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FORMAL STRATEGIES FOR OPTIMAL OBSERVING SYSTEM DESIGN

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What is optimal observing system design?

A range of computational tools to support science applications,

where experimental / observational approaches are …

- ***too costly / slow / dangerous,***
- ***or impossible***

Problem statement:

What is an optimal sampling strategy using given or hypothetical observational assets to best constrain a **Quantity of Interest (QoI)**?

- When a QoI ***is unobserved*** (different variable, different location, different time) – an ubiquitous problem!
- Or when the QoI ***is a forecast***
- Or ***model parameters***

What are “Quantities of Interest” (QoI)

They are oceanic/atmospheric/climate metrics that we seek to quantify

Examples:

- Meridional volume/heat/freshwater transport across given section
  - E.g.: AMOC; transports across Drake Passage, Fram Strait, ITF, …
- Regional ocean heat content (OHC), or its convergence/divergence
  - E.g.: Greenland margin subsurface OHC, Nordic Seas OHC, …
- Climate indices, such as SST, Sea Level Anomaly, …
  - E.g.: Nino3.4 index; US East Coast SLA; …
- Forecast skill: Arctic sea ice cover, …

Simulation-based strategies of observing system design

- Observing System Experiments (OSEs)
- Observing System Simulation Experiments (OSSEs)
- Forecast Sensitivity Observation Impacts (FSOI)
- ***Optimal Experimental Design (OED) / Quantitative Network Design (QND)***

Most of these approaches take place in the context of data assimilation & prediction systems

Why?

A major goal of DA:

"Ideally, all observational data streams are interpreted simultaneously [for calibration] with the process information provided by the model, [which leads to] a consistent picture of the state of the Arctic system that balances all the observational constraints, taking into account the respective uncertainty ranges."

Kaminski et al., The Cryosphere, 2015

Approaches

Some covered in OceanObs'19 CWP:

- Y. Fujii et al., *Front. Mar. Sci.* (2019)
- P. Heimbach et al., *Front. Mar. Sci.* (2019)
- C. Lee et al., *Front. Mar. Sci.* (2019)
- A. Moore et al., *Front. Mar. Sci.* (2019)
- G. Smith et al., *Front. Mar. Sci.* (2019)
- Subramanian et al., *Front. Mar. Sci.* (2019)

Approaches:
Observing System Experiments (OSEs)

a.k.a. **Observation Withholding/Denial Experiments**

- A data assimilative run in which a certain observation-type is withheld from, or added to, the regularly assimilated data.
- The impact of these withheld/added data is assessed by comparing the OSE with the control simulation in which only regular data are assimilated

Some drawbacks:

- The error reduction cannot be estimated accurately because the true state is not known.
- Can only be used to evaluate preexisting, not future, observing systems

Approaches:
Observing System Simulation Experiments (OSSEs)

- Synthetic data, intended to mimic observations from the proposed observing system, are generated from a model simulation that is intended to represent the "true" ocean, thus called the "Nature Run", with observation errors added based on prior information.
- Impact of synthetic data on forecast improvement is assessed from the error reduction in OSSEs when assimilating the new data

Some drawbacks:

- nature runs may not be good enough to realistically model the true ocean and the phenomena of interest
- results may be system-dependent, or results may only apply within the used OSSE system, but are not connected to the real world

Approaches:
Adjoint-based sensitivity methods

Uncover teleconnections, physical/dynamical relationships and causal chains that connect the observed quantities to the rest of the global ocean

1. Adjoint sensitivities
2. Observation sensitivities & FSOI
3. Hessian-based uncertainty quantification (UQ)
4. Hessian-based optimal experimental design (OED)

Main point:

They are related, but vary substantially in degree of sophistication and required computational needs. Level 3 *rarely*, and level 4 probably *never* used so far in context of ocean/climate/NWP context.

Approaches:
Adjoint-based sensitivity methods

Application in parameter & state estimation (PSE)

Objective function is weighted least-squares model-data misfit function

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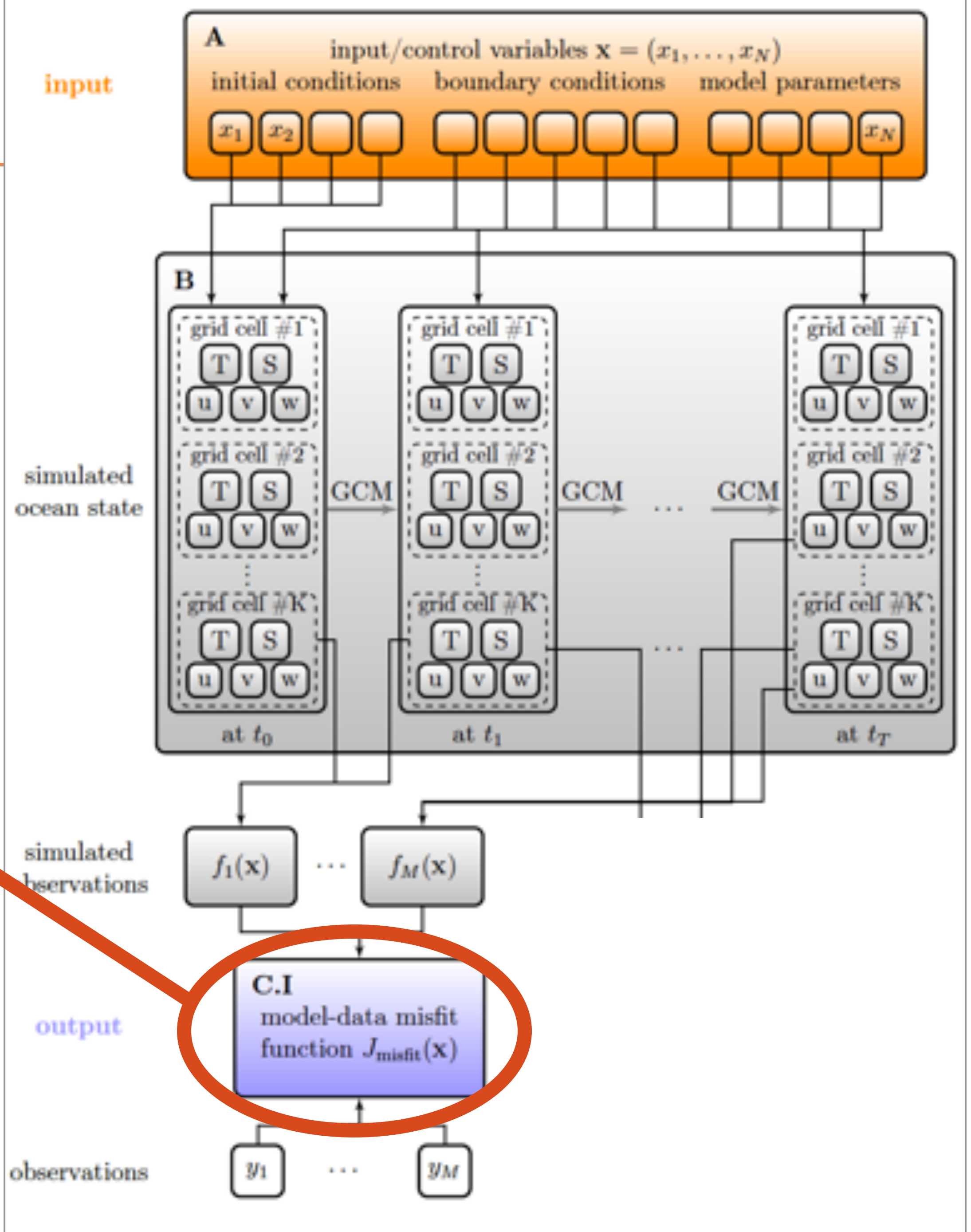


