ODEN INSTITUTE
FOR COMPUTATIONAL ENGINEERING & SCIENCES

DESIGN OF AN OCEAN CLIMATE OBSERVING NETWORK IN THE SUBPOLAR NORTH ATLANTIC VIA HESSIAN UNCERTAINTY QUANTIFICATION

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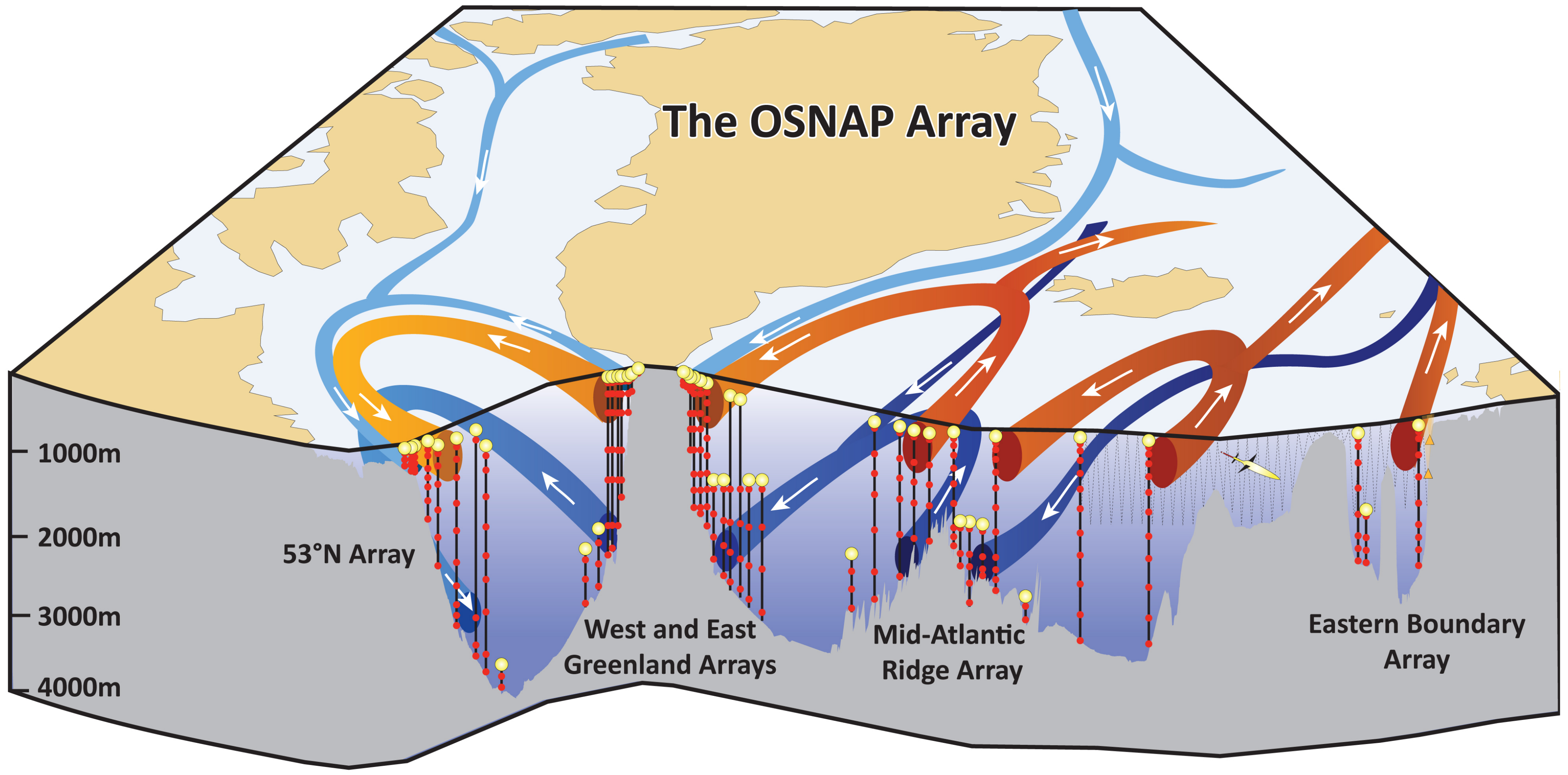
Ocean Observing Systems



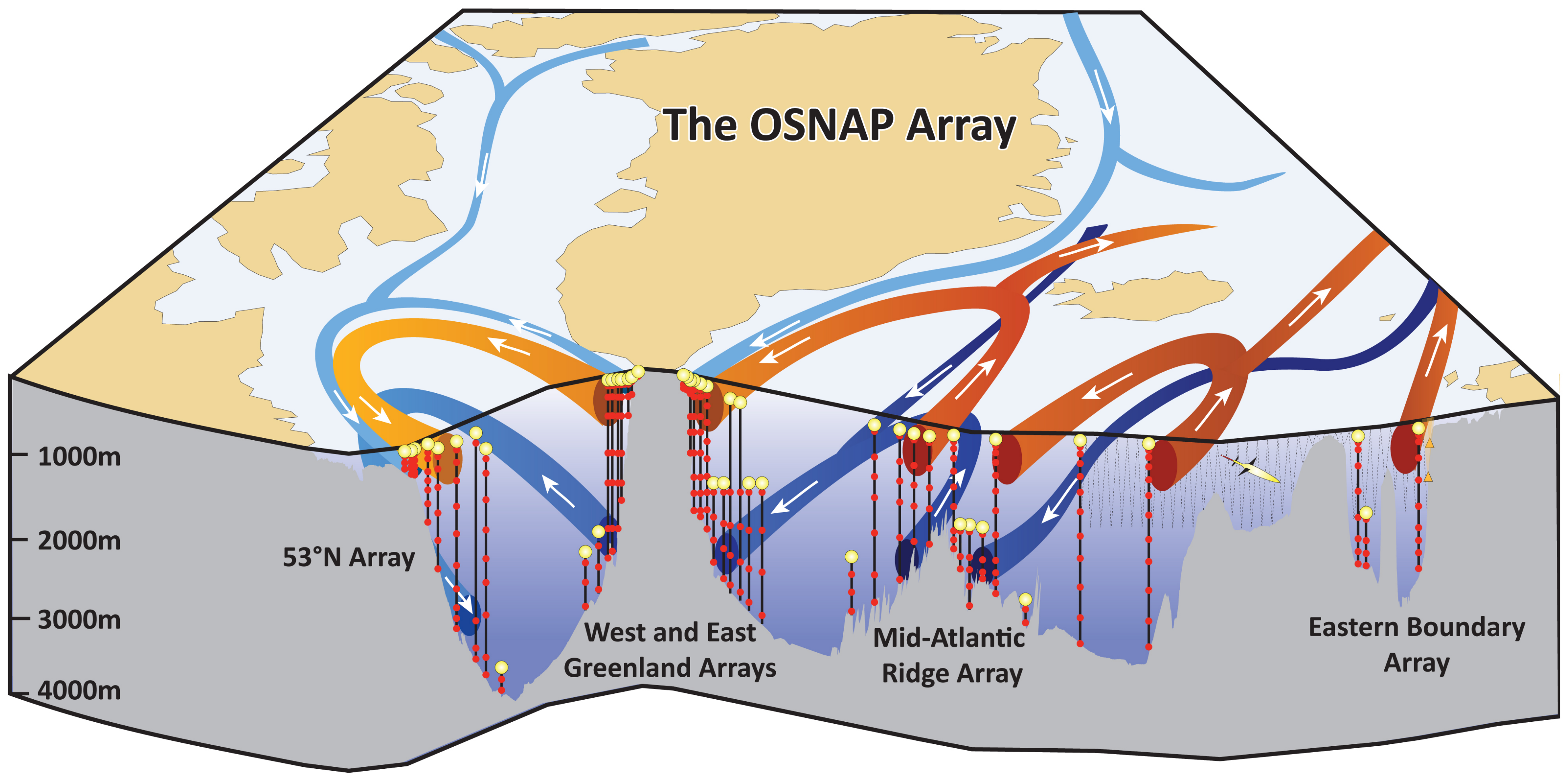
… are crucial for understanding the ocean's role in climate
… but are difficult & expensive to build and maintain

Overturning in the Subpolar North Atlantic Program (OSNAP)

http://www.o-snap.org (since Fall 2014)

Lozier et al., Science (2019)

Ocean Observing Systems



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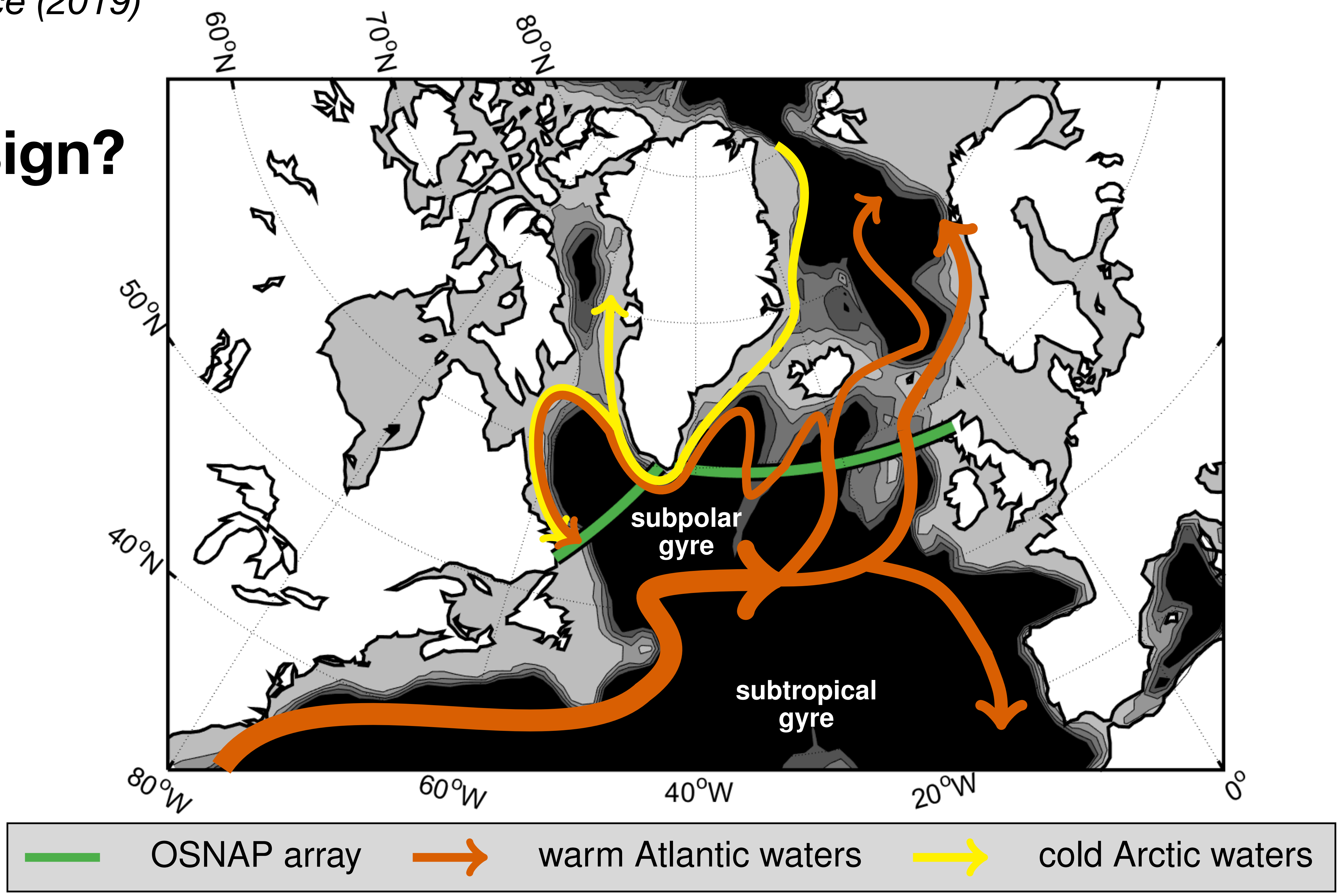
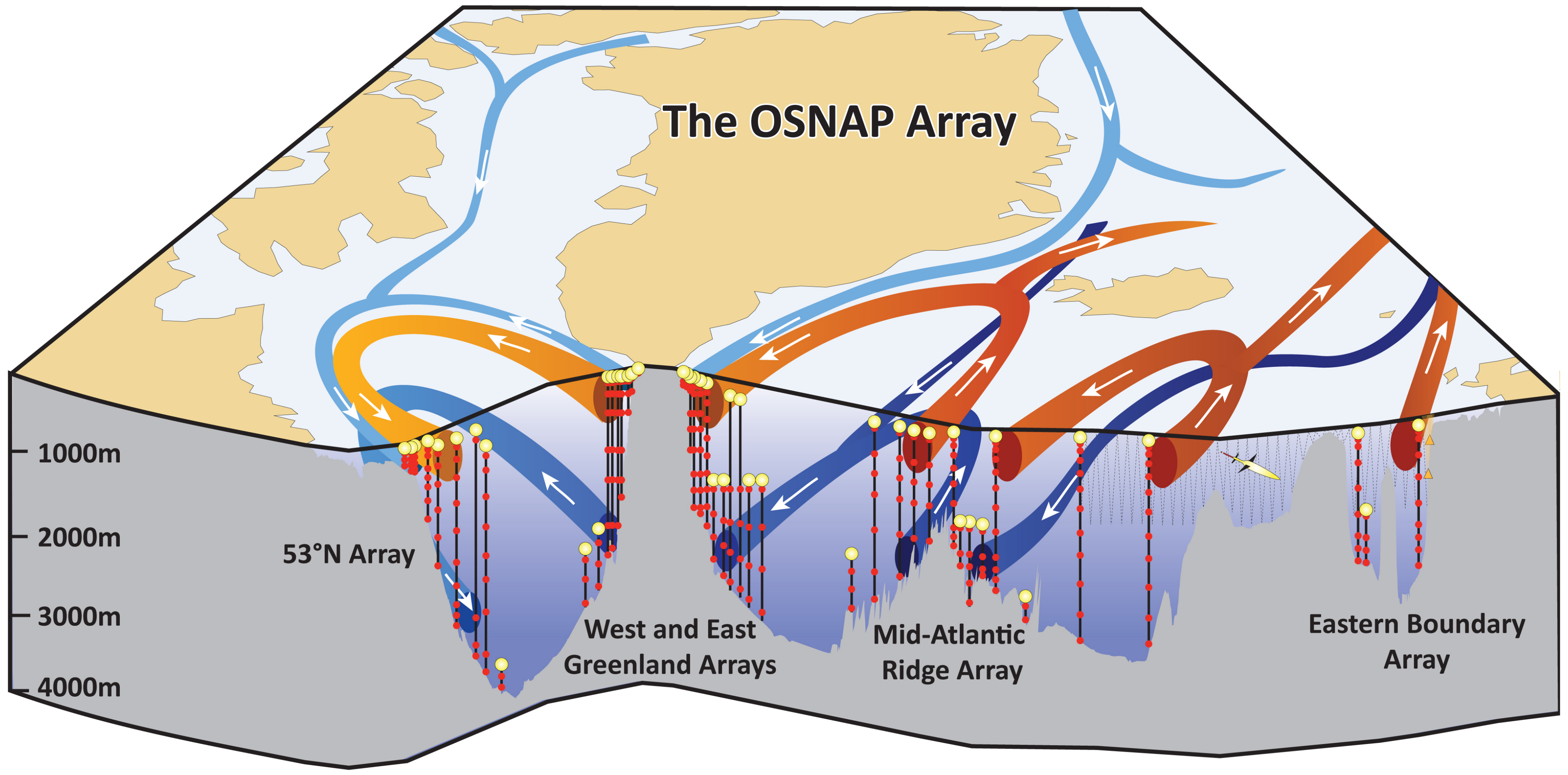
How can ocean models inform observing system design?



Ocean Observing Systems



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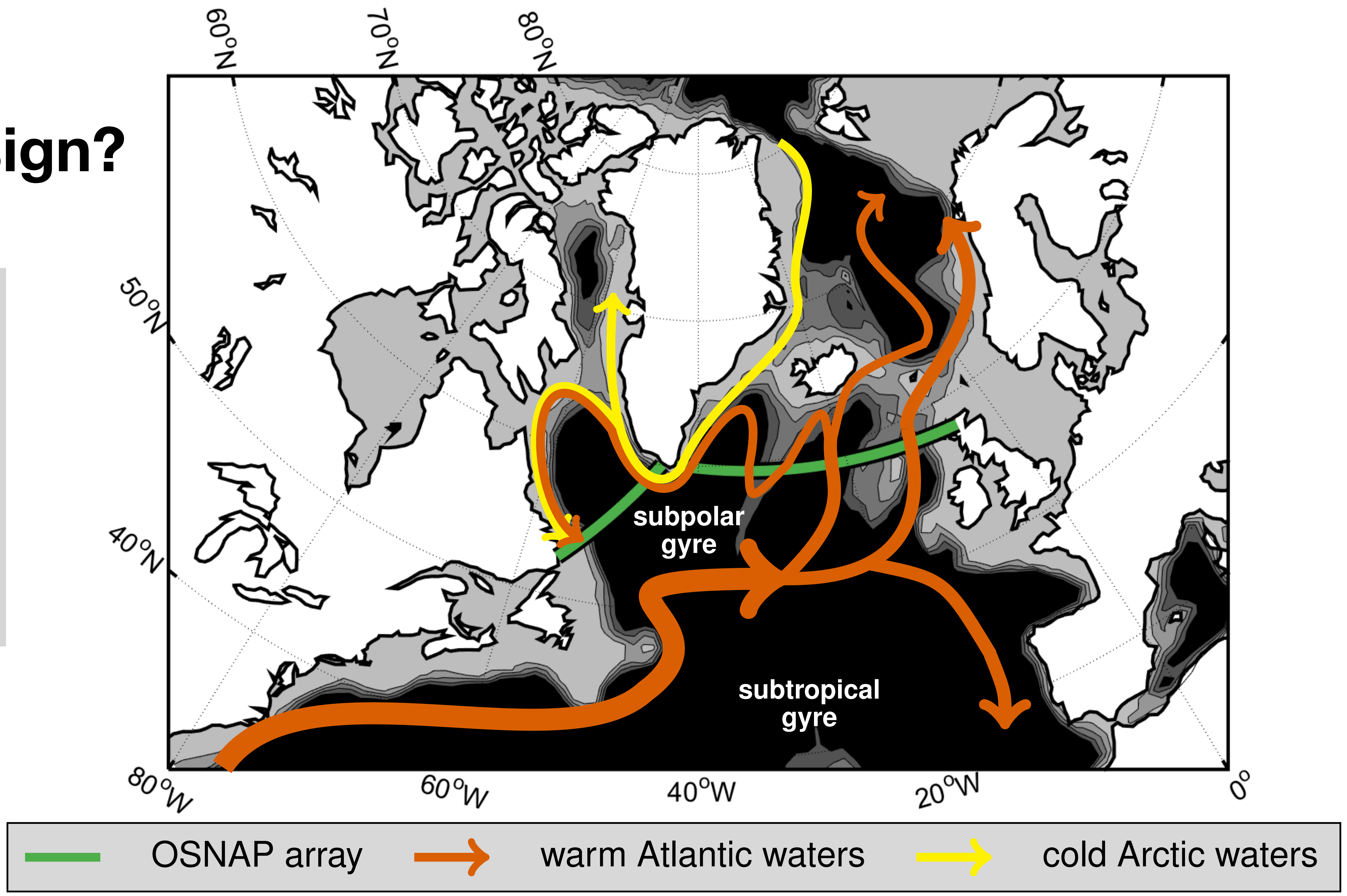
How can ocean models inform observing system design?

