Scalability of Data Assimilation at ECMWF

Yannick Trémolet

ECMWF

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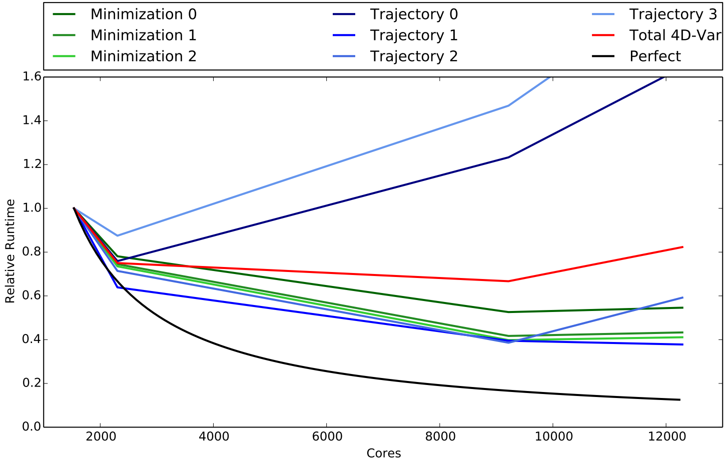
The Ugly Part: Scalability of 4D-Var Today



IFS (41r1), T1279C, T255/T255/T399 on Cray XC30

Our current 4D-Var implementation is not scalable enough for the future.

Improving 4D-Var Scalability

- Data assimilation specific code optimizations:
  - Reduce input observations to the ones actually assimilated (COPE),
  - Reduce I/O (linearization state, preconditioner, ODB): single executable.
- The forecast model is one important component of the data assimilation system (80% of runtime): improvements in the model (and TL/AD) will benefit data assimilation directly.
- The same code adaptations as in the model will be used in other parts of the system (observation operators, covariance matrices, ...)
- However, the lower resolution of most of the data assimilation system ($\approx$20 times less grid-points) makes scalability more problematic.
  - Sequential nature of the minimization algorithm.

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- We get it from the model: as long as the forecast model delivers the same forecast days per day, 4D-Var will run in the same wall clock time.
- Do we need more scalability?
  - Yes, if we want to do better than 4D-Var (better science, better analysis, better forecasts...)

Hybrid Data Assimilation

- Today's best data assimilation algorithms are hybrid.
  - Ensemble DA system for computing background error covariances,
  - Variational DA system to provide the high resolution analysis.

- Hybrid data assimilation systems are very complex.

- There is a choice of ensemble DA methods to choose from.

- 4D-Var provides the best high resolution analysis:
  - one trend is to remove the variational component,
  - another is to improve it (scientifically) and make it more scalable.

Ensemble Data Assimilation

- ECMWF uses an ensemble of 4D-Vars to estimate background error statistics.
- An alternative: EnKF
  - Approximation of a Kalman filter with covariances projected on ensemble space, with issues related to localisation and inflation.
  - A research implementation is maintained at ECMWF.
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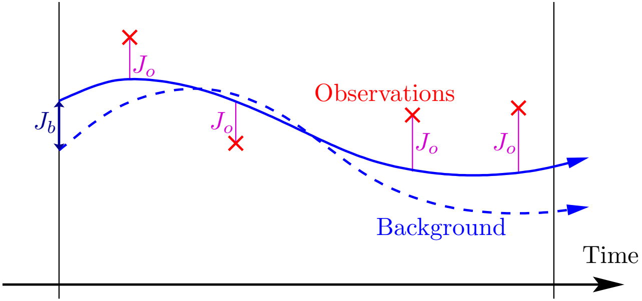
  - Available in OOPS.
- All ensemble DA algorithms require running the members and combining information:
  - The ensemble part scale with the number of members.
  - The combining of information is cheap in computing but expensive in memory and/or I/O. Is that good for the future?
  - The overall cost varies but so far scalability is good.

Parallelism in 4D-Var

- Some aspects of data assimilation that are not available in the forecast model can be exploited.



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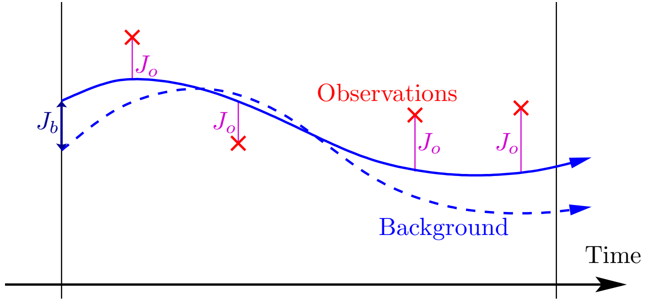
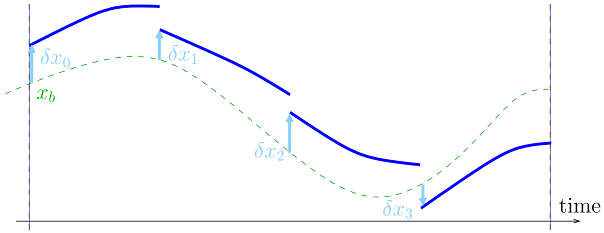


- The observations and background state are available throughout the whole window when we start the assimilation: it is possible to envisage parallelism in the time dimension.
- Assimilation should be considered a 4D problem, not an initial value problem.

