Joint Effort for Data assimilation Integration

Object Oriented Prediction System (OOPS)

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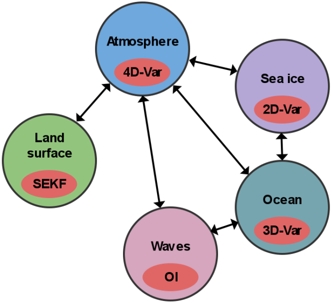
Outline

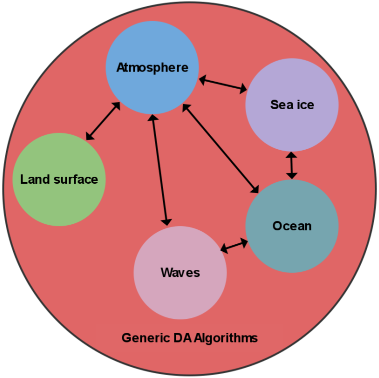
Evolution of Forecasting

- The expectations of society for better weather (and related) forecasts are pushing us to account for more of the Earth system.
- Science and models have progressed in many areas:
  - Atmosphere,
  - Land surface,
  - Ocean,
  - Sea ice,
  - Atmospheric composition...
- Each model is becoming more and more complex as science progresses.
- The models are becoming more and more coupled to account for interactions between all these aspects.

Earth System Data Assimilation

- Data assimilation systems have been developped for each model.





- Coupled data assimilation requires some common infrastructure.

Evolution of Data Assimilation

- Data assimilation algorithms have become very complex over the years:
  - Number and types of observations,
  - Minimisation and preconditioning,
  - Observation bias correction,
  - Sophisticated TL/AD models,
  - Sophisticated observation operators,
  - Wavelet J_b...
  - It is still being developped and improved (weak constraint).
- Today's best data assimilation algorithms are hybrid.
  - Ensemble DA (EDA, 4D-En-Var, EVIL, EnKF) system for computing background error covariances and initializing ensemble forecasts,
  - Variational DA system to provide the high resolution (or *best*) analysis.
- Data assimilation systems have become so complex that comparing all options is almost impossible.

Scalability

Scalability is the ability of a system, network, or process to handle a growing amount of work in a capable manner or its ability to be enlarged to accommodate that growth (wikipedia)

- This applies to running on increasly large number of processors
- It also applies to:
  - the number of code units
  - the number of developers/users/institutions involved

Outline

Flexible

- It should be easy to modify the system (new science, new functionality, better scalability...)

- A requirement is that a change to one aspect should not imply changes all over the place.
  - No code duplication: same modification in many places but also difficult to find and leads to bugs.
  - No global variables: a modification might have unforeseen consequences anywhere.
  - Think of it in terms of *locality* in the source code (as opposed to discontinous code that jumps all over the place).

Reliable

- The code must run without crashing.
- Additional aspects of reliablity are application dependent. For a complex system, the code must do what the user thinks it does:
  - Many experiments are wasted because it is not always the case.
  - The code must run with the user supplied value (namelist, json, yaml...) or abort.
- A controlled abort with a clear error message is not a crash: it saves computer and user time (our time).
- Lots of testing:
  - Internal consistency and correctness of results (this is not meteorological evaluation),
  - Mecanism to run all the tests easily,
  - Tests run automatically on push to source repository.

Modular

- The weather forecasting problem can be broken into manageable pieces:
  - Data assimilation (or ensemble prediction) can be described without knowing the specifics of a model or observations.
  - Minimisation algorithms can be written without knowing the details of the matrices and vectors involved.
  - Development of a dynamical core on a new model grid should not require knowledge of the data assimilation algorithm.
- Separation of concerns:
  - All aspects exist but scientists focus on one aspect at a time.
  - Different concepts should be treated in different parts of the code.
- Unfortunately, in most cases, Fortran modules don't lead to modular codes.

Object-Oriented Programming

- We need a very flexible, reliable, efficient, readable and modular code.
  - Readability improves staff efficiency: it is as important as computational efficiency (it's just more difficult to measure).
  - Modularity improves staff scalability: it is as important as computational scalability (it's just more difficult to measure).

- This is not specific to the IFS: the techniques that have emerged in the software industry to answer these needs are called **generic** and **object-oriented** programming.

- Object-oriented programming does not solve scientific problems in itself: it provides a more powerful way to tell the computer what to do.

Outline

1. Scalability and Complexity
2. What can we do?
3. OOPS design
   - OOPS Design: Abstract Level
   - Implementing the Abstract Design: Applications
4. From old to new

Outline

OOPS Analysis and Design

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- We don't need to know how these operations are performed, how the states are represented or how the observations are stored.

OOPS Analysis and Design

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + \frac{1}{2}\sum_{i=0}^{n}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]^T \mathbf{R}_i^{-1}[\mathcal{H}(\mathbf{x}_i) - \mathbf{y}_i]$$

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- Covariance matrices:
  - Setup,
  - Multiply by matrix (and possibly its inverse).

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- The 4D-Var problem, and the algorithm to solve it, can be described with a very limited number of entities:
  - Vectors: $\mathbf{x}$, $\mathbf{y}$, $\mathbf{g}$ and $\delta\mathbf{x}$.
  - Covariances matrices: $\mathbf{B}$, $\mathbf{R}$ (and eventually $\mathbf{Q}$).
  - Two operators and their linearised counterparts: $\mathcal{M}$, $\mathbf{M}$, $\mathbf{M}^T$, $\mathcal{H}$, $\mathbf{H}$, $\mathbf{H}^T$.
- All data assimilation schemes manipulate the same limited number of entities.
- For future (unknown) developments these entities should be easily available and reusable.
- We have not mentioned any details about how any of the operations are performed, how data is stored or what the model represents.

