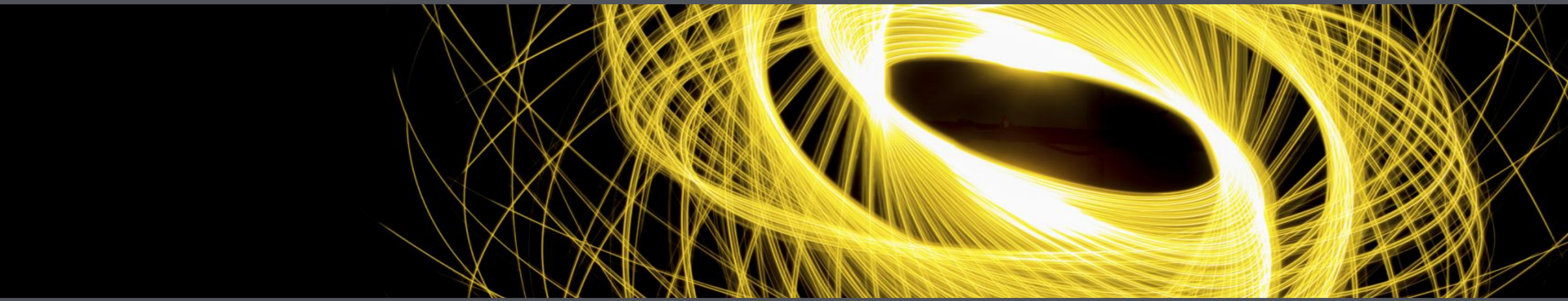
Department of Meteorology
Data assimilation research centre (DARC)

Data Assimilation Research Centre

National Centre for Earth Observation
NATURAL ENVIRONMENT RESEARCH COUNCIL

University of Reading

Data assimilation software (general)



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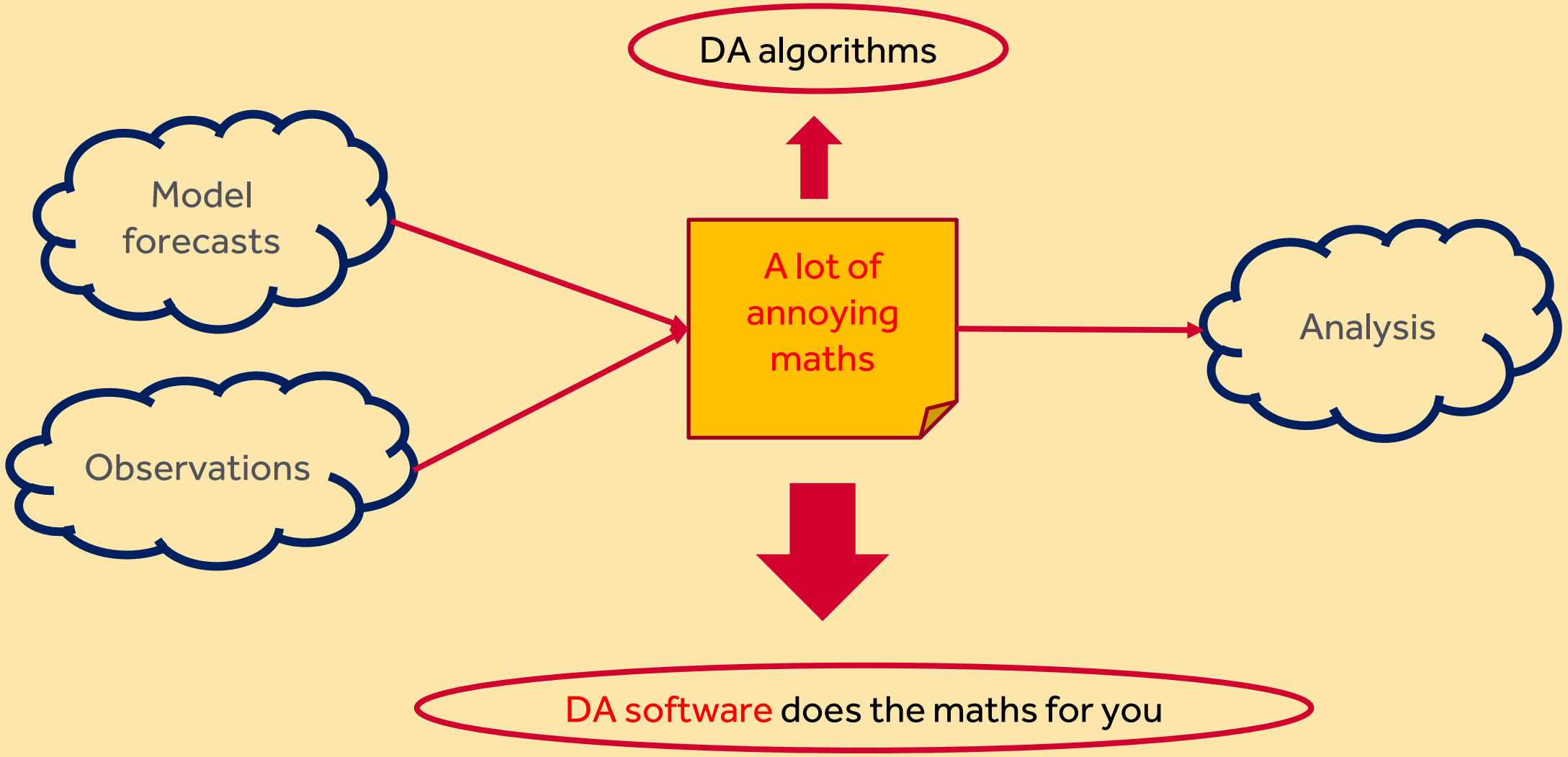
DA algorithms
Model forecasts
Observations
A lot of annoying maths
Analysis
DA software does the maths for you

