# PDAF Tutorial

## Implementation of the analysis step in online mode with a serial model

http://pdaf.awi.de

PDAF Parallel Data Assimilation Framework

V1.8 – 2023-02-20

# Implementation Tutorial for PDAF online with serial model

We demonstrate the implementation

of an online analysis step with PDAF

with a model that is itself not parallelized

using the template routines provided by PDAF

The example code is part of the PDAF source code package
downloadable at http://pdaf.awi.de

(This tutorial is compatible with PDAF V2.1 and later)

PDAF Parallel Data Assimilation Framework

# Implementation Tutorial for PDAF online / serial model

This is just an example!

For the complete documentation of PDAF's interface

see the documentation

at http://pdaf.awi.de

# Overview

Focus on Error Subspace Transform Kalman Filter
(ESTKF, Nerger et al., Mon. Wea. Rev. 2012)

**2 Parts**

a) Global filter

b) Localized filter
(and OpenMP-parallelization)

We recommend to first implement the global filter. The localized filter re-uses routines of the global filter.

In this tutorial we only cover the case of a serial model. The implementation with a parallelized model is described in a separate tutorial.

# Contents


0a) Files for the tutorial

0b) The model without parallelization

0c) State vector and observation vector

0d) PDAF online mode

0e) Inserting subroutine calls

0f) Forecast phase

1a) Global filter

1b) Local filter without parallelization

1b.1) Use local filters with OpenMP-parallelization

2) Hints for adaptions for real models


PDAF Parallel Data Assimilation Framework

# 0a) Files for the Tutorial

# Tutorial implementation

Files are in the PDAF package

Directory:

`/tutorial/classical/online_2D_serialmodel`

- Fully working implementations of user codes
- PDAF core files are in `/src`
  Makefile refers to it and compiles the PDAF library
- Only need to specify the compile settings (compiler, etc.) by environment variable PDAF_ARCH. Then compile with ‘make’.

# Template files for online mode

Directory: `/templates/online`

- Contains all required files
- Contains also
  command line parser
  (convenient but not required)

To generate your own implementation:

1. Copy content of directory
   e.g. into sub-directory of model source code
2. Add calls to interface routines to model code
3. Complete user-routines for your model
4. Adapt compilation (e.g. Makefile) and compile
5. Run with assimilation options

# PDAF library

Directory: `/src`

- The PDAF library is not part of the template
- PDAF is compiled separately as a library
  and linked when the assimilation program is compiled
- Makefile includes a compile step for the PDAF library
- One can also cd to `/src` and run 'make' there
  (requires setting of PDAF_ARCH)

`$PDAF_ARCH`

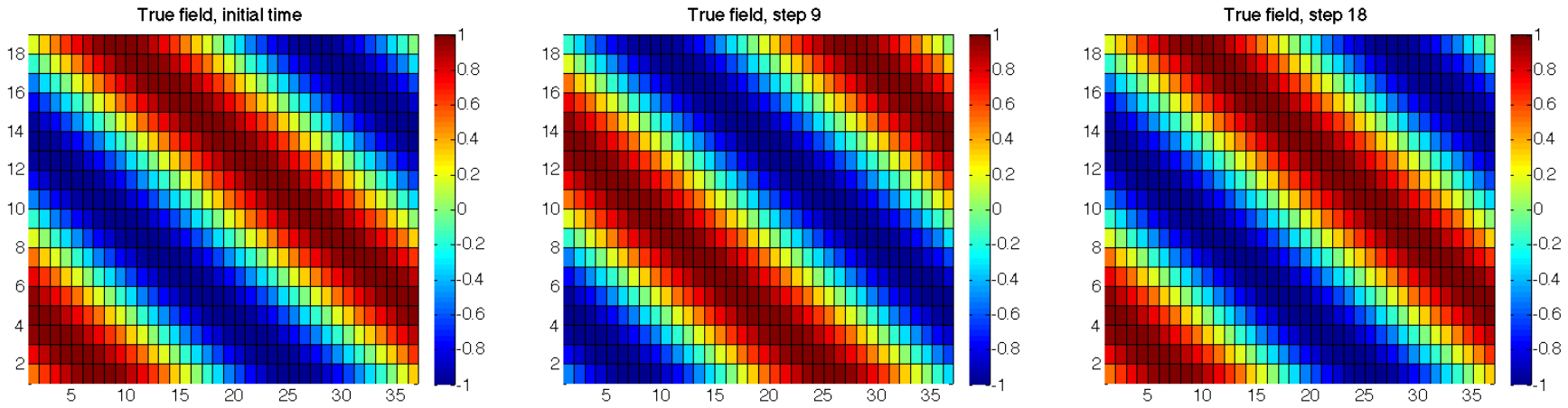
- Environment variable to specify the compile specifications
- Definition files in `/make.arch`
- Define by, e.g.
  `setenv PDAF_ARCH linux_gfortran` (tcsh/csh)
  `export PDAF_ARCH=linux_gfortran` (bash)

# 0b) The model without parallelization

# 2D „Model“

- See the separate tutorial slides about the model

- Simple 2-dimensional grid domain
- 36 x 18 grid points (longitude x latitude)
- True state: sine wave in diagonal direction (periodic for consistent time stepping)



# `Model`: Files

The model source code consists of the following files:

- mod_model.F90
- main.F90
- initialize.F90
- integrate.F90

For clarity, the implementation with PDAF is found in

- main_pdaf.F90
- integrate_pdaf.F90

It allows for easy comparison of the implementations

# 0c) state vector and observation vector

# State vector – some terminology used later

- PDAF performs computations on state vectors
- **State vector**
  - Stores model fields in a single vector
  - Tutorial shows this for one 2-dimensional field
  - Multiple fields are just concatenated into the vector
  - All fields that should be modified by the assimilation have to be in the state vector
- **State dimension**
  - Is the length of the state vector
    (the sum of the sizes of the model fields in the vector)
- **Ensemble array**
  - Rank-2 array which stores state vectors in its columns

# Observation vector

- **Observation vector**
  - Stores all observations in a single vector
  - Tutorial shows this for one 2-dimensional field
  - Multiple observed fields are just concatenated into the vector
- **Observation dimension**
  - Is the length of the observation vector
    (sum of the observations over all observed fields in the vector)
- **Observation operator**
  - Operation that computes the observed part of a state vector
  - Tutorial only selects observed grid points
  - The operation can involve interpolation or integration
    depending on type of observation