Weak Constraint 4D-Var

- The control variable is 4D, with some flexibility w.r.t. the resolution in time (it is already the case in the spatial dimensions).



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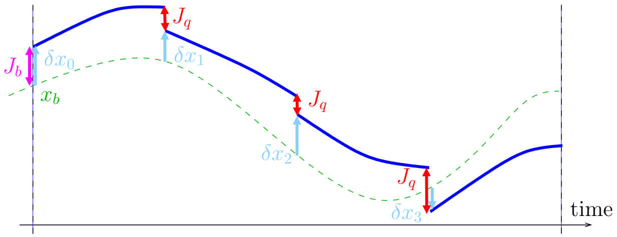

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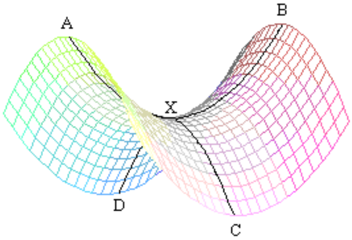
- The additional model error terms (J_q) make the minimization and preconditioning more complex: we need to explore dual (i.e. observation) or mixed primal/dual space algorithms.

- It is also a theoretical improvement of 4D-Var (accounting for model error).

Saddle-Point Formulation of 4D-Var

- The weak constraint 4D-Var problem can be written as a constrained minimisation problem.
- The inner loop minimization problem is replaced by a saddle point optimization problem (Lagrange multiplier approach).
- A few interesting properties are:
  - The inverses of the covariance matrices are not needed,
  - The parallelism over sub-windows is preserved,
  - The tangent linear and adjoint models can run in parallel.



Saddle-Point Formulation of 4D-Var

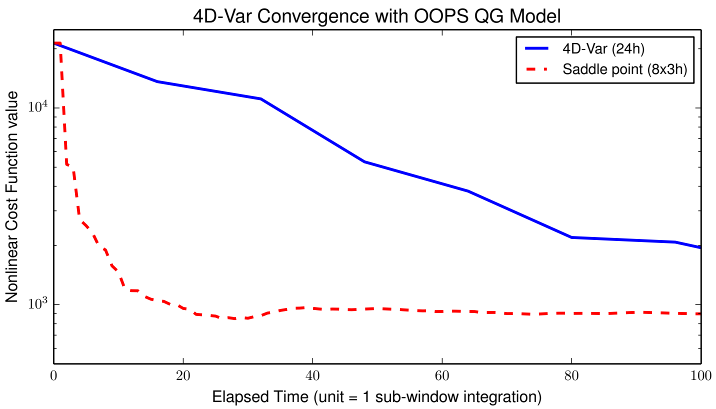


Figure from S. Gürol

- The saddle point formulation of 4D-Var is more scalable.
- Weak constraint 4D-Var is also theoretically better then strong constraint 4D-Var although some questions remain (model error covariance matrix).

Object-Oriented Programming

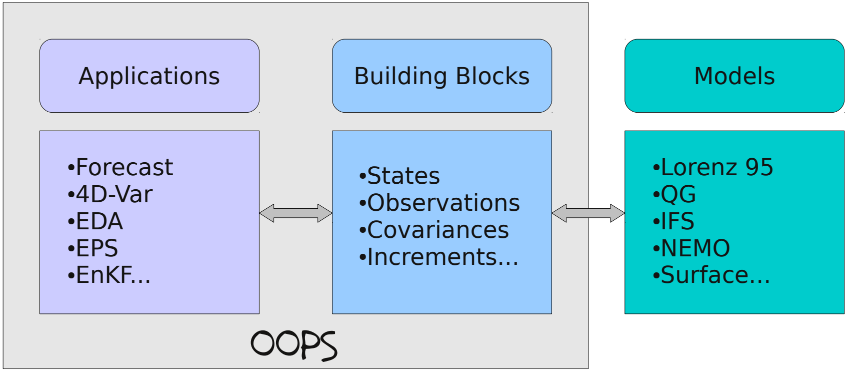
- Exploring parallelism in new directions, through hybrid methods, weak constraint 4D-Var, new minimization algorithms or other techniques, requires considerable changes in the high level data assimilation algorithm.

- All that while getting ready for potential dramatic changes in the model...

- 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 Prediction System



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

From IFS to OOPS

- 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.

OOPS Benefits

- 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.
  - Explore and improve scalability.
  - Changes in one application do not affect other applications.
  - Ability to handle different models opens the door for coupled DA.
- OOPS does not solve scientific problems in itself: it provides a more powerful way to “tell the computer what to do”.
  - 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).

Summary

4D-Var doesn't scale well at the moment.

It is not as bad as it seems.

There are lots of interesting scientific directions to explore to make data assimilation better **and** more scalable!