# Introducing time parallelisation within data assimilation using parareal

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## Introduction

## Motivation

- Numerical weather prediction (NWP) heavily relies on the use of high performance architectures to give forecasts in reasonable time
- Example: A climate simulation problem with 50,000 unknowns given 10,000 cores. Using  $10 \times 10$  unknowns for the horizontal domain would use 500 cores.
  - ▶ More cores ⇒ performance loss
- Data assimilation (DA) is a highly sequential algorithm, why not exploit PinT methods...?

In this talk

- Coupling parareal with the data assimilation framework
- Tuning the precision levels in minimisation for running parareal adaptively
- results with a 1D shallow-water model and a theoretical speedup check
- Some of the possible improvements and future work

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In terms of NWP, the aim is to retrieve the *optimal* initial condition which describes the true state of the atmosphere to give an improved forecast



source: dwd.de

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## Data assimilation

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Available information (pressure, temperature, wind speed,...)

- numerical model describing the governing laws/physics
  - $\blacktriangleright$  state vector of order  $10^8 10^9$
- in-situ measurements, satellite data etc
  - $\blacktriangleright$  observation vector of order  $10^6-10^7$



source: dwd.de

Discrete nonlinear model  ${\mathcal F}$  with state variable  ${\boldsymbol x}$ 

$$\begin{aligned} \mathbf{x}(t_0) &= \mathbf{x}_0 \\ \mathbf{x}_i &= \mathcal{F}_{t_{i-1} \to t_i}(\mathbf{x}_{i-1}) \quad i = 1, ..., N \end{aligned} \qquad \qquad N \text{ - no. of time windows} \end{aligned}$$

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- background state x<sup>b</sup><sub>0</sub>
- observations y<sub>i</sub>
- $\bullet$  observation operator  ${\cal H}$
- covariance matrices **B** and **R**



$$\min_{\mathbf{x}_{0} \in \mathbb{R}^{n}} \mathcal{J}(\mathbf{x}_{0}) = \underbrace{\frac{1}{2} \|\mathbf{x}_{0} - \mathbf{x}_{0}^{b}\|_{\mathbf{B}^{-1}}^{2}}_{\mathcal{J}_{b}(\mathbf{x}_{0})} + \underbrace{\frac{1}{2} \sum_{i=0}^{N} \|\mathbf{y}_{i} - \mathcal{H}_{i}(\mathbf{x}_{i})\|_{\mathbf{R}_{i}^{-1}}^{2}}_{\mathcal{J}_{o}(\mathbf{x}_{0})}$$
(2)

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Bhatt, Debreu, and Vidard

## Adjoint - why do we care?

minimisation algorithms involve lots of function and gradient evaluations

 $\mathcal{J}(\mathbf{x}_0) \rightarrow \text{ one model run}$ 

$$\nabla \mathcal{J}(\mathbf{x}_0) = \begin{pmatrix} \frac{\partial \mathcal{J}}{\partial x_1}(\mathbf{x}_0) \\ \vdots \\ \frac{\partial \mathcal{J}}{\partial x_n}(\mathbf{x}_0) \end{pmatrix} \simeq \begin{pmatrix} \frac{\mathcal{J}(\mathbf{x}_0 + \alpha \mathbf{e}_1) - \mathcal{J}(\mathbf{x}_0)}{\alpha} \\ \vdots \\ \frac{\mathcal{J}(\mathbf{x}_0 + \alpha \mathbf{e}_n) - \mathcal{J}(\mathbf{x}_0)}{\alpha} \end{pmatrix} \to n + 1 \text{ model runs}$$

