

Preconditioning Saddle-Point Formulation of the variational data assimilation

M. Fisher¹, S. Gratton^{2,3}, S. Gürol³

¹ECMWF, Reading, UK

²ENSEEIH, Toulouse, France

³CERFACS, Toulouse, France

Colloque National sur l'Assimilation de données, Toulouse, France

1 December 2014

From Mike's presentation we have seen that:

- Incremental 4D-Var suffers from parallelization in the time dimension.
- Solution: Saddle-point approach

From Mike's presentation we have seen that:

- Incremental 4D-Var suffers from parallelization in the time dimension.
- Solution: Saddle-point approach

What will we discuss in this talk?

- Can we maintain good convergence properties of 4D-Var?
- Can we further accelerate the convergence rate?

Preconditioning of saddle point approach

Outline

- Saddle point approach of 4D-Var
- Preconditioning of saddle point formulation
- Numerical results
- Conclusions

Saddle Point Approach

- Let us consider weak-constraint 4D-Var as a constrained problem and write the Lagrangian function. Then the **stationary point** of \mathcal{L} satisfies the system of equations that can be written in a matrix form as:

$$\begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \\ \delta \mathbf{x} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{0} \end{pmatrix}$$

- This system is called the **saddle-point formulation of 4D-Var**.

- $\mathbf{L} = \begin{pmatrix} I & & & & \\ -M_1 & I & & & \\ & -M_2 & I & & \\ & & \ddots & \ddots & \\ & & & -M_N & I \end{pmatrix}$ is an n-by-n matrix.

- $\mathbf{H} = \text{diag}(\mathbf{H}_0, \mathbf{H}_1, \dots, \mathbf{H}_N)$ is an n-by-m matrix.
- $\mathbf{D} = \text{diag}(\mathbf{B}, \mathbf{Q}_1, \dots, \mathbf{Q}_N)$ is an n-by-n matrix.
- $\mathbf{R} = \text{diag}(\mathbf{R}_0, \mathbf{R}_1, \dots, \mathbf{R}_N)$ is an m-by-m matrix.

Saddle Point Approach

- In matrix form:

$$\underbrace{\begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix}}_{\mathcal{A}} \begin{pmatrix} \lambda \\ \mu \\ \delta \mathbf{x} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{0} \end{pmatrix}$$

where \mathcal{A} is a $(2n + m)$ -by- $(2n + m)$ **indefinite symmetric** matrix.

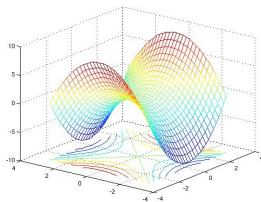
Saddle Point Approach

- In matrix form:

$$\underbrace{\begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix}}_{\mathcal{A}} \begin{pmatrix} \lambda \\ \mu \\ \delta \mathbf{x} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{0} \end{pmatrix}$$

where \mathcal{A} is a $(2n + m)$ -by- $(2n + m)$ **indefinite symmetric** matrix.

- The solution of this problem is a saddle point



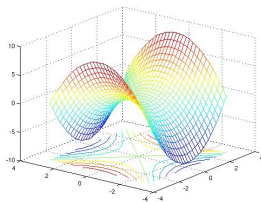
Saddle Point Approach

- In matrix form:

$$\underbrace{\begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix}}_{\mathcal{A}} \begin{pmatrix} \lambda \\ \mu \\ \delta \mathbf{x} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{0} \end{pmatrix}$$

where \mathcal{A} is a $(2n + m)$ -by- $(2n + m)$ **indefinite symmetric** matrix.

- The solution of this problem is a saddle point



→ This approach is **time-parallel**.

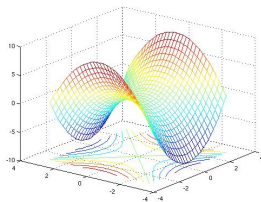
Saddle Point Approach

- In matrix form:

$$\underbrace{\begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix}}_{\mathcal{A}} \begin{pmatrix} \lambda \\ \mu \\ \delta \mathbf{x} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{0} \end{pmatrix}$$

where \mathcal{A} is a $(2n + m)$ -by- $(2n + m)$ **indefinite symmetric** matrix.

- The solution of this problem is a saddle point



→ This approach is **time-parallel**.

→ Solution algorithm: GMRES method with a preconditioner.

Outline

- Saddle point approach of 4D-Var
- Preconditioning of saddle point formulation
- Numerical results
- Conclusions

Preconditioning

- A preconditioner attempts to **improve the spectral properties** of the system matrix \mathcal{A} .

Preconditioning

- A preconditioner attempts to **improve the spectral properties** of the system matrix \mathcal{A} .
- When using GMRES, a **clustered spectrum** often results in **rapid convergence**, especially the departure from normality of the preconditioned matrix is not too high (Benzi et. al 2005).