Idea:

- Use *oceanic teleconnections* that propagate observational constraints over long distances and can be exposed via the adjoint state
- Combine *adjoint-based estimation framework* with *Hessian-based* uncertainty quantification

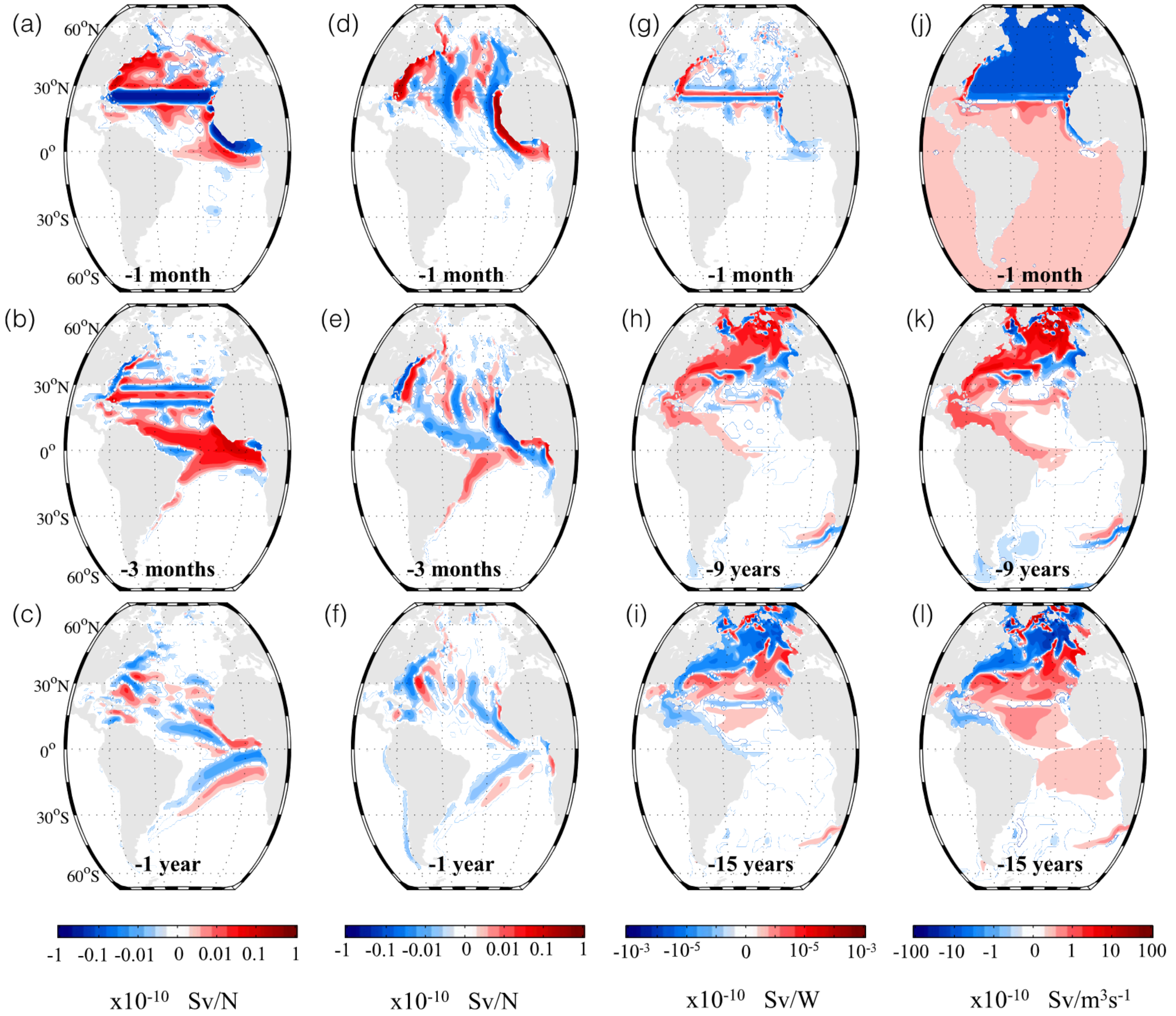


→ **Quantitative design of ocean observing systems**

Oceanic teleconnections

linear adjustment processes:

- oceanic Kelvin & Rossby waves
- exposed by the adjoint state as "time-reversed" waves, reflecting the *<u>sensitivity of a Quantity of Interest (QoI) to perturbations</u>*, (here: volume transport across 26N)
  - back in time, and
  - anywhere in space



Johnson & Marshall, J.Phys. Oceanogr. (2002)
Heimbach et al. Deep Sea Res. (2011)
Pillar et al., J. Clim. (2016)

Oceanic teleconnections

linear adjustment processes:

$$\mu_0 = \frac{\partial J}{\partial x_0} = \sum_{1 \le t \le t_f} \frac{\partial x_t}{\partial x_0} \left(\frac{\partial J}{\partial x_t} \right)$$

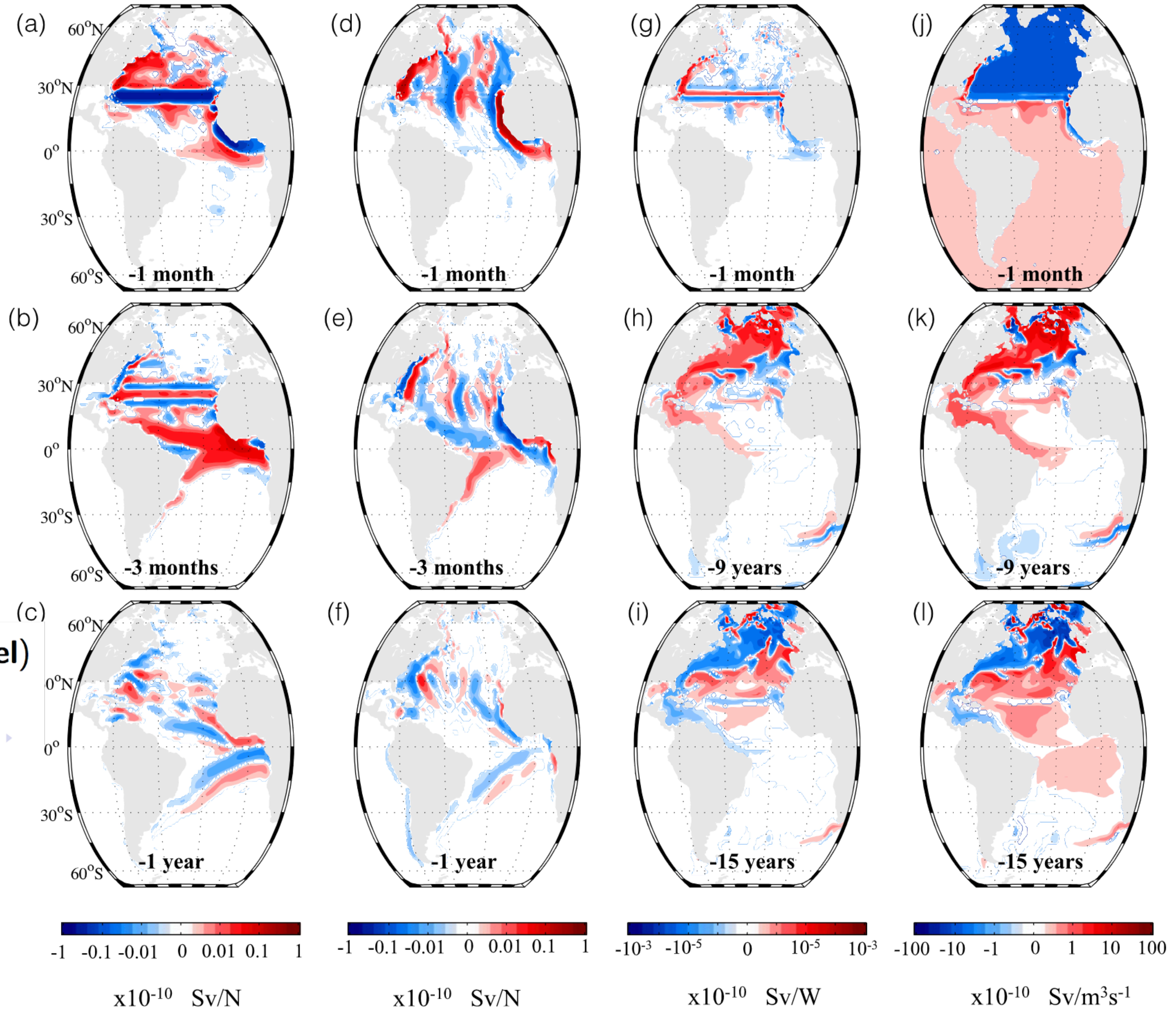
$$= \frac{\partial x_1}{\partial x_0} \left(\frac{\partial J}{\partial x_1} \right) + \frac{\partial x_1}{\partial x_0} \frac{\partial x_2}{\partial x_1} \left(\frac{\partial J}{\partial x_2} \right)$$

$$+ \ldots + \frac{\partial x_1}{\partial x_0} \cdots \frac{\partial x_{t_f}}{\partial x_{t_f - 1}} \left(\frac{\partial J}{\partial x_{t_f}} \right)$$

$$= \mathbf{L}^T \frac{\partial J}{\partial x_1} + \mathbf{L}^T \mathbf{L}^T \frac{\partial J}{\partial x_2} + \ldots + \mathbf{L}^T \cdots \mathbf{L}^T \frac{\partial J}{\partial x_{t_f}}$$

$\mathbf{L}^T$: is the **adjoint model** (and $\mathbf{L}$ is the **tangent linear model**)

$\mu_k = \left(\frac{\partial J}{\partial x_k} \right)$: **Lagrange multipliers** or **gradients**



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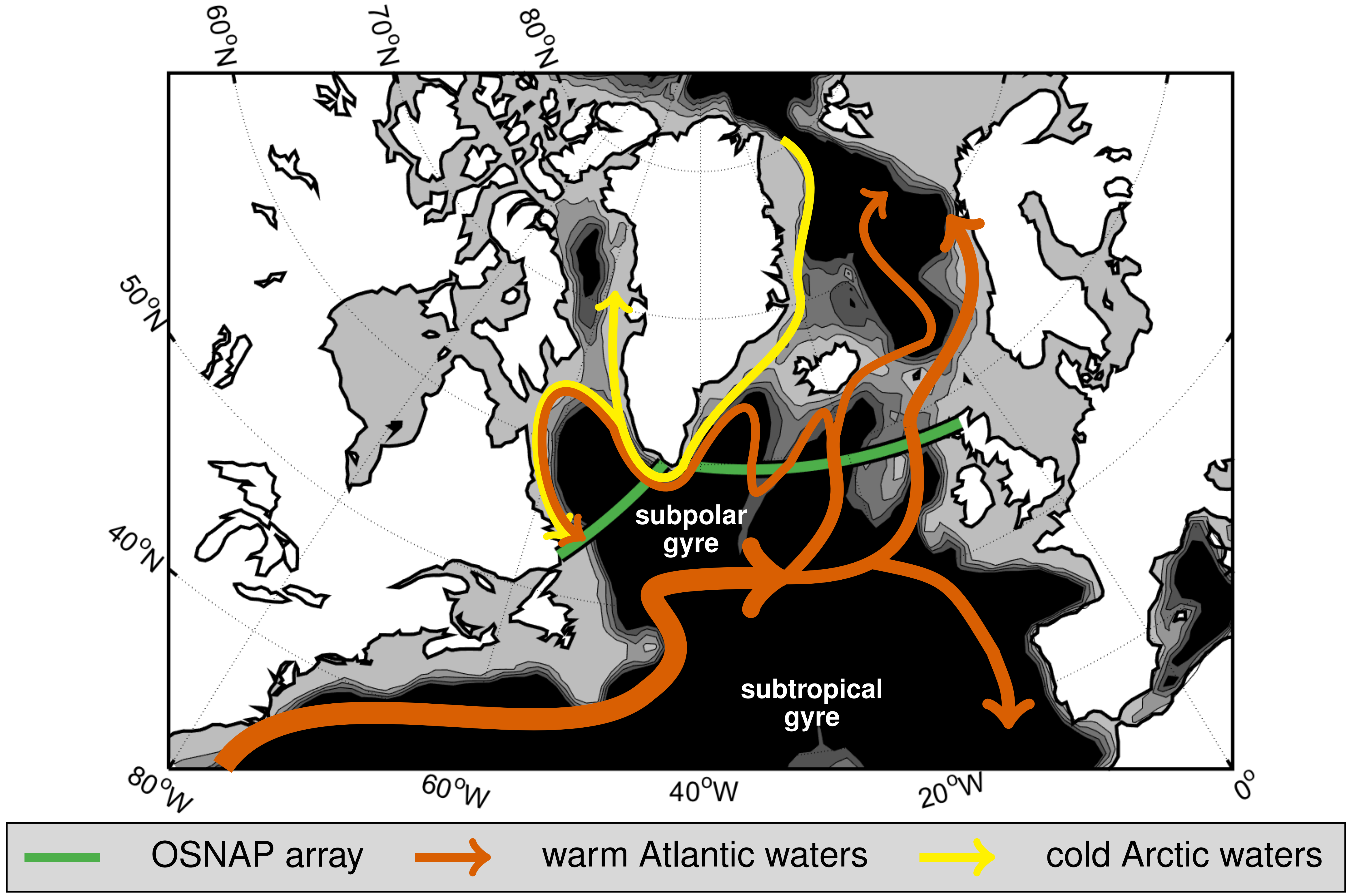
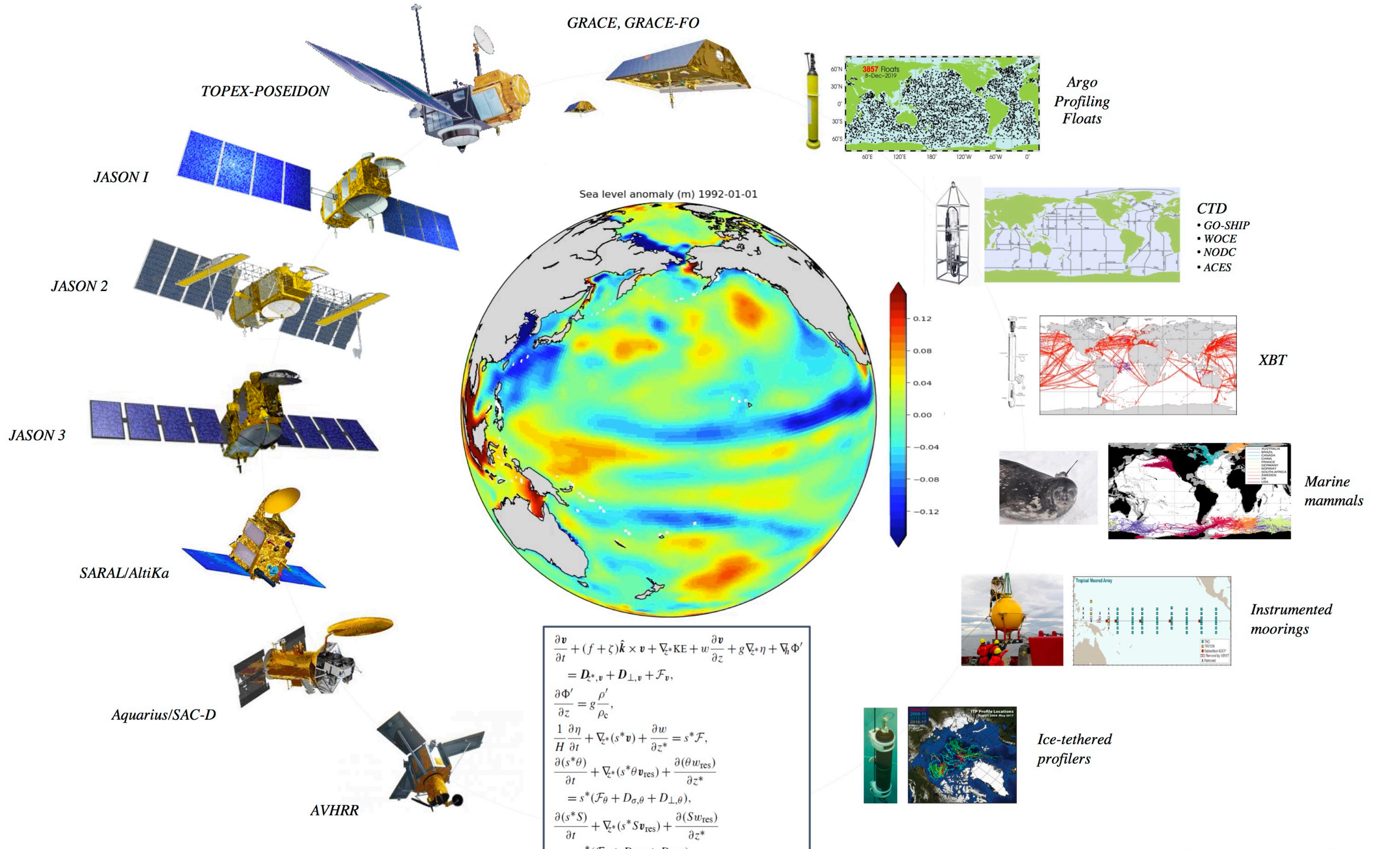
Algorithmic approach

Formulate
Quantity of Interest (QoI)

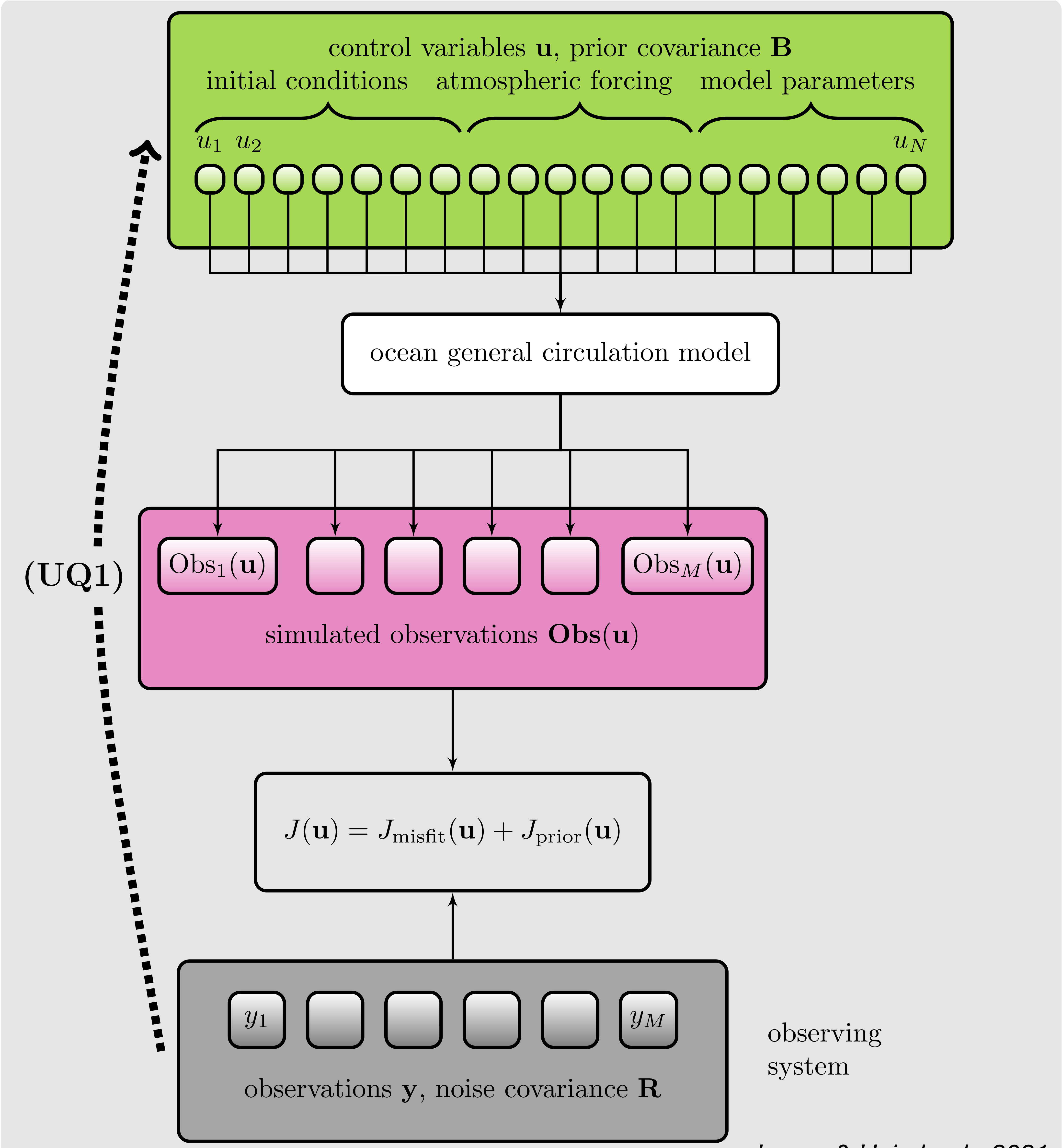


Leverage adjoint-based data assimilation framework: ECCO



Courtesy of Ian Fenty

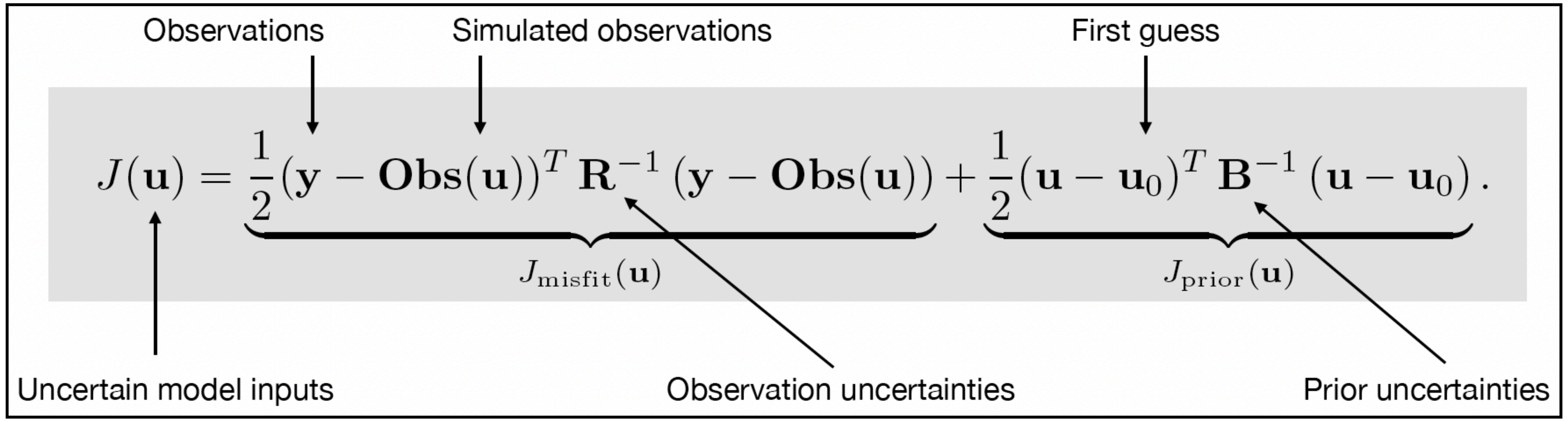
Uncertainty Quantification (UQ)