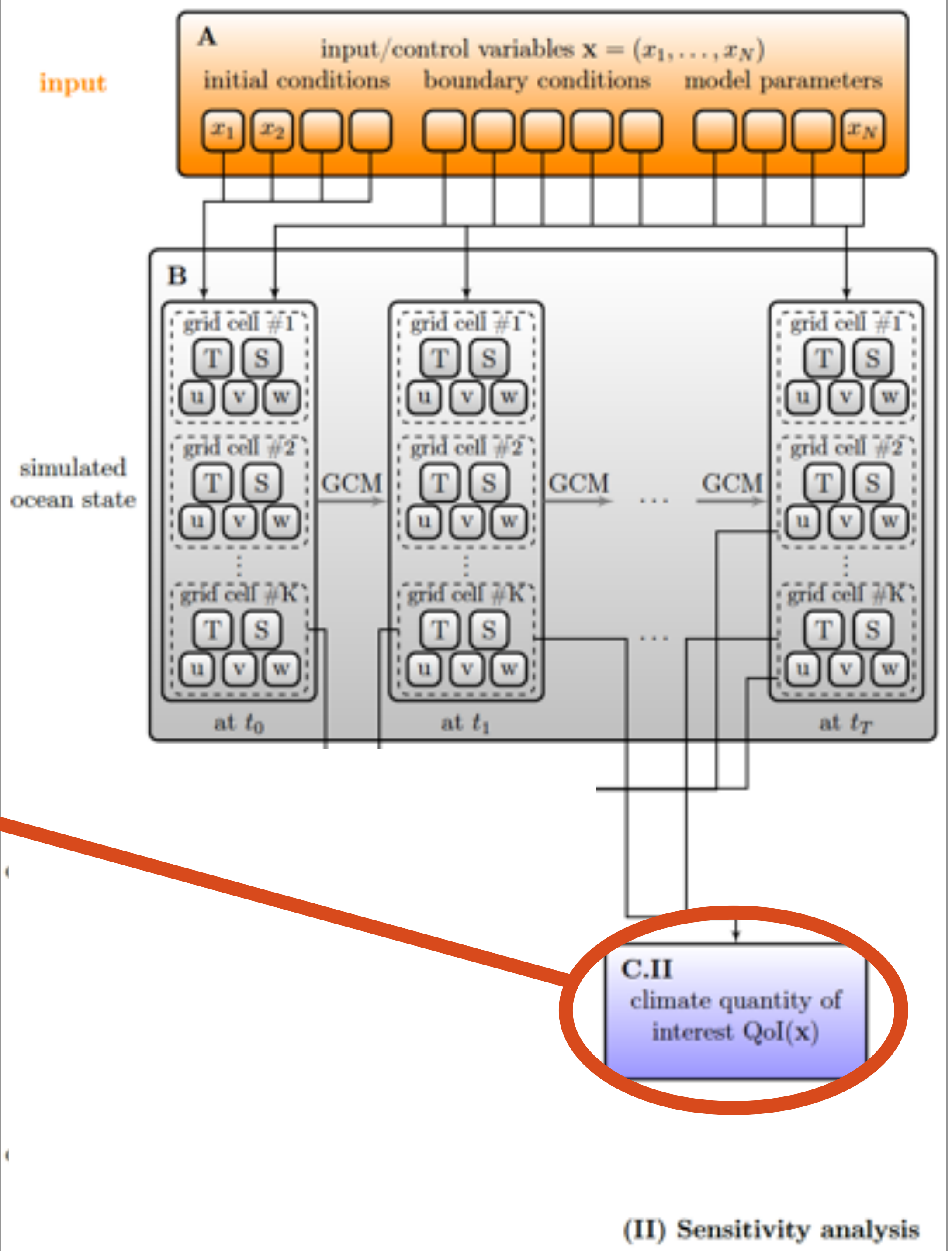
(I) State estimation

Approaches:
Adjoint-based sensitivity methods

Application in sensitivity analysis

Objective function is scalar-valued

Quantity of Interest (QoI), metric, …



Courtesy
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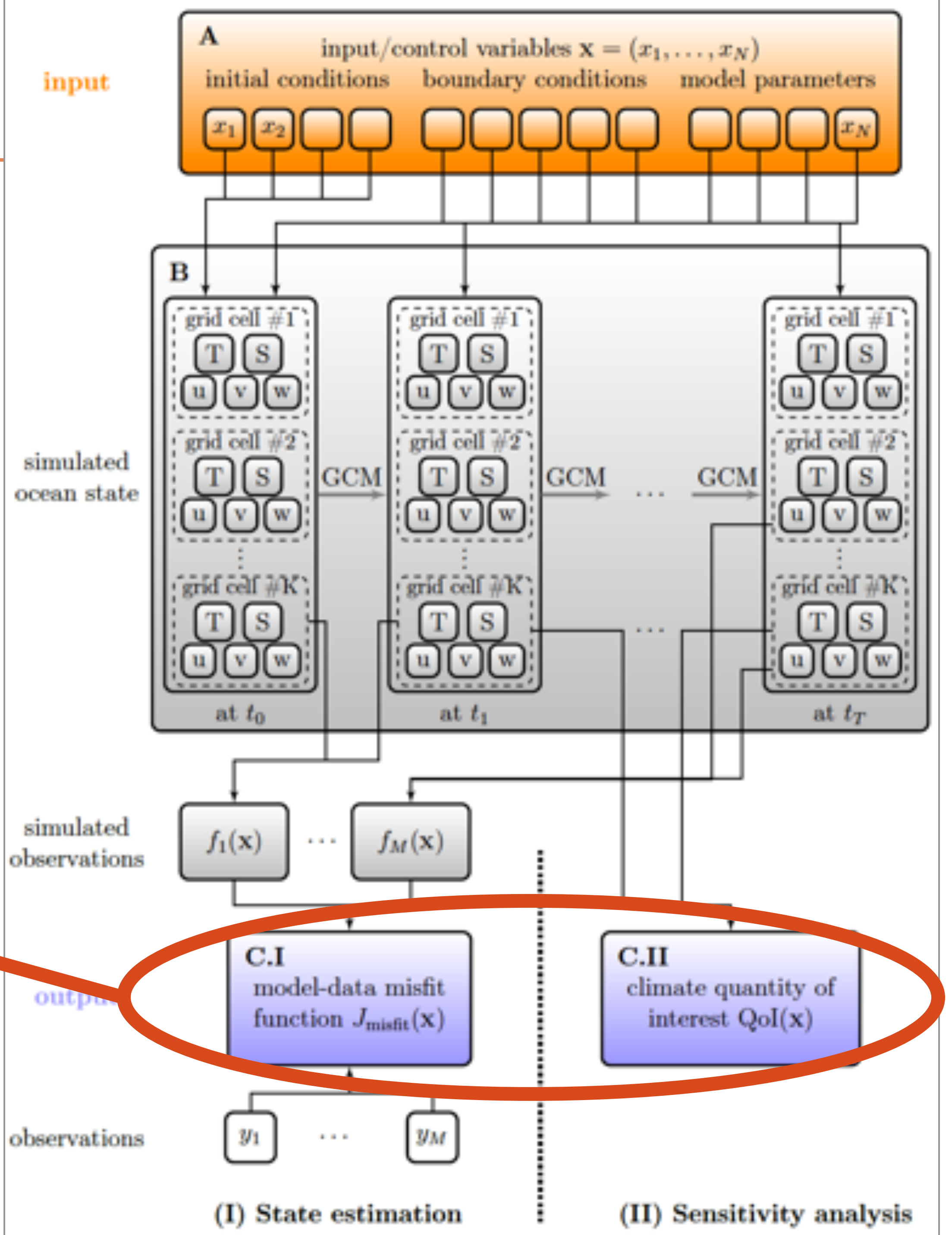
Approaches:
Adjoint-based sensitivity methods

How to combine?