Preconditioning

- A preconditioner attempts to **improve the spectral properties** of the system matrix \mathcal{A} .
- When using GMRES, a **clustered spectrum** often results in **rapid convergence**, especially the departure from normality of the preconditioned matrix is not too high (Benzi et. al 2005).

→ When solving an indefinite saddle point system with GMRES, it is crucial to find an efficient preconditioner.

Preconditioning

- A preconditioner attempts to **improve the spectral properties** of the system matrix \mathcal{A} .
- When using GMRES, a **clustered spectrum** often results in **rapid convergence**, especially the departure from normality of the preconditioned matrix is not too high (Benzi et. al 2005).

→ When solving an indefinite saddle point system with GMRES, it is crucial to find an efficient preconditioner.

Efficient preconditioner \mathcal{P}

- is an approximation to \mathcal{A}
- the cost of constructing and applying the preconditioner should be less than the gain in computational cost
- exploits the block structure of the problem for saddle point systems

Preconditioning

- A preconditioner attempts to **improve the spectral properties** of the system matrix \mathcal{A} .
- When using GMRES, a **clustered spectrum** often results in **rapid convergence**, especially the departure from normality of the preconditioned matrix is not too high (Benzi et. al 2005).

→ When solving an indefinite saddle point system with GMRES, it is crucial to find an efficient preconditioner.

Efficient preconditioner \mathcal{P}

- is an approximation to \mathcal{A}
- the cost of constructing and applying the preconditioner should be less than the gain in computational cost
- exploits the block structure of the problem for saddle point systems

Implementation

- Solving a system $\mathcal{A}\mathbf{u} = \mathbf{f}$ with a preconditioner \mathcal{P} requires solving

$$(\mathcal{P}^{-1}\mathcal{A})\mathbf{u} = \mathcal{P}^{-1}\mathbf{f}$$

Preconditioning Saddle Point Systems

$$\mathcal{A} = \begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix}$$

- Block preconditioners (Kuznetsov (1995), Murphy, Golub and Wathen (2000), Bramble and Pasciak (1988))

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & -\mathbf{S} \end{pmatrix}, \quad \mathcal{P} = \begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{0} & \mathbf{S} \end{pmatrix}$$

where $\mathbf{S} = \mathbf{B}\mathbf{A}^{-1}\mathbf{B}^T$ is the Schur complement (the unpreconditioned 4D-Var Hessian).

- Constraint preconditioners (Bergamaschi et. al (2004), Gould and Wathen (2000), Benzi et al. 2005)

$$\mathcal{P} = \begin{pmatrix} \tilde{\mathbf{A}} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix}$$

It is assumed that solving the system involving \mathcal{P} is significantly easier than solving the original system.

- Hermitian and skew Hermitian splitting of \mathcal{A} , stationary iterative methods, multilevel methods, ... (Benzi et al (2005))

Preconditioning Saddle Point Formulation of 4D-Var

$$\mathcal{A} = \begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix}$$

- The **inexact constraint preconditioner** proposed by (Bergamaschi et. al. 2005) is promising for our application. The preconditioner can be chosen as:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{D} & \mathbf{0} & \tilde{\mathbf{L}} \\ \mathbf{0} & \mathbf{R} & \mathbf{0} \\ \tilde{\mathbf{L}}^T & \mathbf{0} & \mathbf{0} \end{pmatrix}$$

where

- $\tilde{\mathbf{L}}$ is an approximation to the matrix \mathbf{L}
- $\tilde{\mathbf{B}} = [\tilde{\mathbf{L}}^T \quad \mathbf{0}]$ is a full row rank approximation of the matrix $\mathbf{B} \in \mathbb{R}^{n \times (m+n)}$

Preconditioning Saddle Point Formulation of 4D-Var

$$\underbrace{\begin{pmatrix} \mathbf{D} & \mathbf{0} & \mathbf{L} \\ \mathbf{0} & \mathbf{R} & \mathbf{H} \\ \mathbf{L}^T & \mathbf{H}^T & \mathbf{0} \end{pmatrix}}_{\mathcal{A}_k} \underbrace{\begin{pmatrix} \lambda \\ \mu \\ \delta \mathbf{x} \end{pmatrix}}_{\mathbf{u}} = \underbrace{\begin{pmatrix} \mathbf{b} \\ \mathbf{d} \\ \mathbf{0} \end{pmatrix}}_{\mathbf{f}_k}$$

When solving a **sequence of saddle point systems**, can we **further improve the preconditioning** for the outer loops $k > 1$?

Can we find **low-rank updates** for the inexact constraint preconditioner that approximates \mathcal{A}^{-1} or its effect on a vector?