Loose & Heimbach, 2021

(UQ1): Inverse uncertainty propagation

From prior to posterior uncertainty



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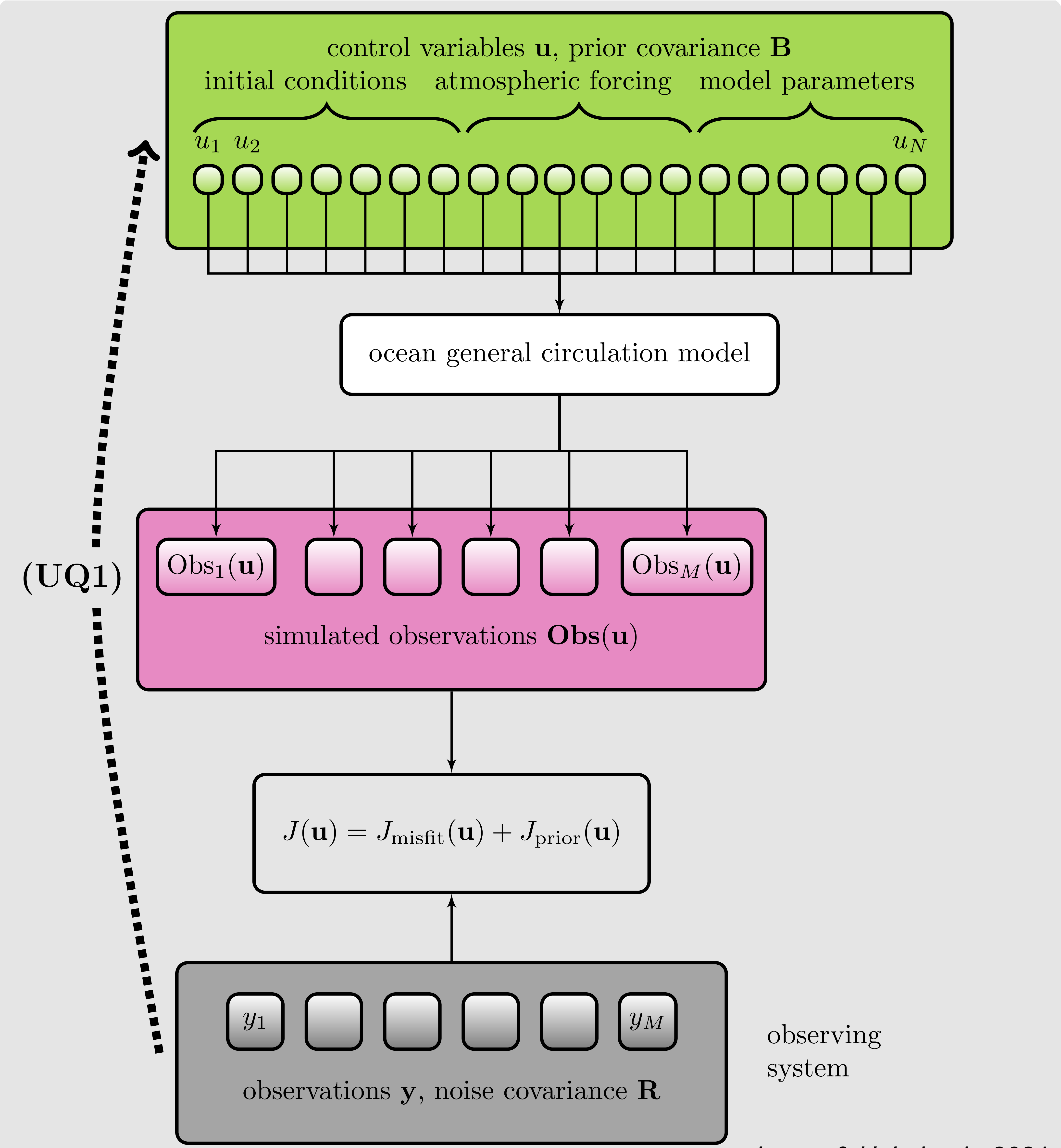
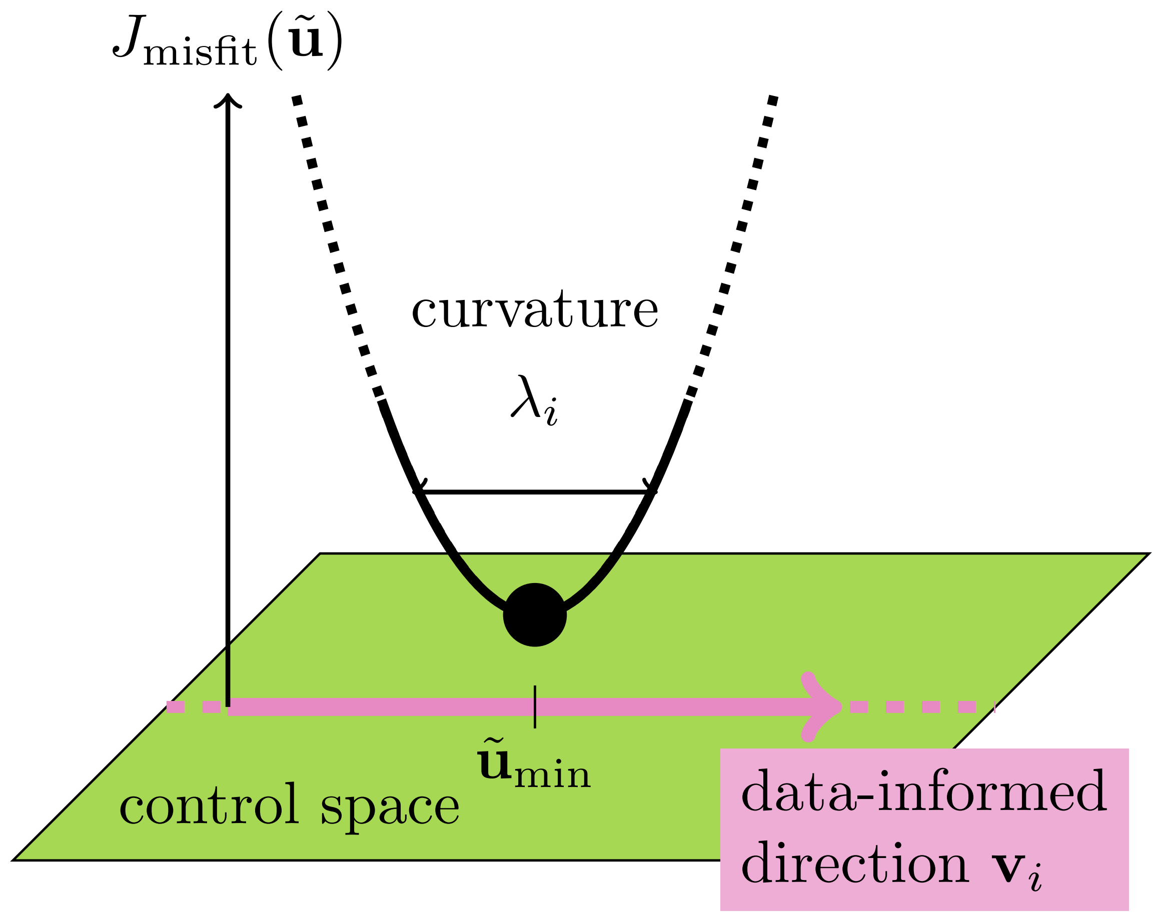


Loose & Heimbach, 2021

Observations — Simulated observations — First guess

$$J(\mathbf{u}) = \underbrace{\frac{1}{2}(\mathbf{y} - \mathbf{Obs}(\mathbf{u}))^T\,\mathbf{R}^{-1}\,(\mathbf{y} - \mathbf{Obs}(\mathbf{u}))}_{J_{\text{misfit}}(\mathbf{u})} + \underbrace{\frac{1}{2}(\mathbf{u} - \mathbf{u}_0)^T\,\mathbf{B}^{-1}\,(\mathbf{u} - \mathbf{u}_0)}_{J_{\text{prior}}(\mathbf{u})}\,.$$

Uncertain model inputs — Observation uncertainties — Prior uncertainties



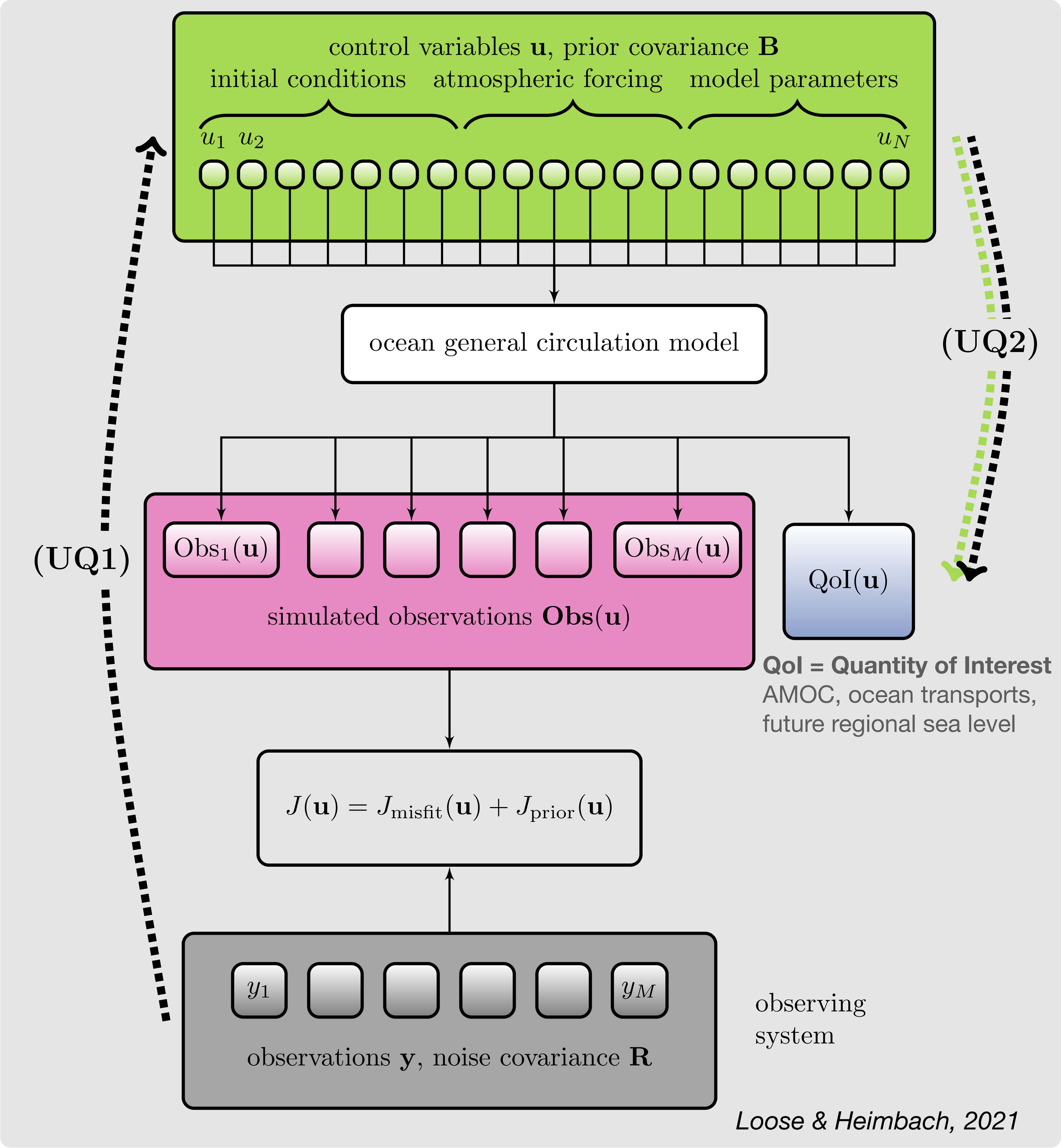
Hessian of cost function J

$$\mathbf{H}_J \approx \sum_{i=1}^{M} \lambda_i \mathbf{v}_i \mathbf{v}_i^T$$

Thacker, 1989

posterior uncertainty *~ inverse Hessian of J*

Uncertainty Quantification (UQ)



QoI = Quantity of Interest
AMOC, ocean transports, future regional sea level

Loose & Heimbach, 2021

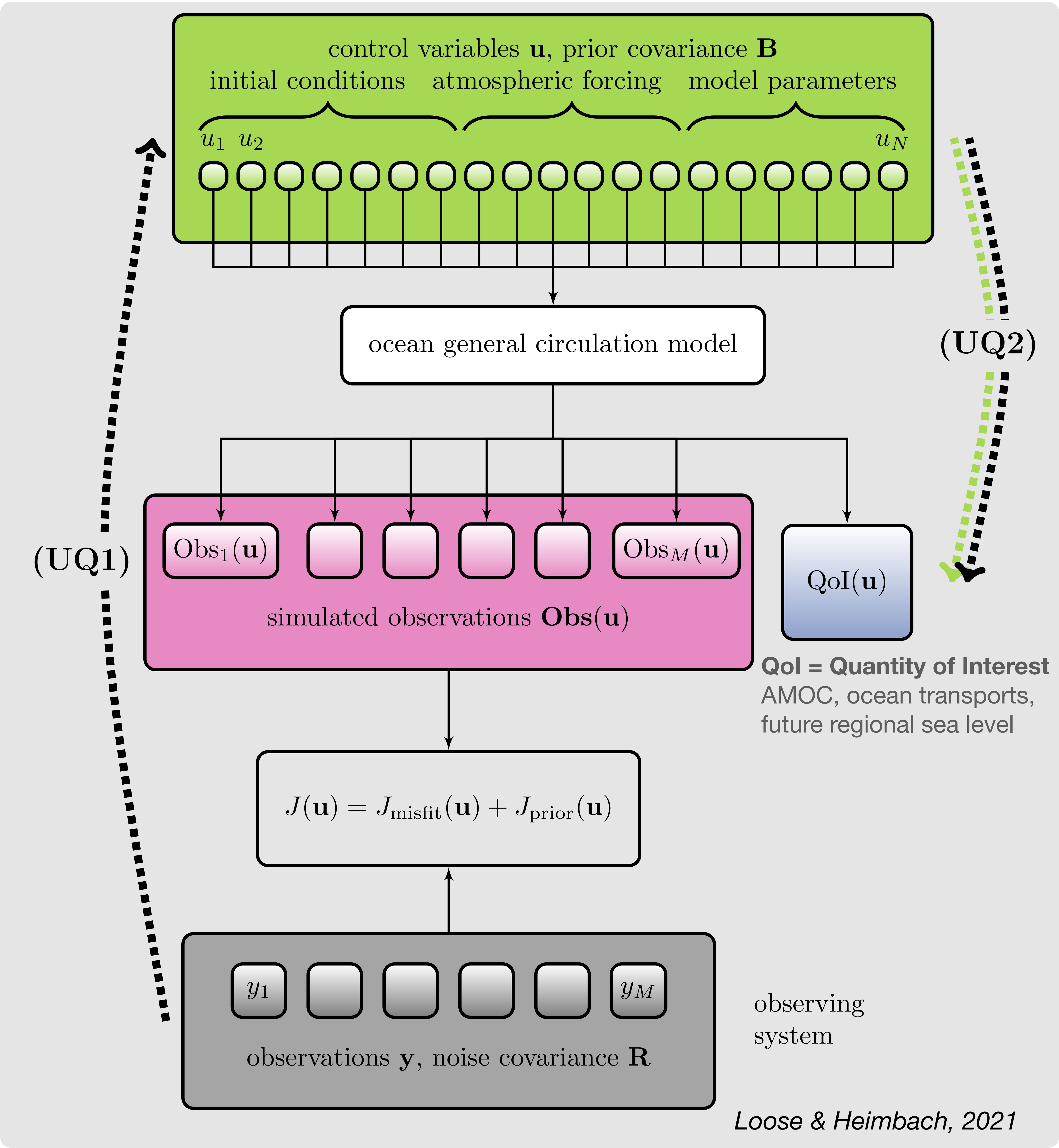
(UQ2): Forward uncertainty propagation

From posterior to QoI uncertainty

Uncertainty reduction in quantity of interest (QoI) by observing system:

$$\sum_{i=1}^{M} \frac{\lambda_i}{\lambda_i + 1} (\mathbf{q} \bullet \mathbf{v}_i)^2 \in [0, 1) \quad \text{where} \quad \mathbf{q} = \frac{\mathbf{B}^{T/2}\, \nabla_u \mathrm{QoI}}{\left\| \mathbf{B}^{T/2}\, \nabla_u \mathrm{QoI} \right\|}$$

Uncertainty Quantification (UQ)



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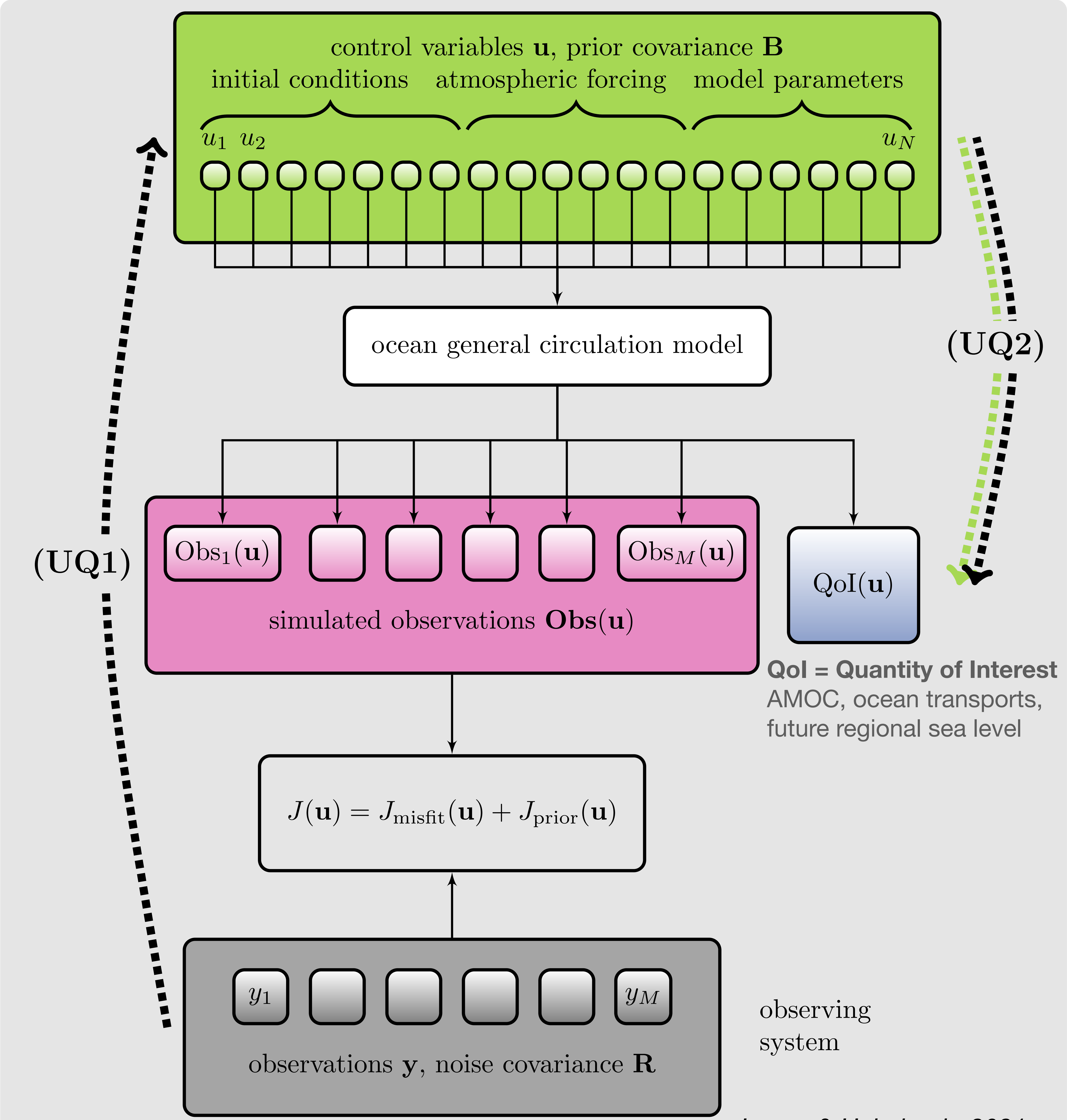
$(\mathbf{q} \bullet \mathbf{v}_i)^2$ = Degree of shared adjustment mechanisms between observing system and QoI

Uncertainty Quantification (UQ)



Loose & Heimbach, 2021

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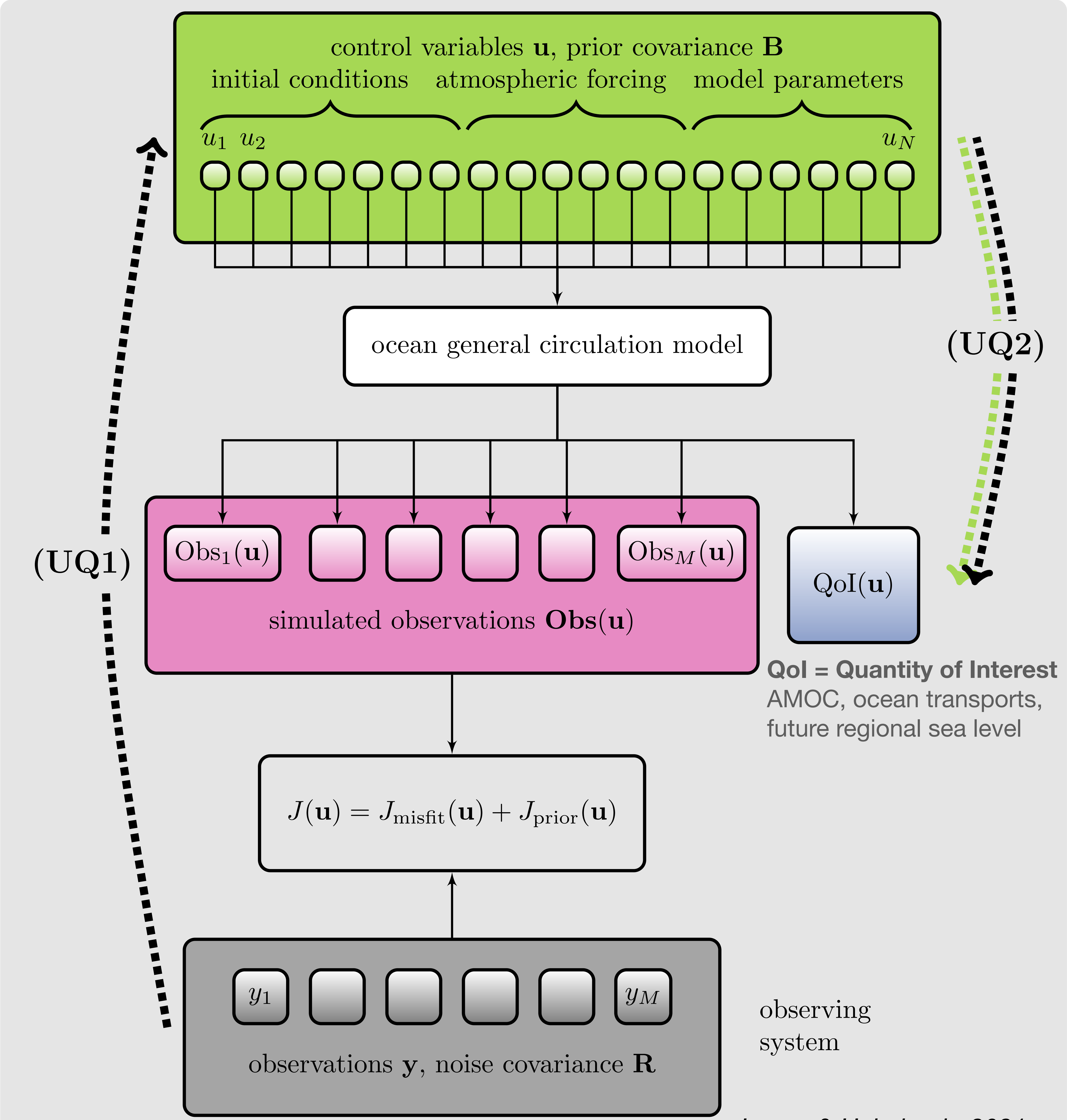
$(\mathbf{q} \bullet \mathbf{v}_i)^2$ = Degree of shared adjustment mechanisms between observing system and QoI