I.e., how do the observations used to constrain the PSE aid to reduce the uncertainty in the QoI

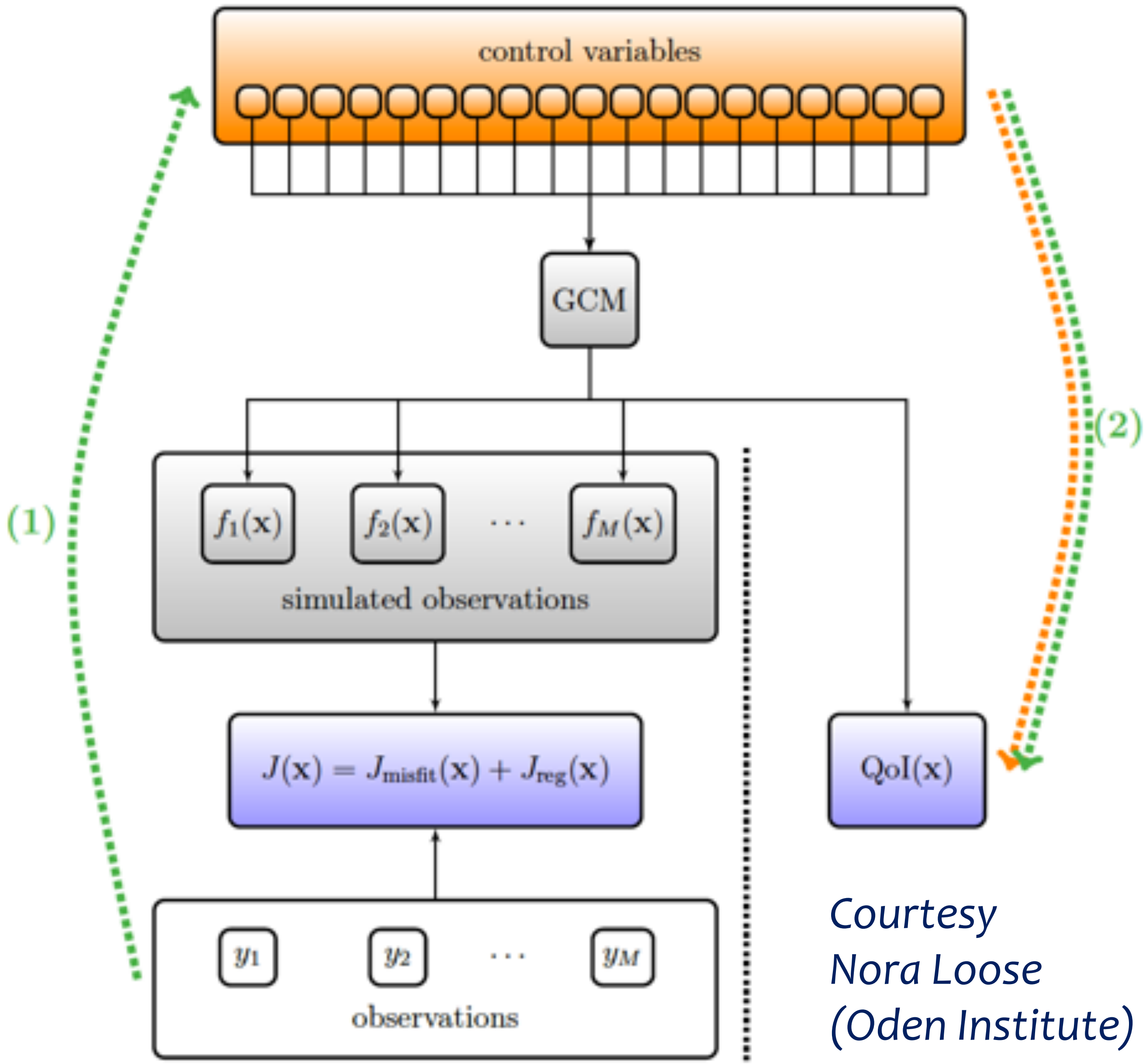
?

Courtesy Nora Loose (Oden Institute)



Optimal Observing System Design

The uncertainty propagation & optimal design problem



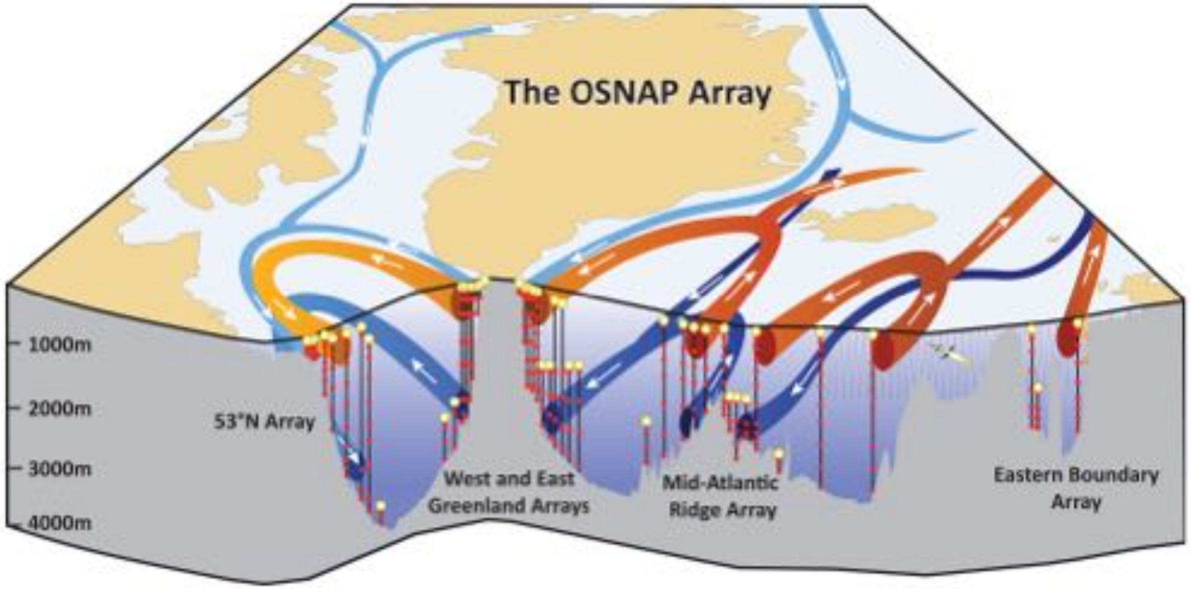
Courtesy Nora Loose (Oden Institute)

Formalize:

- the uncertainty reduction of the PSE provided by observations
  - Information *provided* by the observation
- How the reduced uncertainties in the PSE help to reduce the uncertainty in the QoI
  - Information *required* by the QoI

Both are achieved with the adjoint!

