PDAF Tutorial

Implementation of the analysis step in online mode with a parallel model using PDAF-OMI

http://pdaf.awi.de

PDAF Parallel Data Assimilation Framework

V1.13 – 2024-08-28

Implementation Tutorial for PDAF online with serial model

We demonstrate the implementation

of an online analysis step with PDAF

with a model that is 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 V2.3 and later)

PDAF Parallel Data Assimilation Framework

Implementation Tutorial for PDAF online / parallel 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

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 parallel model. The implementation using a model without parallelization is described in a separate tutorial.

We mark the differences to the case without parallelization in blue

Contents

0a) Files for the tutorial	6
0b) The model with parallelization	10
0c) State vector and observation vector	13
0d) PDAF online mode	16
0e) Inserting subroutine calls	22
0f) Forecast phase	32
1a) Global filter	43
1b) Local filter	64
2) Hints for adaptions for real models	82

0a) Files for the Tutorial

Tutorial implementation

Files are in the PDAF package

Directory:

`/tutorial/online_2D_parallelmodel`

- 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_omi`

- 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`

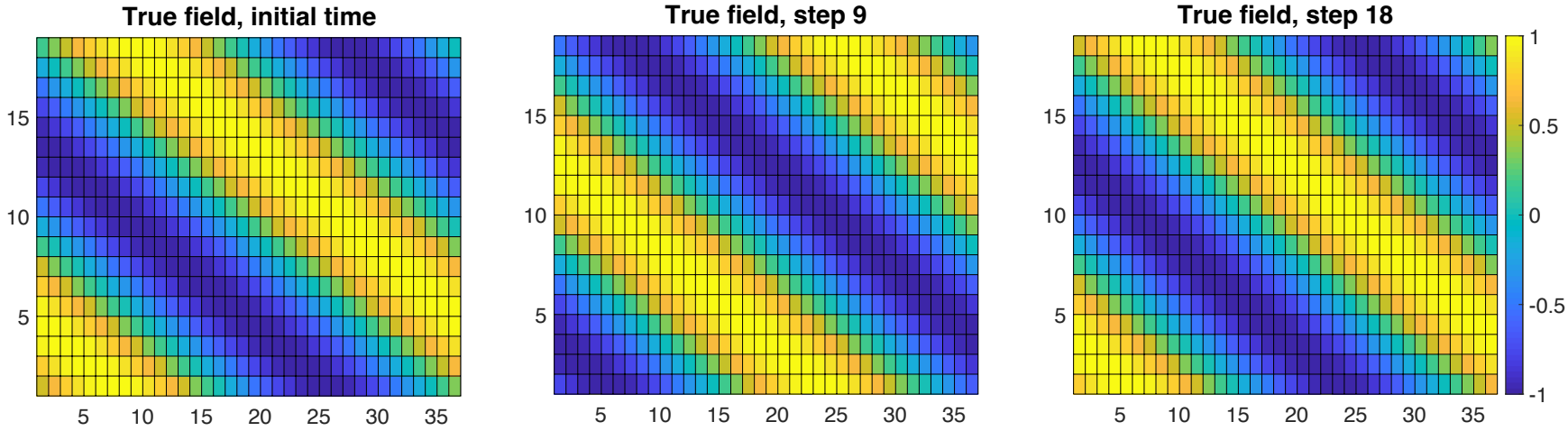
- Environment variable to specify the compile specifications
- Definition files in `/make.arch`
- Define by, e.g.
  `setenv PDAF_ARCH linux_gfortran` (tcsh/csh)
  `export PDAF_ARCH=linux_gfortran` (bash)

0b) The parallelized model

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)



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Parallel `Model`: Files

The source code of the parallel model consists of the following files:

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

Note: One can nicely compare the source codes of the model without and with parallelization

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`	- revise 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