Eigenvalues reflect **"sensitivity-to-noise" ratio** of observations

$$\lambda = \frac{\left\| \mathbf{B}^{T/2}\, \nabla_u \mathrm{Obs} \right\|^2}{\varepsilon_{\mathrm{Obs}}^2}$$

Uncertainty Quantification (UQ)



Loose & Heimbach, 2021

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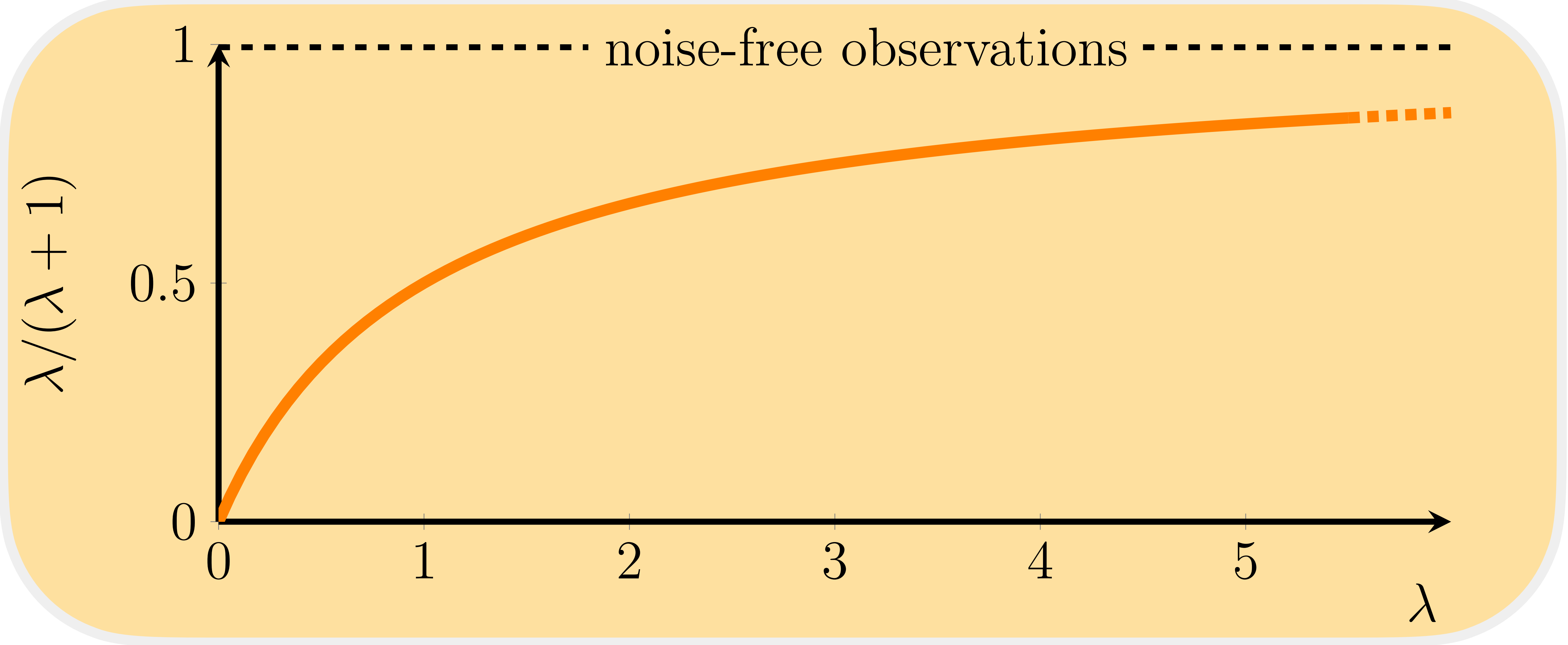

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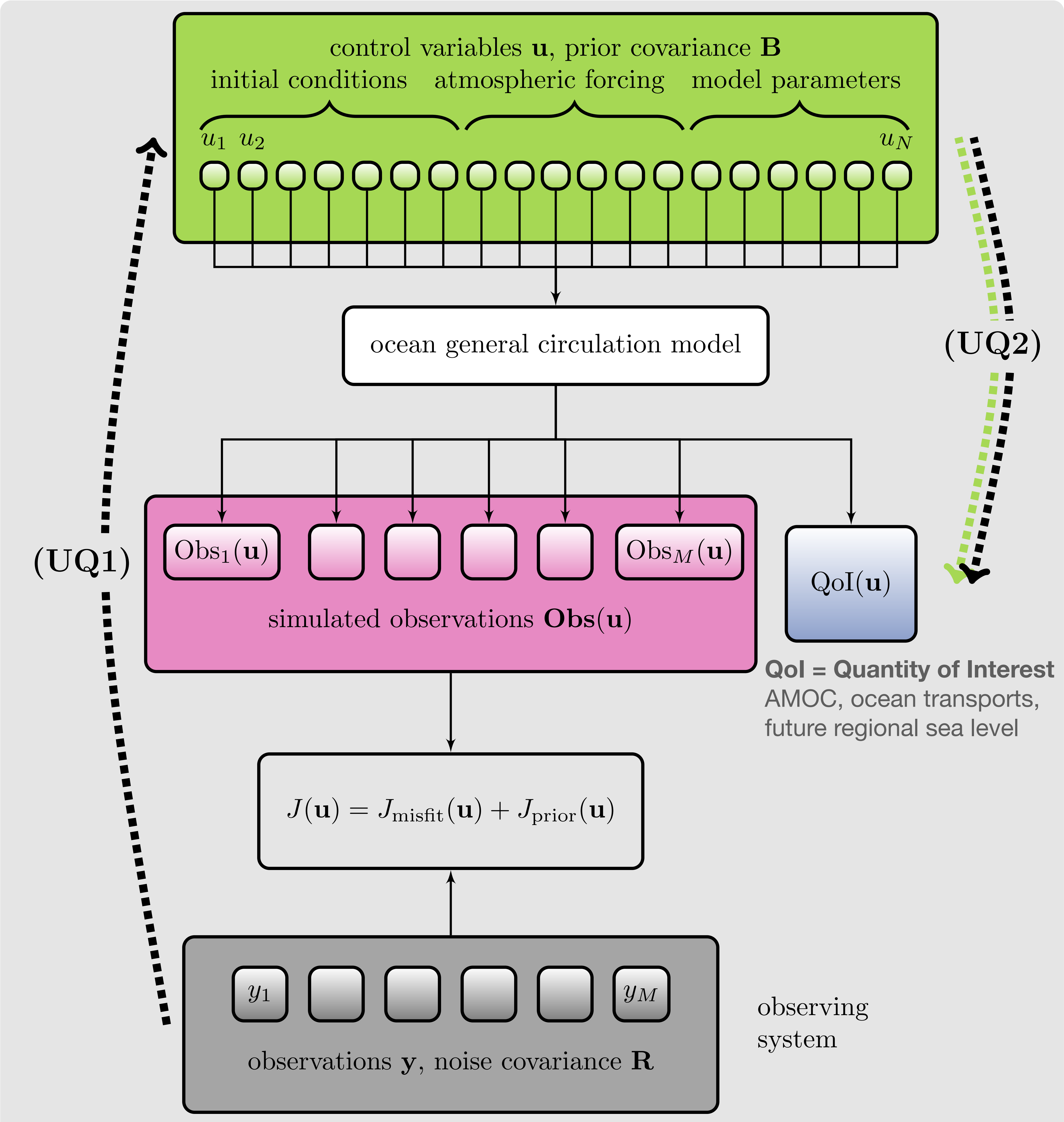
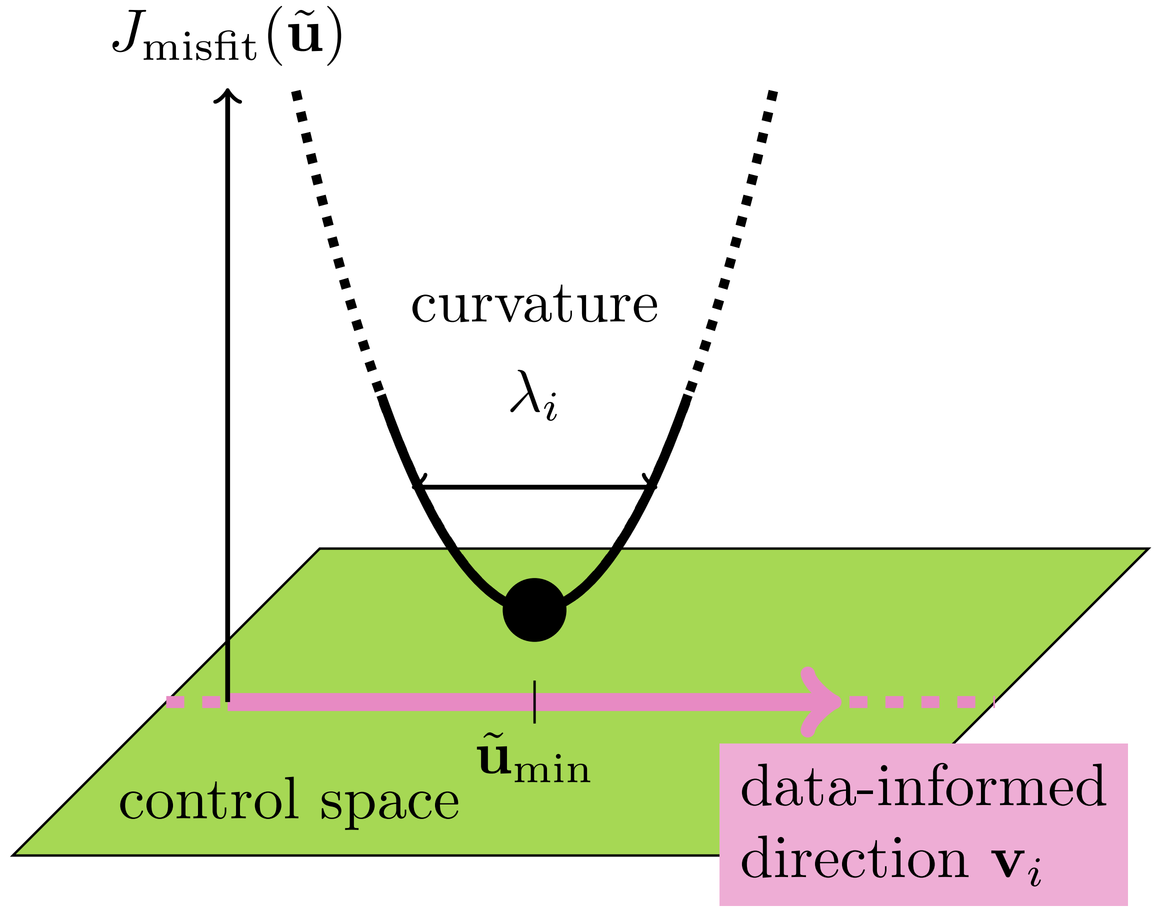


Loose & Heimbach, 2021

(UQ1): Inverse uncertainty propagation



Hessian of cost function J

$$\mathbf{H}_J \approx \sum_{i=1}^{M} \lambda_i \mathbf{v}_i \mathbf{v}_i^T$$

Thacker, 1989

(UQ2): Forward uncertainty propagation

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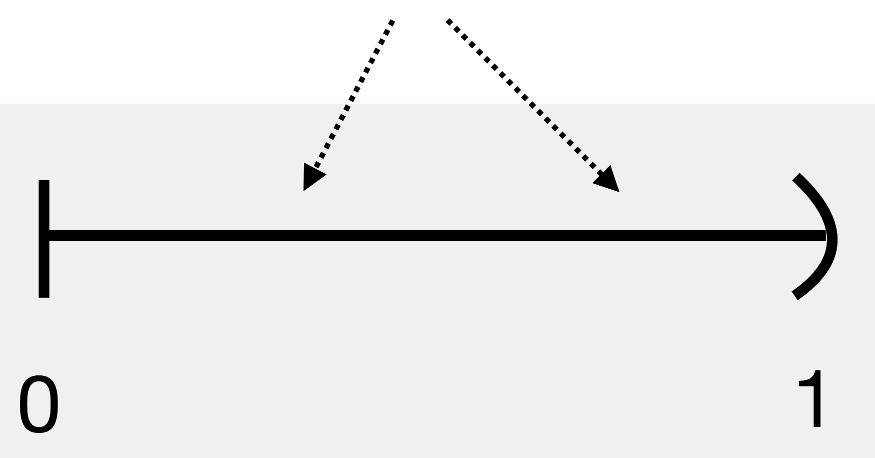
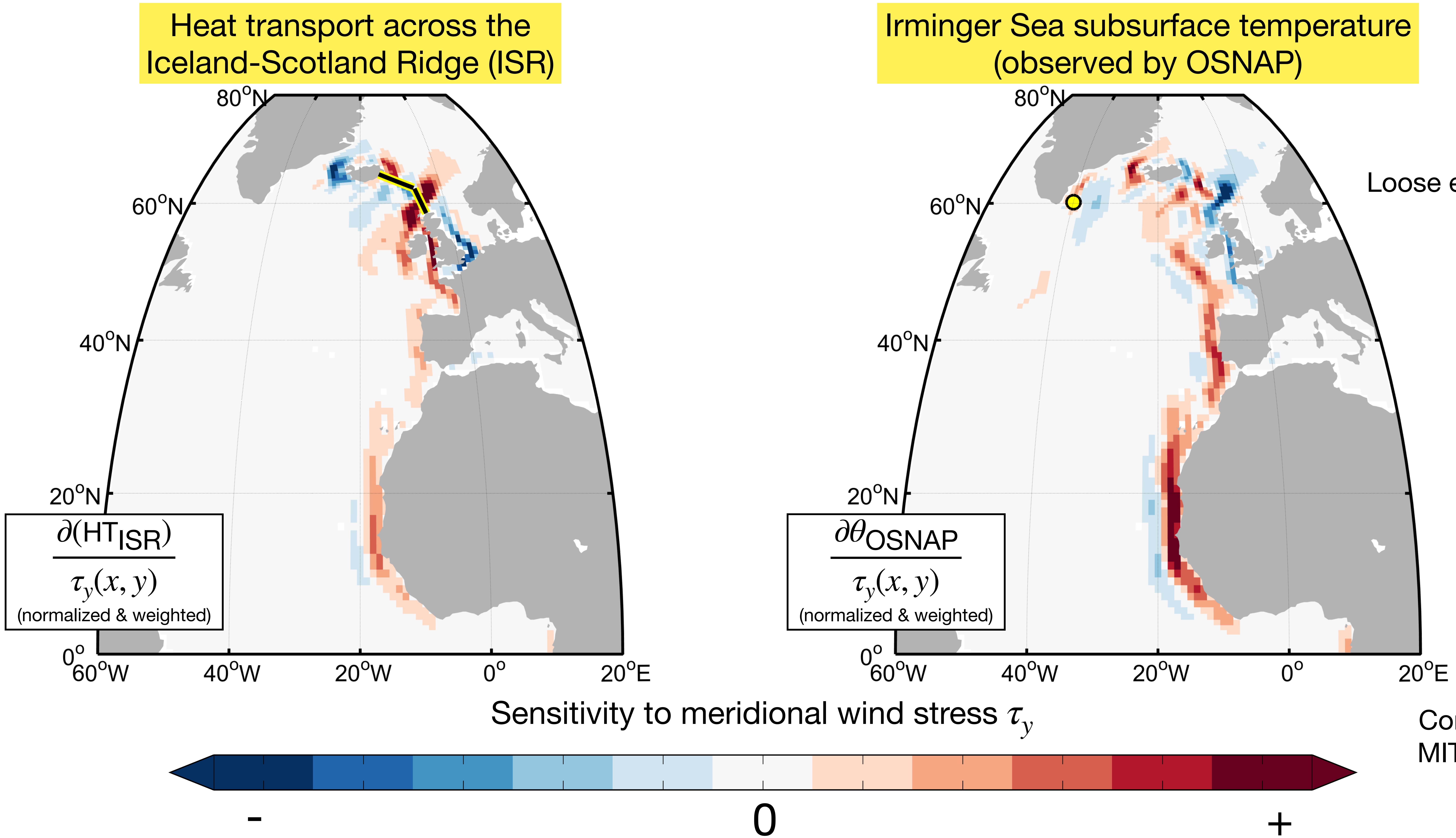


Observing system **provides no new constraints** **is optimal** **for QoI chosen**

Sensitivity maps identify shared adjustment mechanisms & pathways

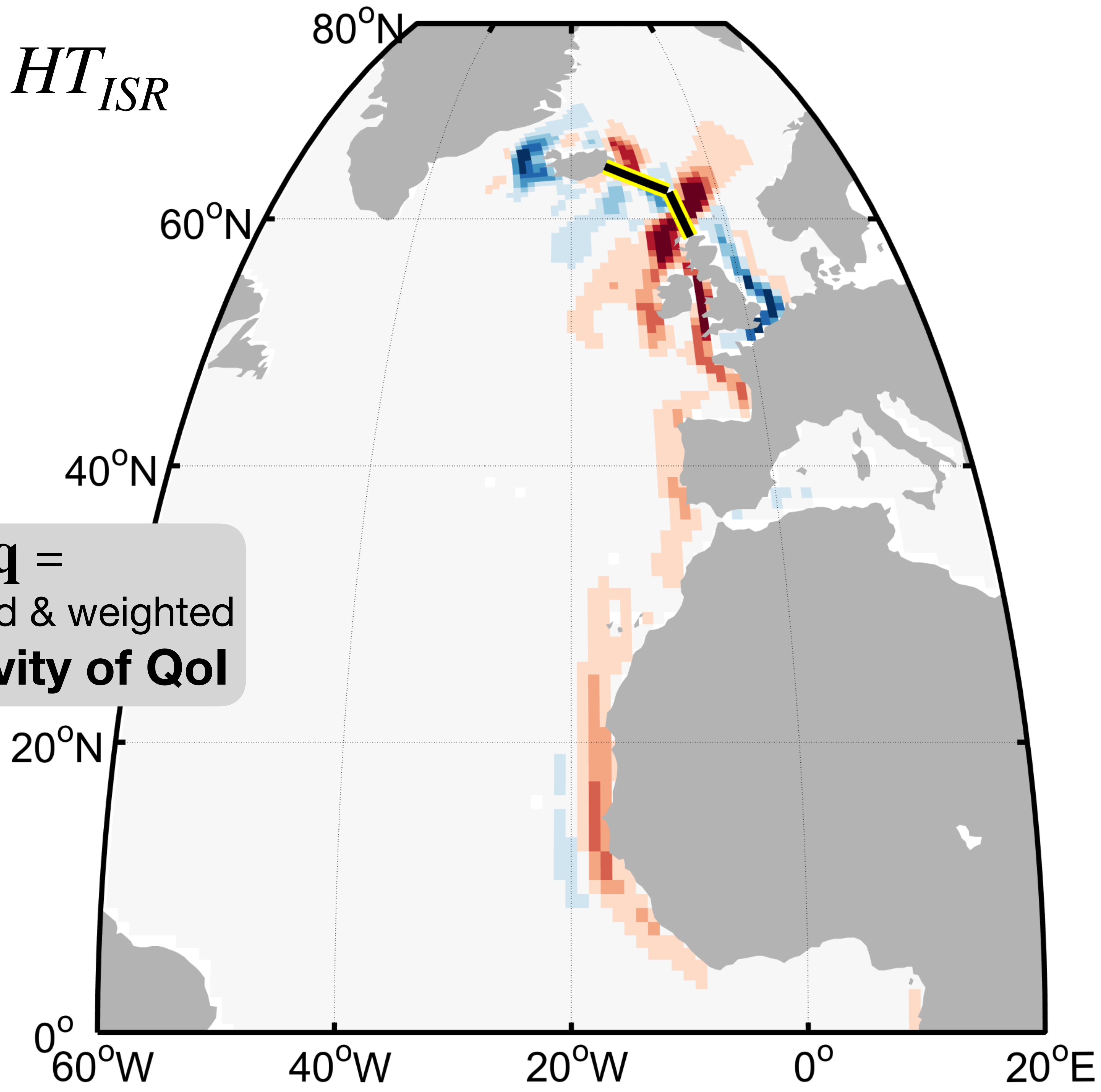


Loose et al., 2020

Computed with MITgcm adjoint model

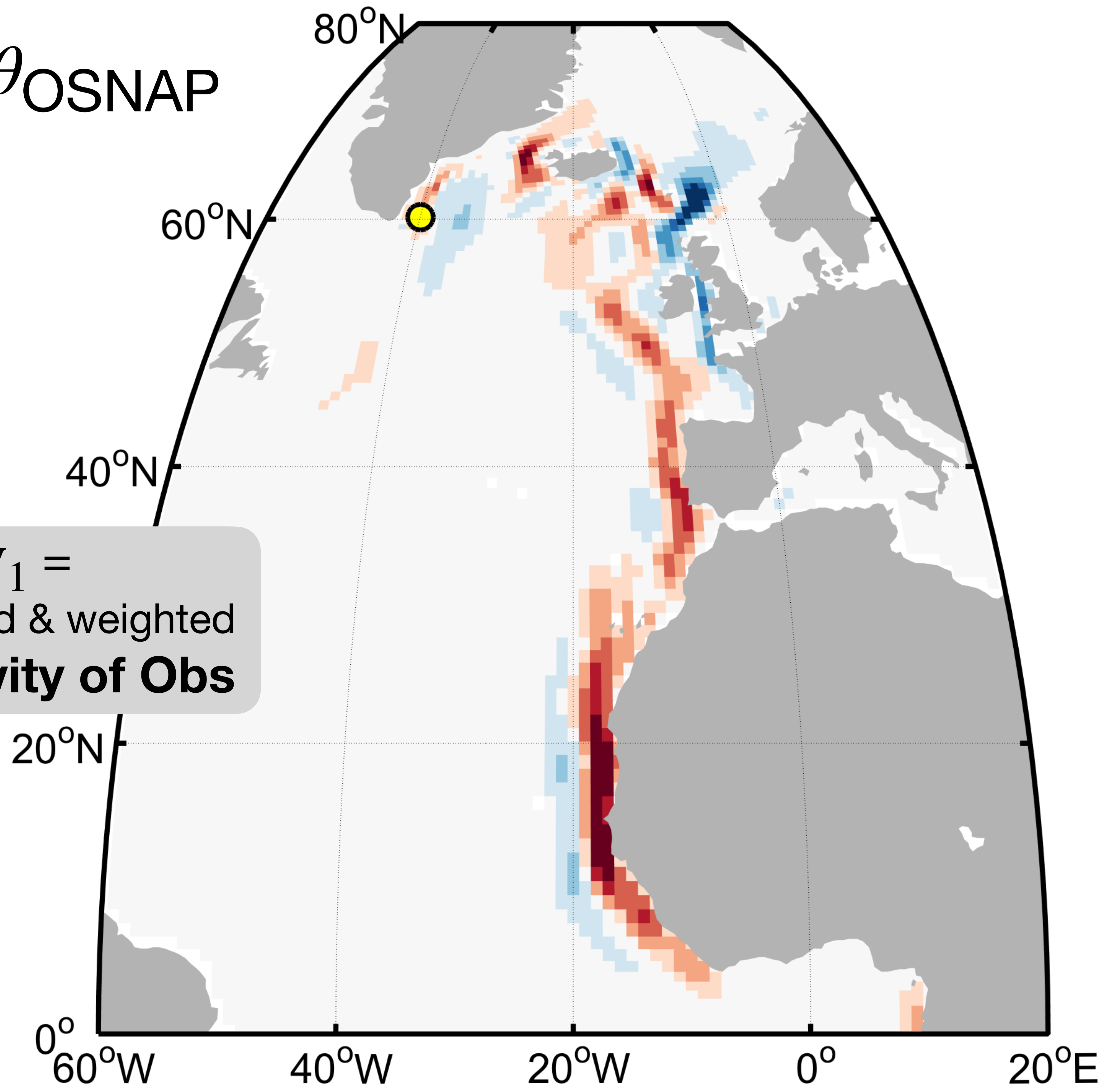
Sensitivity maps re-interpreted in the context of UQ