Bayesian UQ in large-scale inverse problems based on (low-rank) Hessians



Overturning in the Subpolar North Atlantic Program (OSNAP)

http://www.o-snap.org

Lozier et al., BAMS (2017)

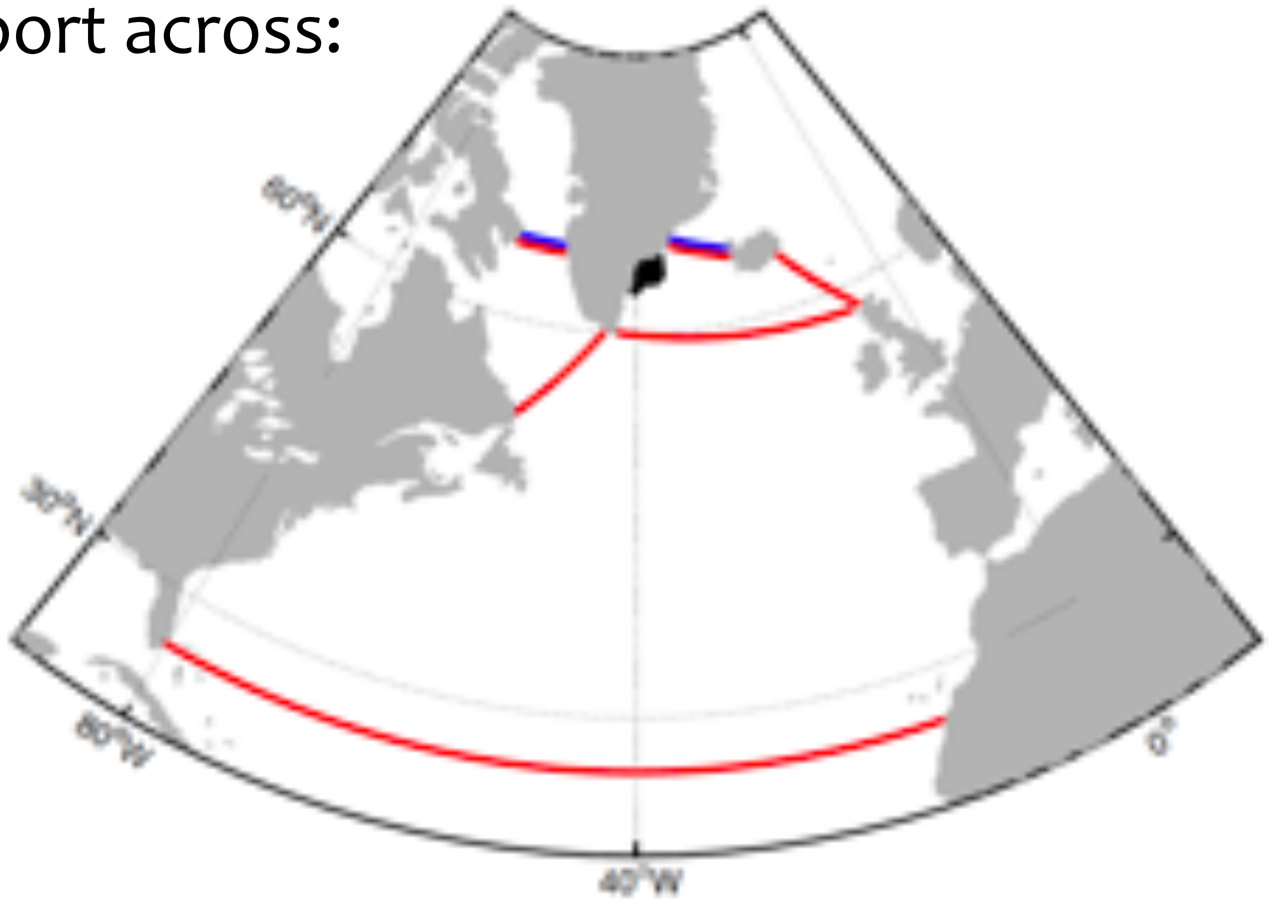
Lozier et al., Science (2019)

N. Loose, PhD thesis (2019)

Bayesian UQ in large-scale inverse problems based on (low-rank) Hessians

Observations: heat & volume transport across:

- Iceland-Scotland Ridge
- RAPID array (26N)
- OSNAP West
- OSNAP East
- Davis Strait



Quantity of Interest (QoI):

subsurface heat content outside of Sermilik Fjord & Helheim Glacier (Southeast Greenland)

N. Loose, PhD thesis (2019)

Bayesian UQ in large-scale inverse problems based on (low-rank) Hessians

Prior & posterior variances of Quantity of Interest Q

$$\mu_{prior} = \left(\frac{\partial Q}{\partial x}\right)^T B \left(\frac{\partial Q}{\partial x}\right), \quad \mu_{post} = \left(\frac{\partial Q}{\partial x}\right)^T P \left(\frac{\partial Q}{\partial x}\right)$$

Uncertainty reduction

$$1 - \frac{\mu_{post}}{\mu_{prior}} = \sum_{i=1}^{N_{obs}} d_i < q\,,\, v_i >^2$$

where

Prior-weighted QoI sensitivity
Information required by QoI

•

Prior-weighted misfit sensitivity
Information transmitted by obs.

Prior & posterior variances of Quantity of Interest Q

$$\mu_{prior} = \left(\frac{\partial Q}{\partial x}\right)^T B \left(\frac{\partial Q}{\partial x}\right), \quad \mu_{post} = \left(\frac{\partial Q}{\partial x}\right)^T P \left(\frac{\partial Q}{\partial x}\right)$$

N.B.:

Almost everything is contained in that posterior error covariance

$\boldsymbol{P}$

Bayesian UQ in large-scale inverse problems based on (low-rank) Hessians

Prior & posterior variances of Quantity of Interest Q

$$\mu_{prior} = \left(\frac{\partial Q}{\partial x}\right)^T B \left(\frac{\partial Q}{\partial x}\right), \quad \mu_{post} = \left(\frac{\partial Q}{\partial x}\right)^T P \left(\frac{\partial Q}{\partial x}\right)$$

with Λ_r , V_r truncated eigenvalues & eigenvector matrix

$$P = B^{1/2}\left(I - V_r D_r V_r^T\right) B^{1/2}, \quad D_r = \mathrm{diag}\left(\frac{\lambda_i}{\lambda_i + 1}\right)$$

$$= B^{1/2}\left\{I - \sum_{i=1}^{N_{obs}} d_i \, v_i \, v_i^T\right\} B^{1/2}, \quad d_i = \frac{\lambda_i}{\lambda_i + 1}$$

How well does each observing system constrain the solution & relevant QoIs?