Preconditioning Saddle Point Formulation of 4D-Var

- For $k = 1$, we have the inexact constraint preconditioner:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix}$$

Preconditioning Saddle Point Formulation of 4D-Var

- For $k = 1$, we have the inexact constraint preconditioner:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix}$$

- For $k > 1$, we want to find a low-rank update $\Delta \mathbf{B} = \mathbf{B} - \tilde{\mathbf{B}}$ and use the updated preconditioner:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix}$$

Preconditioning Saddle Point Formulation of 4D-Var

- For $k = 1$, we have the inexact constraint preconditioner:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix}$$

- For $k > 1$, we want to find a low-rank update $\Delta \mathbf{B} = \mathbf{B} - \tilde{\mathbf{B}}$ and use the updated preconditioner:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix}$$

→ GMRES performs matrix-vector products with \mathcal{A} :

$$\underbrace{\begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix}}_{\mathcal{A}_k} \underbrace{\begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix}}_{\mathbf{u}_j^{(k)}} = \underbrace{\begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix}}_{\mathbf{f}_j^{(k)}}$$

Preconditioning Saddle Point Formulation of 4D-Var

- For $k = 1$, we have the inexact constraint preconditioner:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix}$$

- For $k > 1$, we want to find a low-rank update $\Delta \mathbf{B} = \mathbf{B} - \tilde{\mathbf{B}}$ and use the updated preconditioner:

$$\mathcal{P} = \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix}$$

→ GMRES performs matrix-vector products with \mathcal{A} :

$$\underbrace{\begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix}}_{\mathcal{A}_k} \underbrace{\begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix}}_{\mathbf{u}_j^{(k)}} = \underbrace{\begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix}}_{\mathbf{f}_j^{(k)}}$$

→ We can use the pairs $(\mathbf{u}_j^{(k)}, \mathbf{f}_j^{(k)})$ to find an update $\Delta \mathbf{B}$.

Preconditioning Saddle Point Formulation of 4D-Var

$$\begin{aligned}
 \begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} &= \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \\
 &\Rightarrow \quad \begin{pmatrix} \mathbf{A}\mathbf{u}_1 + \tilde{\mathbf{B}}^T\mathbf{u}_2 \\ \tilde{\mathbf{B}}\mathbf{u}_1 \end{pmatrix} + \begin{pmatrix} \Delta \mathbf{B}^T\mathbf{u}_2 \\ \Delta \mathbf{B}\mathbf{u}_1 \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \\
 &\Rightarrow \quad \begin{pmatrix} \Delta \mathbf{B}^T\mathbf{u}_2 \\ \Delta \mathbf{B}\mathbf{u}_1 \end{pmatrix} = \begin{pmatrix} \mathbf{b} - \mathbf{A}\mathbf{u}_1 - \tilde{\mathbf{B}}^T\mathbf{u}_2 \\ \mathbf{c} - \tilde{\mathbf{B}}\mathbf{u}_1 \end{pmatrix}
 \end{aligned}$$

Preconditioning Saddle Point Formulation of 4D-Var

$$\begin{aligned}
 \begin{pmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} &= \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \Rightarrow \begin{pmatrix} \mathbf{A} & \tilde{\mathbf{B}}^T \\ \tilde{\mathbf{B}} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \\
 &\Rightarrow \begin{pmatrix} \mathbf{A}\mathbf{u}_1 + \tilde{\mathbf{B}}^T\mathbf{u}_2 \\ \tilde{\mathbf{B}}\mathbf{u}_1 \end{pmatrix} + \begin{pmatrix} \Delta \mathbf{B}^T\mathbf{u}_2 \\ \Delta \mathbf{B}\mathbf{u}_1 \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix} \\
 &\Rightarrow \begin{pmatrix} \Delta \mathbf{B}^T\mathbf{u}_2 \\ \Delta \mathbf{B}\mathbf{u}_1 \end{pmatrix} = \begin{pmatrix} \mathbf{b} - \mathbf{A}\mathbf{u}_1 - \tilde{\mathbf{B}}^T\mathbf{u}_2 \\ \mathbf{c} - \tilde{\mathbf{B}}\mathbf{u}_1 \end{pmatrix}
 \end{aligned}$$

- Let's define the vectors \mathbf{r}_b and \mathbf{r}_c as

$$\mathbf{r}_b = \mathbf{b} - \mathbf{A}\mathbf{u}_1 - \tilde{\mathbf{B}}^T\mathbf{u}_2$$

$$\mathbf{r}_c = \mathbf{c} - \tilde{\mathbf{B}}\mathbf{u}_1$$

- Then we have

$$\Delta \mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b \tag{1}$$

$$\Delta \mathbf{B} \mathbf{u}_1 = \mathbf{r}_c \tag{2}$$

→ We want to find an update $\Delta \mathbf{B}$ satisfying these equations.

Preconditioning Saddle Point Formulation of 4D-Var

- A rank-1 update to $\Delta \mathbf{B}$ can be given by

$$\Delta \mathbf{B} = \alpha \mathbf{v} \mathbf{w}^T$$

where $\mathbf{v} \in \mathbb{R}^n$ and $\mathbf{w} \in \mathbb{R}^{n+m}$.