# 0d) PDAF online mode

# Online mode

- Combine model with PDAF into single program
  - `"model_pdaf"`

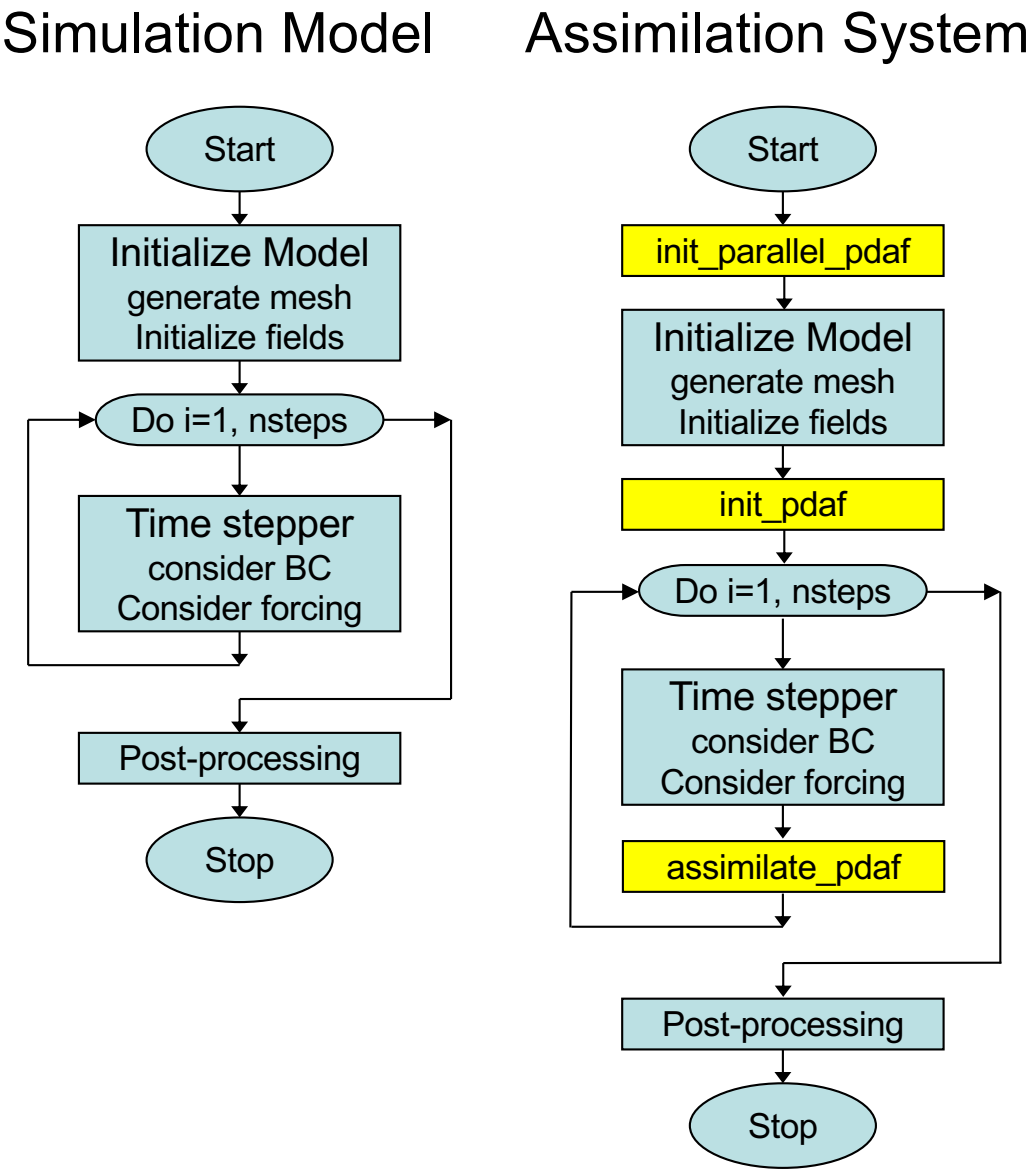
- Add 3 subroutine calls:

| | |
|---|---|
| `init_parallel_pdaf` | - add parallelization |
| `init_pdaf` | - initialize assimilation |
| `assimilate_pdaf` | - perform assimilation |

- Implement user-supplied routines, e.g. for
  - observation operator
  - initialization of observation vector
  - transfer between state vector and model fields

PDAF Parallel Data Assimilation Framework

# Program flow with model extended for data assimilation




*Legend*

Model

Extension for data assimilation

PDAF Parallel Data Assimilation Framework

# Fully parallel configuration

- Tutorial shows implementation for a fully parallel case

  ➜ Number of processes equals ensemble size!

- For a more flexible (and complicated) configuration see PDAF's online guide

# `model_pdaf`: General program structure

```
program main_pdaf
   init_parallel_pdaf    - initialize parallelization
   initialize            - initialize model information
   init_pdaf             - initialize parameters for PDAF
                           and read ensemble
   integrate             - time stepping loop
      assimilate_pdaf    - compute analysis step
                           (called inside stepping loop)
end program
```

Note:
In the example code, we use different files main.F90 and main_pdaf.F90 to allow for easy comparison

# mod_assimilation.F90

Fortran module

- Declares the parameters used to configure PDAF
- Will be included (with '`use`') in the user-written routines
- Additions to template necessary for observation handling

# 0e) Inserting subroutine calls

# Where to insert subroutine calls?

`init_parallel_pdaf`

➜ at the start of the program
(first operations to be executed)

`init_pdaf`

➜ after the initialization of the model
i.e. directly before the time stepping loop

`assimilate_pdaf`

➜ Last operation in the time stepping loop
i.e. just before the '`END DO`'

Note: One can add the routines one after the other:
First insert `init_parallel_pdaf` and test the program,
then add `init_pdaf`, etc.

# init_parallel_pdaf.F90

- It is fully implemented template
- Parallelization variables are declared in Fortran module

  `mod_parallel_pdaf`
- Required adaption:
  - un-comment the second `use model_parallel_pdaf` (includes variables that are declared by the model if it's parallelized)
  - remove local declaration of `mype_world` & `npes_world`
- Important variable:

  `n_modeltasks`
  - Defines number of concurrent model integrations.
  - Has to be equal to ensemble size
  - In the example: Read as 'dim_ens' from command line (using subroutine 'parse')

# init_parallel_pdaf.F90 (2) - Example

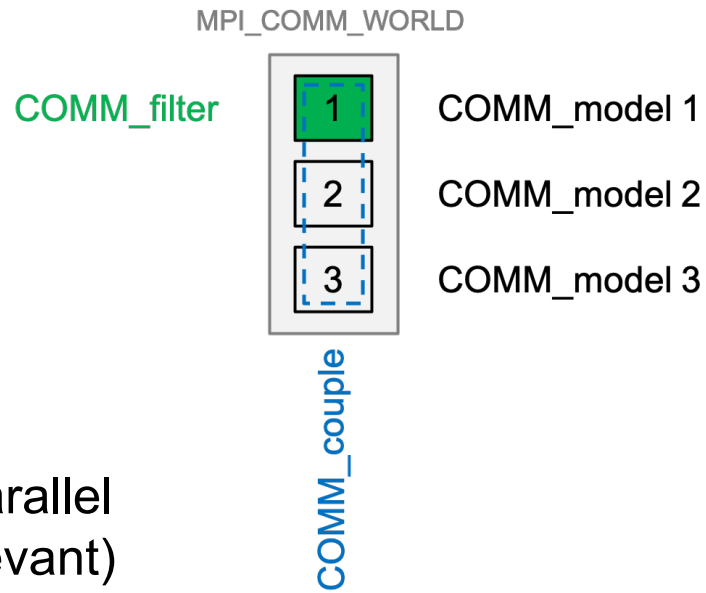
The routine initializes 3 groups of communicators

- COMM_model: Used to run the parallel model forecasts
- COMM_filter: Used to compute the filter
- COMM_couple: Coupling between model and filter processes

These are provided to PDAF when calling PDAF_init

The figure shows an example

- 3 processes in total
- 3 model tasks in parallel each using 1 process in its COMM_model
- COMM_couple links the 3 processes to distribute and collect ensemble states
- The filter process uses model task 1




(See also the tutorial for the online mode with a parallel model where the configuration becomes more relevant)

init_parallel_pdaf is coded to provide this configuration when running with 3 processes and setting dim_ens=3

# init_pdaf.F90

Routine sets parameters for PDAF, calls `PDAF_init` to initialize the data assimilation, and calls `PDAF_get_state` to prepare the ensemble integrations:

Template contains list of available parameters (declared in and used from `mod_assimilation`)

Independent of the filter algorithm:

- Include information on size of model fields from model
- Define dimension of state vector

```
dim_state_p = nx * ny
```

In call to `PDAF_init`, the name of the user-supplied routine for ensemble initialization routine is specified:

```
init_ens_pdaf
```

# init_pdaf.F90 (II)

In call to PDAF_get_state, the names of 3 user-supplied routines are specified:

`next_observation_pdaf`
- Set number of time steps in forecast phase

`distribute_state_pdaf`
- Initialize model fields from state vector

`prepoststep_ens_pdaf`
- poststep routine (compute estimated errors, write state estimate, etc.)