**Tangent linear model** of  $\mathcal{F}$  (for initial perturbation  $\delta \mathbf{x}_0$ )

$$\delta \mathbf{x}_{i+1} = F_i \delta \mathbf{x}$$

Corresponding adjoint equations:

$$\lambda_{N} = H_{N}^{T} \mathbf{R}_{N}^{-1} [\mathbf{y}_{N} - \mathcal{H}_{N}(\mathbf{x}_{N})]$$

$$\lambda_{i} = F_{i}^{T} \lambda_{i+1} + H_{i}^{T} \mathbf{R}_{i}^{-1} [\mathbf{y}_{i} - \mathcal{H}_{i}(\mathbf{x}_{i})] \qquad i = N - 1, \dots, 1$$

$$\lambda_{0} = F_{0}^{T} \lambda_{1} + \mathbf{B}^{-1} (\mathbf{x}_{0} - \mathbf{x}_{0}^{b}) + H_{0}^{T} \mathbf{R}_{0}^{-1} [\mathbf{y}_{0} - \mathcal{H}_{0}(\mathbf{x}_{0})]$$
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Solving (3) gives  $\delta \mathcal{J} = (\lambda_0)^T \delta \mathbf{x}_0 \rightsquigarrow \text{cost around 3 times running forward model}$ 

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- Solve small sub-minimisations by sucessive approximations
- Gives a quadratic J

**Tangent linear approximations** (around  $\mathbf{x}^{(k)}$ )

$$\mathcal{F}(\mathbf{x}^{(k)} + \delta \mathbf{x}^{(k)}) \simeq \mathcal{F}(\mathbf{x}^{(k)}) + F|_{\mathbf{x}^{(k)}} \delta \mathbf{x}^{(k)}$$
  
$$\mathcal{H}(\mathbf{x}^{(k)} + \delta \mathbf{x}^{(k)}) \simeq \mathcal{H}(\mathbf{x}^{(k)}) + H|_{\mathcal{F}(\mathbf{x}^{(k)})} \delta \mathbf{x}^{(k)}$$
(4)



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• At *k*th minimisation solve

$$J^{k}(\delta \mathbf{x}_{0}^{(k)}) = \frac{1}{2} \|\delta \mathbf{x}_{0}^{(k)} - (\mathbf{x}_{0}^{b} - \mathbf{x}_{0}^{(k)})\|_{\mathbf{B}^{-1}}^{2} + \frac{1}{2} \sum_{i=0}^{N} \|\mathbf{y}_{i} - \mathcal{H}_{i} \circ \mathcal{F}(\mathbf{x}_{0}^{(k)} + \delta \mathbf{x}_{0}^{(k)})\|_{\mathbf{R}^{-1}}^{2}$$
(5)

- Innovation vector :  $\mathbf{d}_i = \mathbf{y}_i \mathcal{H}_i \circ \mathcal{F}(\mathbf{x}_0^{(\kappa)})$
- lncrement vector :  $\delta x_0^{(k)} = x_0^{(k+1)} x_0^{(k)}$

<sup>1</sup>Courtier, Thépaut, Hollingsworth (1994)

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$$\begin{aligned} \mathbf{x}(t_0) &= \mathbf{x}_0 \\ \mathbf{x}_{i+1} &= F\mathbf{x}_i \quad i = 1, \dots, N \end{aligned} \qquad \qquad N \text{ - no, of time windows} \end{aligned} \tag{6}$$

#### Description:



- Fine solver computations in parallel
- Nice convergence for parabolic problems, not so good for hyperbolic

#### Error:

With parareal integrator P(k) at iteration k such that  $P(k) {f x}_0 = {f x}_N^k$ , we can write  $^2$ 

$$F^{N} - P(k) = \sum_{p=k+1}^{N} C_{p}^{N} (F - G)^{p} G^{N-p}$$
(7)

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Staff and Ronquist

<sup>3</sup>J. Lions, Y. Maday, and G. Turinici (2001)

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Data assimilation problem: with no background info  $(\mathbf{x}_0^b)$ , a true observation  $\mathbf{y}$  at  $t_N = T$  and H = I.