Prior & posterior variances of Quantity of Interest $\mathcal{Q}$

$$\mu_{prior} = \left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T B \left(\frac{\partial \mathcal{Q}}{\partial x}\right), \quad \mu_{post} = \left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T P \left(\frac{\partial \mathcal{Q}}{\partial x}\right)$$

Case of only 1 observation:

Uncertainty reduction of QoI $\mathcal{Q}$ through observation $\mathcal{J}$

$$1 - \frac{\mu_{post}}{\mu_{prior}} = d_1 \left\langle \frac{B^{1/2}\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T}{\|B^{1/2}\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T\|}, \frac{B^{1/2}\left(\frac{\partial \mathcal{J}}{\partial x}\right)^T}{\|B^{1/2}\left(\frac{\partial \mathcal{J}}{\partial x}\right)^T\|} \right\rangle$$

$$= d_1 < \text{info required by } \mathcal{Q}, \text{ info transmitted by } \mathcal{J} >$$

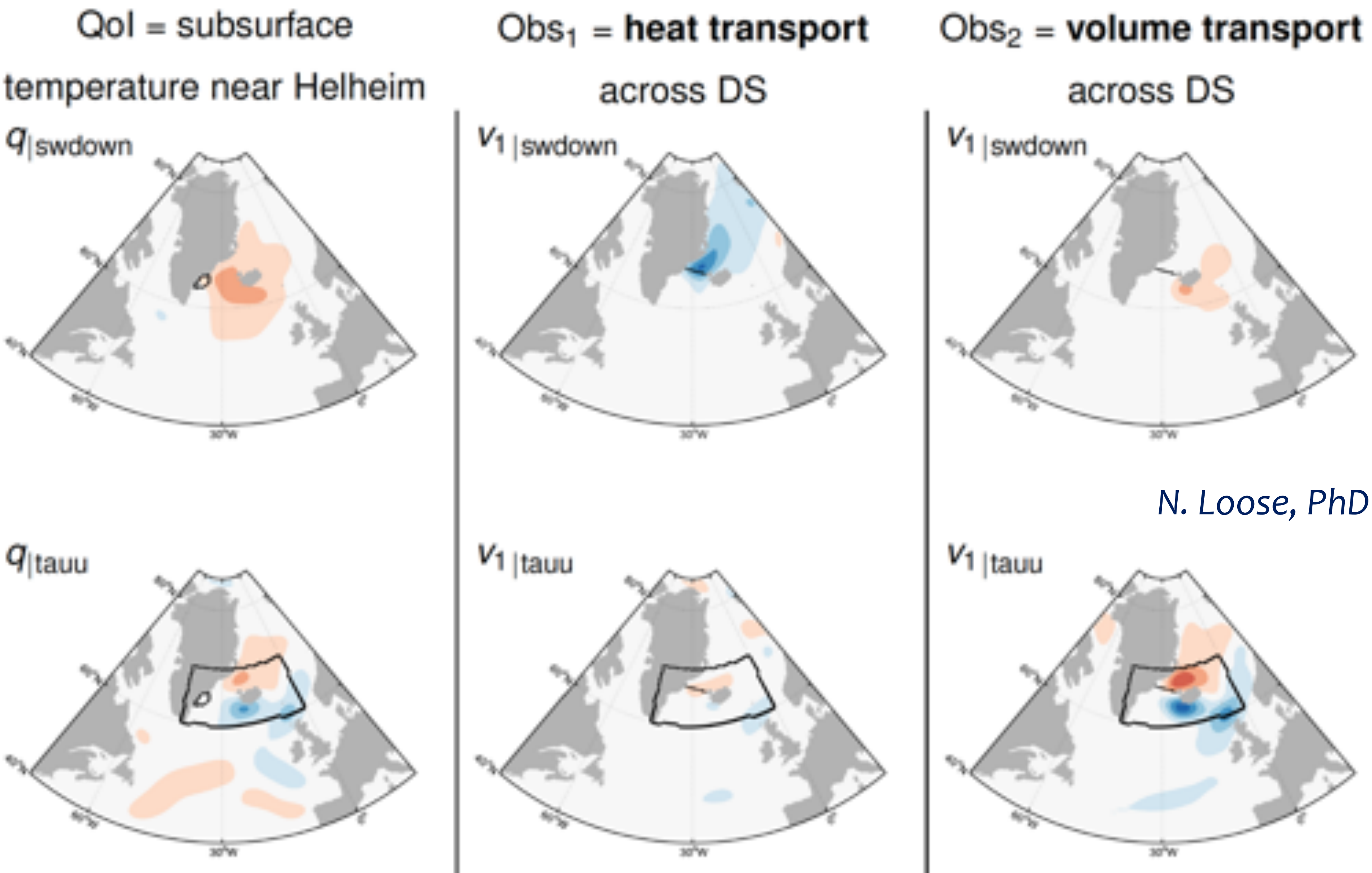
How well does each observing system constrain the solution & relevant QoIs?

Uncertainty reduction of QoI $\mathcal{Q}$ through observation $\mathcal{J}$

$$
\begin{aligned}
1 - \frac{\mu_{post}}{\mu_{prior}} &= d_1 \left\langle \frac{B^{1/2}\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T}{\left\|B^{1/2}\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T\right\|}, \frac{B^{1/2}\left(\frac{\partial \mathcal{J}}{\partial x}\right)^T}{\left\|B^{1/2}\left(\frac{\partial \mathcal{J}}{\partial x}\right)^T\right\|} \right\rangle \\
&= d_1 < \text{info required by } \mathcal{Q}, \text{ info transmitted by } \mathcal{J} >
\end{aligned}
$$

- **Hypothetical proxy potential of observation:**
  - Projection of information communicated (via model dynamics) by observation (***J***) onto information required by QoI (**Q**) via scalar product
- **Effective proxy potential of observation:**
  - Multiplication of scalar product by a scaling factor ***d***

How well does each observing system constrain the solution & relevant QoIs?



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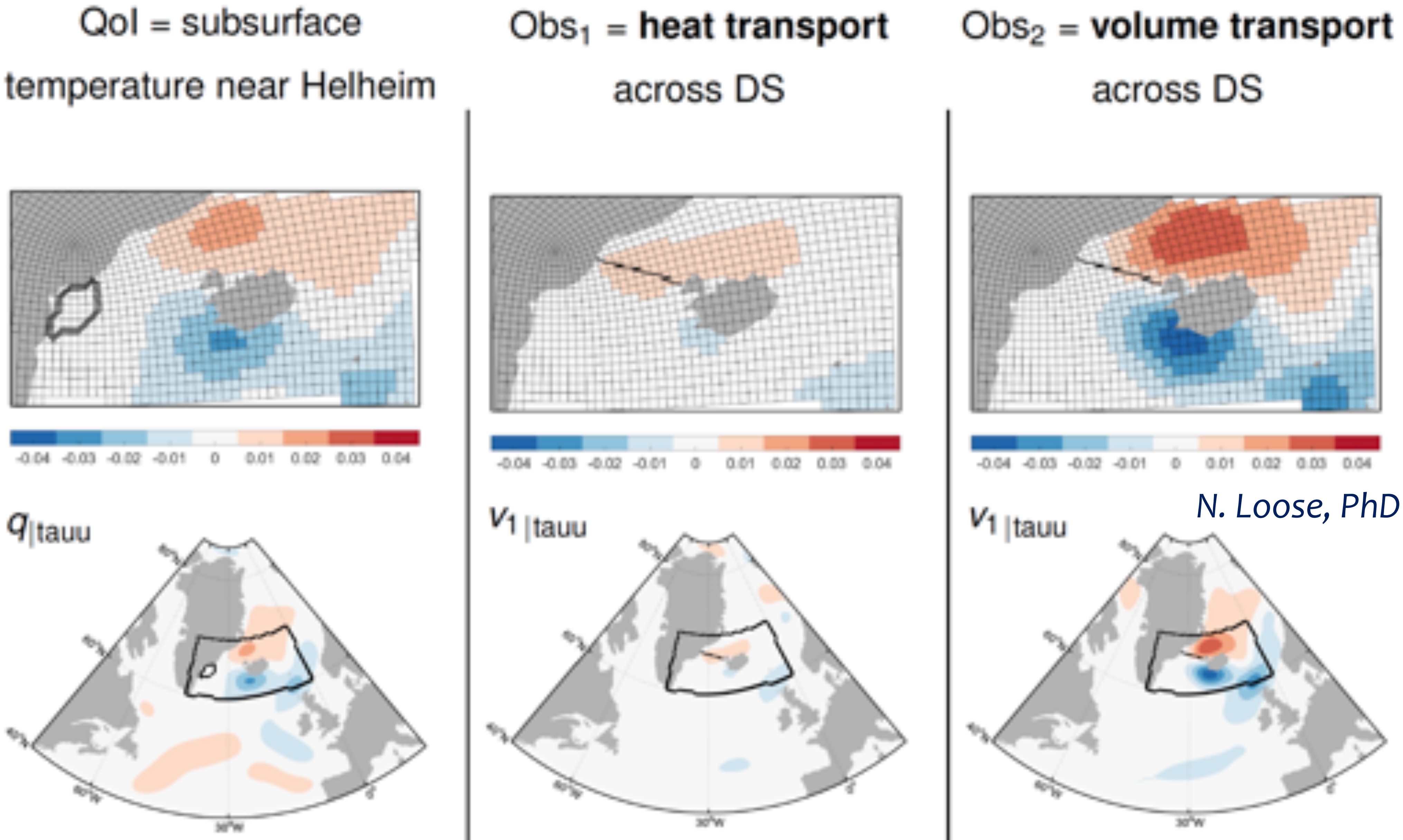
How well does each observing system constrain the solution & relevant QoIs?