Initially, one can just copy the template routines. One can adapt them later to the particular application.

# assimilate_pdaf.F90

Routine just calls a filter-specific routine like

```
PDAF_assimilate_estkf
```

We don't insert `PDAF_assimilate_estkf` directly into the model code

➜ because, we need to declare all user-supplied routines as 'EXTERNAL'. This could clutter the model code.

Filter-specific user routines are described next. Initially, one can just copy the template routines.

Note: Template contains calls for `PDAF_assimilate_estkf` and `PDAF_assimilate_lestkf`. Need to adapt for other filters.

# Differences online and offline

- If you've studied the tutorial for offline mode

**Offline**

- Separate programs for model and assimilation
- Needed to implement routine `intialize`
- Grid dimensions declared in `mod_assimilation`
- Ensemble information read from files
- `mod_assimilation` contains all field and assimilation variables

**Online**

- Extend model program for assimilation
- Operations in `initialize` given by model; no changes for assimilation!
- Grid dimensions defined in model code (`mod_model`)
- Ensemble information provided by model fields
- `mod_assimilation` only contains variables for assimilation

PDAF Parallel Data Assimilation Framework

# Optional routine: finalize_pdaf.F90

Call to `finalize_pdaf` can be inserted at the end of the model

Routine contains two calls to PDAF_print info:

```
CALL PDAF_print_info(2)
```

– display information on allocated memory inside PDAF

```
CALL PDAF_print_info(1)
```

– display timing information
(values 3 and 4 also possible for more detailed timers)

Note: finalize_pdaf only prints the information for mype_world==0

In addition there is

```
CALL PDAF_deallocate()
```

which deallocates internal arrays in PDAF

# 0f) Forecast phase

# Files for PDAF

Template contains all required files

- just need to be filled with functionality

```
init_pdaf.F90
init_ens_pdaf.F90
next_observation_pdaf.F90
distribute_state_pdaf.F90
collect_state_pdaf.F90
init_dim_obs_pdaf.F90
obs_op_pdaf.F90
init_obs_pdaf.F90
prodrinva_pdaf.F90
prepoststep_ens_pdaf.F90
```

initialization

ensemble forecast

analysis step

post step

PDAF Parallel Data Assimilation Framework

# init_pdaf.F90

Routine sets parameters for PDAF and calls `PDAF_init` to initialize the data assimilation:

Template contains list of available parameters (declared in and used from `mod_assimilation`)

For the example set :

1. `dim_ens = 9`
2. `rms_obs = sqrt(0.5)`
3. `filtertype = 6` (for ESTKF)
4. `delt_obs = 2` (assimilate afer each 2nd time step)

In call to PDAF_init, the name of the ensemble initialization routine is specified:

`init_ens_pdaf`

# init_ens_pdaf.F90

A *call-back* routine called by PDAF_init:

- Implemented by the user
- Its name is specified in the call to PDAF_init
- It is called by PDAF through a defined interface:

```
SUBROUTINE init_ens_pdaf(filtertype, dim_p,
       dim_ens, state_p, Uinv, ens_p, flag)
```

Declarations in header of the routine shows “intent” (input, output):

```
REAL, INTENT(out)    :: ens_p(dim_p, dim_ens)
```

Note:
All call-back routines have a defined interface and show the intent of the variables. Their header comment explains what is to be done in the routine.

# init_ens_pdaf.F90 (2)

Initialize ensemble matrix `ens_p` for the start time of the assimilation

1. Include `nx, ny` with `use mod_model`
2. Declare and allocate `real :: field(ny, nx)`
3. Loop over ensemble files `(i=1,dim_ens)`

   for each file:

   - read ensemble state into `field`
   - store contents of `field` in column `i` of `ens_p`
4. Deallocate `field`

Note:
Columns of `ens_p` are state vectors.
Store following storage of field in memory (column-wise in Fortran)

# The forecast phase

At this point the initialization of PDAF is complete:

- Initial Ensemble of model states is initialized
- Filter algorithm and its parameters are chosen

Next:

- Implement user-routines for forecast phase
- All are call-back routines:
  - ➢ User-written, but called by PDAF

Note:
Some variables end with `_p`.
It means that the variable is specific for a process.
(Not relevant until we do parallelization in the analysis step)

# next_observation_pdaf.F90

Routine to

- Set number of time steps in next forecast phase
- Set flag to control exit from forecasts (`doexit`)

Most simple setting:

include `delt_obs` from `mod_assimilation`

```
nsteps = delt_obs
doexit = 0
```

Note: The assimilation program stops when the maximum number of time steps of the model is reached, even if doexit=0

# next_observation_pdaf.F90 (II)

More sophisticated setting:

- Utilize `stepnow` (current time step) and `total_steps` (total number of time steps given by model).

```
IF (stepnow + nsteps <= total_steps) THEN
      nsteps = delt_obs        ! Forecast length
      doexit = 0               ! Continue assimilation
ELSE
      nsteps = 0               ! No more steps
      doexit = 1               ! Exit assimilation
END IF
```

Note: In the example `doexit=1` is used only inside PDAF and avoids some screen output.

# distribute_state_pdaf.F90

Routine to

- Initialize model fields from a state vector
- Routine is provided with the state vector `vector_p`

For the example:

1. Access `nx, ny` and `field` with `use mod_model`
2. Initialize model field from state vector:

```
DO j = 1, nx
 field(1:ny, j) = state_p(1+(j-1)*ny : j*ny)
END DO
```

# prepoststep_ens_pdaf.F90

Post-step routine for the online mode:

Already there in the template:

1. Compute ensemble mean state `state_p`
2. Compute estimated variance vector `variance`
3. Compute estimated root mean square error `rmserror_est`

Possible extensions:

4. Write analysis state (ensemble mean, `state_step*_ana.txt`)
5. Write analysis ensemble into files
   (Analogous to reading in `init_ens_pdaf`)
6. Analogously one can write the forecast fields

# Completion of forecast phase

At this point the implementation of the forecast phase is practically complete:

- Initial ensemble and PDAF's parameters are set
- The ensemble forecast can be computed

One can now compile the program model_pdaf (make model_pdaf) to check whether it runs.

Note: It is recommended to compile PDAF with –DPDAF_NO_UPDATE at this point as the routine for the analysis step are not yet implemented.