When do we want to write our own code?

- Not very complicated algorithms
- Learning details of an algorithm
- Sense of control
- Easier modifications
- Tailored to our own applications
- Fewer dependent libraries

...

Why bother with DA software?

$$\mathcal{J}(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{i=0}^{N}(\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i)$$

Algorithm 1.2 4D-Var in its basic form

$j = 0$, $\mathbf{x} = \mathbf{x}_0$
while $||\nabla J|| > \epsilon$ **or** $j \leq j_{\max}$
  (1) compute J with the direct model M and H
  (2) compute ∇J with adjoint model $\mathbf{M}^{\mathrm{T}}$ and $\mathbf{H}^{\mathrm{T}}$ (reverse mode)
  gradient descent and update of $\mathbf{x}_{j+1}$
  $j = j + 1$
end

Source: Data Assimilation: Methods, Algorithms, and Applications by Maëlle Nodet, Marc Bocquet, Mark Asch

- Convenience
  - Prefer np.mean to writing loops
- Optimised and efficient
- Well-maintained and reliable
- Focus on the scientific questions
- Ensures reproducible and consistent scientific research

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Why bother with DA software?

One may even argue that we can build a DA system without a team using good software.

Example DA software/libraries/framework

Name	Developers	Primary Language
JEDI	JCSDA + collaborators	C++
PDAF	AWI	Fortran
DART	NCAR	Fortran
NEDAS	NERSC	Python
MIDAS	ECCC	Fortran
…		

Name	Developers	Primary Language
DAPPER	NERSC	Python
EnKF-C	Sakov	C
TorchDA	Cheng	Python
…		

There is also software for specific purposes, e.g. land DA, snow DA, weather DA, etc.