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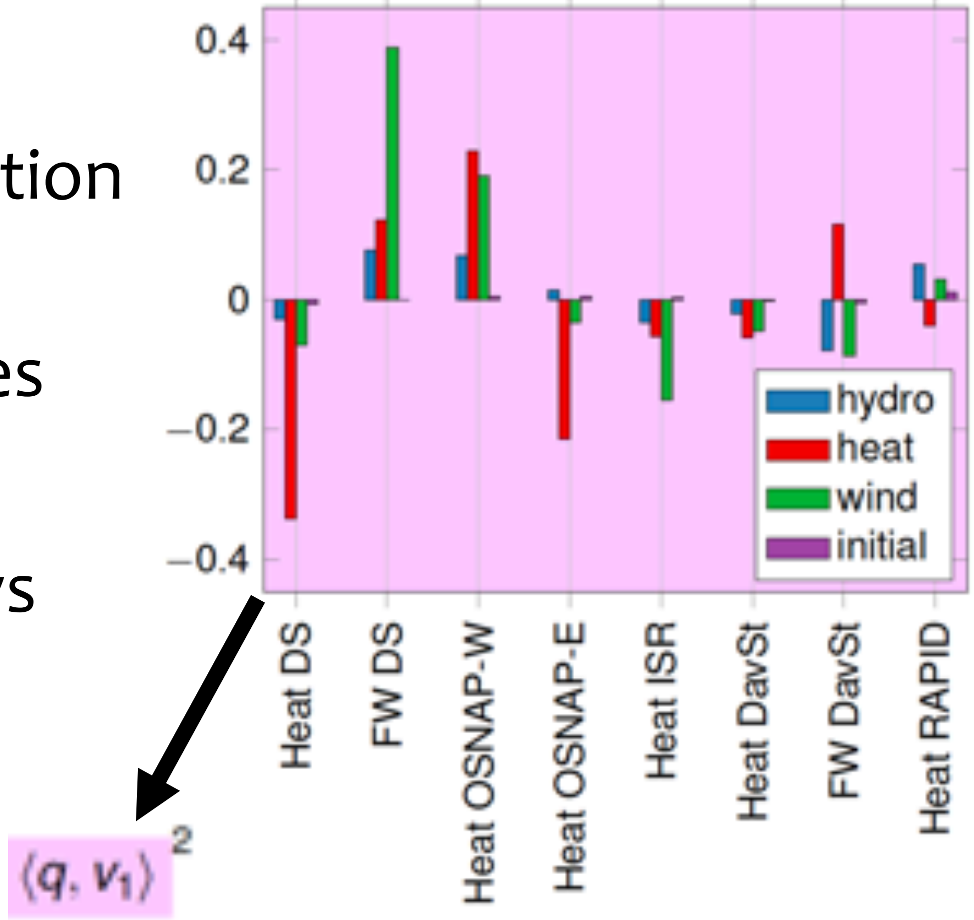
Hypothetical proxy potential

from scalar product / projection of all observation sensitivities with QoI sensitivities

- Accounts for propagation of all uncertainties
- Accounts for observational redundancy
- Accounts for all dynamically viable pathways between observed and QoI location



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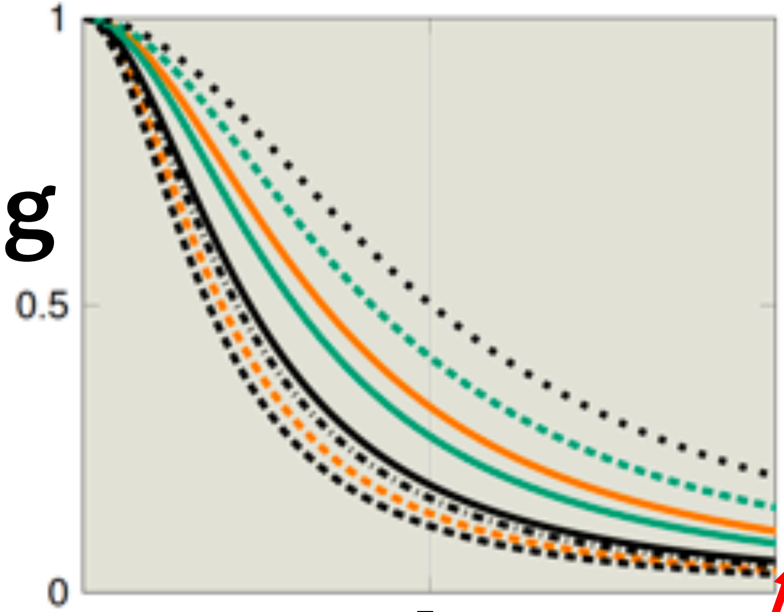
How well does each observing system constrain the solution & relevant QoIs?

Information transfer/damping factor:

- Accounts for obs. Errors (rho)
- Accounts for prior knowledge / uncertainties (beta)



$$= \frac{\left\| \mathbf{B}^{1/2} \left[\frac{\partial(\mathrm{Obs})}{\partial \mathbf{x}} \right]^T \right\|^2}{\left(\left\| \mathbf{B}^{1/2} \left[\frac{\partial(\mathrm{Obs})}{\partial \mathbf{x}} \right]^T \right\|^2 + \frac{\rho^2}{\beta^2} {}^2 \right)}$$

Ratio of observation to prior error uncertainty:

