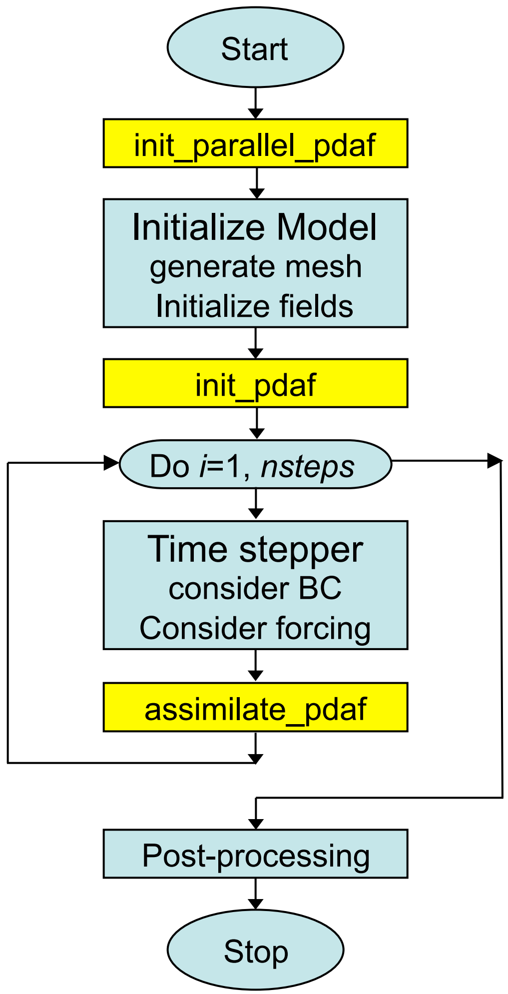
Features of online program

- minimal changes to model code when combining model with filter algorithm
- model not required to be a subroutine
- no change to model numerics!
- model-sided control of assimilation program (user-supplied routines in model context)
- observation handling in model-context
- filter method encapsulated in subroutine
- complete parallelism in model, filter, and ensemble integrations

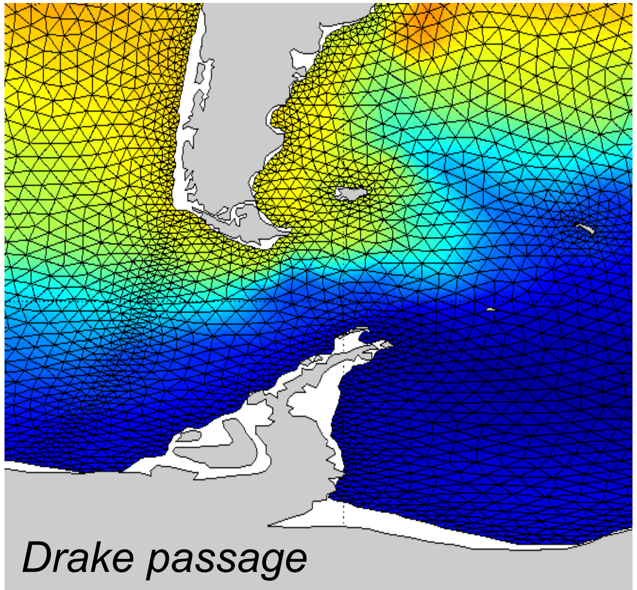


Parallel Performance

Global ocean model

FESOM (Finite Element Sea-ice Ocean model, Danilov et al. 2004)

- Uses unstructured triangular grid



Global configuration

- 1.3^{o} resolution, 40 levels
- horizontal refinement at equator
- state vector size 10^7

Setup used for assimilation of sea surface height data

Parallel Performance

Use between 64 and 4096 processor cores of SGI Altix ICE cluster (HLRN-II)

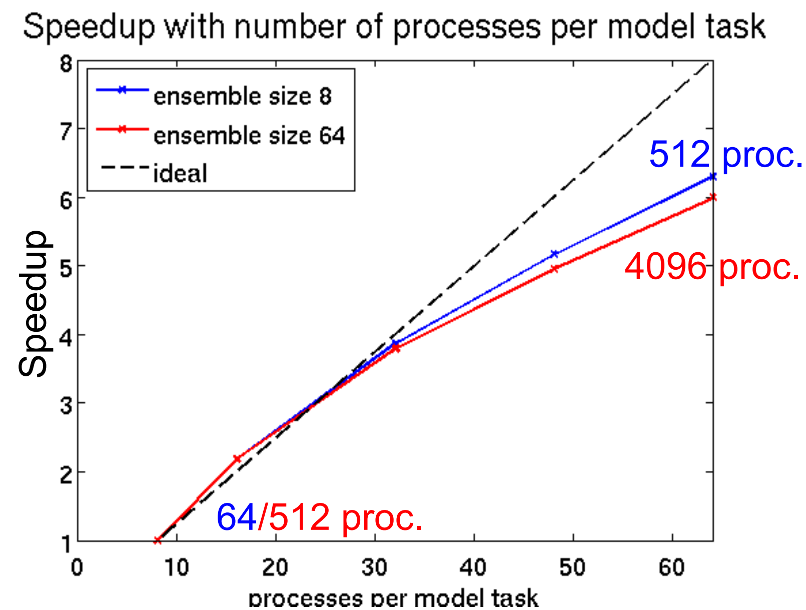
94-99% of computing time in model integrations