Data Assimilation with Python: a Package for Experimental Research (DAPPER)

- DAPPER is a set of templates to provide a benchmark for different DA methods
- The typical set-up is a synthetic (twin) experiment
- Ease of adding new DA methods and models
- Pure Python implementation with multiprocessing support
- It is not suited for very big models (>60k unknowns)

Method	Literature reproduced
EnKF [1]	Sakov08, Hoteit15, Grudzien2020
EnKF-N	Bocquet12, Bocquet15
EnKS, EnRTS	Raanes2016
iEnKS / iEnKF / EnRML / ES-MDA [2]	Sakov12, Bocquet12, Bocquet14
LETKF, local & serial EAKF	Bocquet11
Sqrt. model noise methods	Raanes2014
Particle filter (bootstrap) [3]	Bocquet10
Optimal/implicit Particle filter [3]	Bocquet10
NETF	Tödter15, Wiljes16
Rank histogram filter (RHF)	Anderson10
4D-Var	
3D-Var	
Extended KF	
Optimal interpolation	
Climatology	

https://github.com/nansencenter/DAPPER

Data Assimilation with Python: a Package for Experimental Research (DAPPER)

Model setup

Obs. setup

Time steps, observation frequency, etc.

```
import dapper.mods as modelling
import dapper.da_methods as da

HMM = modelling.HiddenMarkovModel(dyn, obs, tseq, x0)
xx, yy = HMM.simulate()

xp = da.EnKF("Sqrt", N=10, infl=1.02)
xp.assimilate(HMM, xx, yy)
```

Initial condition

Truth (xx) and synthetic observations (yy)

DA set up and run DA

Check model-specific configuration files for setting up dyn, obs, tseq, x0

Using DA for large models: JEDI or PDAF

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Functionalities	PDAF	JEDI
Methods	Focuses on EnKF; also supports (Hybrid) 3DVar and nonlinear filters	EnKF + Var + Hybrid
Language	Fortran/Python	Primarily C++
Model Coupling	Adjustments in user-supplied functions. Non-intrusive to the model.	C++ interface class which needs to wrap the model components + YAML files manipulation.
Observation operator	User-defined by user-supplied code (can utilise existing Fortran code)	Various built-in operators and QC processes
Error covariance modelling	Ensemble generation method	Ensemble and parametric B-matrix modelling
Software installation	Minimal dependencies	Requires specific machine or correct container configuration
Communities	Research-driven	Operational centres but also used by the research community

PDAF Parallel Data Assimilation Framework

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Parallel Data Assimilation Framework (PDAF)

- Suitable for weather and climate models, e.g. AWI-CM, MITgcm, MPI-ESM, NEMO, etc.
- Implementation is in general efficient and reliable
- Good protocols and well-documented to be used with any models and observations
- Recently PDAF version 3.0 is released

	Global filter	Local filter	Smoother
EnKF	ETKF	✓	✓
	ESTKF	✓	✓
	EnKF	✓	✓
	SEIK	✓	✓
	SEEK		
Nonlinear filtering	NETKF	✓	✓
	Particle filter		
3DVar	3DVar		
	3DEnVar		
	Hyb3DVar		

https://pdaf.awi.de/trac/wiki

PDAF Parallel Data Assimilation Framework

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Parallel Data Assimilation Framework (PDAF)

- A typical workflow of PDAF:

Initialise PDAF

```
CALL PDAF_init(filtertype, subtype, 0,  filter_param_i, 2, filter_param_r, 1,
COMM_model, COMM_filter, COMM_couple,  task_id, n_modeltasks,
filterpe, init_ens,  screen, status_pdaf)
CALL PDAF_init_forecast(next_observation, distribute_state,  prepoststep,
status_pdaf)
```