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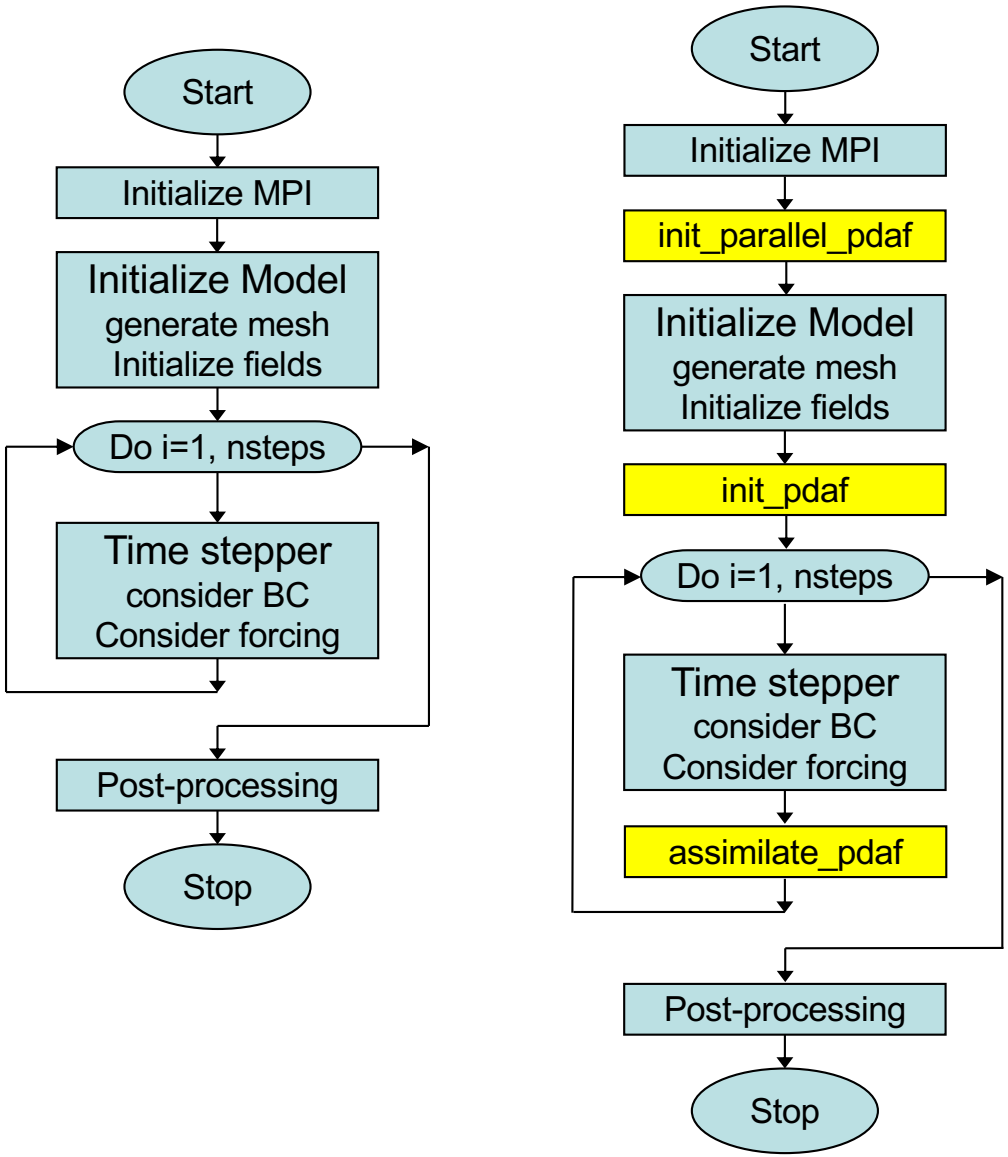
Program flow with model extended for data assimilation



Legend

Model

Extension for data assimilation

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Fully parallel configuration

- Tutorial shows implementation for a fully parallel case

  ➜ Number of processes equals ensemble size times number of processes used for a single model task!

- 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, but after the MPI_Init performed in the code of the parallel model

`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 usable with small adaptions
- Required adaptions
  - Include MPI variables from module of the model:
    MPI_COMM_WORLD, COMM_model, mype_model, npes_model
    (the latter three variables might be named differently in a model)
  - init_parallel_pdaf defines a model communicator
    `comm_model`
    (actually it's a set for communicators, one for each model task)
  - Set communicator of the parallel model to comm_model at the end
    if init_parallel_pdaf:
    `"my_models_communicator" = comm_model`
    (include my_models_communicator from module of model)
  - Set variables for number of processes in model and rank of a process (`npes_model, mype_model`) at end of routine

init_parallel_pdaf.F90 (2)

- Parallelization variables for PDAF are declared in Fortran module

  `mod_parallel_pdaf`

- 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’)

- **Important:** If the parallel model uses MPI_COMM_WORLD, this has to be replaced! (MPI_COMM_WORLD denotes always all processes in the program)