OOPS Abstract Design

- OOPS is independent of the model and the physical system it represents.
- Flexibility (including yet unknown future development) requires that this goes both ways.
- The Models do not know about the high level algorithm currently being run:
  - All actions are driven by the top level code,
  - All data, input and output, is passed by arguments.
- Models interfaces must be general enough to cater for all cases, and detailed enough to be able to perform the required actions.
- OOPS currently stops at the level of the calls to the forecast model and observation operators but the same principle could be applied at any level.

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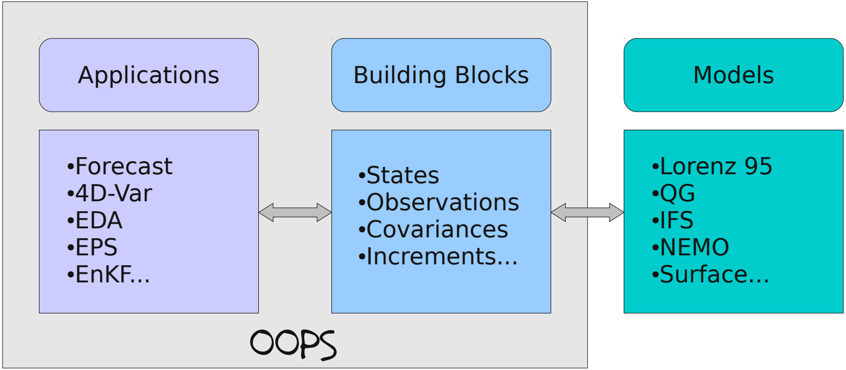

- The high levels Applications use abstract building blocks.
- The Models implement the building blocks.
- OOPS is independent of the Model being driven.

Outline

State-Observations Interactions

- Two classes make the link between the model and observation spaces:
  - Locations
  - ModelAtLocations
- The computation of observations equivalents is done in a `PostProcessor`:
  1. Ask the Observations for a list of locations where there are observations (at the current time)
  2. Ask the State for the model values at these locations
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- Preserves encapsulation (model grid not visible in observation operator).
- But it's up to each model implementation: OOPS does not prevent copying the full State in the GOM...

Cost Function Design

- Naive approach:
  - One object for each term of the cost function.
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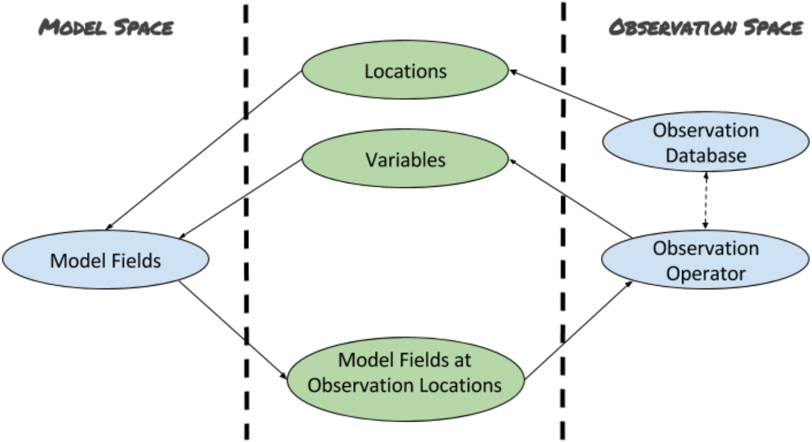
  - Problem: The full 4D state is too big (for us).
- A feasible approach:
  - Run the model once.
  - Compute each term (or gradient) on the fly while the model is running.
  - Add all the terms together.

Cost Function Implementation

- One class for each term (more flexible).
- Call a method on each object on the fly while the model is running.
  - Uses the `PostProcessor` structure already in place (observer pattern).
  - Finalize each term and add the terms together at the end.
  - Saving the model linearization trajectory is also the responsibility of a PostProcessor.
- Each formulation derives from an abstract CostFunction base class.
  - Code duplication between strong and weak constraint 4D-Var: use in the same derived class (weak constraint) or write the weak constraint 4D-Var as a sum of strong constraint terms for each sub-window.
  - It was decided to keep 3D-Var and 4D-Var for readability reasons.
- The terms can be re-used (or not), 4D-Ens-Var was added in a few hours.
  - OO is not magic and will not solve scientific questions by itself.
  - Scientific questions (localization) remain but scientific work can start.
  - Weeks of work would have been necessary in the IFS.

Generic UFO



- Classes have to be compatible
- Generic but not polymorphic

Outline

From (IFS, GSI, NavDAS...) to (OOPS, JEDI)

- The main idea is to keep the computational parts of the existing code and reuse them in a re-designed flexible structure.
- This can be achieved by a top-down and bottom-up approach.
  - From the top: Develop a new, modern, flexible structure (C++).
  - From the bottom: Progressively create self-contained units of code (Fortran).
  - Put the two together: Extract self-contained parts of the IFS and plug them into OOPS.
- From a Fortran point of view, this implies:
  - No global variables,
  - Control via interfaces (derived types passed by arguments).
- This is done at high level in the code.
  - It complements work on code optimisation done at lower level.
- The OO layer developed for the simple models is not only a proof of concept: the same code is re-used to drive the IFS (generic).