Assimilation in model time stepping

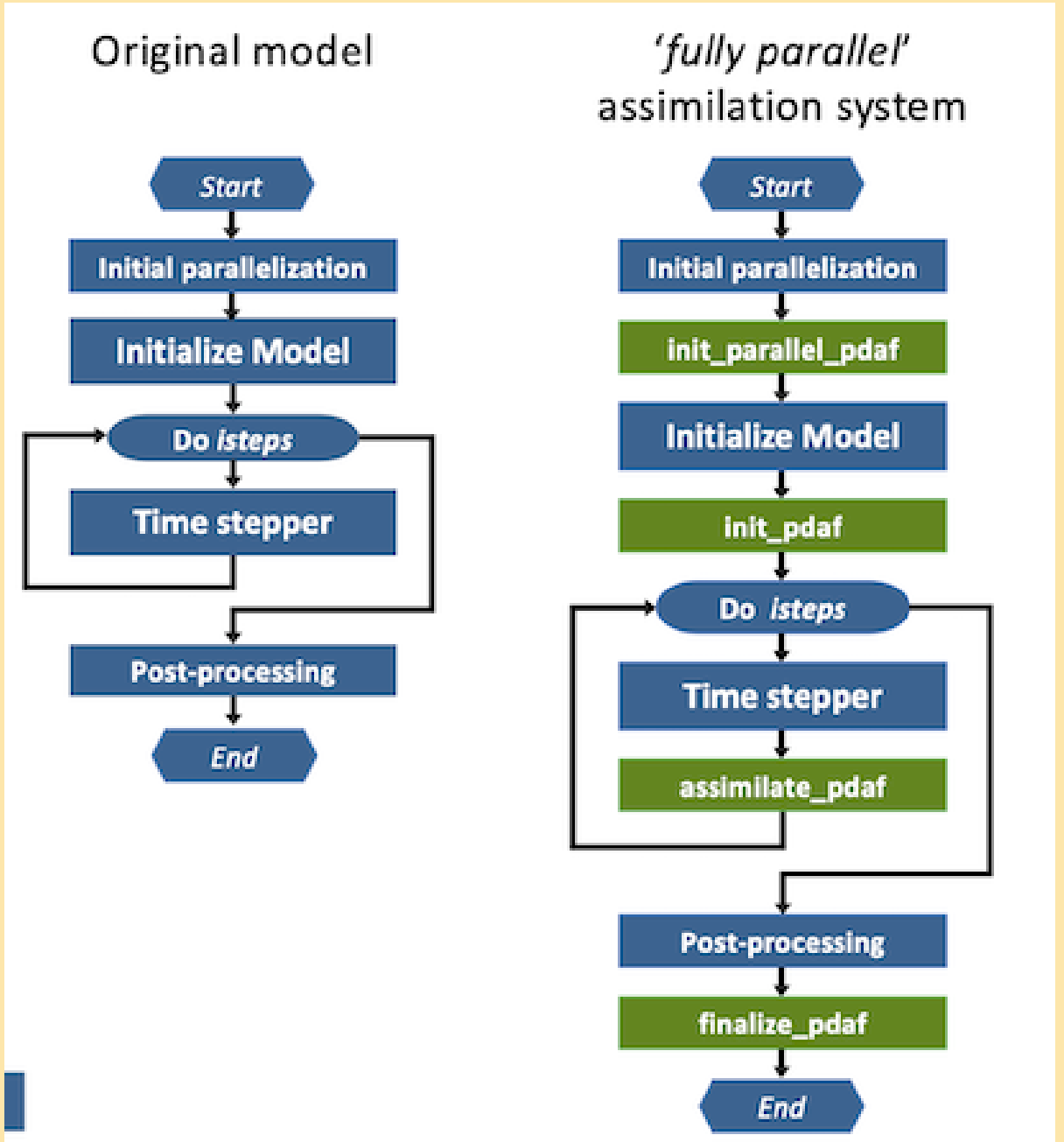
```
CALL PDAF3_assimilate(collect_state, distribute_state, init_dim_obs,
obs_op,  init_n_domains, init_dim_l, init_dim_obs_l,  prepoststep,
next_observation, status_pdaf)
```

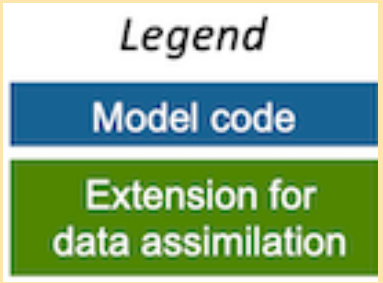
Finalise PDAF

```
CALL finalize_pdaf()
```