Note: For now, `prepoststep_ens_pdaf` only lets you test the initial ensemble. Testing the forecast fields need implementation of routine `collect_state_pdaf`

# 1a) Global filter

# Running the tutorial program

- cd `to /tutorial/classical/online_2D_serialmodel`
- Set environment variable `PDAF_ARCH` or set it in Makefile
  (e.g. `linux_gfortran_openmpi`)
- Compile by running `'make model_pdaf'`
  (next slide will discuss possible compile issues)
- Run the program with

```
mpirun -np 9 ./model_pdaf -dim_ens 9
```

- Inputs are read in from `/tutorial/inputs_online`
- Outputs are written in `/tutorial/classical/online_2D_serialmodel`
- Plot result, e.g with 'octave':

```
load state_step10_ana.txt

pcolor(state_step10_ana)
```

# Requirements for compiling PDAF

PDAF requires libraries for BLAS and LAPACK

- Libraries to be linked are specified in the include file for make in `/make.arch` (file according to `PDAF_ARCH`)
- For `$PDAF_ARCH=linux_gfortran_openmpi` the specification is

  ```
  LINK_LIBS =-L/usr/lib -llapack  -lblas   -lm
  ```

- If the libraries are at another non-default location, one has to change the directory name (`/usr/lib`)
- Some systems or compilers have special libraries (e.g. MKL for ifort compiler, or ESSL on IBM/AIX)

PDAF needs to be compiled for double precision

- Needs to be set at compiler time in the include file for make:
- For gfortran: `OPT = -O3 -fdefault-real-8`

# Files in the tutorial implementation

`/tutorial/inputs_online`

- `true_stepY.txt` — true state
- `state_ini.txt` — initial estimate (ensemble mean)
- `obs_stepY.txt` — observations
- `ens_X.txt` — initial ensemble members

`/tutorial/classical/online_2D_serialmodel`

(after running model_pdaf)

- `state_stepY_ana.txt` — analysis state estimate
- `ens_X_stepY_ana.txt` — analysis ensemble members

X=1,…,9: ensemble member index

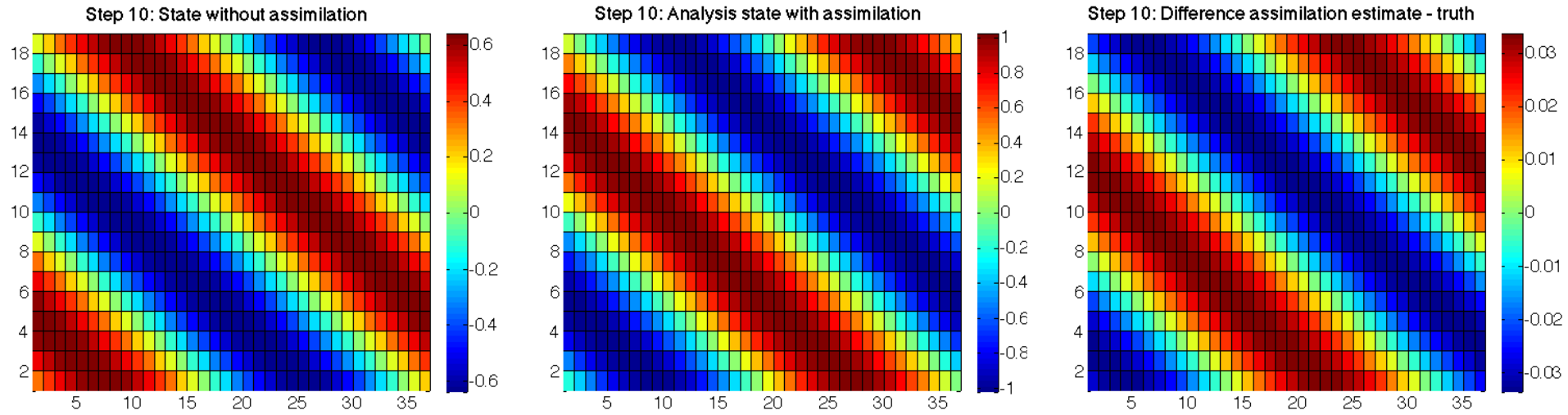
Y=1,…,18: time step index

Note: Files *_for.txt contain forecast fields

# Result of the global assimilation

For example, at step 10

- The analysis state (center) is closer to the true field than without assimilation (left)
- Truth and analysis are nearly identical (right)






PDAF Parallel Data Assimilation Framework

# The analysis step

Next: Implement user-routines for the analysis step

The analysis step needs several user-supplied routines for operations like

- write forecast model fields into state vector
- determine number of available observations
- observation operator acting on a state vector
- initialization of the vector of observations

# collect_state_pdaf.F90

Routine to

- Fill state vector with forecasted model fields
- Routine is provided with the state vector `vector_p`

For the example:

1. Access `nx, ny` and `field` with `use mod_model`
2. Initialize state vector from model field:

```
DO j = 1, nx
  state_p(1+(j-1)*ny : j*ny) = field(1:ny, j)
END DO
```

**Note:** The routine independent of the filter!

# init_dim_obs_pdaf.F90

Routine to

- read observation file
- count number of available observations
  (direct output to PDAF: **`dim_obs_p`**)

Optional, also

- initialize array holding available observations
- initialize index array telling index of observation point
  in full state vector

The most complicated routine in the example!
(but less than 100 lines)

# init_dim_obs_pdaf.F90 (2)

Preparations and reading of observation file:

1. Include `nx, ny` with `use mod_model`
2. declare and allocate real array `obs_field(ny, nx)`
3. read observation file for current time step:

Initialize string '`stepstr`' for time step

```
OPEN (12, &
    file='inputs_online/obs'//stepstr//'.txt', &
    status='old')
DO i = 1, ny
    READ (12, *) obs_field(i, :)
END DO
CLOSE (12)
```

# init_dim_obs_pdaf.F90 (3)

Count available observations (**dim_obs_p**):

1. Declare `integer :: cnt, cnt0`
2. Now count

```
cnt = 0
DO j = 1, nx
  DO i= 1, ny
     IF (obs_field(i,j) > -999.0) cnt = cnt + 1
  END DO
END DO
dim_obs_p = cnt
```

# init_dim_obs_pdaf.F90 (4)

Initialize observation vector (`obs`)
and index array (`obs_index`):

1. Include `obs_p` and `obs_index_p`
   with `use mod_assimilation`

2. Allocate
   `obs_p(dim_obs_p), obs_index_p(dim_obs_p)`
   (If already allocated, deallocate first)

3. Now initialize …

Note:
The arrays only contain information about valid observations;
one could store observations already in files in this way.

# init_dim_obs_pdaf.F90 (5)

3. Now initialize

```
cnt0 = 0                    ! Count grid points
cnt = 0                     ! Count observations
DO j = 1, nx
  DO i= 1, ny
    cnt0 = cnt0 + 1
    IF (obs_field(i,j) > -999.0) THEN
      cnt = cnt + 1
      obs_index_p(cnt) = cnt0        ! Index
      obs_p(cnt) = obs_field(i, j) ! observations
    END IF
  END DO
END DO
```

# obs_op_pdaf.F90

Implementation of observation operator
acting one some state vector

Input: state vector `state_p`

Output: observed state vector `m_state_p`

1. Include `obs_index_p` with `use mod_assimilation`
2. Select observed grid points from state vector:

```
DO i = 1, dim_obs_p
  m_state_p(i) = state_p(obs_index_p(i))
END DO
```

Note:
`dim_obs_p` is an input argument of the routine

# init_obs_pdaf.F90

Fill PDAF's observation vector

Output: vector of observations `observation_p`

1. Include `obs_p` by `use mod_assimilation`
2. Initialize `observation_p`:

```
observation_p = obs_p
```

Note:
This is trivial, because of the preparations in `init_dim_obs_pdaf`!