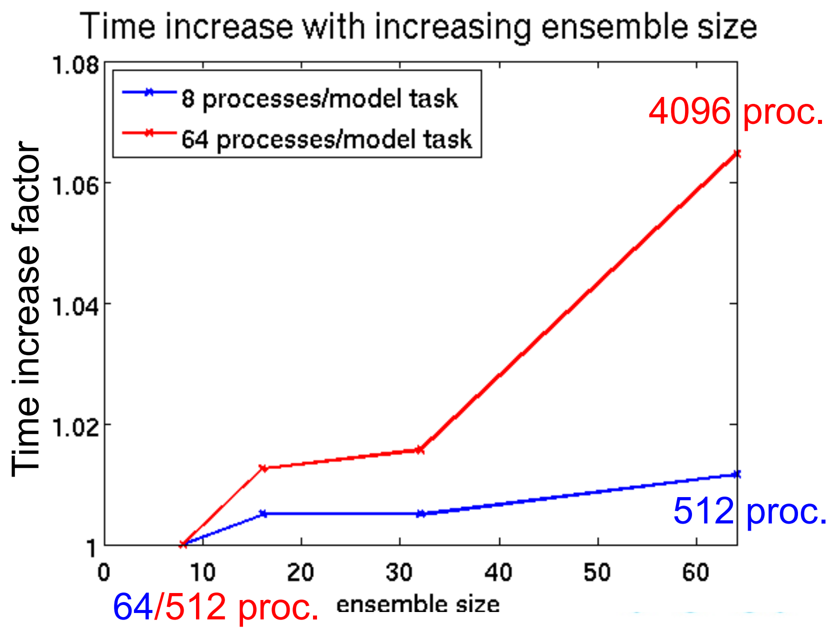
Speedup: Increase number of processes for each model task, fixed ensemble size

- factor 6 for 8x processes/model task
- one reason: time stepping solver needs more iterations

Scalability: Increase ensemble size, fixed number of processes per model task

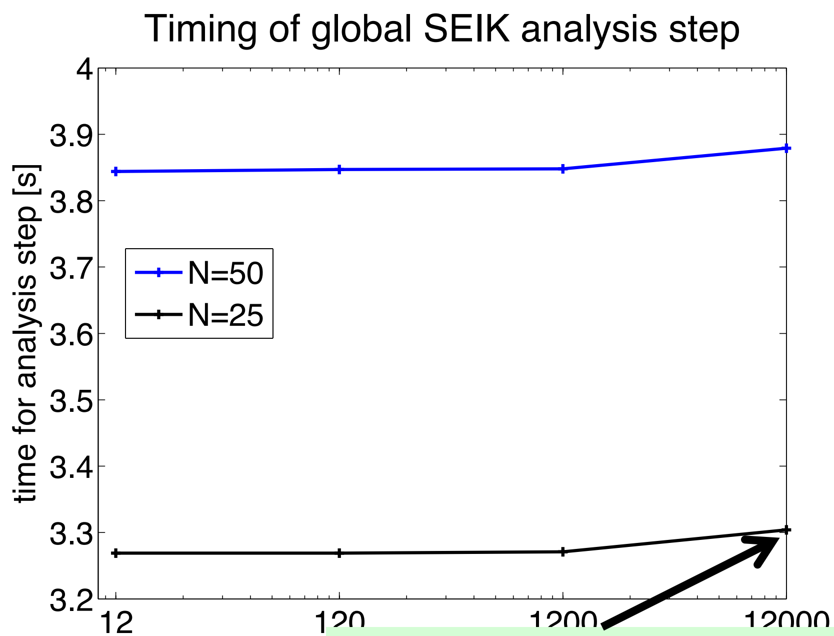
- increase by ~7% from 512 to 4096 processes (8x ensemble size)
- one reason: more communication on the network





Very big test case

- 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
- 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%)
- Didn’t try to run a real ensemble of largest state size (no model yet)

Summary

- Simplify building data assimilation systems
- Efficient online coupling
  with minimal changes to model code
- Generic model interface
  and case-specific call-back routines
- Parallelization allows for ensemble forecasts
- Data assimilation framework PDAF (http://pdaf.awi.de)
  supports high-dimensional models
- Coding you own Ensemble Kalman filter or Particle Filter
  usually not necessary

Thank you !