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Optimality condition:  $\nabla J(\mathbf{x}_0) = 0 \implies$  Solving linear system  $\underbrace{(F^N)^T F^N}_{A^*} \mathbf{x}_0 = \underbrace{(F^N)^T \mathbf{y}}_{\mathbf{b}}$ 

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Idea:

Parareal for forward integration i.e.  $F^N \approx P(k)$ 

$$abla J(\mathbf{x}_0) \approx (F^N)^T (P(k) \mathbf{x}_0 - \mathbf{y})$$

Solve 
$$\longrightarrow \underbrace{(F^N)^T P(k)}_A \mathbf{x}_0 = \underbrace{(F^N)^T \mathbf{y}}_{\mathbf{b}}$$



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 $\rightarrow$  Conjugate gradient for minimisation as  $A^*$  is symmetric

#### Inexact matrix-vector multiplication (a costly operation!)

$$E(k) = A - A^* = -(F^N)^T(F^N - P(k))$$

$$\|E_j p_j\|_{A^{-1}} \le \omega_j \left( \|\mathbf{b}\|_{A^{-1}}, \|\mathbf{p}_j\|_A, \|\mathbf{r}\|_{A^{-1}} \right)$$

$$\|\underbrace{\mathbf{r}(\mathbf{x}_j) - \mathbf{r}_j}_{\text{recidual range}} \|_{A^{-1}} \le \frac{\sqrt{\epsilon}}{2} \|\mathbf{b}\|_{A^{-1}}$$
(10)

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$$J(\mathbf{x}_j) - J(\mathbf{x}_*) \le \epsilon J(\mathbf{x}_*)$$

- Inexact matrix-vector multiplication (a costly operation!)
- By gradually increasing the inexactness of the mat-vec product, one could still produce the exact version's level of accuracy.
- In our case, the perturbation matrix is

$$E(k) = A - A^* = -(F^N)^T (F^N - P(k))$$

**Theorem in nutshell (a bit modified...)**: At icg-iteration *j* if

$$\|E_{j}p_{j}\|_{A^{-1}} \leq \omega_{j}(\|\mathbf{b}\|_{A^{-1}}, \|\mathbf{p}_{j}\|_{A}, \|\mathbf{r}\|_{A^{-1}})$$

then

$$\|\underbrace{\mathbf{r}(\mathbf{x}_j) - \mathbf{r}_j}_{\text{residual rap}}\|_{A^{-1}} \le \frac{\sqrt{\epsilon}}{2} \|\mathbf{b}\|_{A^{-1}}$$
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**p** - direction vector

**r** - inexact residual

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residual gap

If additionally

then the cost function can be monitored as

$$J(\mathbf{x}_j) - J(\mathbf{x}_*) \le \epsilon J(\mathbf{x}_*)$$

- Inexact matrix-vector multiplication (a costly operation!)
- By gradually increasing the inexactness of the mat-vec product, one could still produce the exact version's level of accuracy.
- In our case, the perturbation matrix is

$$E(k) = A - A^* = -(F^N)^T (F^N - P(k))$$

**Theorem in nutshell (a bit modified...)**: At icg-iteration *j* if

$$\|E_j p_j\|_{A^{-1}} \le \omega_j (\|\mathbf{b}\|_{A^{-1}}, \|\mathbf{p}_j\|_A, \|\mathbf{r}\|_{A^{-1}})$$

then

$$\|\underbrace{\mathbf{r}(\mathbf{x}_j) - \mathbf{r}_j}_{\mathbf{r}_j}\|_{A^{-1}} \le \frac{\sqrt{\epsilon}}{2} \|\mathbf{b}\|_{A^{-1}}$$
(10)

**p** - direction vector

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<sup>&</sup>lt;sup>4</sup>Gratton et al, 2021

- In real problems A has a huge size  $\implies$  impractical estimates.
- Gratton et al approximated  $\|\mathbf{p}_j\|_{\mathcal{A}}, J(\mathbf{x}_j), \|\mathbf{b}\|_{\mathcal{A}^{-1}}$  and the termination test (11) by easily computable quantities.
  - $||\mathbf{p}_j||_A \approx \sqrt{\frac{1}{n}} \mathrm{Tr}(A) ||\mathbf{p}_j||_2$
  - $\blacktriangleright J(\mathbf{x}_j) \approx J_j \stackrel{\text{def}}{=} -\frac{1}{2} b^T \mathbf{x}_j$
  - ►  $\|\mathbf{b}\|_{A^{-1}} \approx \frac{\|\mathbf{b}\|_2}{\sqrt{\lambda_{\max}}}$   $j = 0, \mathbf{x}_0 = 0$  and  $\|\mathbf{b}\|_{A^{-1}} \approx \sqrt{2|J_j|}$   $j = 1, 2, ..., j_{\max}$
  - ▶  $\|\mathbf{r}_j\|_{A^{-1}} \le \frac{\epsilon}{2} \|\mathbf{b}\|_{A^{-1}}$  by  $J_{j-d} J_j \le \frac{1}{4} \epsilon |J_j|$  for some integer d
- But now  $||E_i\mathbf{p}_i||_{A^{-1}}$  also needs an approximation!