Preconditioning Saddle Point Formulation of 4D-Var

- A rank-1 update to $\Delta \mathbf{B}$ can be given by

$$\Delta \mathbf{B} = \alpha \mathbf{v} \mathbf{w}^T$$

where $\mathbf{v} \in \mathbb{R}^n$ and $\mathbf{w} \in \mathbb{R}^{n+m}$.

- Substituting this relation into equations (1) and (2), we get

$$\Delta \mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b \Leftrightarrow \alpha \mathbf{w} \mathbf{v}^T \mathbf{u}_2 = \mathbf{r}_b$$

$$\Delta \mathbf{B} \mathbf{u}_1 = \mathbf{r}_c \Leftrightarrow \alpha \mathbf{v} \mathbf{w}^T \mathbf{u}_1 = \mathbf{r}_c$$

from which we obtain that

$$\mathbf{w} = \mathbf{r}_b / \alpha \mathbf{v}^T \mathbf{u}_2$$

$$\mathbf{v} = \mathbf{r}_c / \alpha \mathbf{w}^T \mathbf{u}_1$$

Preconditioning Saddle Point Formulation of 4D-Var

- A rank-1 update to $\Delta \mathbf{B}$ can be given by

$$\Delta \mathbf{B} = \alpha \mathbf{v} \mathbf{w}^T$$

where $\mathbf{v} \in \mathbb{R}^n$ and $\mathbf{w} \in \mathbb{R}^{n+m}$.

- Substituting this relation into equations (1) and (2), we get

$$\Delta \mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b \Leftrightarrow \alpha \mathbf{w} \mathbf{v}^T \mathbf{u}_2 = \mathbf{r}_b$$

$$\Delta \mathbf{B} \mathbf{u}_1 = \mathbf{r}_c \Leftrightarrow \alpha \mathbf{v} \mathbf{w}^T \mathbf{u}_1 = \mathbf{r}_c$$

from which we obtain that

$$\mathbf{w} = \mathbf{r}_b / \alpha \mathbf{v}^T \mathbf{u}_2$$

$$\mathbf{v} = \mathbf{r}_c / \alpha \mathbf{w}^T \mathbf{u}_1$$

- With the choice of

$$\mathbf{w} = \mathbf{r}_b$$

and

$$\mathbf{v} = \mathbf{r}_c$$

we can show that α is compatible and given as

$$\alpha = 1 / \mathbf{v}^T \mathbf{u}_2 = 1 / \mathbf{w}^T \mathbf{u}_1$$

Preconditioning Saddle Point Formulation of 4D-Var

- As a result, an inexact constraint preconditioner \mathcal{P} can be updated from

$$\mathcal{P}_{j+1} = \mathcal{P}_j + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix} = \mathcal{P}_j + \begin{pmatrix} \mathbf{0} & \alpha \mathbf{w} \mathbf{v}^T \\ \alpha \mathbf{v} \mathbf{w}^T & \mathbf{0} \end{pmatrix},$$

where $\mathbf{w} = \mathbf{r}_b$, $\mathbf{v} = \mathbf{r}_c$ and $\alpha = 1/\mathbf{v}^T \mathbf{u}_2$.

Preconditioning Saddle Point Formulation of 4D-Var

- As a result, an inexact constraint preconditioner \mathcal{P} can be updated from

$$\mathcal{P}_{j+1} = \mathcal{P}_j + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix} = \mathcal{P}_j + \begin{pmatrix} \mathbf{0} & \alpha \mathbf{w} \mathbf{v}^T \\ \alpha \mathbf{v} \mathbf{w}^T & \mathbf{0} \end{pmatrix},$$

where $\mathbf{w} = \mathbf{r}_b$, $\mathbf{v} = \mathbf{r}_c$ and $\alpha = 1/\mathbf{v}^T \mathbf{u}_2$.

- We can rewrite this formula as

$$\mathcal{P}_{j+1} = \mathcal{P}_j + \underbrace{\begin{pmatrix} \mathbf{0} & \mathbf{w} \\ \mathbf{v} & \mathbf{0} \end{pmatrix}}_{\mathbf{F}} \underbrace{\begin{pmatrix} \alpha \mathbf{w}^T & \mathbf{0} \\ \mathbf{0} & \alpha \mathbf{v}^T \end{pmatrix}}_{\mathbf{G}}$$

where \mathbf{F} is an $(2n + m)$ -by-2 matrix and \mathbf{G} is an 2-by- $(2n + m)$ matrix.

Preconditioning Saddle Point Formulation of 4D-Var

- As a result, an inexact constraint preconditioner \mathcal{P} can be updated from

$$\mathcal{P}_{j+1} = \mathcal{P}_j + \begin{pmatrix} \mathbf{0} & \Delta \mathbf{B}^T \\ \Delta \mathbf{B} & \mathbf{0} \end{pmatrix} = \mathcal{P}_j + \begin{pmatrix} \mathbf{0} & \alpha \mathbf{w} \mathbf{v}^T \\ \alpha \mathbf{v} \mathbf{w}^T & \mathbf{0} \end{pmatrix},$$

where $\mathbf{w} = \mathbf{r}_b$, $\mathbf{v} = \mathbf{r}_c$ and $\alpha = 1/\mathbf{v}^T \mathbf{u}_2$.