QoI: HT_{ISR}



$\mathbf{q}$ =
normalized & weighted
sensitivity of QoI

Obs: θ_{OSNAP}

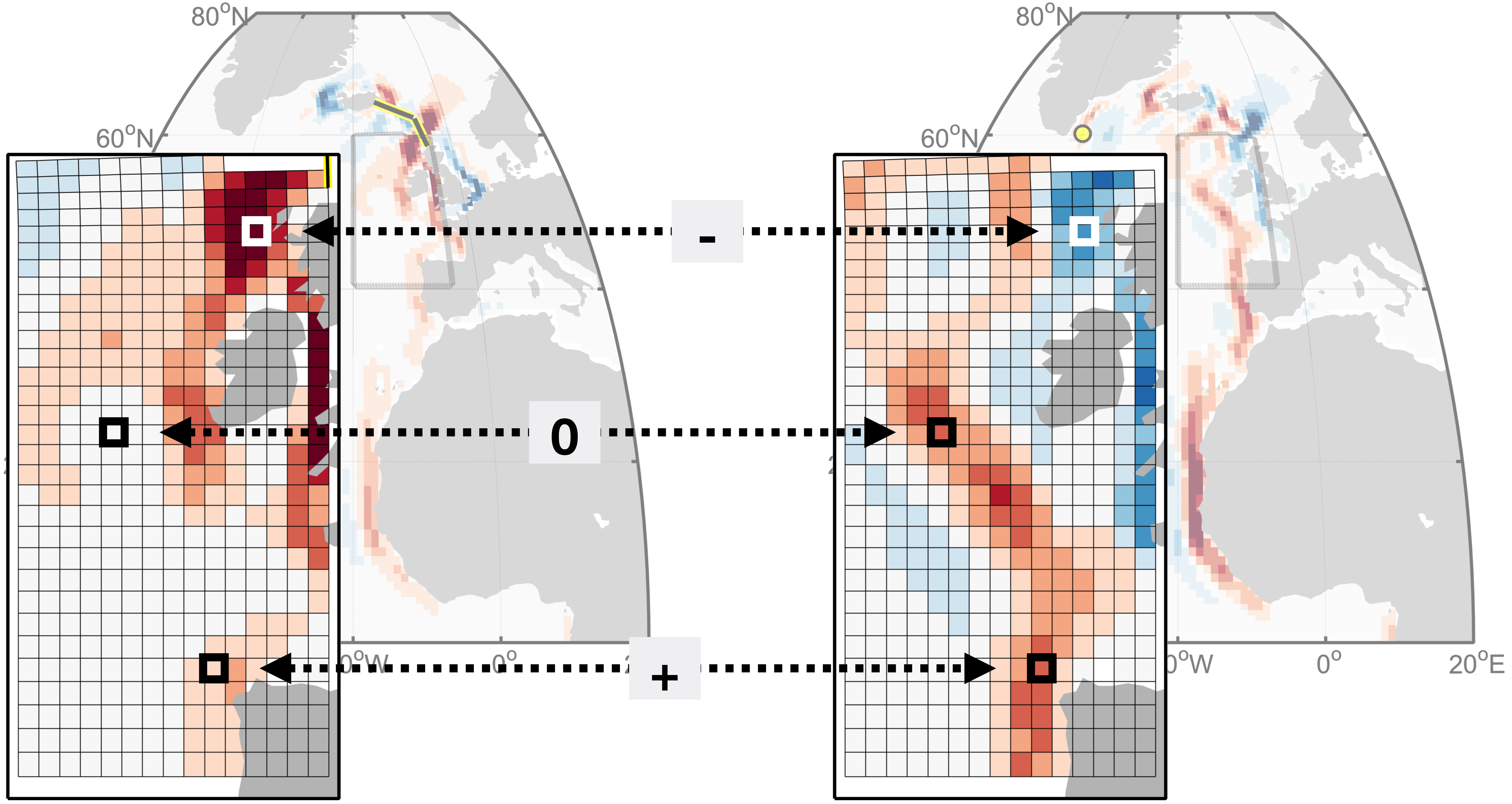


$\mathbf{v}_1$ =
normalized & weighted
sensitivity of Obs

$\mathbf{v}_1$ = **Hessian eigenvector** (in ECCO)

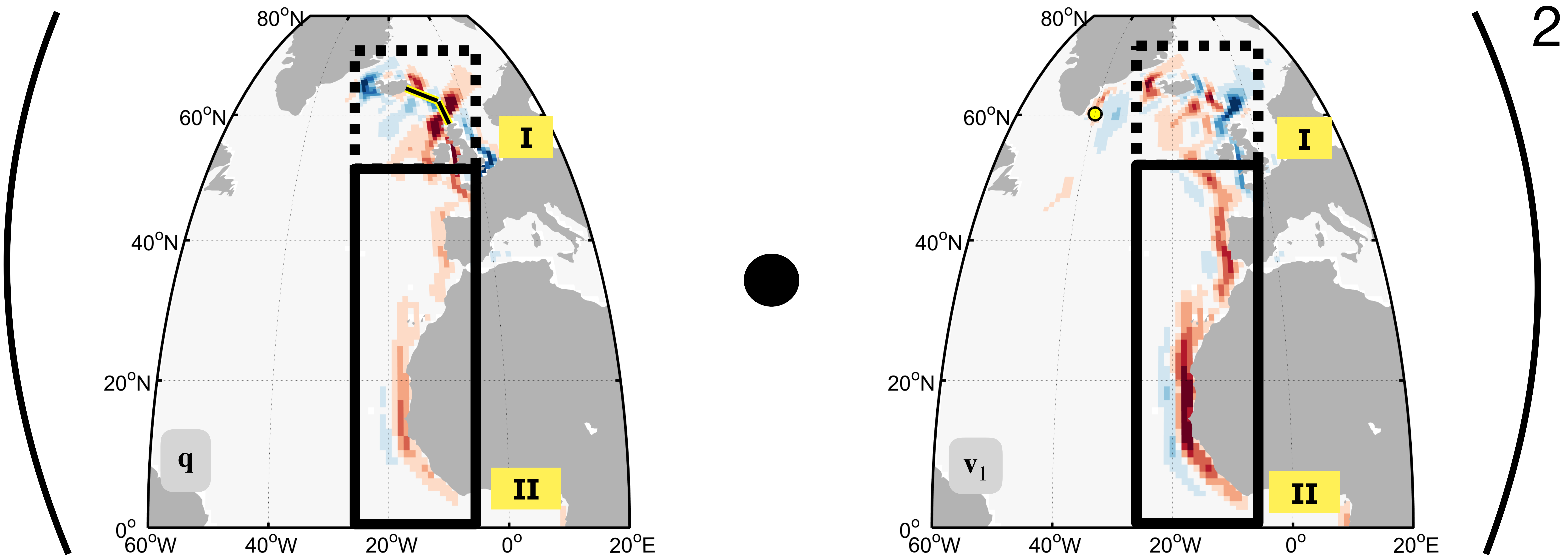
$(\mathbf{q} \bullet \mathbf{v}_1)^2$ = uncertainty reduction in HT_{ISR} by noise-free θ_{OSNAP} observation

Computing $(\mathbf{q} \bullet \mathbf{v}_1)$



$$(\mathbf{q} \bullet \mathbf{v}_1) = \left([\mathbf{q} \bullet \mathbf{v}_1]_+ + [\mathbf{q} \bullet \mathbf{v}_1]_- + \cancel{[\mathbf{q} \bullet \mathbf{v}_1]_0} \right)$$

Uncertainty reduction via oceanic teleconnections

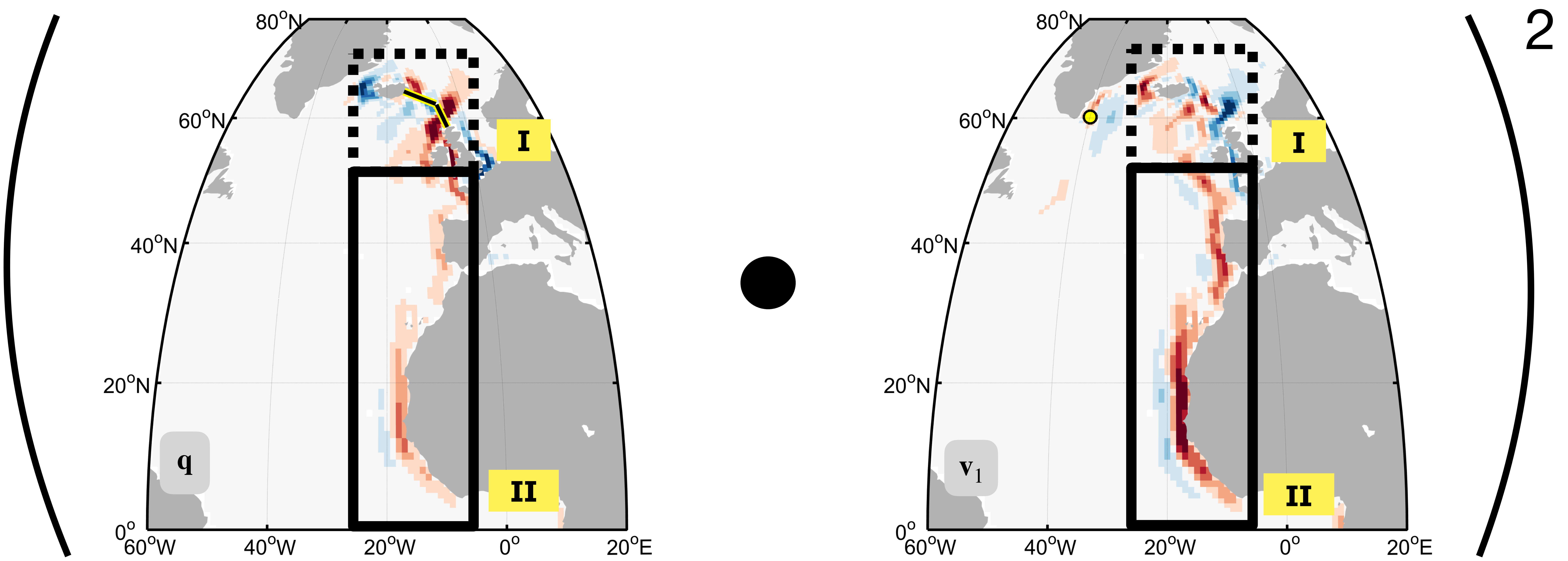


Uncertainty reduction in HT_{ISR} by noise-free θ_{OSNAP} observation:

$$(\mathbf{q} \bullet \mathbf{v}_1)^2 = ([\mathbf{q} \bullet \mathbf{v}_1]_+ + [\mathbf{q} \bullet \mathbf{v}_1]_-)^2 = (0.15 + (-0.59))^2 = (-0.44)^2 = 19\%$$

II I

Uncertainty reduction via oceanic teleconnections



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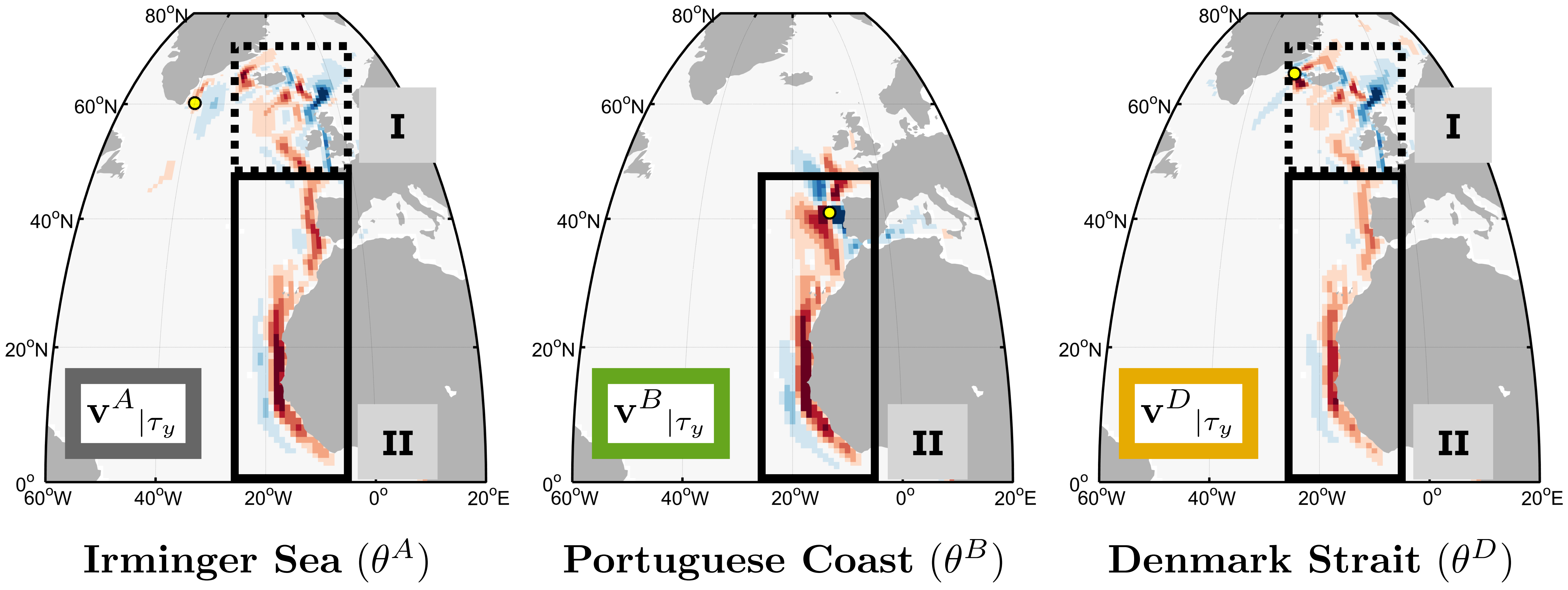
II I

- **Shared adjustment mechanisms lead to large uncertainty reduction**
- **BUT: destructive interference is possible**

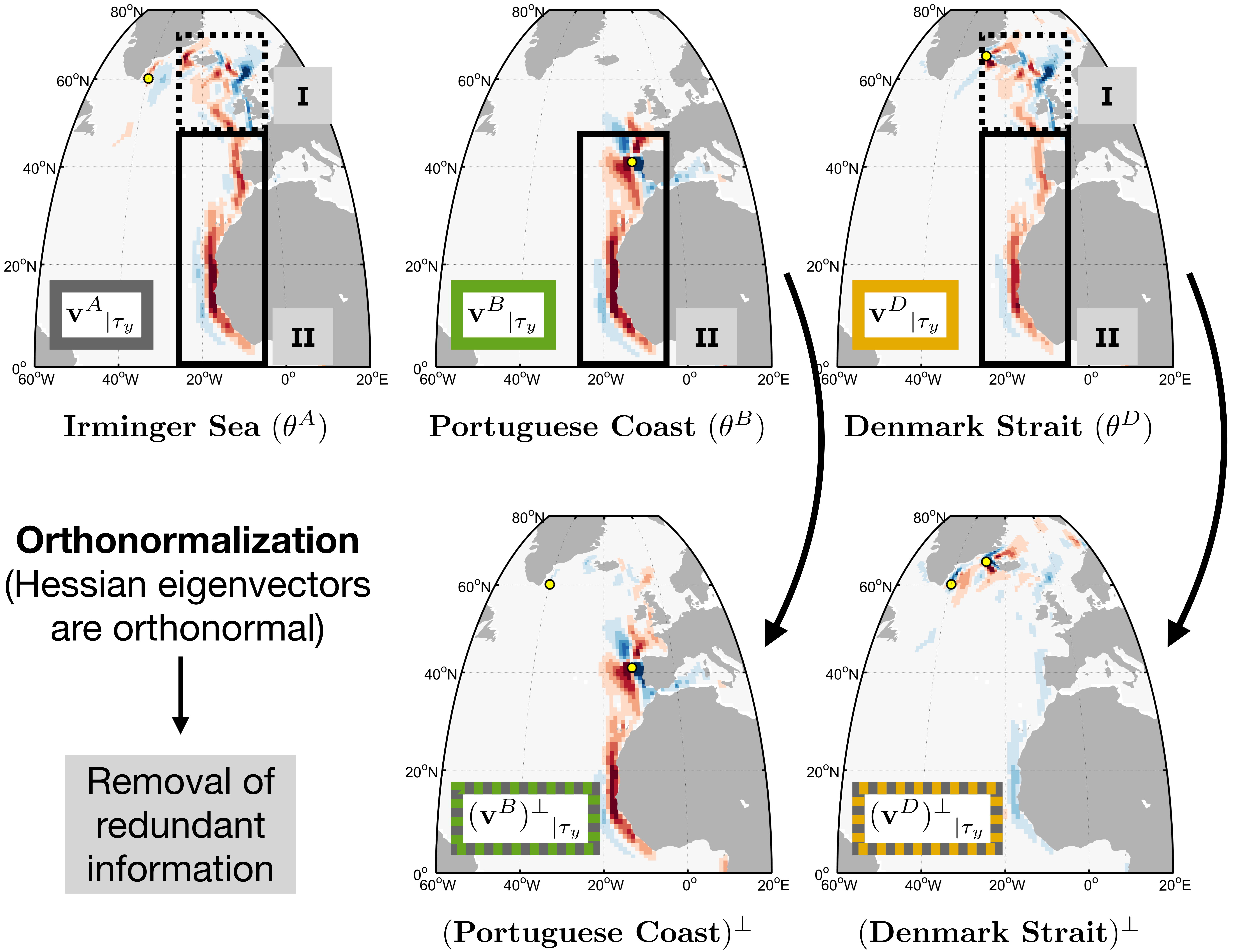
Assessing data redundancy



No actual data needed ⟶ can test future observing systems

Loose & Heimbach, 2021

Assessing data redundancy



Orthonormalization
(Hessian eigenvectors are orthonormal)

