Software Infrastructure for Numerical Weather Prediction

OOPS Project

Yannick Trémolet

ECMWF

November 2015

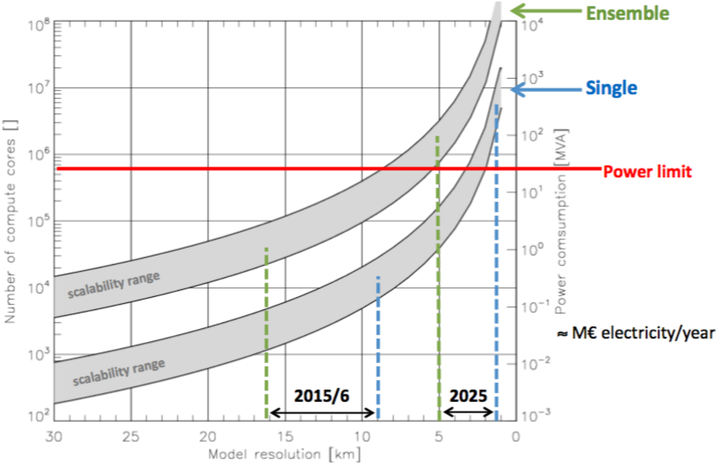
OOPS contributors: P. Bauer, W. Deconinck, M. Fisher, A. Geer, M. Hamrud, P. Lean, O. Marsden, F. Pierfederici, F. Rabier, D. Salmond, J.N. Thépaut, T. Wilhelmson and external collaborators...

Outline

Outline

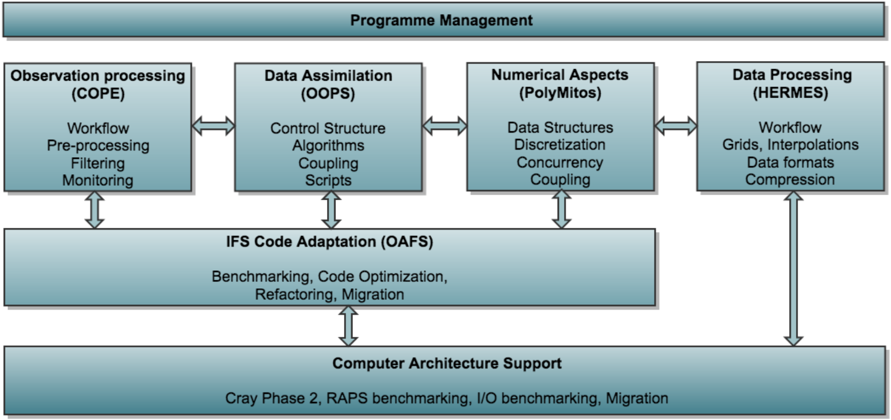
The Scalability Question

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)



Reducing power consumption will require complex architectures

ECMWF Scalability Programme



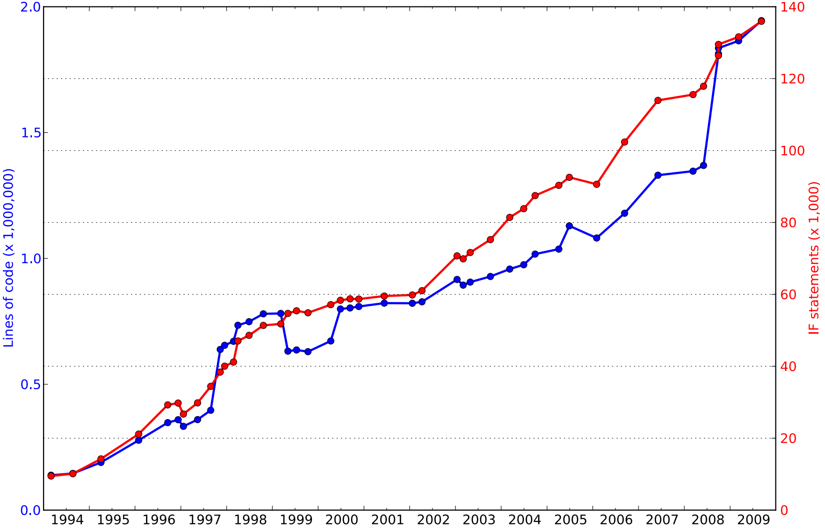
- Implement a formal structure at ECMWF to coordinate science and software activities across departments for efficient exa-scale computing/archiving.
- Include and coordinate all components of the system, including data assimilation, model, data pre- and post-processing and archiving.