- We can rewrite this formula as

$$\mathcal{P}_{j+1} = \mathcal{P}_j + \underbrace{\begin{pmatrix} \mathbf{0} & \mathbf{w} \\ \mathbf{v} & \mathbf{0} \end{pmatrix}}_{\mathbf{F}} \underbrace{\begin{pmatrix} \alpha \mathbf{w}^T & \mathbf{0} \\ \mathbf{0} & \alpha \mathbf{v}^T \end{pmatrix}}_{\mathbf{G}}$$

where \mathbf{F} is an $(2n + m)$ -by-2 matrix and \mathbf{G} is an 2-by- $(2n + m)$ matrix.

- Using the Sherman-Morrison-Woodbury formula on this equation gives the inverse update as

$$\mathcal{P}_{j+1}^{-1} = \mathcal{P}_j^{-1} - \mathcal{P}_j^{-1} \mathbf{F} (\mathbf{I}_2 + \mathbf{G} \mathcal{P}_j^{-1} \mathbf{F})^{-1} \mathbf{G} \mathcal{P}_j^{-1}$$

Preconditioning Saddle Point Formulation of 4D-Var

- We have shown that it is possible to find a **low-cost low-rank update** for the inexact constraint preconditioner.

Preconditioning Saddle Point Formulation of 4D-Var

- We have shown that it is possible to find a **low-cost low-rank update** for the inexact constraint preconditioner.
- This update amounts to the **two-sided-rank-one (TR1)** update proposed by Griewank and Walther (2002).

TR1 update:

- It generalizes the classical symmetric rank-one update.
- It maintains the validity of all previous secant conditions.
- It is invariant with respect to linear transformations

Preconditioning Saddle Point Formulation of 4D-Var

- We have shown that it is possible to find a **low-cost low-rank update** for the inexact constraint preconditioner.
- This update amounts to the **two-sided-rank-one (TR1)** update proposed by Griewank and Walther (2002).

TR1 update:

- It generalizes the classical symmetric rank-one update.
- It maintains the validity of all previous secant conditions.
- It is invariant with respect to linear transformations
- **It has no least change characterization in terms of any particular matrix norm.**

Preconditioning Saddle Point Formulation of 4D-Var

- We have shown that it is possible to find a **low-cost low-rank update** for the inexact constraint preconditioner.
- This update amounts to the **two-sided-rank-one (TR1)** update proposed by Griewank and Walther (2002).

TR1 update:

- It generalizes the classical symmetric rank-one update.
- It maintains the validity of all previous secant conditions.
- It is invariant with respect to linear transformations
- **It has no least change characterization in terms of any particular matrix norm.**

→ Next slides are dedicated to find the **least-Frobenius norm update**.

$$\text{Frobenius norm : } \|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}^2|}$$

Preconditioning Saddle Point Formulation of 4D-Var

- Remember that we want to find an update such that

$$\Delta \mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b \quad (1)$$

$$\Delta \mathbf{B} \mathbf{u}_1 = \mathbf{r}_c \quad (2)$$

Preconditioning Saddle Point Formulation of 4D-Var

- Remember that we want to find an update such that

$$\Delta \mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b \quad (1)$$

$$\Delta \mathbf{B} \mathbf{u}_1 = \mathbf{r}_c \quad (2)$$

- Any solution $\Delta \mathbf{B}$ satisfying Equation (1) can be written as [Lemma 2.1](Sun 1999)

$$\Delta \mathbf{B}^T = \mathbf{r}_b \mathbf{u}_2^\dagger + \mathbf{S}(\mathbf{I} - \mathbf{u}_2 \mathbf{u}_2^\dagger),$$

where \dagger denotes the pseudo-inverse and \mathbf{S} is an $(n + m) \times n$ matrix. Inserting this relation into (2) yields

$$\mathbf{u}_2^{T\dagger} \mathbf{r}_b^T \mathbf{u}_1 + (\mathbf{I} - \mathbf{u}_2^{T\dagger} \mathbf{u}_2^T) \mathbf{S}^T \mathbf{u}_1 = \mathbf{r}_c.$$