Blue: user-supplied functions

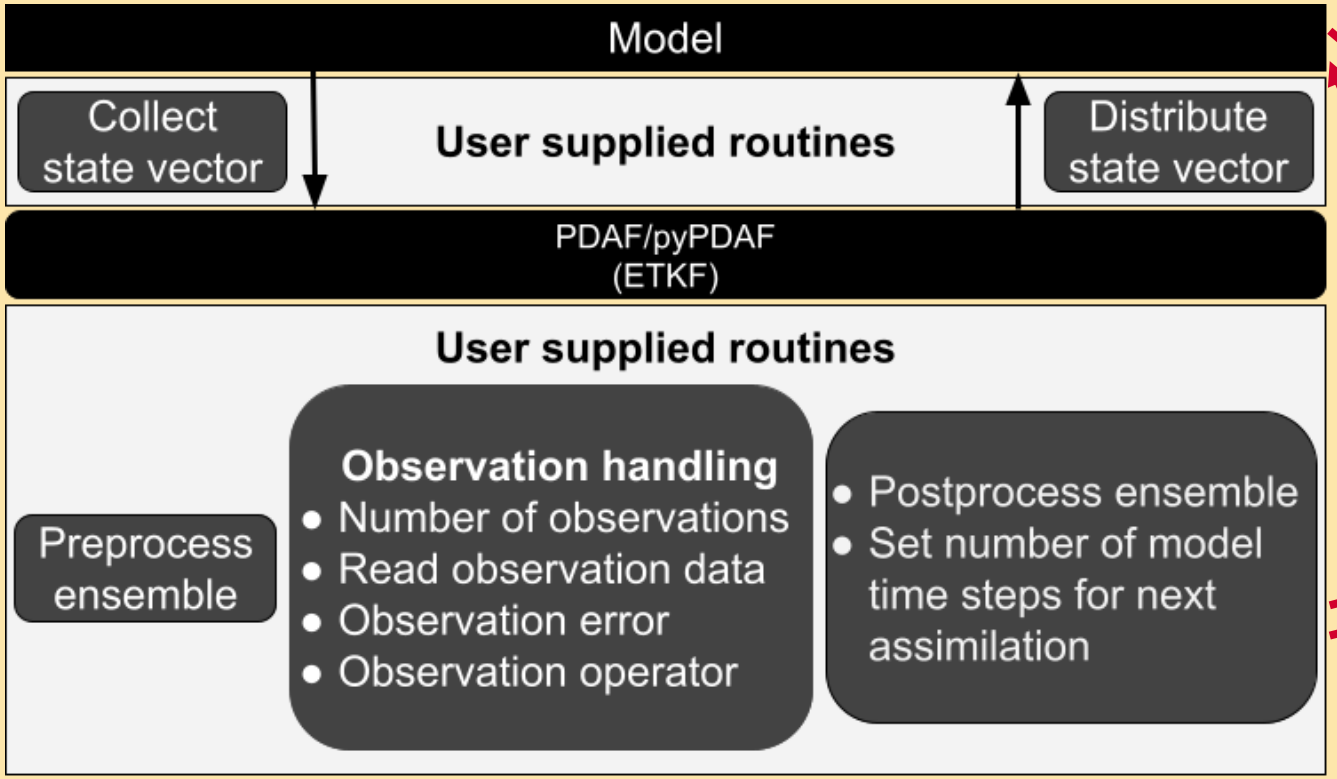
- Adding addition subroutines with limited subroutine calls in existing model





Parallel Data Assimilation Framework (PDAF)

- Flexibility of PDAF relies on user-supplied routines (grey boxes)



$$\mathbf{x}_{\mathrm{a}}^{i} = \mathbf{x}_{\mathrm{b}}^{i} + \mathbf{K}^{i}\left(\mathbf{y}^{i} - h\left(\mathbf{x}_{\mathrm{b}}^{i}\right)\right)$$

- Types of user-supplied routines vary for different filters; check the PDAF website for references.

PDAF Parallel Data Assimilation Framework

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Parallel Data Assimilation Framework (PDAF)

- PDAF also has a Python version, pyPDAF:
  - https://github.com/yumengch/pypdaf
- Build a simple DA system using pyPDAF:
  - https://colab.research.google.com/github/yumengch/pyPDAF/
  - If you run the notebook on your local computer:
    - conda create -n pypdaf -c conda-forge yumengch::pypdaf jupyter matplotlib
  - Any feedback on pyPDAF and the tutorials are welcome!