Outline

Evolution of Forecasting: Earth System Modelling

- 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.

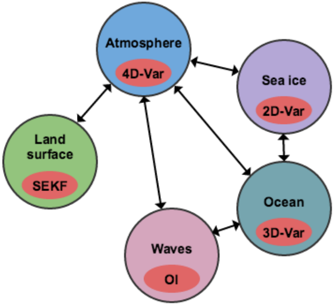
An example: IFS complexity

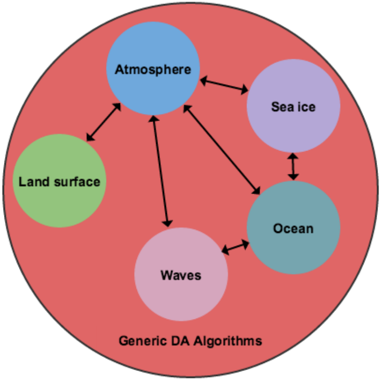


It means growth of maintenance, development costs, and number of bugs.

Earth System Data Assimilation

- Data assimilation systems have been developped for each model.





- Coupled data assimilation requires a common framework.

Outline

Evolution of Data Assimilation

- 4D-Var has been the main staple of data assimilation at ECMWF since 1997.
- The algorithm has progressed to become more complex over the years. It is still being developped and improved (weak constraint, saddle point).
- ECMWF uses an ensemble of 4D-Vars to estimate background error statistics. There are alternatives:
  - EnKF, 4D-En-Var, EVIL...
- Today's best data assimilation algorithms are hybrid:
  - Again, there are a number of options for combining the variational and ensemble aspects
- The data assimilation scene is uncertain but complex...

Complexity

- Computing
- Models
- Data Assimilation
- More and more people are working with the same codes
- Complexity needs to be managed

Outline

Flexible + Reliable = Modular?

- Flexibility:
  - It should be easy to modify the system (new science, new functionality, better scalability...)
- Reliability:
  - The code must run without crashing.
  - For a system like the IFS, the code must do what the user thinks it does.
- Modularity is the answer!
- And 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.
  - Development of a dynamical core on a new model grid should not require knowledge of the data assimilation algorithm.

Flexible + Reliable = Modular?

- Flexibility:
  - It should be easy to modify the system (new science, new functionality, better scalability...)
- Reliability:
  - The code must run without crashing.
  - For a system like the IFS, the code must do what the user thinks it does.
- Modularity is the answer!
- And 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.
  - Development of a dynamical core on a new model grid should not require knowledge of the data assimilation algorithm.
- 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.

- It promotes 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.

Outline

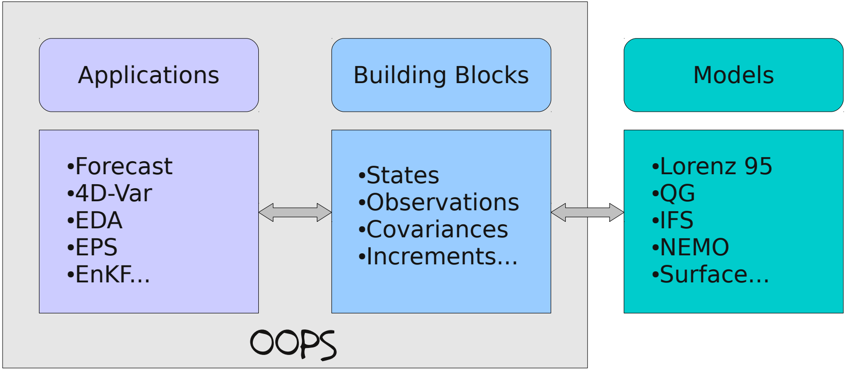
Outline

OOPS Abstract Design

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

- 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



- The high levels Applications use abstract building blocks.
- The Models implement the building blocks.
- OOPS is independent of the Model being driven.
- Models interfaces must be general enough to cater for all cases, and detailed enough to be able to perform the required actions.