Preconditioning Saddle Point Formulation of 4D-Var

- Remember that we want to find an update such that

$$\Delta \mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b \quad (1)$$

$$\Delta \mathbf{B} \mathbf{u}_1 = \mathbf{r}_c \quad (2)$$

- Any solution $\Delta \mathbf{B}$ satisfying Equation (1) can be written as [Lemma 2.1](Sun 1999)

$$\Delta \mathbf{B}^T = \mathbf{r}_b \mathbf{u}_2^\dagger + \mathbf{S}(\mathbf{I} - \mathbf{u}_2 \mathbf{u}_2^\dagger),$$

where \dagger denotes the pseudo-inverse and \mathbf{S} is an $(n + m) \times n$ matrix. Inserting this relation into (2) yields

$$\mathbf{u}_2^{T\dagger} \mathbf{r}_b^T \mathbf{u}_1 + (\mathbf{I} - \mathbf{u}_2^{T\dagger} \mathbf{u}_2^T) \mathbf{S}^T \mathbf{u}_1 = \mathbf{r}_c.$$

- If this equation admits one solution, its **least Frobenius norm solution**,

$$\min_{\mathbf{S}^T \in \mathbb{R}^{m \times n}} \|(\mathbf{r}_c - \mathbf{u}_2^{T\dagger} \mathbf{r}_b^T \mathbf{u}_1) - (\mathbf{I} - \mathbf{u}_2^{T\dagger} \mathbf{u}_2^T) \mathbf{S}^T \mathbf{u}_1\|_F,$$

can be written as [Lemma 2.3](Sun 1999)

$$(\mathbf{S}^T)^* = (\mathbf{I} - \mathbf{u}_2^{T\dagger} \mathbf{u}_2^T)^\dagger (\mathbf{r}_c - \mathbf{u}_2^{T\dagger} \mathbf{r}_b^T \mathbf{u}_1) \mathbf{u}_1^\dagger.$$

Preconditioning Saddle Point Formulation of 4D-Var

- Substituting the solution for \mathbf{S} into $\Delta\mathbf{B}$ yields that

$$\Delta\mathbf{B}^* = \mathbf{u}_2^{\text{T}\dagger} \mathbf{r}_b^{\text{T}} + (\mathbf{I} - \mathbf{u}_2^{\text{T}\dagger} \mathbf{u}_2^{\text{T}}) \mathbf{r}_c \mathbf{u}_1^{\dagger}$$

Preconditioning Saddle Point Formulation of 4D-Var

- Substituting the solution for \mathbf{S} into $\Delta\mathbf{B}$ yields that

$$\Delta\mathbf{B}^* = \mathbf{u}_2^{\text{T}\dagger} \mathbf{r}_b^{\text{T}} + (\mathbf{I} - \mathbf{u}_2^{\text{T}\dagger} \mathbf{u}_2^{\text{T}}) \mathbf{r}_c \mathbf{u}_1^{\dagger}$$

- This formula is not invariant with respect to linear transformations.

Preconditioning Saddle Point Formulation of 4D-Var

- Substituting the solution for \mathbf{S} into $\Delta\mathbf{B}$ yields that

$$\Delta\mathbf{B}^* = \mathbf{u}_2^{T\dagger} \mathbf{r}_b^T + (\mathbf{I} - \mathbf{u}_2^{T\dagger} \mathbf{u}_2^T) \mathbf{r}_c \mathbf{u}_1^\dagger$$

- This formula is not invariant with respect to linear transformations.
- We want to find such a formula by solving the following variational problem:

$$\min \|\mathbf{W}_1^{-1} \Delta\mathbf{B} \mathbf{W}_2^{-1}\|_F$$

$$\text{s.t. } \Delta\mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b$$

$$\Delta\mathbf{B} \mathbf{u}_1 = \mathbf{r}_c$$

where \mathbf{W}_1 is any symmetric positive definite matrix such that $\mathbf{W}_1 \mathbf{W}_1^T \mathbf{u}_2 = \mathbf{c}$, and \mathbf{W}_2 is any symmetric positive definite matrix such that $\mathbf{W}_2^T \mathbf{W}_2 \mathbf{u}_1 = \mathbf{b}$. For instance, \mathbf{W}_1 can be considered as $\mathbf{B} \mathbf{A}^{-1} \mathbf{B}^T$ and \mathbf{W}_2 can be considered as \mathbf{A} .

Preconditioning Saddle Point Formulation of 4D-Var

- Substituting the solution for \mathbf{S} into $\Delta\mathbf{B}$ yields that

$$\Delta\mathbf{B}^* = \mathbf{u}_2^{\top\dagger} \mathbf{r}_b^{\top} + (\mathbf{I} - \mathbf{u}_2^{\top\dagger} \mathbf{u}_2^{\top}) \mathbf{r}_c \mathbf{u}_1^{\dagger}$$

- This formula is not invariant with respect to linear transformations.
- We want to find such a formula by solving the following variational problem:

$$\min \|\mathbf{W}_1^{-1} \Delta\mathbf{B} \mathbf{W}_2^{-1}\|_F$$

$$\text{s.t. } \Delta\mathbf{B}^T \mathbf{u}_2 = \mathbf{r}_b$$

$$\Delta\mathbf{B} \mathbf{u}_1 = \mathbf{r}_c$$

where \mathbf{W}_1 is any symmetric positive definite matrix such that $\mathbf{W}_1 \mathbf{W}_1^T \mathbf{u}_2 = \mathbf{c}$, and \mathbf{W}_2 is any symmetric positive definite matrix such that $\mathbf{W}_2^T \mathbf{W}_2 \mathbf{u}_1 = \mathbf{b}$. For instance, \mathbf{W}_1 can be considered as $\mathbf{B} \mathbf{A}^{-1} \mathbf{B}^T$ and \mathbf{W}_2 can be considered as \mathbf{A} .