init_parallel_pdaf.F90 (3) - Example

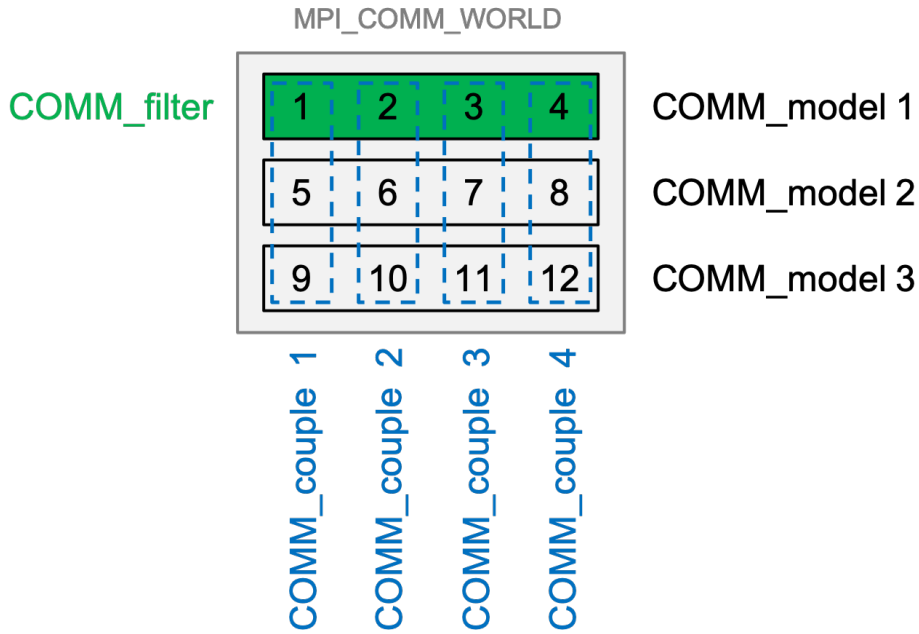
The routine initializes 3 groups of communicators

- 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

- 12 processes in total
- 3 model tasks in parallel
- Each model task uses 4 processes in its COMM_model
- Each COMM_couple links groups of 3 processes to distribute and collect ensemble states
- The filter processes use model task 1



init_parallel_pdaf is coded to provide this configuration when running with 12 processes and setting dim_ens=3

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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 decomposed state vector

```
dim_state_p = nx_p * 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 an interface routine like

```
PDAFomi_assimilate_global
```

We don't insert `PDAFomi_assimilate_global` 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: The template contains calls for all 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

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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
callback_obs_pdafomi.F90
obs_A_pdafomi.F90
prepoststep_ens_pdaf.F90
```

initialization

ensemble forecast

analysis step

post step

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`)

Include variables for observation 'A' with

```
USE obs_A_pdafomi, ONLY: assim_A, rms_obs_A
```

For the example set :

1. `dim_ens = 9`
2. `rms_obs_A = 0.5`
3. `assim_A = .true.`
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, nx_p` 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 local part of `field` in column `i` of `ens_p` (columns nx_p*mype_model+1 : nx_p*mype_model+nx_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
(its values are different for each process)

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_p`, `ny` and `field_p` with `use mod_model`
2. Initialize model field from state vector:

```
DO j = 1, nx_p
  field_p(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/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 18 ./model_pdaf -dim_ens 9
```

- Inputs are read in from `/tutorial/inputs_online`
- Outputs are written in `/tutorial/online_2D_parallelmodel`
- 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/online_2D_parallelmodel` (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

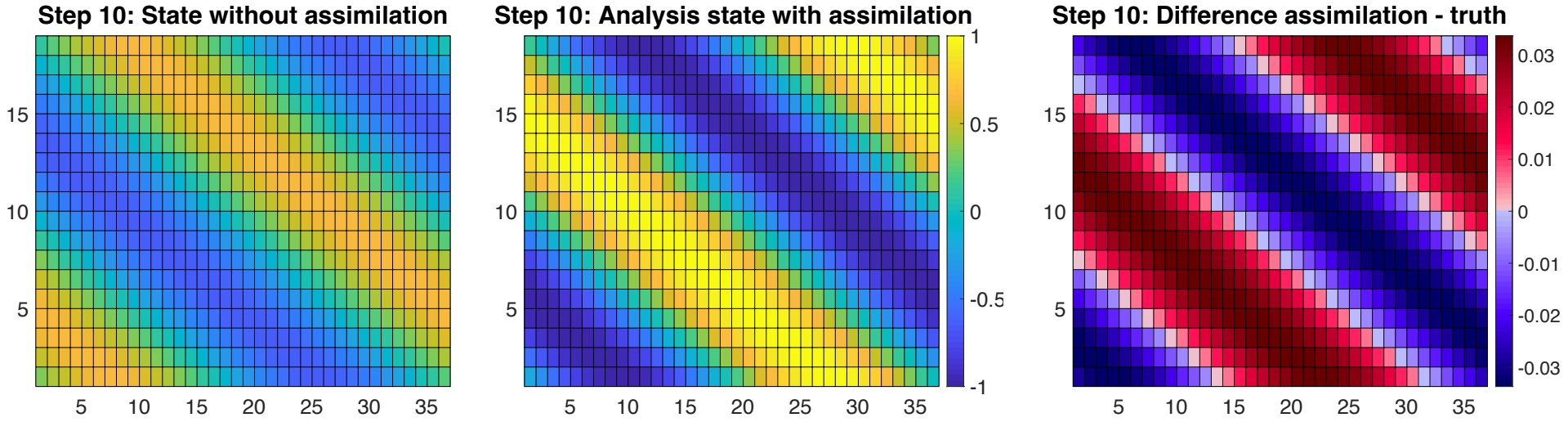
Y=1,…,18: time step index

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)
  (this is a special result caused by the chosen ensemble. A smaller ensemble (dim_ens 4) leads to much higher difference)