Outline

OOPS Classes

- OOPS requires a consistent set of classes that work together with predefined interfaces:

– In model space:

1. Geometry
2. State
3. Increment
4. Model
5. LinearModel (TLM and adjoint)

– In observation space:

6. ObservationSpace
7. ObsVector
8. ObsOperator
9. LinearObsOperator

– To make the link:

10. Locations
11. ModelAtLocations
12. Variables

– Covariance matrices (if generic ones are not used):

13. Model space (**B** and **Q**)
14. Observation space (**R**)
15. Localization (4D-Ens-Var)

- Approximately 100 methods to be implemented (in Fortran or not).

- Observation and model errors (biases) can also be defined.

Model Trait Definition

Actual implementation ⇓ Name used in OOPS ⇓

```
struct QgTraits {
  typedef qg::QgGeometry                Geometry;
  typedef qg::QgState                   State;
  typedef qg::QgIncrement               Increment;
  typedef qg::QgModel                   Model;
  typedef qg::QgTLM                     LinearModel;

  typedef qg::ObsSpaceQG                ObsSpace;
  typedef qg::QgObservation             ObsOperator;
  typedef qg::LinearObsOp               LinearObsOperator;
  typedef qg::ObsVecQG                  ObsVector;

  typedef qg::ObsBias                   ObsAuxControl;
  typedef qg::ObsBiasIncrement          ObsAuxIncrement;
  typedef qg::ObsBiasCovariance         ObsAuxCovariance;

  typedef qg::GomQG                     ModelAtLocations;
  typedef qg::LocQG                     Locations;
  typedef qg::VarQG                     Variables;

  typedef qg::QgErrorCovariance         Covariance;
  typedef qg::LocalizationMatrixQG      LocalizationMatrix;
};
```

The trait is used as a template argument <MODEL>: compile time polymorphism.

Model Trait Definition

Actual implementation ⇓ Name used in OOPS ⇓

```
struct IfsTraits {
  typedef ifs::GeometryIFS              Geometry;
  typedef ifs::StateIFS                 State;
  typedef ifs::IncrementIFS             Increment;
  typedef ifs::ModelIFS                 Model;
  typedef ifs::LinearModelIFS           LinearModel;

  typedef ifs::ODBwrapper               ObsSpace;
  typedef ifs::AllObs                   ObsOperator;
  typedef ifs::AllObsTLAD               LinearObsOperator;
  typedef ifs::ObsVector                ObsVector;

  typedef ifs::ObsBias                  ObsAuxControl;
  typedef ifs::ObsBiasIncrement         ObsAuxIncrement;
  typedef ifs::ObsBiasCovariance        ObsAuxCovariance;

  typedef ifs::GomsIFS                  ModelAtLocations;
  typedef ifs::LocationsIFS             Locations;
  typedef ifs::VariablesIFS             Variables;

  typedef ifs::ErrorCovariance3D        Covariance;
  typedef ifs::LocalizationMatrixIFS    LocalizationMatrix;
};
```

The trait is used as a template argument <MODEL>: compile time polymorphism.

Running a forecast

```
template<typename MODEL>
void Model<MODEL>::forecast(const ModelAuxCtrl_ & mctl,
          const util::Duration & len, PostProcessor<State_> & post) {
    const util::DateTime end(validTime() + len);

    post.initialize(validTime(), end, model_.timestep());
    this->init(model_);
    post.process(*this);

    while (validTime() < end) {
      this->step(model_, mctl);
      post.process(*this);
    }

    post.finalize();
}
```

- forecast calls the PostProcessors at each time step (Observer pattern).
- PostProcessors are very generic: I/O, FullPos, print information...
- It is the responsibility of the PostProcessors to know when and what actions are needed, not of the model.
- The responsibility of the model is to move the state in time, nothing else.