- The solution is given as:

$$\Delta\mathbf{B}^* = \frac{\mathbf{c} \mathbf{r}_b^T}{\mathbf{u}_2^T \mathbf{c}} + \frac{\mathbf{r}_c \mathbf{b}^T}{\mathbf{u}_1^T \mathbf{b}} - \frac{\mathbf{u}_2^T \mathbf{r}_c \mathbf{c} \mathbf{b}^T}{\mathbf{u}_2^T \mathbf{c} \mathbf{u}_1^T \mathbf{b}}$$

- This formula can be rewritten as

$$\Delta \mathbf{B} = \begin{bmatrix} \frac{\mathbf{c}}{\mathbf{u}_2^T \mathbf{c}} & \mathbf{r}_c & -\frac{\mathbf{c}}{\mathbf{u}_2^T \mathbf{c}} \end{bmatrix} \begin{bmatrix} \mathbf{r}_b^T \\ \frac{\mathbf{b}^T}{\mathbf{u}_1^T \mathbf{b}} \\ \frac{\mathbf{u}_2^T \mathbf{r}_c \mathbf{b}^T}{\mathbf{u}_1^T \mathbf{b}} \end{bmatrix} = \mathbf{V} \mathbf{W}^T,$$

- This formula can be rewritten as

$$\Delta \mathbf{B} = \begin{bmatrix} \frac{\mathbf{c}}{\mathbf{u}_2^T \mathbf{c}} & \mathbf{r}_c & -\frac{\mathbf{c}}{\mathbf{u}_2^T \mathbf{c}} \end{bmatrix} \begin{bmatrix} \mathbf{r}_b^T \\ \frac{\mathbf{b}^T}{\mathbf{u}_1^T \mathbf{b}} \\ \frac{\mathbf{u}_2^T \mathbf{r}_c \mathbf{b}^T}{\mathbf{u}_1^T \mathbf{b}} \end{bmatrix} = \mathbf{V} \mathbf{W}^T,$$

- The preconditioner can be updated by using the following formula

$$\mathcal{P}_1 = \mathcal{P}_0 + \begin{pmatrix} \mathbf{0} & \mathbf{W} \mathbf{V}^T \\ \mathbf{V} \mathbf{W}^T & \mathbf{0} \end{pmatrix} = \mathcal{P}_0 + \underbrace{\begin{pmatrix} \mathbf{0} & \mathbf{W} \\ \mathbf{V} & \mathbf{0} \end{pmatrix}}_{\mathbf{F}} \underbrace{\begin{pmatrix} \mathbf{W}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{V}^T \end{pmatrix}}_{\mathbf{G}}$$

- The inverse formula is then given by

$$\boxed{\mathcal{P}_F^{-1} = \mathcal{P}_0^{-1} - \mathcal{P}_0^{-1} \mathbf{F} (\mathbf{I}_6 + \mathbf{G} \mathcal{P}_0^{-1} \mathbf{F})^{-1} \mathbf{G} \mathcal{P}_0^{-1}}$$

where \mathbf{F} is an $(2n + m)$ -by-6 matrix and \mathbf{G} is an 6-by- $(2n + m)$ matrix.

Numerical Results

Implementation platform

- We used the Object Oriented Prediction System (OOPS) developed by ECMWF
- OOPS consists of simplified models of a real-system

The model

- It is a two-layer quasi-geostrophic model with 1600 grid-points

Implementation details

- There are 100 observations of stream function every 3 hours, 100 wind observations plus 100 wind-speed observations every 6 hours
- The error covariance matrices are assumed to be horizontally isotropic and homogeneous, with Gaussian spatial structure
- The analysis window is 24 hours, and is divided into 8 subwindows
- 3 outer loops with 10 inner loops each are performed

Methods

- 1 Standard weak-constrained 4D-Var formulation
 - Solution method is preconditioned conjugate-gradients

Methods

- 1 Standard weak-constrained 4D-Var formulation
 - Solution method is preconditioned conjugate-gradients
- 2 Saddle point formulation with an updated inexact constraint preconditioner
 - Solution method is GMRES
 - The initial preconditioner is chosen as

$$\mathcal{P}_0 = \begin{pmatrix} \mathbf{D} & \mathbf{0} & \tilde{\mathbf{L}} \\ \mathbf{0} & \mathbf{R} & \mathbf{0} \\ \tilde{\mathbf{L}}^T & \mathbf{0} & \mathbf{0} \end{pmatrix} \quad \text{with} \quad \tilde{\mathbf{L}} = \begin{pmatrix} \mathbf{I} & & & \\ -\mathbf{I} & \mathbf{I} & & \\ & \ddots & \ddots & \\ & & -\mathbf{I} & \mathbf{I} \end{pmatrix}.$$