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_p
  state_p(1+(j-1)*ny : j*ny) = field_p(1:ny, j)
END DO
```

Note: The routine is independent of the filter!

callback_obs_pdafomi.F90

File collecting interface routines for the observation routines called by PDAF

For each observation type we need to add subroutine calls

- Example observation is just called **A**, defined in `obs_A_pdafomi.F90`

In **init_dim_obs_pdafomi**:

- Insert `USE obs_A_pdafomi, ONLY: assim_A, init_dim_obs_A`
- Declare `INTEGER :: dim_obs_A` and set this to zero
- Insert `IF (assim_A) CALL init_dim_obs_A(step, dim_obs_A)`

In **obs_op_pdafomi**:

- Insert `USE obs_A_pdafomi, ONLY: obs_op_A`
- Insert `CALL obs_op_A(dim_p, dim_obs, state_p, ostate)`

(The other observations (B, C) in the file show how to use multiple observations)

obs_A_pdafomi.F90

PDAF-OMI observation module

- There is a long header with information

Implementation steps from template

- Copy file to name according to observation ('A')
- Replace 'OBSTYPE' by name of observation ('A')
- Implement
  - `init_dim_obs_A`
  - `obs_op_A`

obs_A_pdafomi.F90 (2)

With PDAF-OMI

- Observation Information is stored in Fortran data type `obs_f`

```
TYPE obs_f
   INTEGER :: doassim          ! Whether to assimilate this obs. type
   INTEGER :: disttype         ! Type of distance computation
   INTEGER :: ncoord           ! Number of coordinates
   INTEGER, ALLOCATABLE :: id_obs_p(:,:)
                               ! Indices of observations in state vector
    ...
END TYPE obs_f
```

- It is allocated with generic name `thisobs`
  (Motivated by object-oriented programming)

- A single variable, e.g. `disttype`, is accessed in the form

  `thisobs%disttype`

init_dim_obs_A in obs_A_pdafomi.F90

Main routine to initialize observation information

- read observation file
- count number of available observations
  (direct output to PDAF: **`dim_obs_p`**)
- initialize array holding available observations
- initialize array of index of observation in global state vector
- Call `PDAFomi_gather_obs` to finalize initializations

init_dim_obs_A in obs_A_pdafomi.F90 (2)

First initializations:

- Specify whether observation is assimilated

```
IF (assim_A) thisobs%doassim = 1
```

(assim_A is included with use and set in init_pdaf)

- Specify type of distance computation (0=Cartesian)

```
thisobs%disttype = 0
```

- Number of coordinates used for distance computation

```
thisobs%ncoord = 2
```

Note: Parts of the template that are not needed here are deleted from `init_dim_obs_A`

init_dim_obs_A in obs_A_pdafomi.F90 (3)

Preparations and reading of observation file:

1. Include `nx, ny, nx_p` with `use mod_model`
2. declare and allocate real array `obs_field(ny, nx)`
3. Get offset of local part in global state vector
   `off_p` = Sum over nx_p*ny up to i=mype_filter
4. 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)
```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init_dim_obs_A in obs_A_pdafomi.F90 (4)

Count available process-local observations (**dim_obs_p**):

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

```
cnt0 = 0
cnt_p = 0
DO j = 1, nx
  DO i= 1, ny
   cnt0 = cnt0 + 1
   IF (cnt0>off_p .AND. cnt0<=off_p+nx_p*ny) THEN
     IF (obs_field(i,j) > -999.0) cnt_p = cnt_p + 1
END IF; END DO; END DO
dim_obs_p = cnt_p
```

init_dim_obs_A in obs_A_pdafomi.F90 (5)

Now we need to initialize

- observation vector `obs_p`
- inverse variances `ivar_obs_p`
- index array `thisobs%id_obs_p`
- observation coordinates `ocoord_p`

1. All arrays are declared in the template

2. Allocate
   - `obs_p(dim_obs_p)`
   - `ivar_obs_p(dim_obs_p)`
   - `thisobs%id_obs_p(dim_obs_p)`
   - `ocoord_p(2, dim_obs_p)`

3. Initialize these arrays

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

init_dim_obs_pdaf.F90 (6)

3. Now initialize

```
cnt0_p = 0                    ! Count grid points
cnt_p = 0                     ! Count observations
DO j = 1 + off_nx, nx_p + off_nx
  DO i= 1, ny
     cnt0_p = cnt0_p + 1
    IF (obs_field(i,j) > -999.0) THEN
      cnt_p = cnt_p + 1
       thisobs%id_obs_p(cnt_p) = cnt0_p   ! Index
       obs_p(cnt_p) = obs_field(i, j)   ! observations
       ocoord_p(1, cnt_p) = REAL(j)     ! X-coordinates
       ocoord_p(2, cnt_p) = REAL(i)     ! Y-coordinates
    END IF
  END DO
END DO
ivar_obs_p(:) = 1.0 / (rms_obs_A*rms_obs_A)
```