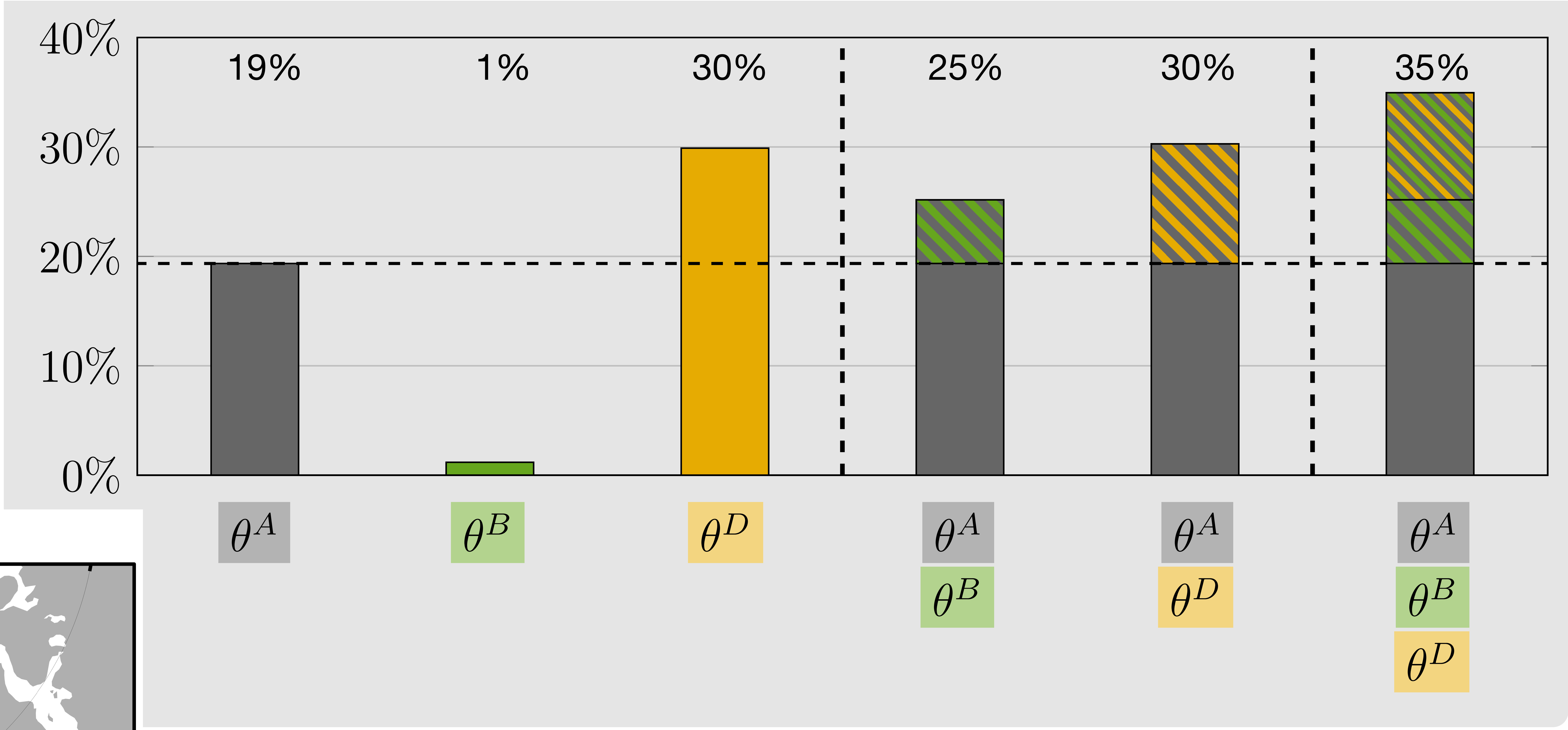
↓

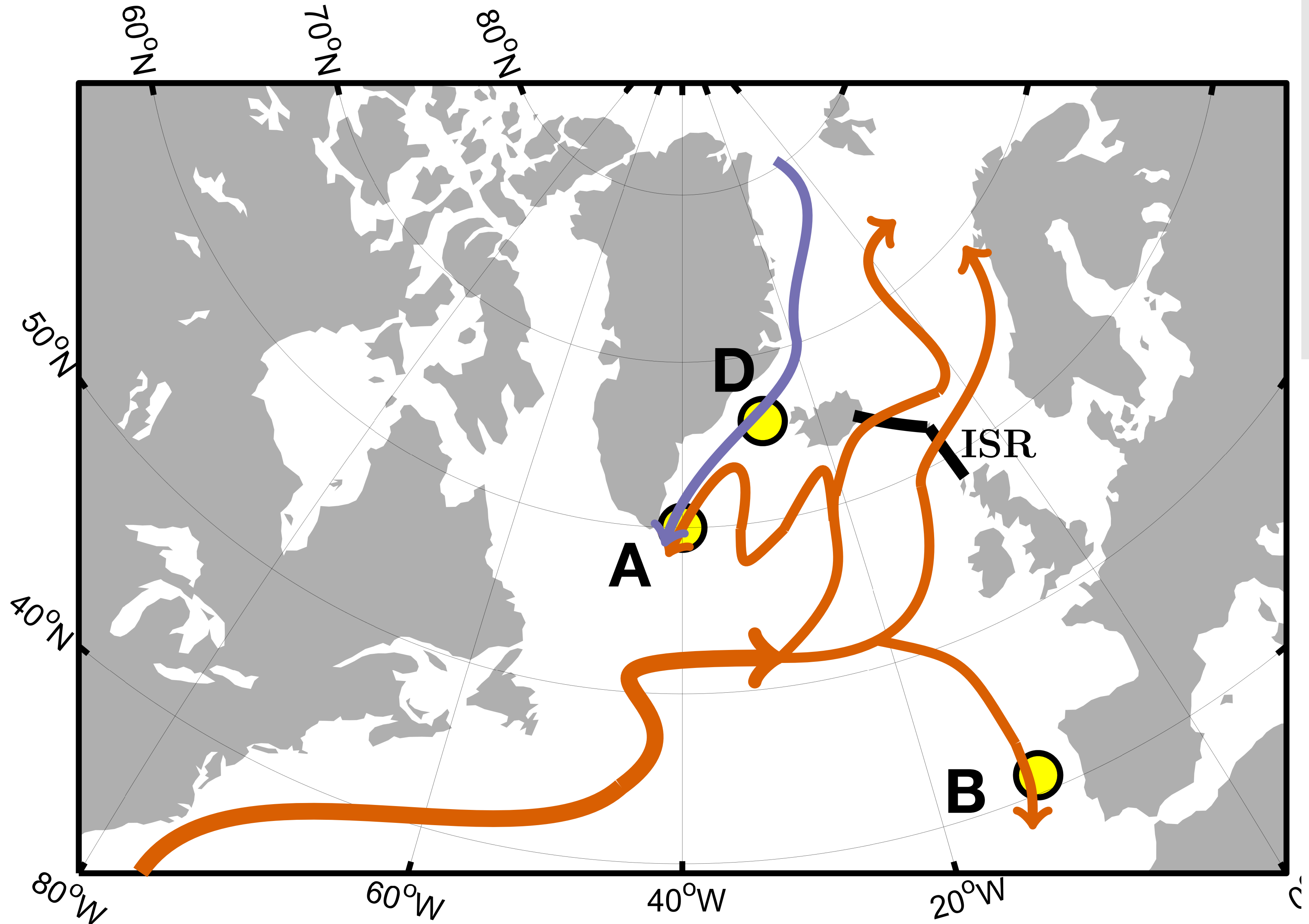
Removal of redundant information

Loose & Heimbach, 2021

Assessing data redundancy

Uncertainty reduction in HT_{ISR} by noise-free observations





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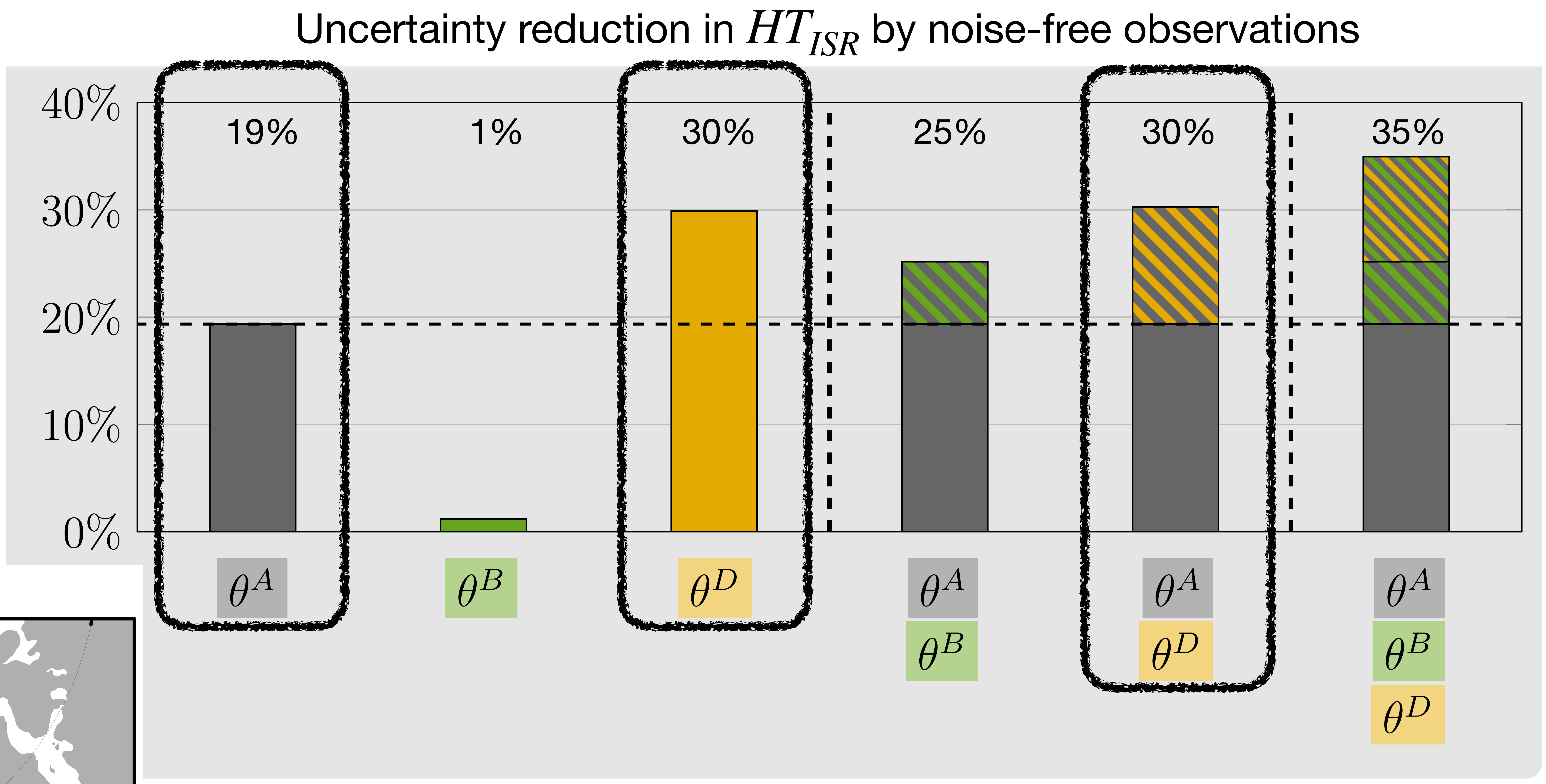
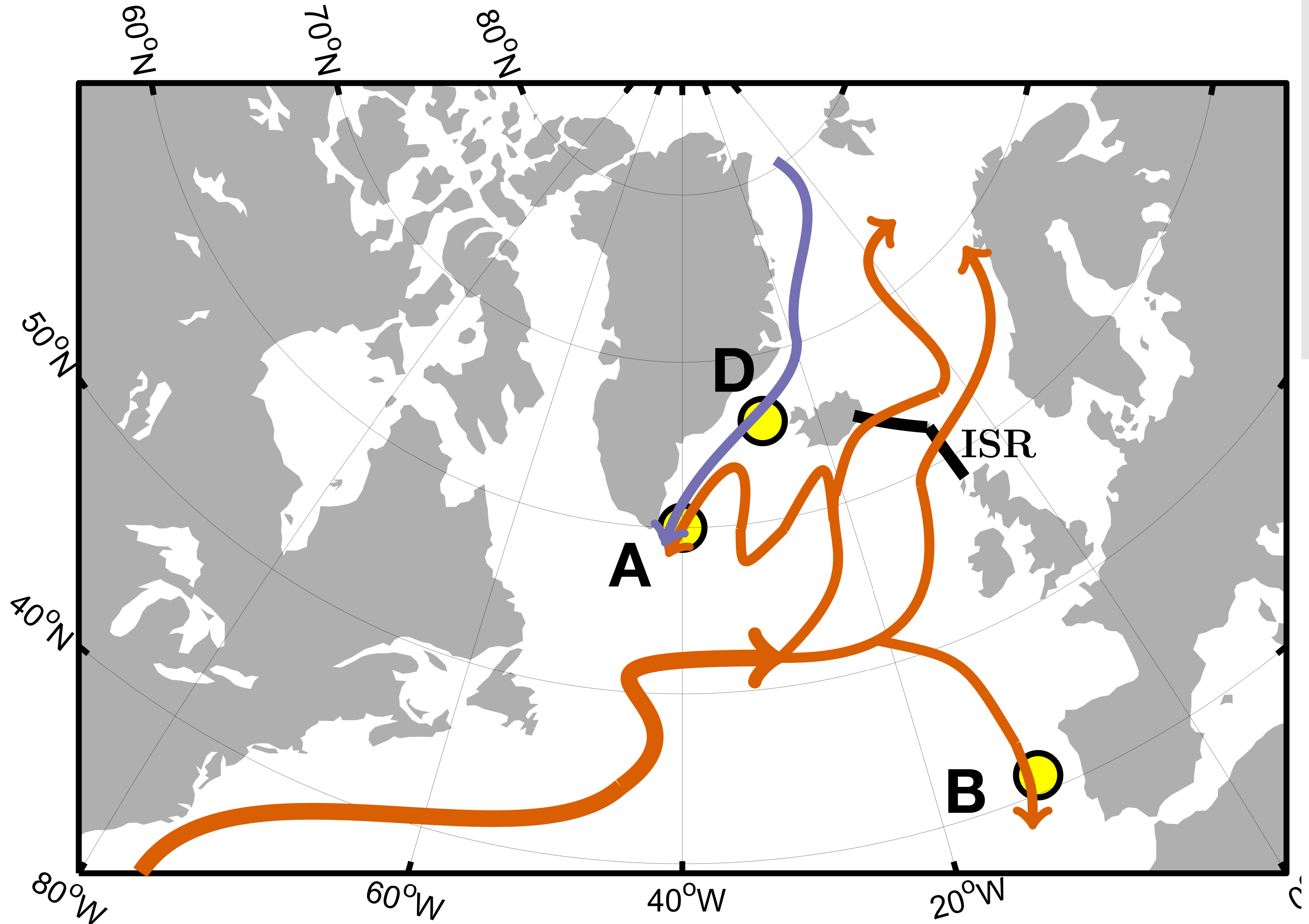
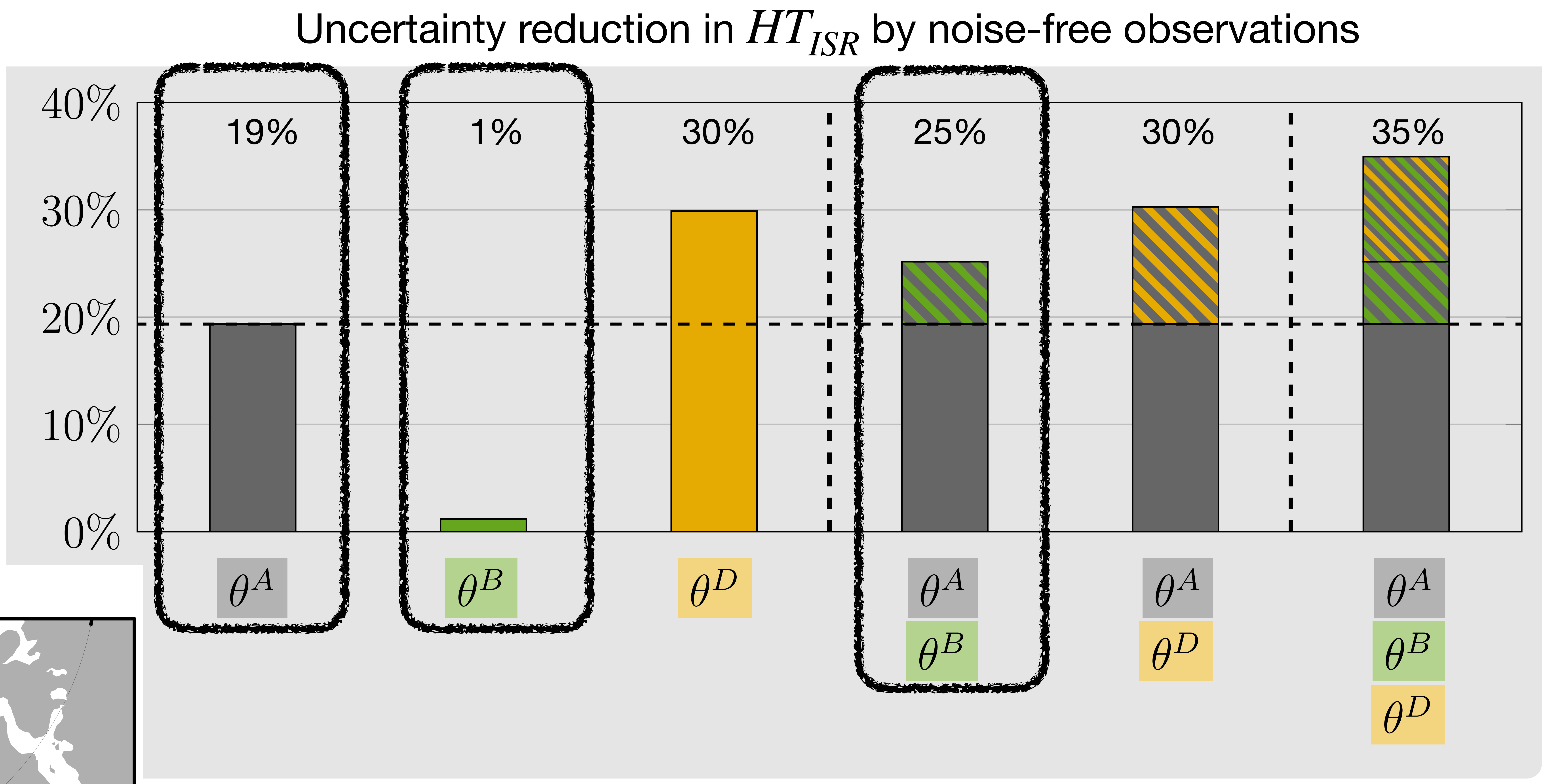
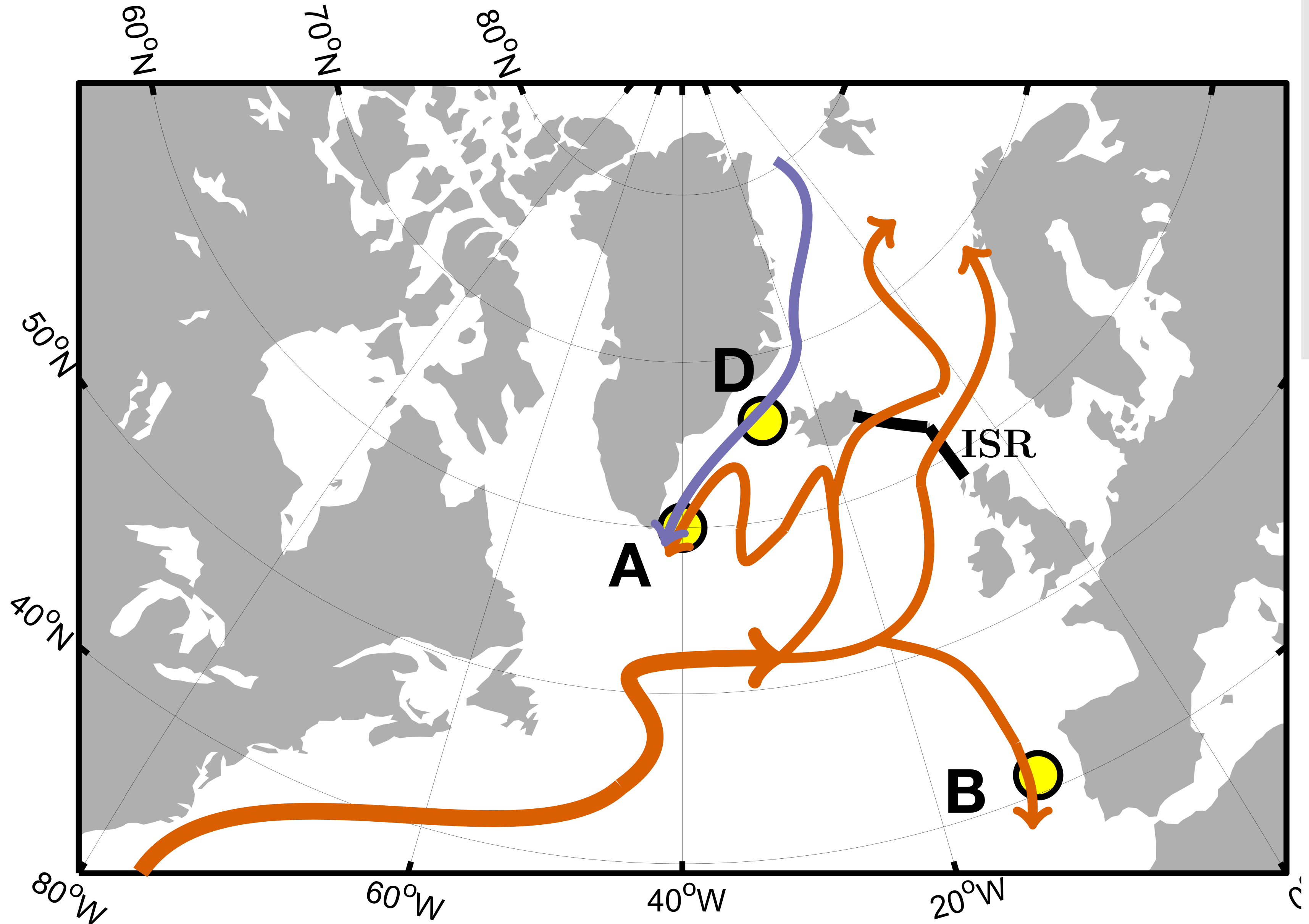




- Adding observation A (in the Irminger Sea) to observation D (in Denmark Strait) gives no extra information due to **data redundancy**