Methods

- 1 Standard weak-constrained 4D-Var formulation
→ Solution method is preconditioned conjugate-gradients
- 2 Saddle point formulation with an updated inexact constraint preconditioner
→ Solution method is GMRES
→ The initial preconditioner is chosen as

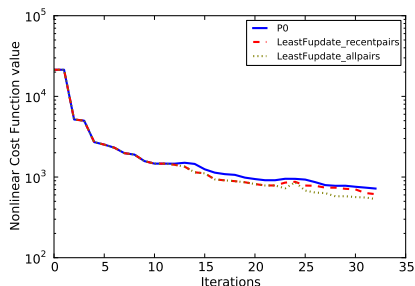
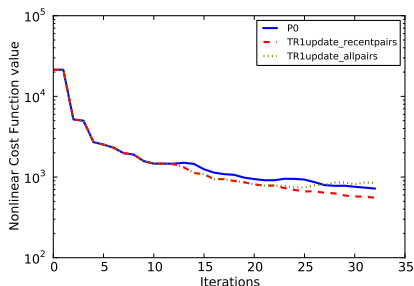
$$\mathcal{P}_0 = \begin{pmatrix} \mathbf{D} & \mathbf{0} & \tilde{\mathbf{L}} \\ \mathbf{0} & \mathbf{R} & \mathbf{0} \\ \tilde{\mathbf{L}}^T & \mathbf{0} & \mathbf{0} \end{pmatrix} \quad \text{with} \quad \tilde{\mathbf{L}} = \begin{pmatrix} \mathbf{I} & & & \\ -\mathbf{I} & \mathbf{I} & & \\ & \ddots & \ddots & \\ & & -\mathbf{I} & \mathbf{I} \end{pmatrix}.$$

$$\mathcal{P}_0^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \tilde{\mathbf{L}}^{-T} \\ \mathbf{0} & \mathbf{R}^{-1} & \mathbf{0} \\ \tilde{\mathbf{L}}^{-1} & \mathbf{0} & -\tilde{\mathbf{L}}^{-1} \mathbf{D} \tilde{\mathbf{L}}^{-T} \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{L}}^{-1} = \begin{pmatrix} \mathbf{I} & & & \\ \mathbf{I} & \mathbf{I} & & \\ \vdots & \ddots & \ddots & \\ \mathbf{I} & \dots & \mathbf{I} & \mathbf{I} \end{pmatrix}.$$

Second-level preconditioners:

- 1 \mathcal{T}_k : The preconditioner obtained by using the TR1 update
- 2 \mathcal{F}_k : The preconditioner obtained by using the least-Frobenius update

The performance of the second level preconditioners



- Second-level preconditioners obtained by using updates may accelerate the convergence
- When all pairs are used the least-Frobenius update is more stable.

Overall performance compared with the standard 4DVar formulation

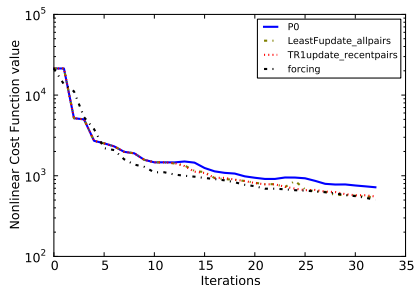


Figure: Nonlinear cost function values along iterations

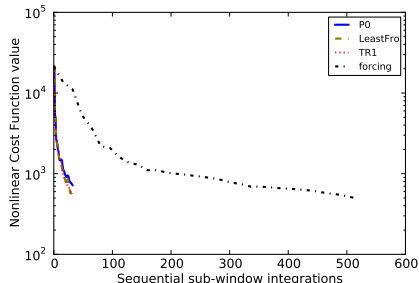


Figure: Nonlinear cost function values along sequential subwindow integrations

- At each iteration the standard 4DVar formulation requires one application of \mathbf{L}^{-1} , followed by one application of \mathbf{L}^{-T} (**16 sequential subwindow integrations**)
- At each iteration of **saddle point formulation** require **one subwindow integration** (provided that \mathbf{L}^{-1} and \mathbf{L}^{-T} are applied simultaneously)

Conclusions

- The saddle point formulation of weak-constraint 4D-Var allows parallelisation in the time dimension.
- Finding an effective preconditioner is a key issue in solving the saddle point systems.
- The inexact constraint preconditioner can be used to precondition the saddle point formulation of 4D-Var.
- When solving a sequence of saddle point systems, a low-rank low-cost update formulas can be found to further improve preconditioning.
- The preconditioned GMRES algorithm for saddle point formulation is competitive with the existing algorithms and has the potential to allow 4D-Var to remain computationally viable on next-generation computer architectures.

Thank you for your attention !