(However, the operations needed to be separate, because PDAF allocates `observations_p` after the call to `init_dim_obs_pdaf`)

# prodrinva_pdaf.F90

Compute the product of the inverse observation error covariance matrix with some other matrix

- Input: Matrix `A_p(dim_obs_p, rank)`
- Output: Product matrix **`C_p`**`(dim_obs_p, rank)`
  (`rank` is typically `dim_ens-1`)

1. Declare and initialize inverse observation error variance

```
ivariance_obs = 1.0 / rms_obs**2
```

2. Compute product:

```
DO j = 1, rank
  DO i = 1, dim_obs_p
     C_p(i, j) = ivariance_obs * A_p(i, j)
  END DO
END DO
```

# Done!

The analysis step in online mode with the serial (non-parallelized) model is fully implemented now

The implementation allows you now to use the global filter ESTKF (ETKF and SEIK are usable by adding a call to the corresponding routines PDAF_assimilate_X in assimilate_pdaf)

Not usable are EnKF and SEEK (The EnKF needs some other user files und SEEK a different ensemble initialization)

# A complete analysis step

We now have a fully functional analysis step
- if no localization is required!

Possible extensions for a real application:

Adapt routines for

- Multiple model fields
  - → Store full fields consecutively in state vector
- Third dimension
  - → Extend state vector
- Different observation types
  - → Store different types consecutively in observation vector
- Other file type (e.g. binary or NetCDF)
  - → Adapt reading/writing routines

# Differences between online and offline modes

For the analysis step in online mode:

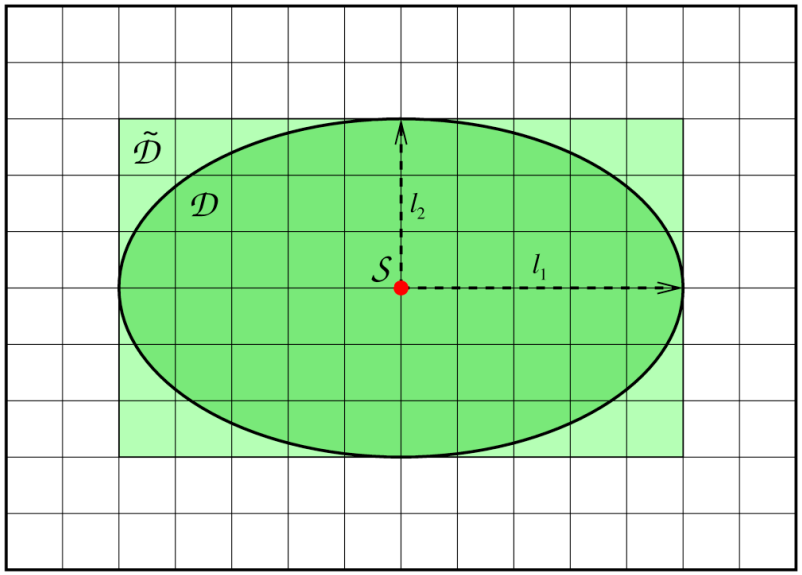
| | |
|---|---|
| `collect_state_pdaf` | - additional routine for online mode |
| `init_dim_obs_pdaf` | - read from file for current time step; include `nx, ny` from `mod_model` instead of `mod_assimilate` |
| `obs_op_pdaf` | - identical in online and offline modes |
| `init_obs_pdaf` | - identical in online and offline modes |
| `prodrinva_pdaf` | - identical in online and offline modes |

# 1b) Local filter without parallelization

# Localization

Localization is usually required for high-dimensional systems

- Update small regions (*S*)
  (e.g. single grid points, single vertical columns)
- Consider only observations within cut-off distance (*D*)
- Weight observations according to distance from *S*



# The FULL observation vector

- A single local analysis at *S* (single grid point) need observations from domain *D*
- A loop of local analyses over all *S* needs all observations
  - This defines the *full* observation vector
- Why distinguish *full* and *all* observations?

  ➔ They can be different in case of parallelization!
  - Example:
    - ➢ Split domain in left and right halves
    - ➢ Some of the analyses in left half need observations from the right side.
    - ➢ Depending on localization radius not all observations from the right side might be needed for the left side analyses

# Running the tutorial program

- Compile as for the global filter
- Run the program with

```
mpirun -np 9 ./model_pdaf -dim_ens 9 OPTIONS
```

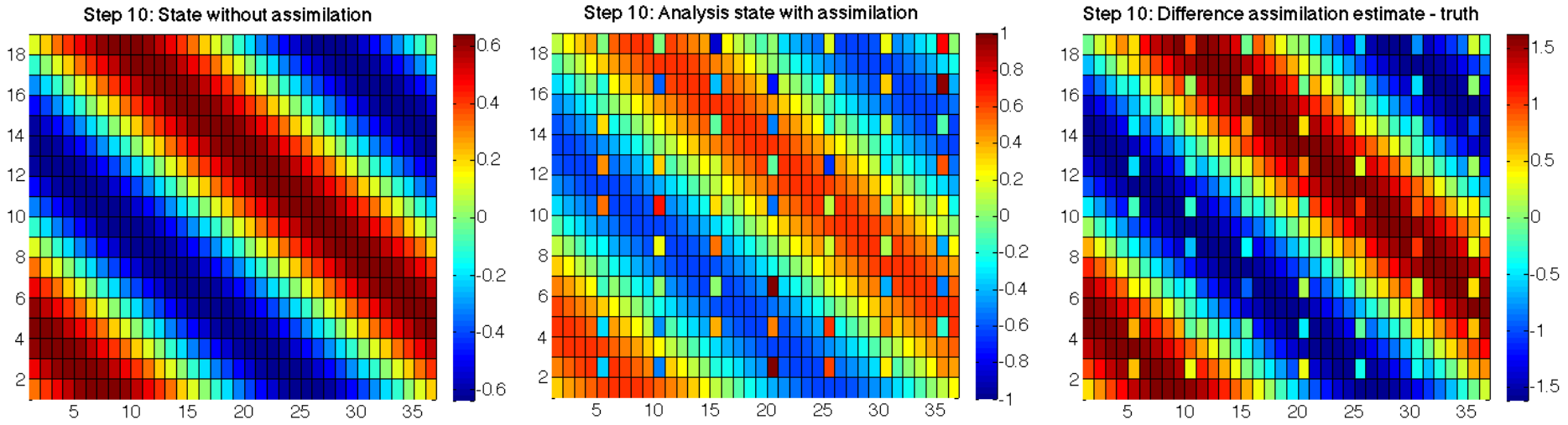
- `OPTIONS` are always of type `-KEYWORD VALUE`
- Possible `OPTIONS` are

| | |
|---|---|
| `-filtertype 7` | (select LESTKF if not set in init_pdaf) |
| `-cradius 5.0` | (set localization radius, 0.0 by default, any positive value should work) |
| `-locweight 2` | (set weight function for localization, default=0 for constant weight of 1; possible are integer values 0 to 4; see `init_pdaf`) |