Assessing data redundancy



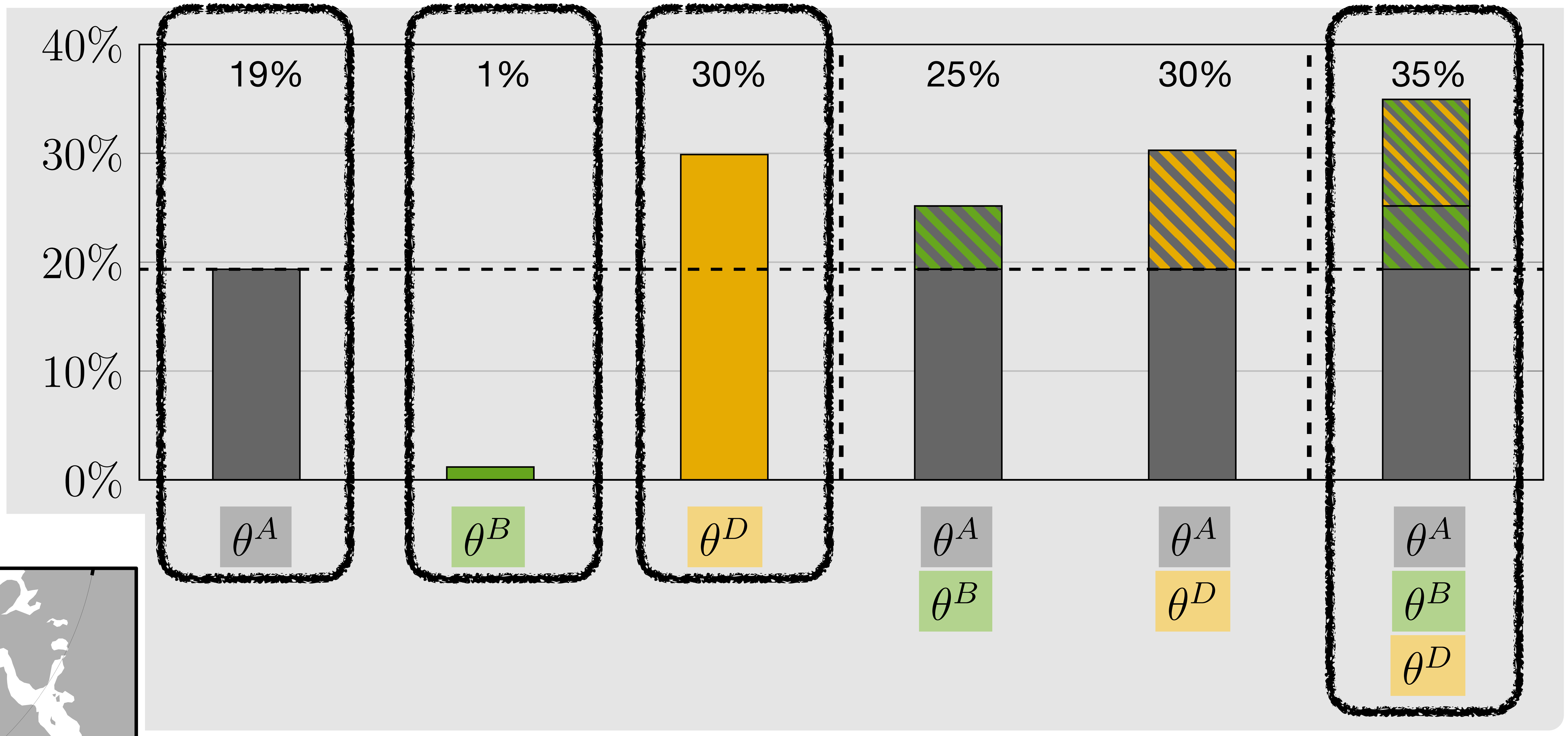


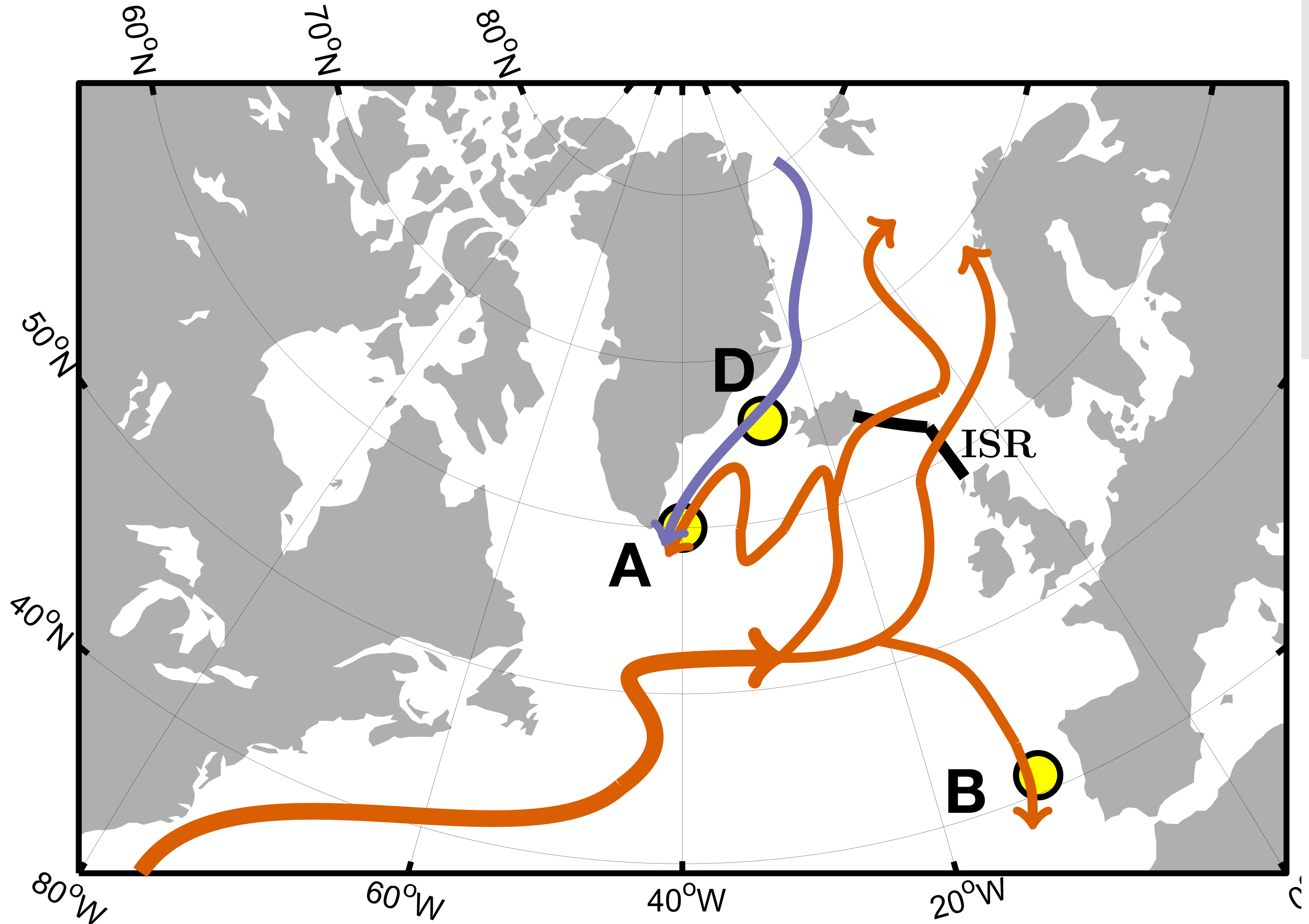
- Adding observation A (in the Irminger Sea) to observation D (in Denmark Strait) gives no extra information due to **data redundancy**

- Observation A (in the Irminger Sea) and observation B (off Portugal) show **data complementarity**

Assessing data redundancy

Uncertainty reduction in HT_{ISR} by noise-free observations





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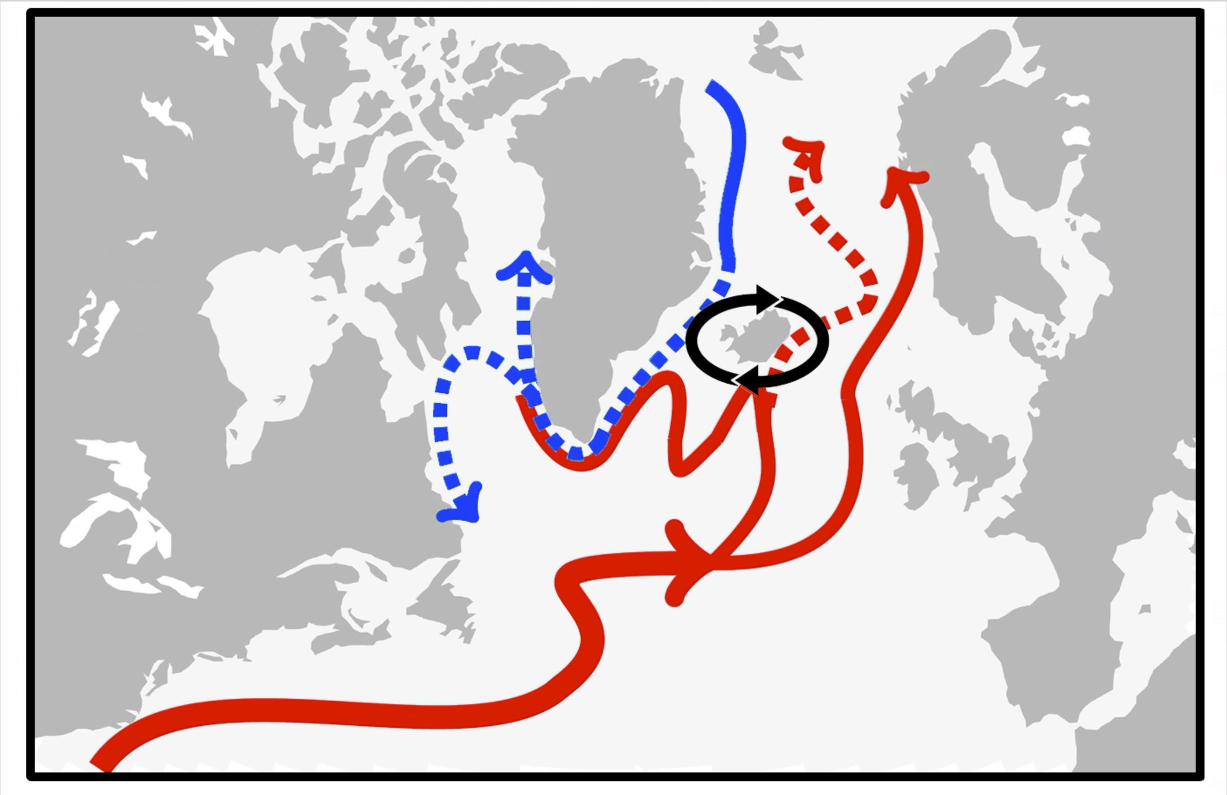
Summary

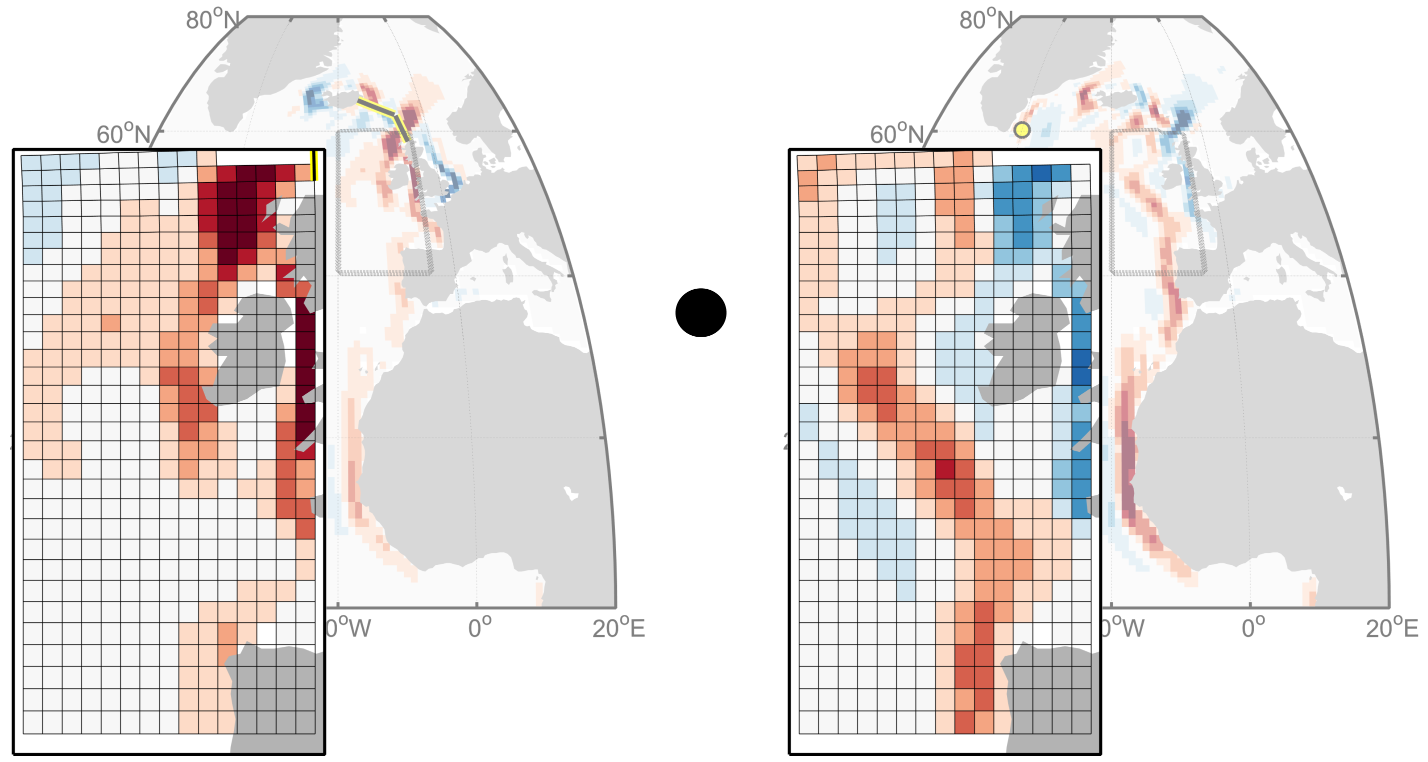
Loose et al., *JGR Oceans* (2020)

Oceanic teleconnections



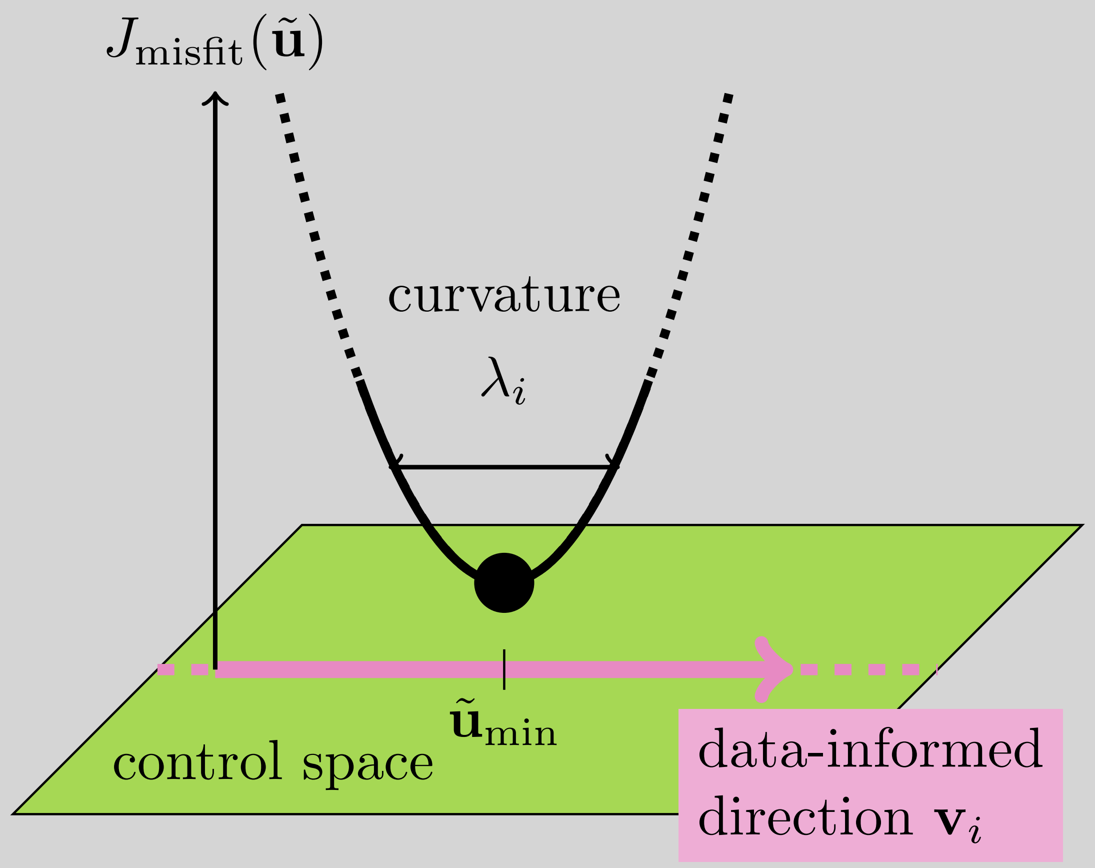
Shared adjustment mechanisms

Adjoint model



Loose & Heimbach, *JAMES* (2021)

Uncertainty Quantification (UQ)



Data redundancy & complementarity

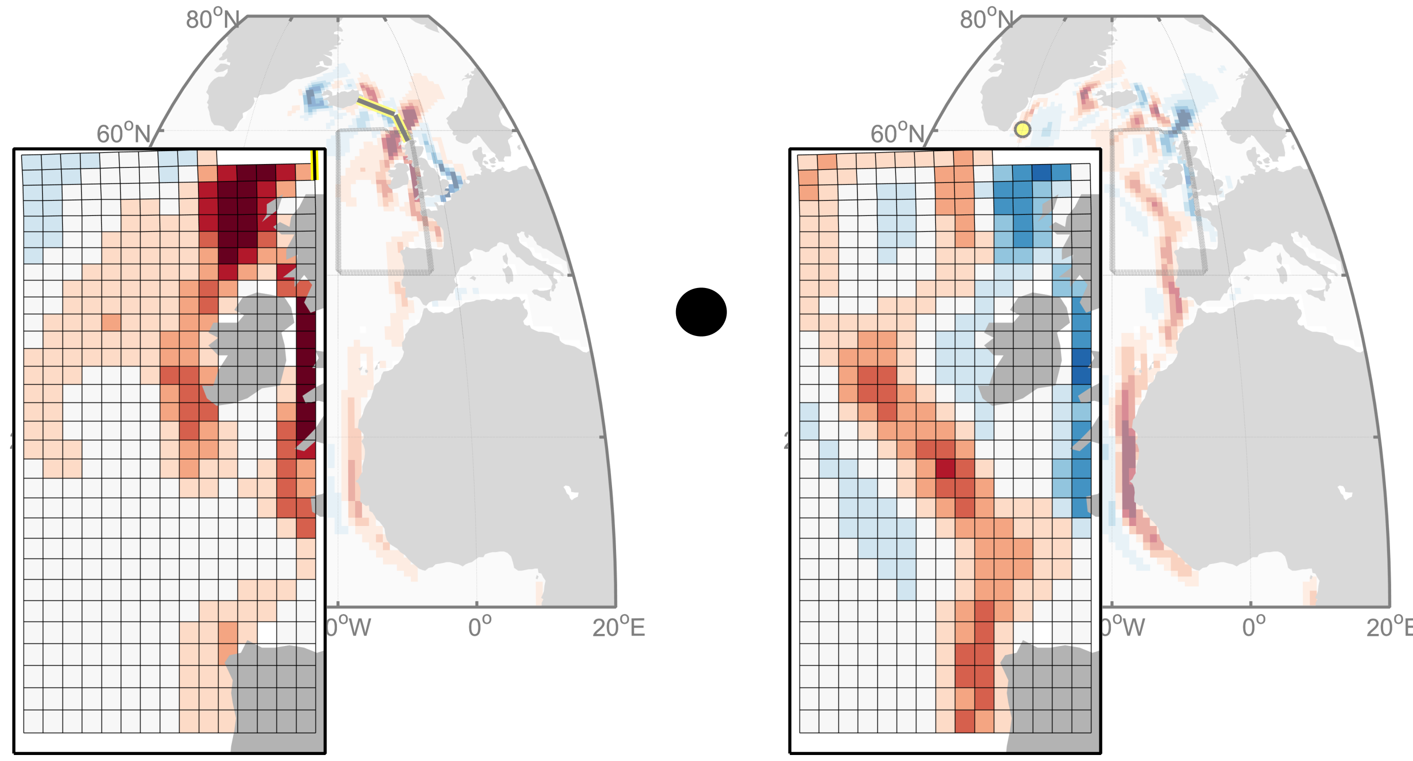
Dynamics-informed & quantitative observing system design