## Result

If F is invertible,  $||E_j(k)\mathbf{p}_j||_{A^{-1}}$  and  $||P(k)\mathbf{p}_j - F^N\mathbf{p}_j||_2$  are rigorously the same whatever the parareal approximation.  $F^N\mathbf{p}_j$  is the corresponding exact solution.

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• similar profile for  $||E_j\mathbf{p}_j||_{A^{-1}}$ 

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• Start with parareal with a reasonable tolerance and then use previous parareal iterates to approximate  $\|\mathbf{p}_i\|$  for subsequent icg-iterations

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- Check that  $\xi_i$  doesn't lie between last two norm values

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## Shallow water model

1d linear shallow water model

$$\frac{\partial \eta}{\partial t} = -H \frac{\partial u}{\partial x} 
\frac{\partial u}{\partial t} = -g \frac{\partial \eta}{\partial x} + \mu \frac{\partial^2 u}{\partial x^2}$$
(12)

Setup: Arakawa C-grid discretisation

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = C\mathbf{x}, \qquad \mathbf{x} = \begin{pmatrix} \eta \\ u \end{pmatrix}$$

Parameters

#### • N = 20

- no. of fine time steps per time window,  $N_f = 100$
- no. of coarse time steps per time window,  $N_g = 20$
- coarse time step,  $\Delta t = 0.05$
- spatial grid-step,  $\Delta x = 1$
- diffusion constant,  $\mu = 0.15$
- average height, H = 0.9



Coarse and fine propagators are defined using theta scheme  $( heta={ extsf{0.51}})$ 

$$F = [(I - \theta \delta tC)^{-1}(I + (1 - \theta) \delta tC)]^{N_f}$$

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# Exact cg

- Initial condition a gaussian at the middle of the basin/domain
- $\bullet\,$  Using exact CG with  $\epsilon_{\rm cg}=10^{-4},$  takes 24 minimisation iterations



# Exact cg with parareal

- $\bullet\,$  Fixed stopping tolerance for parareal  $\epsilon_{\rm p}=10^{-6},\;\epsilon_{\rm cg}=10^{-4}$
- On average 8.125 p-iterations per icg-iteration



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## Inexact cg with practical estimates

- On average 6.36 p-iterations per icg-iteration, nice!
- Theoretical speedup:  $\frac{N}{\text{p-iterations}} = \frac{20}{6.36} = 3.1$

•  $\omega_j$  is the tolerance for the error norm  $\|E_j(k)\|_{A^{-1},A}$ 



## Retreived initial condition and final results



Bhatt, Debreu, and Vidard

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- Reducing the cost of the coarse solver.
  - Using the Krylov enhanced parareal<sup>5</sup> version. Choosing the right vectors for the convergence of Krylov enhanced method because of storage issues.
- Running a parallel version of adjoint running parareal but in reverse direction leading to double degree of parallelism. Similar error analysis for adjoint.
- Current processes work on synchronicity. Introduce asynchronous methods which don't wait for neighbouring processes and are more linked to the spatial discretisation.
- Other ways to couple DA and PinT algorithms solving the forward and backward model together as a system as done in ParaOpt<sup>6</sup>.
- Extension to 2d model

<sup>&</sup>lt;sup>5</sup>Gander and Petcu, 2008

<sup>&</sup>lt;sup>6</sup>Gander, Kwok and Salomon, 2020