# Result of the local assimilation

```
mpirun -np 9./model_pdaf -dim_ens 9 -filtertype 7
```

- Default: zero localization radius (cradius=0.0)
- Change only at observation locations





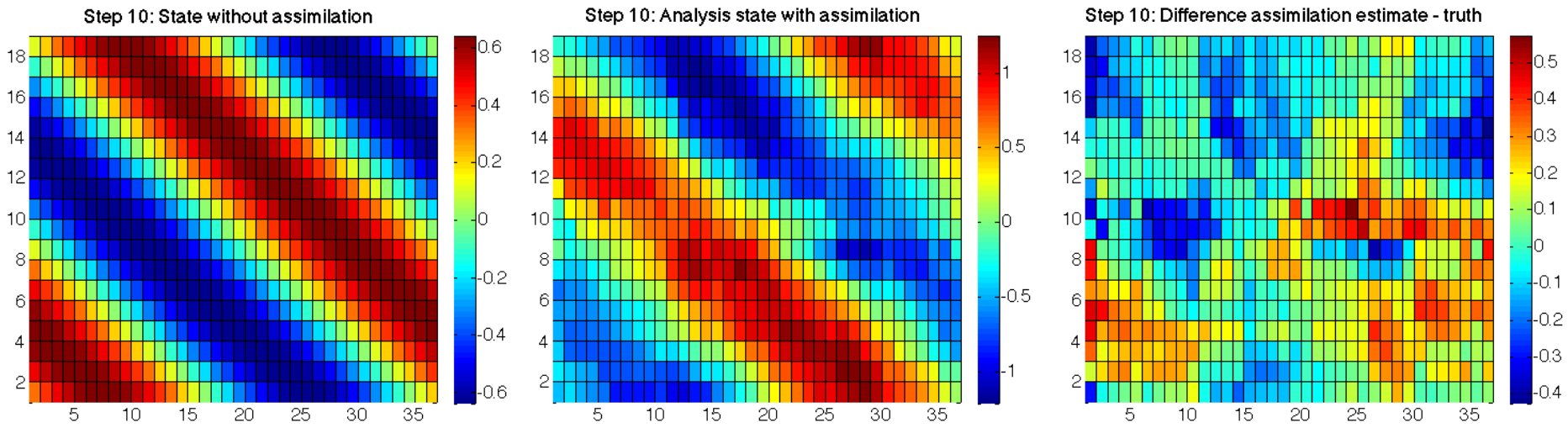

PDAF Parallel Data Assimilation Framework

# Result of the local assimilation (2)

```
… -filtertype 7 -cradius 10.0
```

- All local analysis domains are influenced (all see observations)
- Up to 16 observations in a single local analysis (average 9.6)

Note: The set up of the experiment favors the global filter
because of the shape of the ensemble members



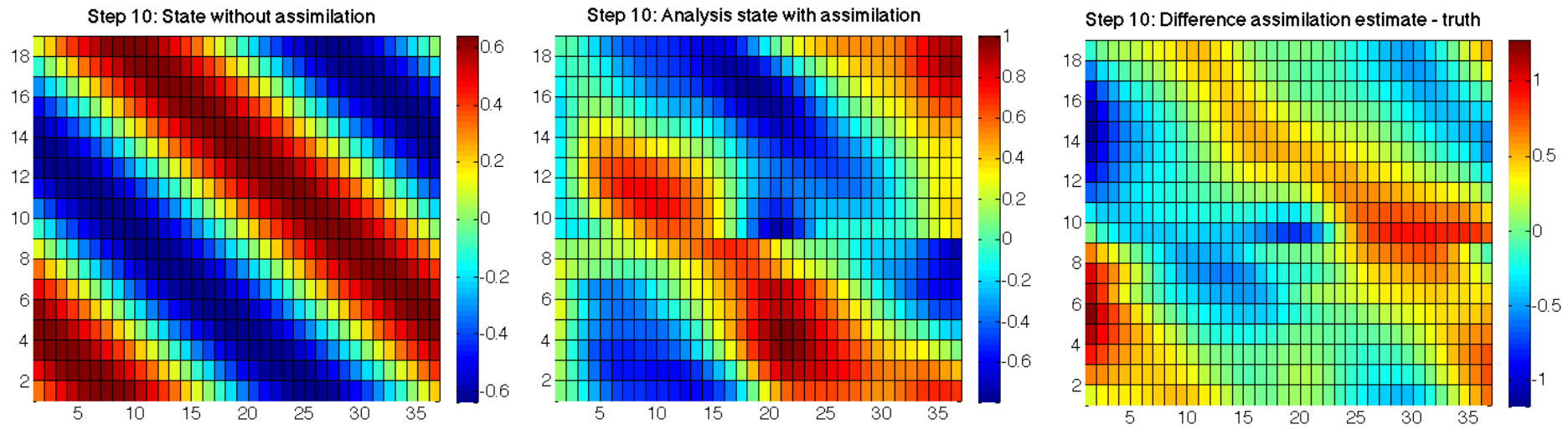



PDAF Parallel Data Assimilation Framework

# Result of the local assimilation (2)

```
… -filtertype 7 -cradius 10.0 -locweight 2
```

- Observation weighting by 5th-order polynomial
- Analysis field is smoother than before (because of weighting)



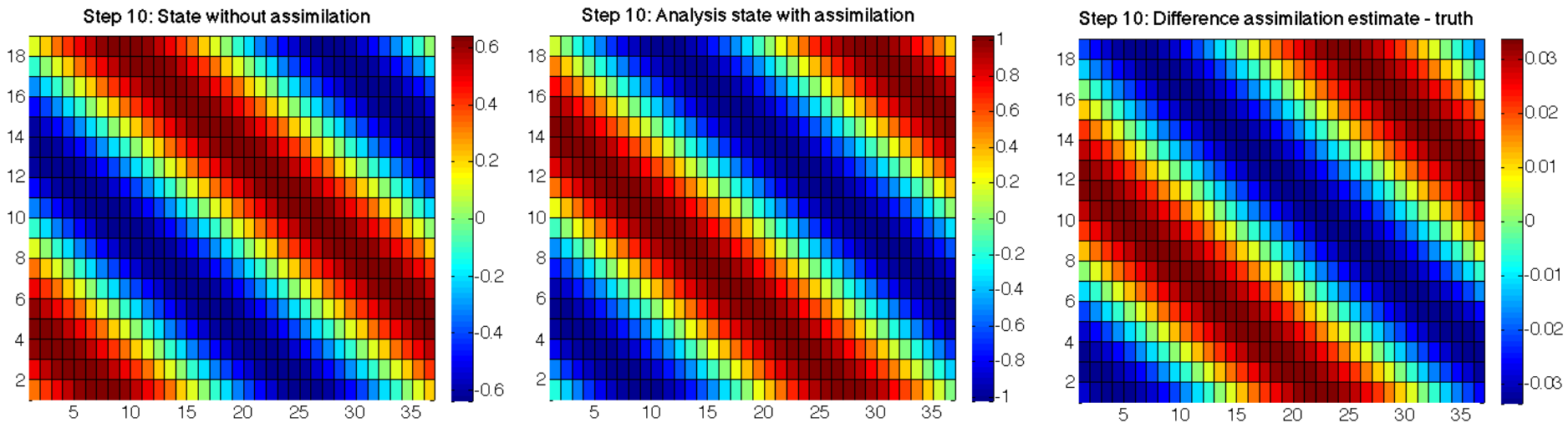



PDAF Parallel Data Assimilation Framework

# Result of the local assimilation (3)

```
… -filtertype 7 -cradius 40.0
```

- Large radius: All local analysis domains see all observations
- Result identical to global filter