Summary

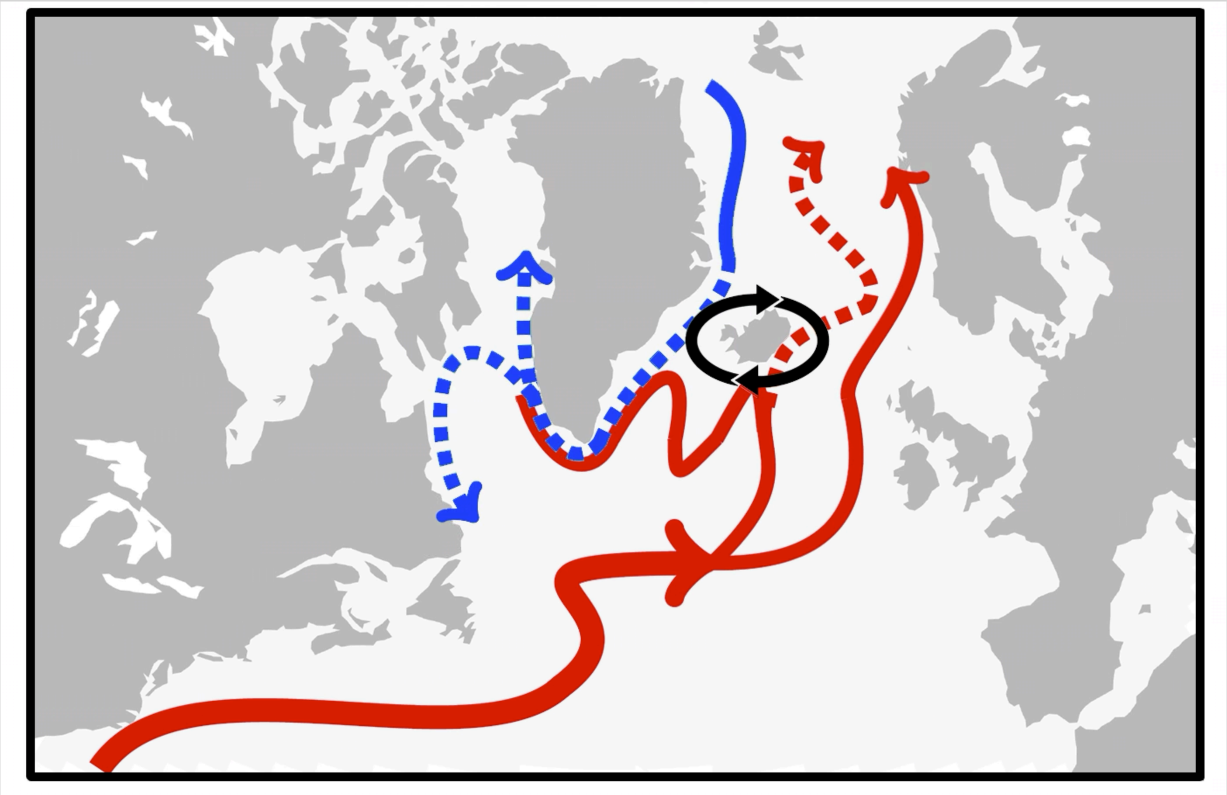
Loose et al., *JGR Oceans* (2020)

Loose & Heimbach, *JAMES* (2021)

Adjoint model

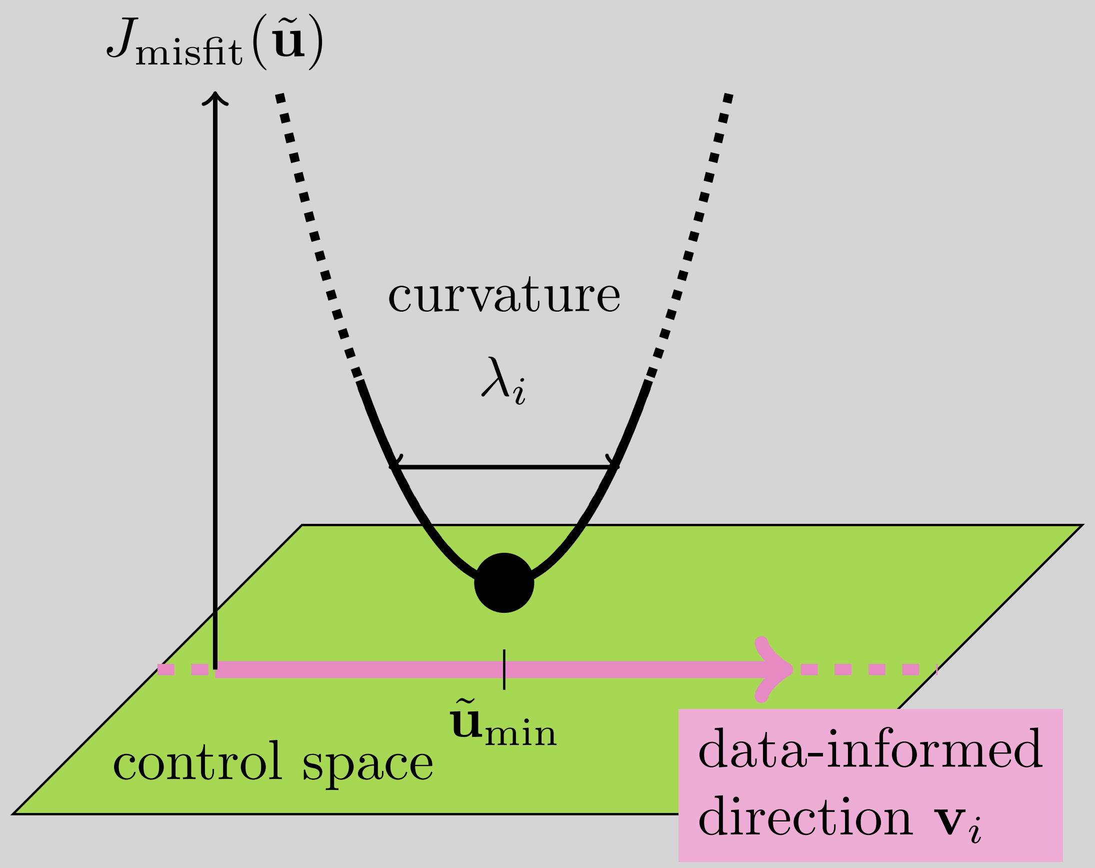


Oceanic teleconnections



Shared adjustment mechanisms

Uncertainty Quantification (UQ)



Data redundancy & complementarity

Dynamics-informed & quantitative observing system design

Limitation: Adjoint only provides linearized approximation of ocean dynamics

Appropriate for: Large-scale dynamics and Gaussian approximation of uncertainty

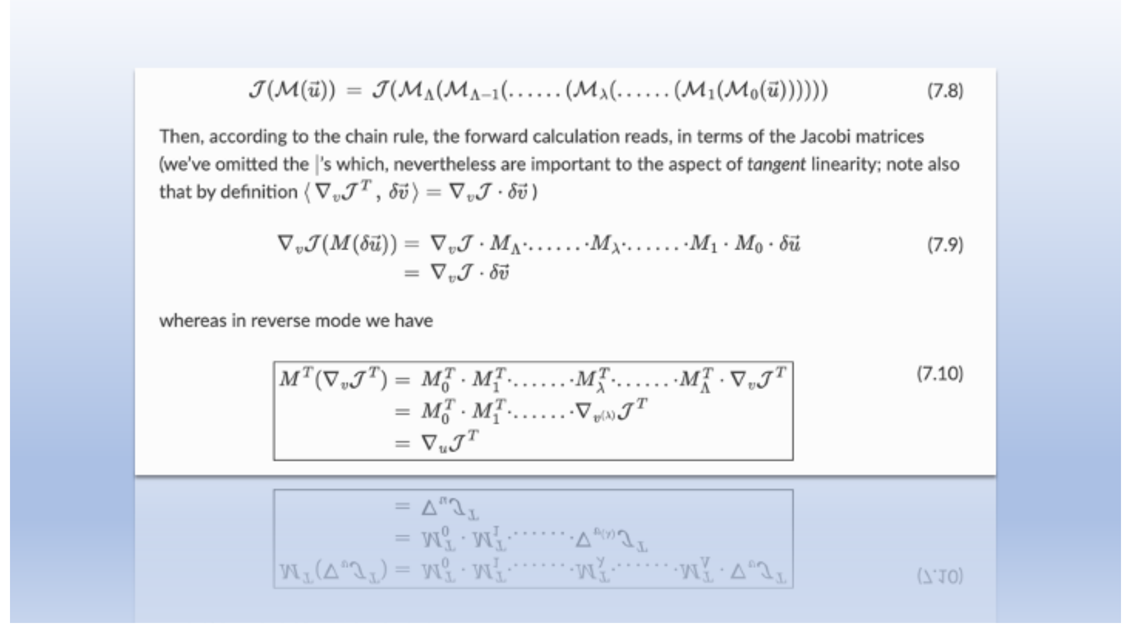
Outlook: How to deal with very nonlinear dynamics & implied uncertainty?

Outlook

DJ4Earth :

Differentiable programming in Julia for Earth system modeling

https://dj4earth.github.io/



$$\mathcal{J}(\mathcal{M}(\vec{u})) = \mathcal{J}(\mathcal{M}_\Lambda(\mathcal{M}_{\Lambda-1}(\ldots\ldots(\mathcal{M}_\lambda(\ldots\ldots(\mathcal{M}_1(\mathcal{M}_0(\vec{u})))))) \quad (7.8)$$

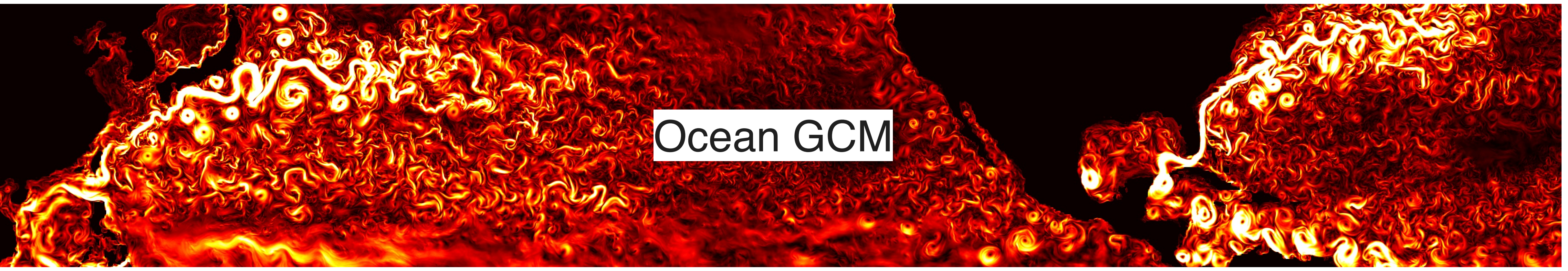
Then, according to the chain rule, the forward calculation reads, in terms of the Jacobi matrices (we've omitted the |'s which, nevertheless are important to the aspect of *tangent* linearity; note also that by definition $\langle \nabla_v \mathcal{J}^T, \delta\vec{v} \rangle = \nabla_v \mathcal{J} \cdot \delta\vec{v}$)

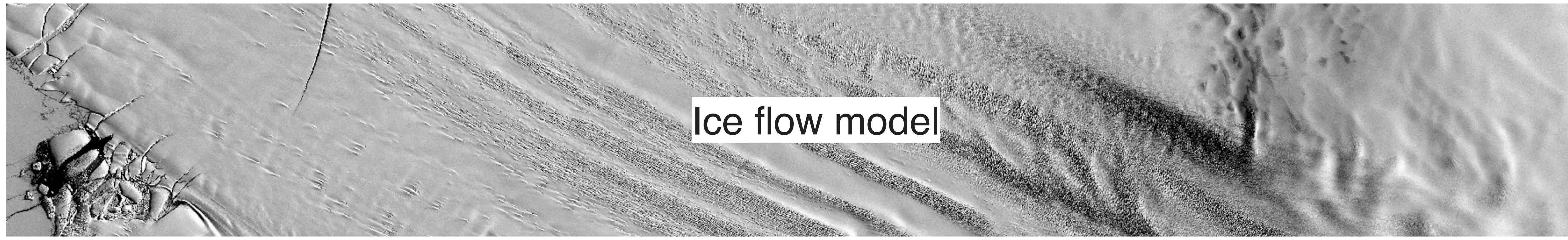
$$\begin{aligned} \nabla_v \mathcal{J}(M(\delta\vec{u})) &= \nabla_v \mathcal{J} \cdot M_\Lambda \cdot \ldots\ldots \cdot M_\lambda \cdot \ldots\ldots \cdot M_1 \cdot M_0 \cdot \delta\vec{u} \\ &= \nabla_v \mathcal{J} \cdot \delta\vec{v} \end{aligned} \quad (7.9)$$

whereas in reverse mode we have

$$\boxed{\begin{aligned} M^T(\nabla_v \mathcal{J}^T) &= M_0^T \cdot M_1^T \cdot \ldots\ldots \cdot M_\lambda^T \cdot \ldots\ldots \cdot M_\Lambda^T \cdot \nabla_v \mathcal{J}^T \\ &= M_0^T \cdot M_1^T \cdot \ldots\ldots \cdot \nabla_{v^{(\lambda)}} \mathcal{J}^T \\ &= \nabla_u \mathcal{J}^T \end{aligned}} \quad (7.10)$$

Earth system flagship applications



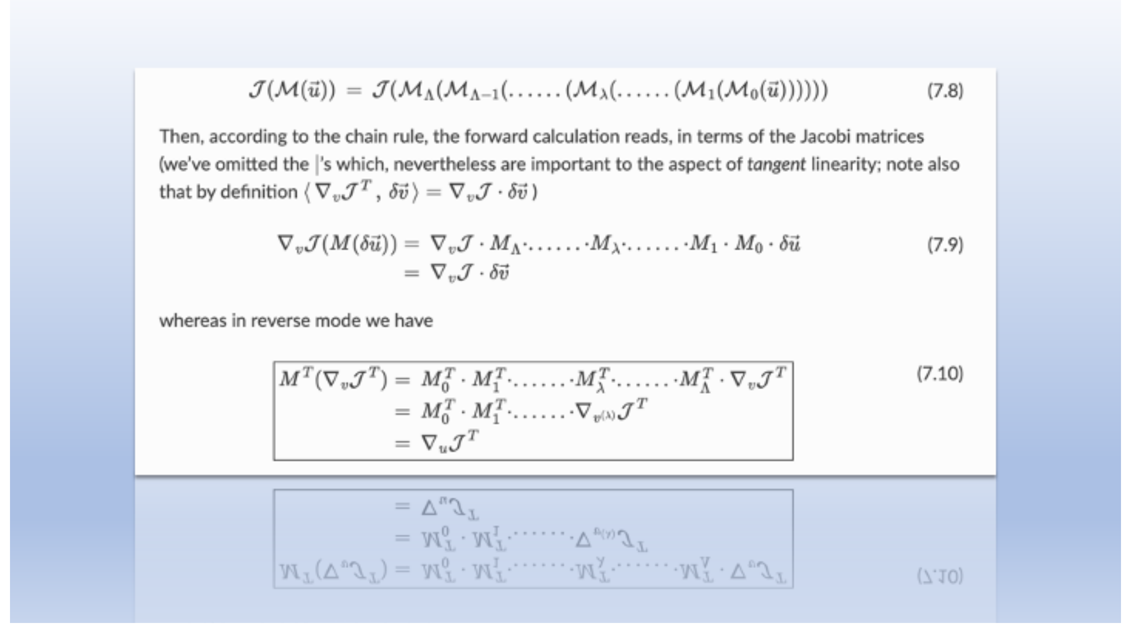


Outlook

DJ4Earth :

Differentiable programming in Julia for Earth system modeling

https://dj4earth.github.io/



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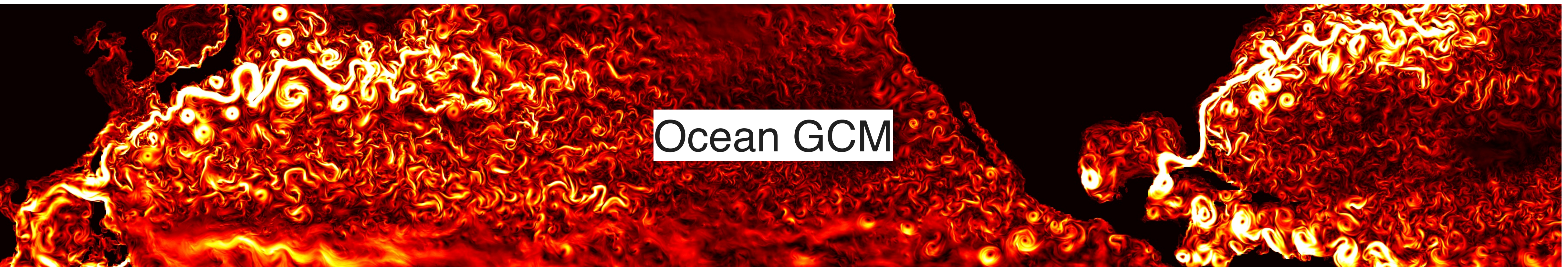
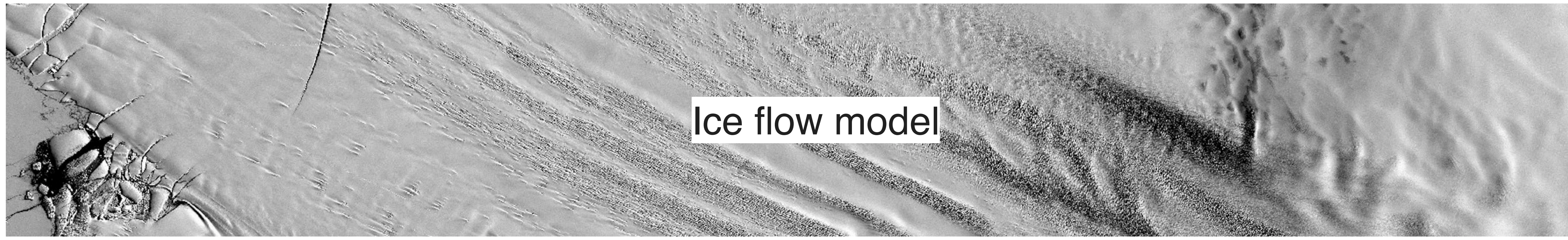
⟷ julia

Earth system flagship applications





Goal: Advance automatic differentiation (AD) to generate adjoint and back-propagation operators in Earth system models

Julia:

Physics model (PDE) & its adjoint

Earth system model

Seamless integration

Machine Learning (ML) & differentiable programming

Outlook

DJ4Earth :

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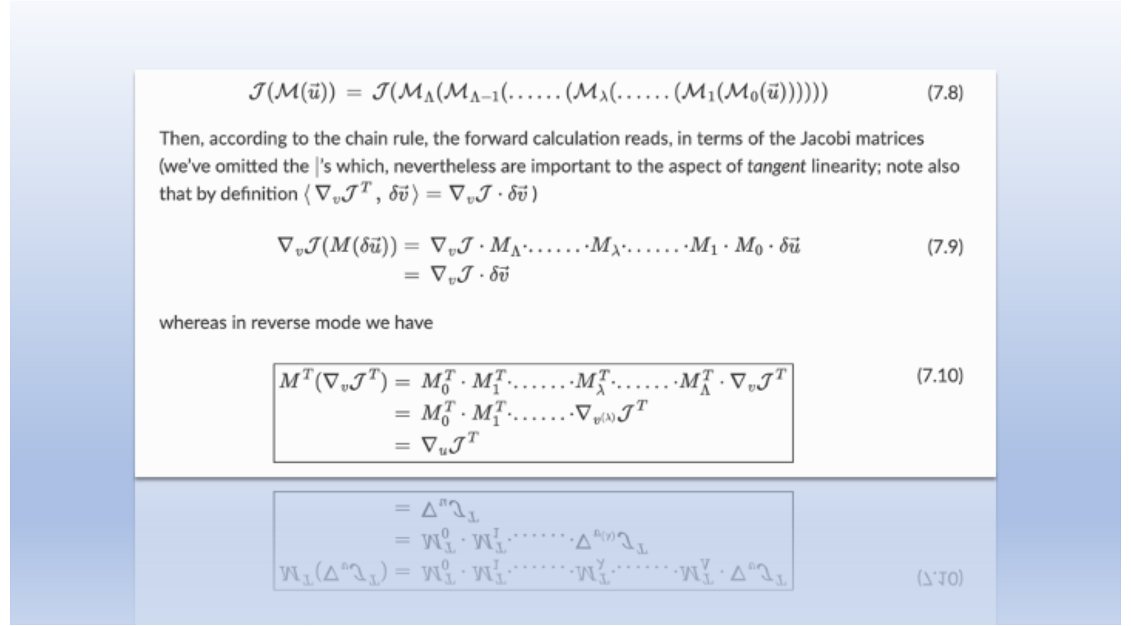

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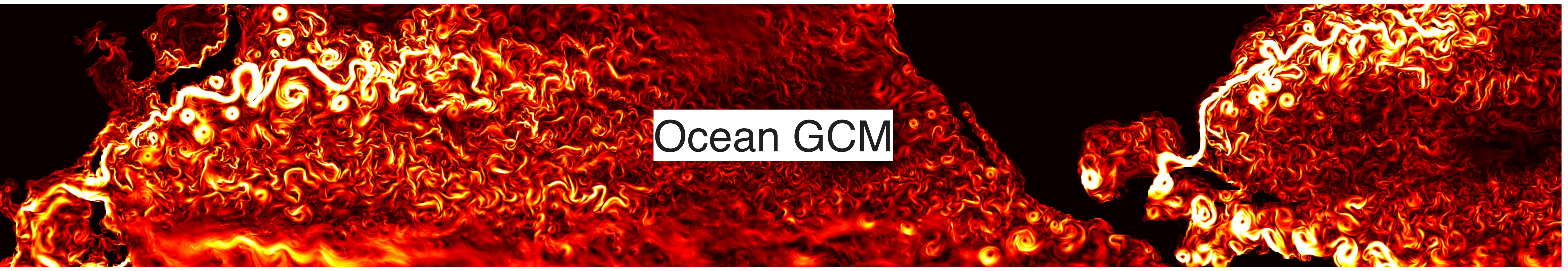
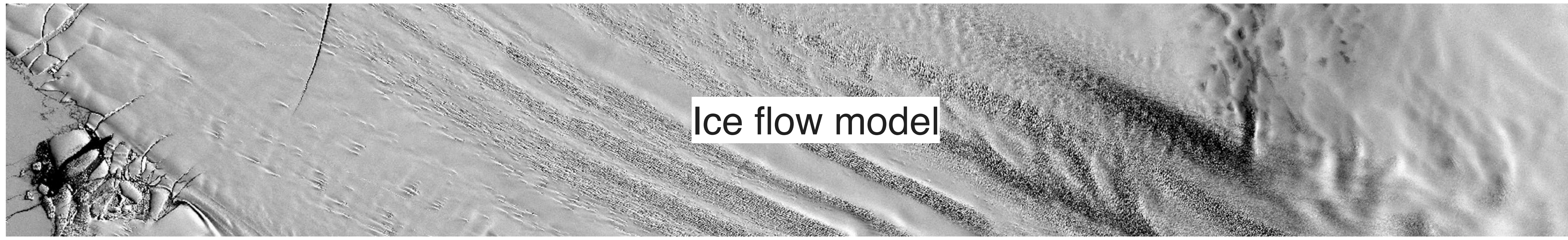
Earth system flagship applications





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Hybrid approaches:

- ML-accelerated sampling for non-Gaussian UQ
- Derivative- and physics-informed ML