PDAF Parallel Data Assimilation Framework

obs_op_A in obs_A_pdafomi.F90

Implementation of observation operator
acting one some state vector

Input: state vector `state_p`

Output: observed state vector `ostate`

`init_dim_obs_A` initialized all required information stored in `'thisobs'`

Observation 'A' is defined at grid points

1. Include observation operator routine:

```
USE PDAFomi, ONLY: PDAFomi_obs_op_gridpoint
```

2. Call observation operator

```
CALL PDAFomi_obs_op_gridpoint(thisobs, state_p, ostate)
```

Note: OMI provides different observation operators,
e.g. for linear interpolation

prepoststep.F90

PDAF-Omi required one small change in prepoststep:

We need to deallocate OMI internal arrays:

For this we insert at the end of the routine

```
CALL deallocate_obs_pdafomi(step)
```

(The routine is included by calback_obs_pdafomi.F90)

Done!

The analysis step in online mode with the parallelized model is fully implemented now

The implementation allows you now to use all global filters! (ESTKF, EKTF, SEIK, EnKF, NETF, PF)

Not usable is SEEK (It's deprecated)

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
  → Tutorial code shows example of 2 observation types
- 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

`callback_obs_pdafomi.F90`
- identical in online and offline modes

`obs_A_pdafomi.F90`:

`init_dim_obs_A` - read from file for current time step; include `nx, ny` from `mod_model` instead of `mod_assimilate`; use `local_dims` to compute offset

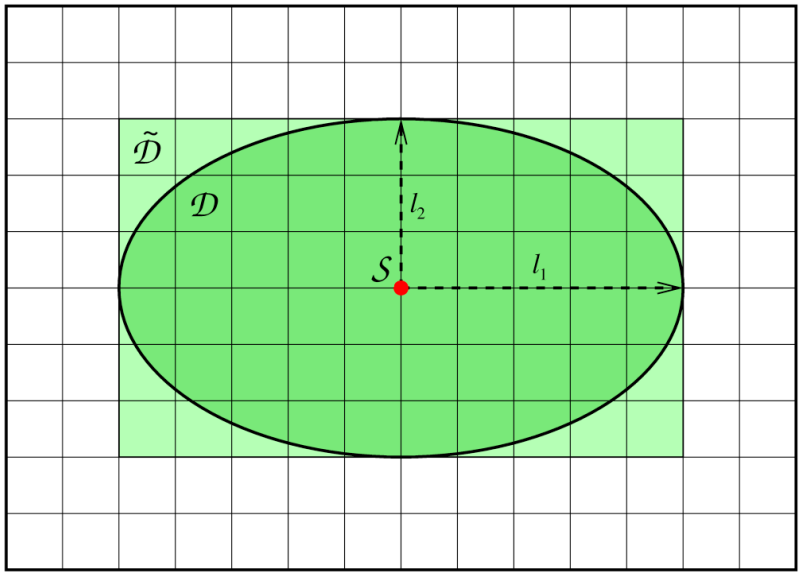
`obs_op_pdaf` - identical in online and offline modes