PDAF Parallel Data Assimilation Framework

# Local filter LESTKF

- Localized filters are a variant of the global filters
- User written files for global filter can be widely re-used
- Additional user-written files to handle local part

- No changes to:

  `initialize.F90`

  `init_ens_pdaf.F90`

  `prepoststep_ens_pdaf.F90`

- Change in `init_pdaf.F90`:

  Set `filtertype = 7`

  (You can also set it later on command line)

# Local filter LESTKF (2)

Adapt files from global analysis

| | | |
|---|---|---|
| `init_dim_obs_pdaf.F90` | ➜ | `init_dim_obs_f_pdaf.F90` |
| `obs_op_pdaf.F90` | ➜ | `obs_op_f_pdaf.F90` |
| `init_obs_pdaf.F90` | ➜ | `init_obs_f_pdaf.F90` |
| `prodrinva_pdaf.F90` | ➜ | `prodrinva_l_pdaf` |

Naming scheme:

`_f_` "full": operate on all required observations
(without parallelization these are all observations)

`_l_` "local": operation in local analysis domain or corresponding local observation domain

# Local filter LESTKF (3)

Additional files for local analysis step

```
init_n_domains_pdaf.F90
init_dim_l_pdaf.F90
g2l_state_pdaf.F90
l2g_state_pdaf.F90
init_dim_obs_l_pdaf.F90
g2l_obs_pdaf.F90
init_obs_l_pdaf.F90
```

localize state vector

localize observations

Discuss now the files in the order they are called

# init_n_domains_pdaf.F90

Routine to set the number of local analysis domains

Output: `n_domains_p`

For the example: number of grid points (nx * ny)

To do:

1. Include `nx, ny` with `use mod_model`
2. Set

```
n_domains_p = nx * ny
```

# init_dim_obs_f_pdaf.F90

Initialize dimension of *full* observation vector

For the local filter:

1. Copy functionality from `init_dim_obs_pdaf.F90`
2. Rename `dim_obs_p` to **`dim_obs_f`**
3. Add storage of observation coordinates
   1. include `coords_obs_f` with `use mod_assimilation`
   2. Where `obs_index_p` is allocated in the routine:
      Allocate also `coords_obs_f(2,cnt)`
   3. In the loop where obs_index_p is initialized add:

```
coords_obs_f(1,cnt)=j
coords_obs_f(2,cnt)=i
```

# obs_op_f_pdaf.F90

Implementation of observation operator
for full observation domain

1. Copy functionality from obs_op_pdaf.F90
2. Rename
   - `dim_obs_p` to `dim_obs_f`
   - `m_state_p` to `m_state_f`

Note:

The renaming is just for consistency. Quantities referring to the full observations should be recognizable by `_f`

# init_obs_f_pdaf.F90

Fill PDAF's full observation vector

1. Copy functionality from init_obs_pdaf.F90
2. Rename
   - `dim_obs_p` to `dim_obs_f`
   - `observation_p` to `observation_f`

Note:

The renaming is just for consistency. Quantities referring to the full observations should be recognizable by `_f`

# init_dim_l_pdaf.F90

Set the vector size `dim_l` of the local analysis domain

Further set the coordinates of the local analysis domain and the indices of the elements of the local state vector in the global state vector

Each single grid point is a local analysis domain in the example

1. Set **`dim_l`** = `1`
2. Compute the coordinates:
   - Include `coords_l` with `use mod_assimilation`

```
coords_l(1) = REAL(CEILING(REAL(domain_p)/REAL(ny)))
coords_l(2) = REAL(domain_p) - (coords_l(1)-1)*REAL(ny)
```

**Note:** `coords_l` will be used later for computing the distance of observations form the local analysis domain in `init_dim_l_pdaf`

# init_dim_l_pdaf.F90 (2)

3. Set indices of the elements of the local state vector in the global state vector

a) Include `id_lstate_in_pstate` with `use mod_assimilation`

b) Allocate `id_lstate_in_pstate(dim_l)` (Deallocate first if already alloced)

c) Specify the index: It's identical to `domain_p` here (because we only have a single model variable)

```
id_lstate_in_pstate(1) = domain_p
```

# init_dim_obs_l_pdaf.F90

Set the size of the observation vector for the local analysis domain

As for the global filter, this is the longest routine (~102 lines)

Only direct output: **`dim_obs_l`**

Operations:

1. Include coordinates `coords_l` with `use mod_assimilation`
2. Determine coordinate range for observations
3. Count observations within prescribed localization radius
4. Set index array for local observations (`id_lobs_in_fobs`) and array of distances of local observations (`distance_l`)

**Note:** The index array in step 4 is re-used for an efficient implementation of g2l_obs_pdaf. The local distance array initialized in step 4 is re-used in prodrinva_l_pdaf avoiding to recompute distances.

# init_dim_obs_l_pdaf.F90 (2)

2. Determine coordinate range for local observations
   1. Declare `real :: limits_x(2), limits_y(2)`
   2. Include `cradius` with `use mod_assimilation`
   3. Set lower and upper limits. E.g. for x-direction

```
limits_x(1) = coords_l(1) - cradius
if (limits_x(1) < 1.0) limits_x(1) = 1.0
limits_x(2) = coords_l(1) + cradius
if (limits_x(2) > real(nx)) limits_x(2) = real(nx)
```

   (analogous for y-direction)

**Note:** Using `limits_x, limits_y` is not strictly required, but it makes the search for local observations more efficient.

If the localization is only based on grid point indices, the coordinates could be handled as integer values

# init_dim_obs_l_pdaf.F90 (3)

3. Count local observations (within distance `cradius`)

```
dim_obs_l = 0
DO i = 1, dim_obs_f
   IF ("coords_obs(:,i) within coordinate limits") THEN
      Compute distance between coords_obs and coords_l
      IF (distance <= cradius) &
           dim_obs_l = dim_obs_l + 1
   END IF
END DO
```

**Note:**
For efficiency, we only compute `distance` for observations within coordinate limits `limits_x, limits_y`. Valid local observations reside within circle of radius `cradius`.

# init_dim_obs_l_pdaf.F90 (4)

4. Set index array for local observations

   - Index of a local observation in the full observation vector

   1. Include `id_obs_in_fobs` and `distance_l` with `use mod_assimilation`
   2. Allocate `id_obs_in_fobs(dim_obs_l)`
   3. Fill index array:

```
cnt = 0
DO i = 1, dim_obs_f
  IF ("coords_obs(:,i) within coordinate limits") THEN
    Compute distance between coords_obs and coords_l
    IF (distance <= cradius) THEN
      cnt = cnt + 1
      id_lobs_in_fobs(cnt) = i
      distance_l(cnt) = distance
END …
```

# g2l_state_pdaf.F90 & l2g_state_pdaf.F90

**g2l_state_pdaf:** Initialize state vector for local analysis domain
from global state vector

**l2g_state_pdaf:** Initialize global state vector
from state vector for local analysis domain

- The templates provide a generic implementation using the array `id_lstate_in_fstate`

→ We use the templates without any changes!