Outline

Cost Function Design

- Naive approach:
  - One object for each term of the cost function.
  - Compute each term (or gradient) and add them together.
  - Problem: The model is run several times (J_o, J_c, J_q)

Cost Function Design

- Naive approach:
  - One object for each term of the cost function.
  - Compute each term (or gradient) and add them together.
  - Problem: The model is run several times (J_o, J_c, J_q)

- Another naive approach:
  - Run the model once and store the full 4D state.
  - Compute each term (or gradient) and add them together.
  - Problem: The full 4D state is too big (for us).

Cost Function Design

- Naive approach:
  - One object for each term of the cost function.
  - Compute each term (or gradient) and add them together.
  - Problem: The model is run several times (J_o, J_c, J_q)
- Another naive approach:
  - Run the model once and store the full 4D state.
  - Compute each term (or gradient) and add them together.
  - 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, using the `PostProcessor` structure already in place.
  - Finalize each term and add the terms together at the end.

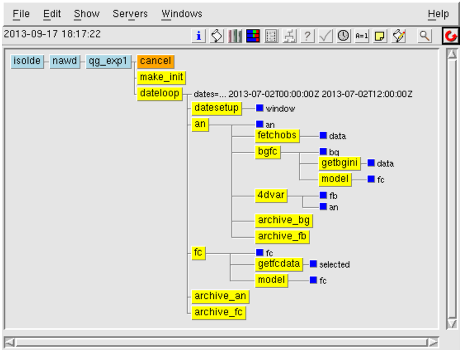
Outline

OOPS Suites and Scripts

- Like the Fortran code, the suite definitions and scripts have become more and more difficult to maintain and develop.
- Complexity will keep increasing in the future:
  - Long overlapping 4D-Var windows,
  - Hybrid data assimilation (EDA and DA coupled two-ways),
  - Coupled ocean-atmosphere models...
- The suite definitions and scripts define the application at the highest level.
  - We should think of them as part of the "system".
- Three levels are mixed together in the suite definitions and scripts:
  - The model (IFS, NEMO...), although the top level of OOPS is generic,
  - The "scientifc" description of the cycling,
  - The workflow "technical" specificity (SMS, ecflow, ...).
- The three levels could be, and should be, isolated from each other.

Prototype with QG toy-model and ecFlow

- A prototype has been implemented in python to test the approach.
- It is organised around tasks whose input and outputs are metadata objects.
- The metadata objects are also used by the workflow to generate the triggers.




```
class Analysis(CompositeTask):

  def compose(self):
    window = self.input('window')

    bg = self.bgfc(window=window)
    obs = self.fetchobs(window=window)
    (an,fb) = self.an4dvar(bg=bg, obs=obs,
                           window=window)
    self.archive_bg(data=bg)
    self.archive_fb(data=fb)

    self.set_output('an', an)
```

- Note that GetBackground is a composite task as well!
- The workflow (ecFlow) is abtracted from the suite definition.

Abstracting the workflow

- Scientists should think as if writing any algorithm.
- Executing the (python) code generates the suite (and scripts).
  - Each component can generate a single task or a family.
  - The workflow is chosen when running the python program.
  - A simple workflow can run the tasks on the fly (toy system on a laptop).
- The workflow can be specialized for Operations to control when the observations are retrieved and the analysis cycle started.
- Everything else is the same: More can be shared between research and operations.

The key is again separation of concerns

Outline

From IFS to OOPS

- The main idea is to keep the efficient 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.

OOPS Summary

- Code components are independent:
  - Components can easily be developed in parallel.
  - Their complexity decreases: less bugs and easier testing and debuging.
- Improved flexibility:
  - Develop new data assimilation (and other) science.
  - Prepares DA for potentially dramatic changes the model (scalability).
  - Explore and improve data assimilation scalability.
  - Changes in one application do not affect other applications.
  - Ability to handle different models opens the door for coupled DA.
- Other projects in the scalability programme are following a similar approach, using OOP (and C++) to abstract low level data structures and architectures.
- The main difficulties are not technical but human...