1b) Local filter with parallelized model

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*



PDAF Parallel Data Assimilation Framework

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 18 ./model_pdaf -dim_ens 9 OPTIONS
```

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

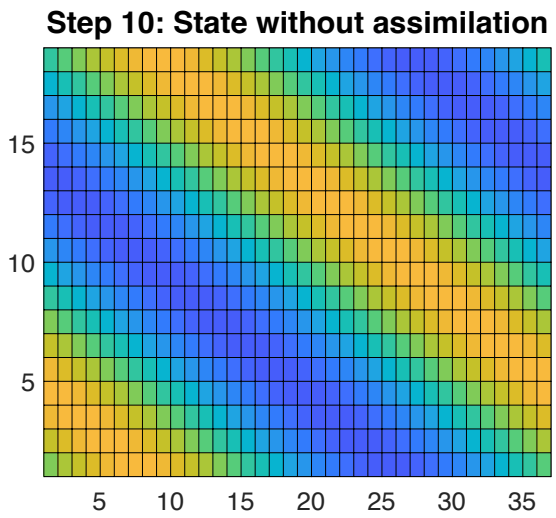
`-filtertype 7`	(select LESTKF if not set in init_pdaf)
`-cradius 5.0`	(set localization radius, 0.0 by default, any positive value should work)
`-locweight 2`	(set weight function for localization, default=0 for constant weight of 1; possible are integer values 0 to 4; see `init_pdaf`)

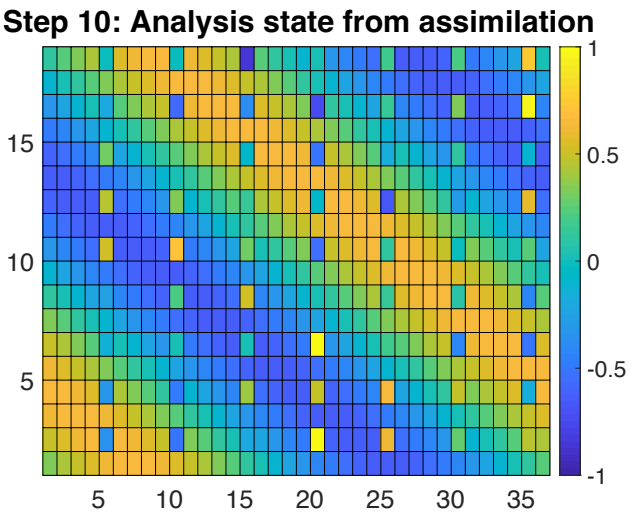
Note: You can run the model e.g. using 18 MPI-processes even on most computers with only 2 processor cores. However, to see a speedup in computing time, you need more physical processors

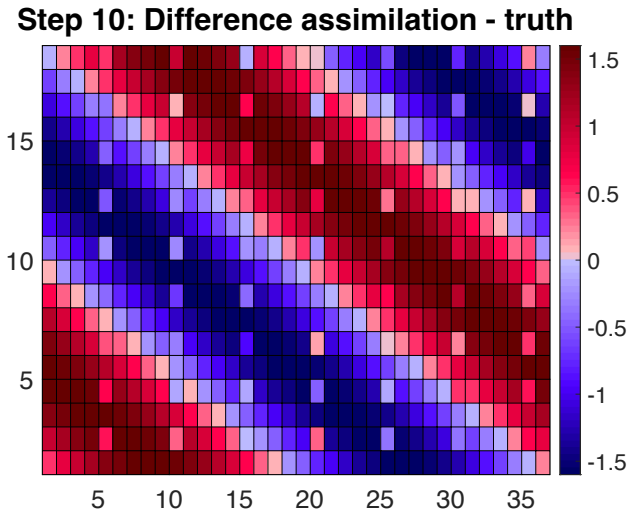
Result of the local assimilation