# g2l_obs_pdaf.F90 & init_obs_l_pdaf.F90

**g2l_obs_pdaf:** Initialize local observed state vector from full observed vector

**init_obs_l_pdaf:** Initialize local vector of observations

- The templates provide a generic implementation using the array `id_lobs_in_fobs`

→ We use the templates with out any changes!

**Note:**

`init_obs_l_pdaf` requires that the full observation vector is stored in the array `obs_f`

# prodrinva_l_pdaf.F90

Compute the product of the inverse observation error covariance matrix with some other matrix

+ apply observation localization (weighting)

- The weighting and the product are fully implemented for a diagonal observation error covariance matrix with constant variance

→ When we re-use the array `distance_l` initialized in `init_dim_obs_l_pdaf`, the template can be used without changes.

# Done!

Now, the analysis step for local ESKTF in offline mode is fully implemented.

The implementation allows you now to use the local filter LESTKF (LETKF, LSEIK can be used after adding calls to PDAF_assimilate_X)

Not usable are EnKF and SEEK (PDAF does not have localization for these filters)

For testing one can vary localization parameters:

`cradius` – the localization cut-off radius

`locweight` – the weighting method

Default are `cradius=0.0` (observation at single grid point) and `locweight=1` (uniform weight)

PDAF Parallel Data Assimilation Framework

# A complete local analysis step

We now have a fully functional analysis step including localization

- It can be adapted to multiple model fields, 3 dimensions, different observations, etc.
- It can be used even with big models
  - if computing time is no concern
  - and if the computer has sufficient memory
    (e.g. ensemble array with dimension $10^7$ and 20 members requires about 1.6 GB)
- Parallelization of the analysis step
  - is required if the problem is too big for a single process
  - is recommended if you used a parallelized model

# 1b.1) Use local filter with OpenMP-parallelization

# OpenMP

- OpenMP is so-called *shared-memory parallelization*
- Support for OpenMP is built into current compilers (needs to be activated by compiler-flag)
- Define OpenMP in the code by compiler directives: `!$OMP ...`
- Shared-memory parallelization:
  - Run several OpenMP "threads" (like processes in MPI)
  - All threads can access the same array in memory, but perform different operations
  - Typical is loop-parallelization: Each thread executes some part of a loop. For example, a fraction of a vector:

```
!$OMP parallel do
DO i = 1, 1000
   a(i) = b(i) + c(i)
ENDDO
```

With 2 threads, typically:
- thread 1 runs i=1 to 500
- thread 2 runs i=501 to 1000

PDAF Parallel Data Assimilation Framework

# OpenMP – what's relevant for PDAF

The local filters (LESTKF, LETKF, LSEIK, LNETF) are parallelized with OpenMP

- The loop over local analysis domains is distributed over threads

To make this work:

- Take into account, whether a variable is
  - *shared* (all treads see the same) or
  - *private* (each thread has it's own copy)
- Variables referring to a local analysis domain (e.g. coords_l) have to be private
- This is ensured using the declaration 'THREADPRIVATE'

# Running the tutorial program

Run analogously to case without parallelization

- cd to `/tutorial/classical/online_2D_serialmodel`
- Set environment variable `PDAF_ARCH` or set it in Makefile (e.g. `linux_gfortran_openmpi`)
- Check and edit the make include file to activate OpenMP
  - for gfortran: `OPT = … -fopenmp`
  - for Intel compiler: `OPT = … -openmp`
- Compile by running `'make'`
- Set the number of OpenMP threads as environment variable, e.g.
  - for bash: `export OMP_NUM_THREADS=2`
  - for tcsh: `setenv OMP_NUM_THREADS 2`
- Run the program as without OpenMP-parallelization

PDAF Parallel Data Assimilation Framework

# Results from running with OpenMP parallelization

The results should be *identical* to those without parallelization

If the program is compiled with activated OpenMP-parallelization, you will see in the output of the analysis step the line

```
--- Use OpenMP parallelization with     2 threads
```

# OpenMP in the local filter LESTKF

PDAF supports the use of OpenMP in the localized filters (LESTKF, LETKF, LSEIK, LNETF)

Settings to make OpenMP work are in two files:

```
prodrinva_l_pdaf.F90
mod_assimilation.F90
```

The template files include the settings for OpenMP

# prodrinva_l_pdaf.F90

Two variables have attribute ‘save’:

```
domain_save        mythread
```

Both variables are set private to the thread by

```
!$OMP THREADPRIVATE(mytread, domain_save)
```

(thus each OpenMP thread has a different value of the variables)

Both variables are used to ensure ‘nice’ screen output.

# mod_assimilation.F90

Last line of `mod_assimilation.F90` is

```
!$OMP THREADPRIVATE(coords_l, id_lstate_in_pstate, id_lobs_in_fobs, …
                                                              distance_l)
```

- These variables are specific for each local analysis domain
- The variables are declared in mod_assimilation.F90
- The declaration ‘THREADPRIVATE’ ensures that each variable can have a different value in the different threads

# 2) Hints for adaptions for real models

# Implementations for real models

- Tutorial demonstrates implementation for simple model
- You can base your own implementation on the tutorial implementation or the templates provided with PDAF
- Need to adapt most routines, e.g.
  - Specify model-specific state vector and its dimension
  - Adapt `distribute_state` and `collect_state`
  - Adapt routines handling observations
- Further required changes
  - Adapt file output (usually only want to write ensemble mean state in `prepoststep_pdaf`; sometimes possible to use output routines from model)

# Multiple fields in state vector

- Tutorial uses a single 2-dimensional field
- All fields that should be updated by the assimilation have to be part of the state vector
- For more fields:
  - concatenate them in the state vector
  - adapt state dimension in `init_pdaf`
  - adapt `init_ens_pdaf`, `collect_state_pdaf`, `distribute_state_pdaf`, `prepoststep_pdaf`
  - For local filters: Adapt full (`_f_`) and local (`_l_`) routines and `g2l_state_pdaf`, `l2g_state_pdaf`, `g2l_obs_pdaf`
- **Note**
  - It can be useful to define a vector storing the offset (position) of each field in the state vector

# Multiple observed fields

- In tutorial: observed one field at some grid points
- For several observed fields adapt observation routines:
  - concatenate observed fields in observation vector
  - adapt all observation-handling routines
- **Note**
  - The observation errors can be set differently for each observed field (e.g. using an array `rms_obs`)
  - The localization radius can be set specific for each observed field (observation search in `init_dim_obs_l_pdaf` would use different `cradius` for different fields)
  - One can use spatially varying observation errors using an array `rms_obs` in `prodrinva(_l)_pdaf`

# The End!

Tutorial described example implementations

- Online mode of PDAF parallelized over ensemble members
- Simple 2D model without parallelization and with OpenMP parallelization
- Square root filter ESTKF
    - global and with localization
- Extension to more realistic cases possible with limited coding
- Applicable also for large-scale problems

For full documentation of PDAF
and the user-implemented routines
see http://pdaf.awi.de

PDAF Parallel Data Assimilation Framework