```
mpirun -np 18 ./model_pdaf -dim_ens 9 -filtertype 7
```

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







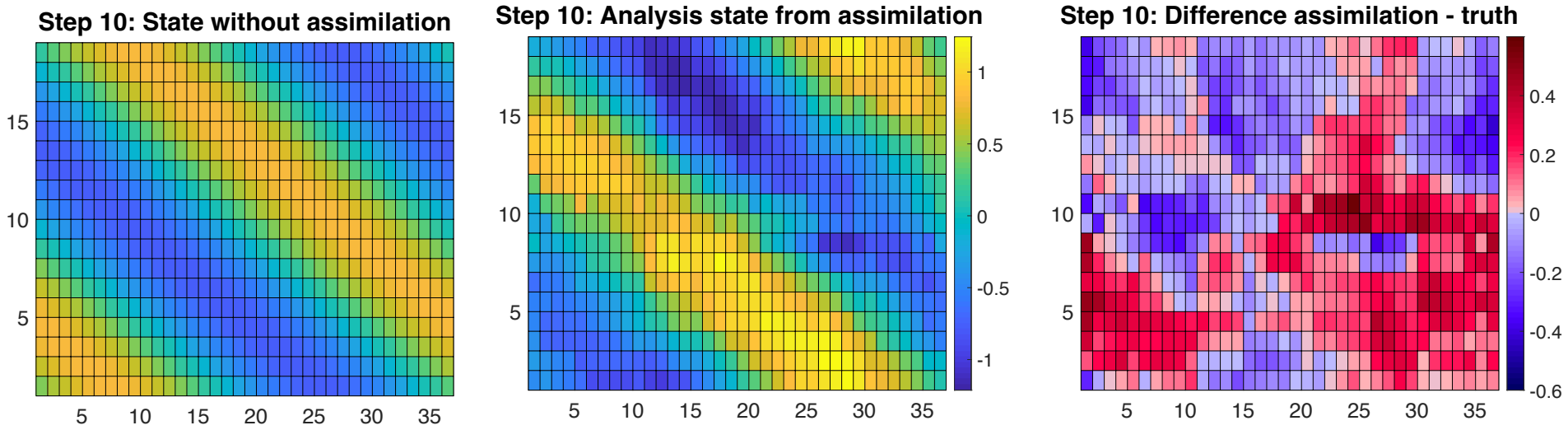
PDAF Parallel Data Assimilation Framework

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

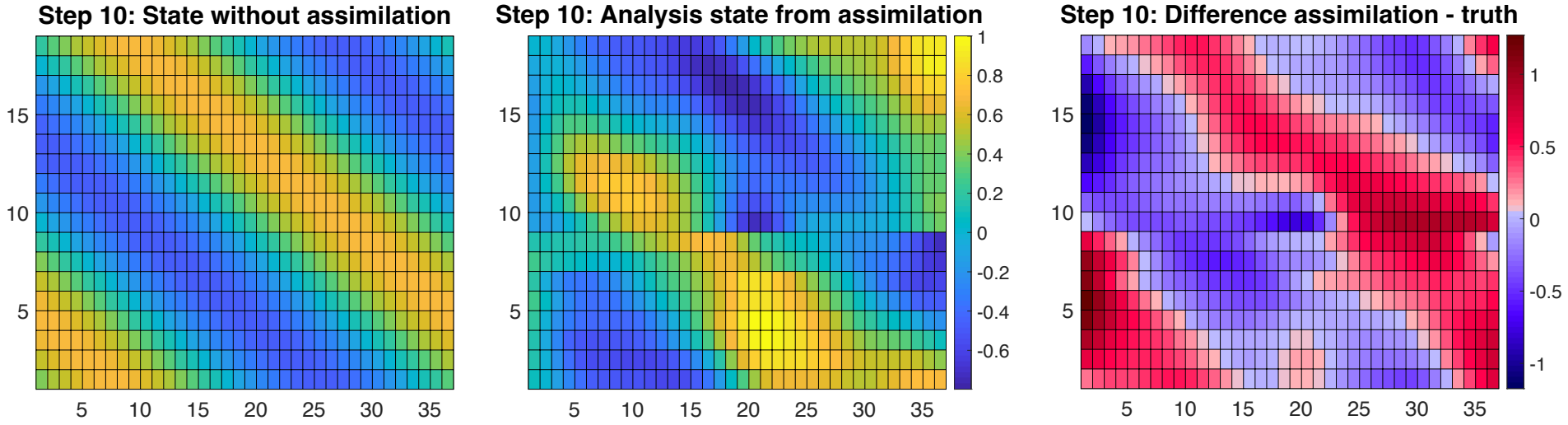


PDAF Parallel Data Assimilation Framework

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)
- The high errors on the left are due to the distance of observations

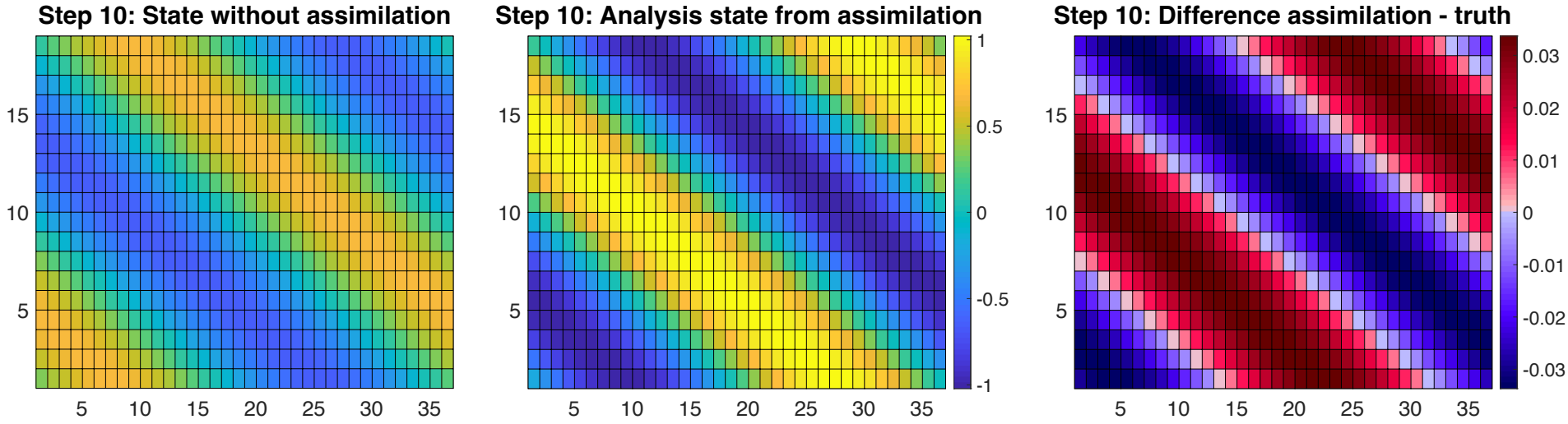


PDAF Parallel Data Assimilation Framework

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)

Additional files for local analysis step

```
init_n_domains_pdaf.F90
init_dim_l_pdaf.F90
```

} localize state vector

Additional routine in callback_obs_pdafomi.F90:

```
init_dim_obs_l_pdafomi
```

} 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 process-local grid points (nx_p * ny)

To do:

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

```
n_domains_p = nx_p * ny
```

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

init_dim_l_pdaf.F90 (2)

2. Determine coordinates of local analysis domain

   1. Compute offset:

      `off_p` = Sum over `nx_p*ny` up to i=mype_filter

   2. Include `coords_l` with `use mod_assimilation`

   3. Include `nx, ny, nx_p` with `use mod_model`

   4. Compute `coords_l` from `nx, ny:`

```
coords_l(1)
  = real(ceiling(real(domain_p + off_p)/real(ny)))
coords_l(2)
  = real(domain_p + off_p) - (coords_l(1)-1)*ny
```

Note: With parallelization the domain numbering begins with 1 for each process. For the coordinates we also need to count the domains from processes with lower process rank using `off_p`

init_dim_l_pdaf.F90 (3)

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

a) Declare
```
INTEGER, ALLOCATABLE :: id_lstate_in_pstate(:)
```

b) Allocate `id_lstate_in_pstate(dim_l)`

c) Specify the index: It is identical to `domain_p` here (because we only have a single model variable):
```
id_lstate_in_pstate(1) = domain_p
```

d) Provide `id_lstate_in_pstate` by calling
```
CALL PDAFlocal_set_indices(dim_l, id_lstate_in_pstate)
```

callback_obs_pdafomi.F90

File collecting interface routines for the observation routines called by PDAF

For each observation type we need to add subroutine calls

- The example observation is just called **A**, defined in `obs_A_pdafomi.F90`

In **init_dim_obs_l_pdafomi**:

- Insert

```
USE obs_A_pdafomi, ONLY: init_dim_obs_l_A
```

- Insert

```
CALL init_dim_obs_l_A(domain_p, step, dim_obs, dim_obs_l)
```

(The other observations (B, C) in the file show how to use multiple observations)

init_dim_obs_l_pdaf.F90

Set size of the observation vector for the local analysis domain and initialize local observation information

Only direct output: **`dim_obs_l`**

Operations:

1. With `use mod_assimilation`
   - Include coordinates `coords_l`
   - Include localization variables (`cradius, locweight, sradius`)
2. Call `PDAFomi_init_dim_obs_l` to perform necessary operations

Note: we use a fixed radius cradius here. One could make it varying with the local analysis domain. Also it could vary with observation type.

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!

Done!

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

The implementation allows you now to use all local filters!
(LESTKF, LETKF, LSEIK, LNETF)

Not usable is LEnKF
(It needs one more routine (localize_covariance_pdafomi) which we don't discuss here; but it's coded in the tutorial code)

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)

2) Hints for adaptions for real models

Implementations for real models

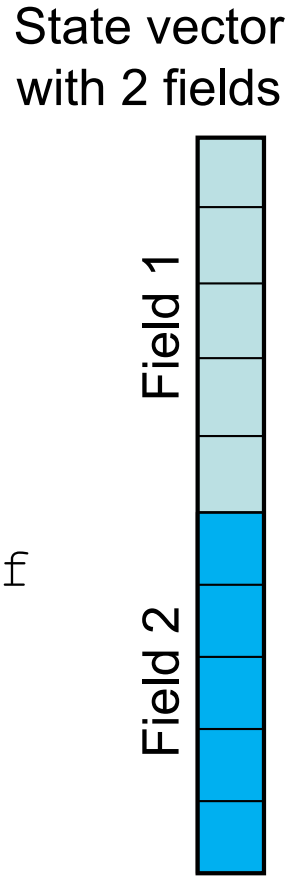
- Tutorial demonstrates implementation for simple model
- You can base your own implementation on the tutorial implementation or the templates provided with PDAF
- Need to adapt most routines, e.g.
  - Specify model-specific state vector and its dimension
  - Adapt `distribute_state` and `collect_state`
  - 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)

Adaptation for 2 fields in state vector

- Both field should be updated by the assimilation have to be part of the state vector

  ➜ see tutorial for online mode with serial model for example of 2 fields

- For two or more fields:
  - concatenate them in the state vector
  - adapt state dimension in `init_pdaf`
  - Add arrays for field offsets and dimensions in `init_pdaf`
  - adapt `init_ens_pdaf`, `collect_state_pdaf`, `distribute_state_pdaf`, `prepoststep_pdaf`
  - For local filters: Adapt `init_dim_l_pdaf`
  - Adapt observation modules (in particular thisobs%is_obs_p)



PDAF Parallel Data Assimilation Framework

Multiple observed fields

- In tutorial:
  - We discussed observations of one field at some grid points
  - Example code shows three different observation types
- For several observed fields adapt observation routines:
  - Create a new observation module (`obs_OBSTYPE_pdafomi.F90`)
  - Add calls to routine in `callback_obs_pdafomi.F90`
- **Note**
  - The observation errors can be set differently for each observed field
  - The localization radius can be set specific for each observed field (use a different variable `cradius_OBSTYPE`)

The End!

Tutorial described example implementations

- Online mode of PDAF
- Simple 2D model with parallelization
- Parallelization over ensemble members at the model itself
- Implementation supports various filters
    - 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