>> 1: large obs. uncertainty, i.e., small reduction

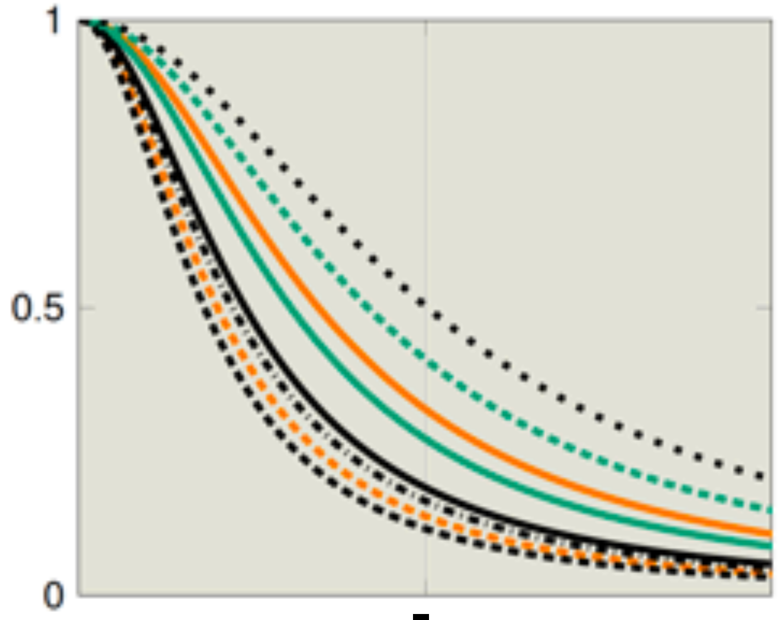
<< 1: small obs. uncertainty, i.e., large reduction

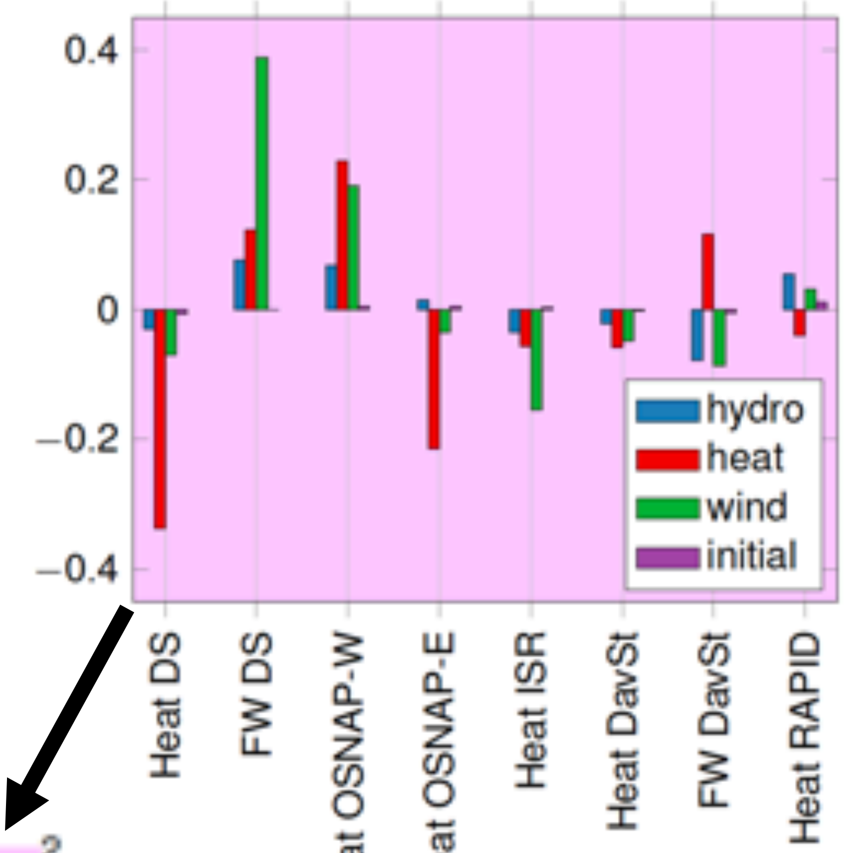
N. Loose, PhD thesis (2019)

How well does each observing system constrain the solution & relevant QoIs?

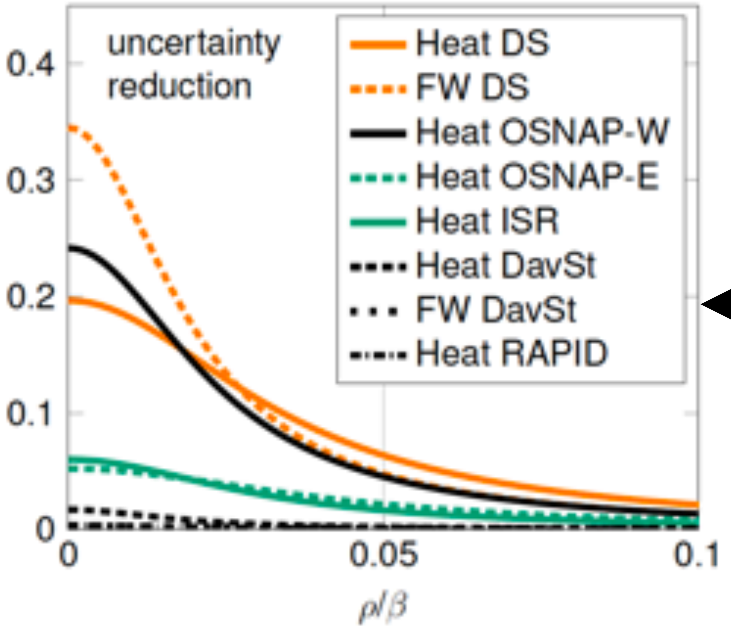
Effective proxy potential

- Accounts for everything





$$\frac{\left\|\mathbf{B}^{1/2}\left[\frac{\partial(\mathrm{Obs})}{\partial \mathbf{x}}\right]^T\right\|^2}{\left(\left\|\mathbf{B}^{1/2}\left[\frac{\partial(\mathrm{Obs})}{\partial \mathbf{x}}\right]^T\right\|^2 + \frac{\rho^2}{\beta^2}\varepsilon^2\right)} \langle q, v_1 \rangle^2$$



N. Loose, PhD thesis (2019)

Effective proxy potential:

- Arises for such observational assets that share the same dynamical adjustment pathways as those of QoIs
- Arises if the information contained in the observation is not masked too strongly by observational noise/error

In Practice:

- Eigen-decomposition of the misfit Hessian is key
  - Leading eigenvectors/values point to most potent obs. constraints, i.e., data-informed directions in control space
  - The eigen-decomposition is also a formal framework for letting the dynamics determine the effective low-order subspace/approximation!

Kaminski et al., The Cryosphere (2015, 2018)

Similar approach, but using a-priori control space reduction via “large region approach”

Obs.:

Operation IceBridge retrievals of sea ice area, ice & snow thicknesses, averaged over “large regions”

QoIs:

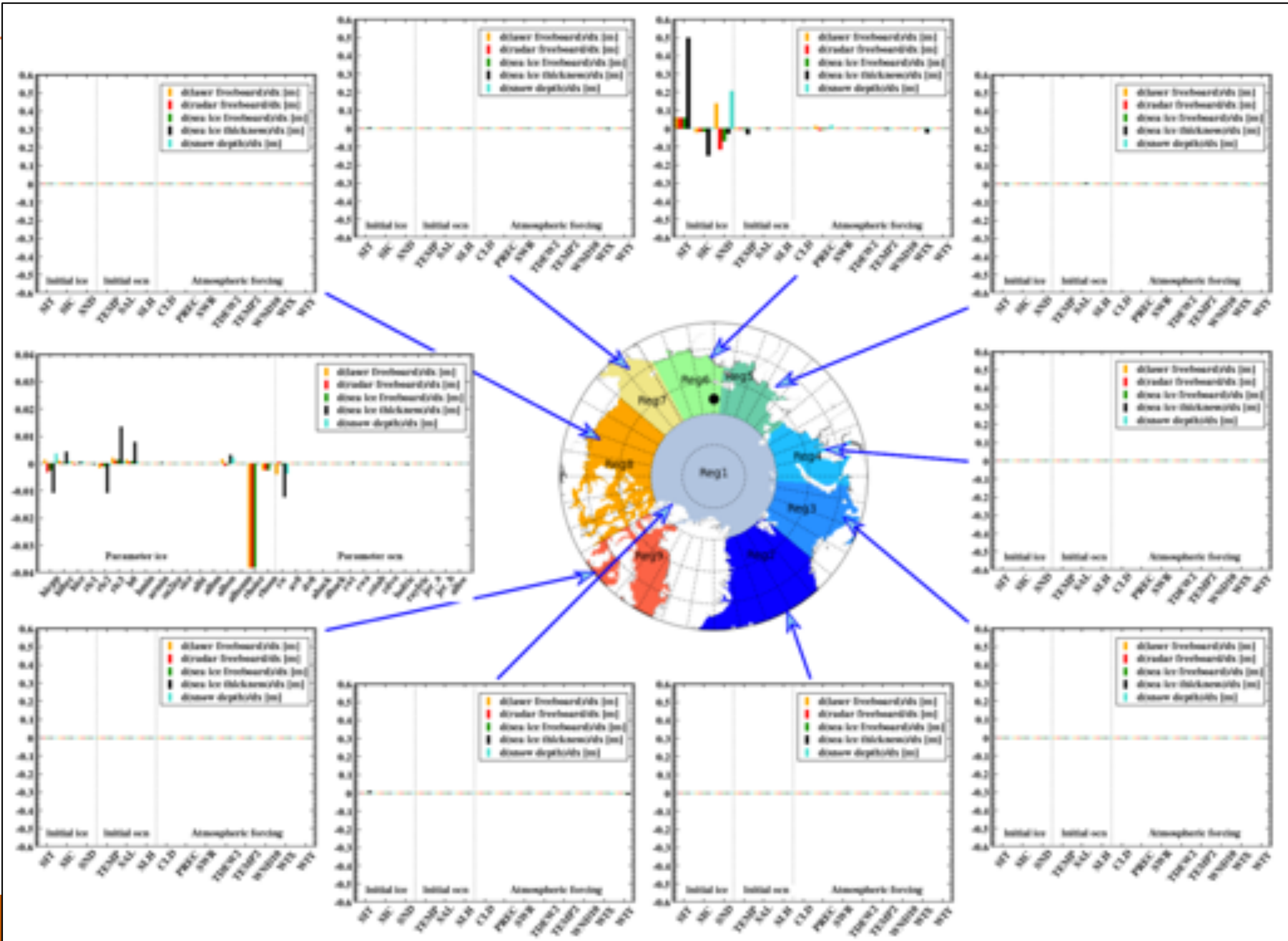
Forecasts of sea ice area & thickness in Chukchi & Beaufort Seas

Index	Name	Type	Meaning	Prior uncertainty (mean)	Start
1	hiccp	p	(alias pstar) ice strength (divided by density)	15(20) $[\mathrm{N\,m^{-2}\,kg^{-1}}]$	1
2	hibcc	p	(alias cstar) ice strength depend. on ice conc.	5.0(20.0)	2
3	hicce	p	(alias eccen) squared yield curve axis ratio	0.5(2.0)	3
4	rlc1	p	extra lead closing (Notz et al., 2013)	0.2(0.25)	4
5	rlc2	p	extra lead closing (Notz et al., 2013)	1.0(3.0)	5
6	rlc3	p	extra lead closing (Notz et al., 2013)	1.0(2.0)	6
7	h_0	p	lead closing	1.0(0.5) (m)	7
8	hmin	p	mimimal ice thickness	0.04(0.05) (m)	8
9	armin	p	minimal ice compactness	0.15(0.15)	9
10	hsntoice	p	limit on flooding	0.45(0.45)	10
11	sice	p	salinity in sea ice	2.0(5.0) $[\mathrm{g\,kg^{-1}}]$	11
12	albi	p	freezing ice albedo	0.1(0.75)	12
13	albm	p	melting ice albedo	0.1(0.70)	13
14	albsn	p	freezing snow albedo	0.1(0.85)	14
15	albsnm	p	melting snow albedo	0.1(0.70)	15
16	rhoice	p	density of sea ice	20(910) $[\mathrm{kg\,m^{-3}}]$	16
17	rhosn	p	density of snow	20(330) $[\mathrm{kg\,m^{-3}}]$	17
18	cw	p	ocean drag coefficient	$2.0\times10^{-3}(4.5\times10^{-3})$	18
19	av0	p	coefficient vertical viscosity	$1.\times10^{-4}(2.\times10^{-4})\,[\mathrm{m^2\,s^{-1}}]$	19
20	dv0	p	coefficient vertical diffusivity	$1.\times10^{-4}(2.\times10^{-4})\,[\mathrm{m^2\,s^{-1}}]$	20
21	aback	p	background coefficient vertical viscosity	$3.\times10^{-5}(5.\times10^{-5})\,[\mathrm{m^2\,s^{-1}}]$	21
22	dback	p	background coefficient vertical diffusivity	$1.\times10^{-5}(1.05\times10^{-5})\,[\mathrm{m^2\,s^{-1}}]$	22
23	cwt	p	vertical wind mixing parameter tracers	$2.0\times10^{-4}(3.5\times10^{-4})\,[\mathrm{m^2\,s^{-1}}]$	23
24	cwa	p	vertical wind mixing parameter momentum	$0.4\times10^{-3}(0.75\times10^{-3})\,[\mathrm{m^2\,s^{-1}}]$	24
25	cstabeps	p	vertical wind mixing stability parameter	0.03(0.06)	25
26	cdvocon	p	coefficient for enhanced vertical diffusivity	0.1(0.15)	26
27	bofric	p	linear bottom friction	$2.\times10^{-4}(3.\times10^{-4})\,[\mathrm{m^2\,s^{-1}}]$	27
28	rayfric	p	quadratic bottom friction	$0.5\times10^{-3}(1.\times10^{-3})\,[\mathrm{m^2\,s^{-1}}]$	28
29	jer_a	p	jerlov atten – ocean-water types	0.04(0.08)	29
30	jer_b	p	jerlov bluefrac – ocean-water types	0.20(0.36)	30
31	albw	p	open water albedo	0.05(0.1)	31
32	SIT	i	initial ice thickness	0.5 (m)	32
33	SIC	i	initial ice concentration	0.1	41
34	SND	i	initial snow thickness	0.2 (m)	50
35	TEMP	i	initial ocean temperature	0.5 [K] (vertically decreasing)	59
36	SAL	i	initial salinity	0.5 $[\mathrm{g\,kg^{-1}}]$ (vertically decreasing)	68
37	SLH	i	initial sea level elevation	0.08 (m)	77
38	CLD	f	cloud cover	0.07	86
39	PREC	f	total precipitation	$0.4\times10^{-8}\,[\mathrm{m\,s^{-1}}]$	95
40	SWR	f	solar downward radiation	6. $[\mathrm{W\,m^{-2}}]$	104
41	TDEW2	f	2 m dew point temperature	1.1 [K]	113
42	TEMP2	f	2 m air temperature	1.2 [K]	122
43	WND10	f	10m scalar wind speed	0.6 $[\mathrm{m\,s^{-1}}]$	131
44	WIX	f	zonal wind stress x component	0.02 $[\mathrm{Nm^2}]$	140
45	WIY	f	meridional wind stress y component	0.02 $[\mathrm{Nm^2}]$	149

Kaminski et al., The Cryosphere (2015, 2018)

Observation sensitivities

(information communicated by observations)



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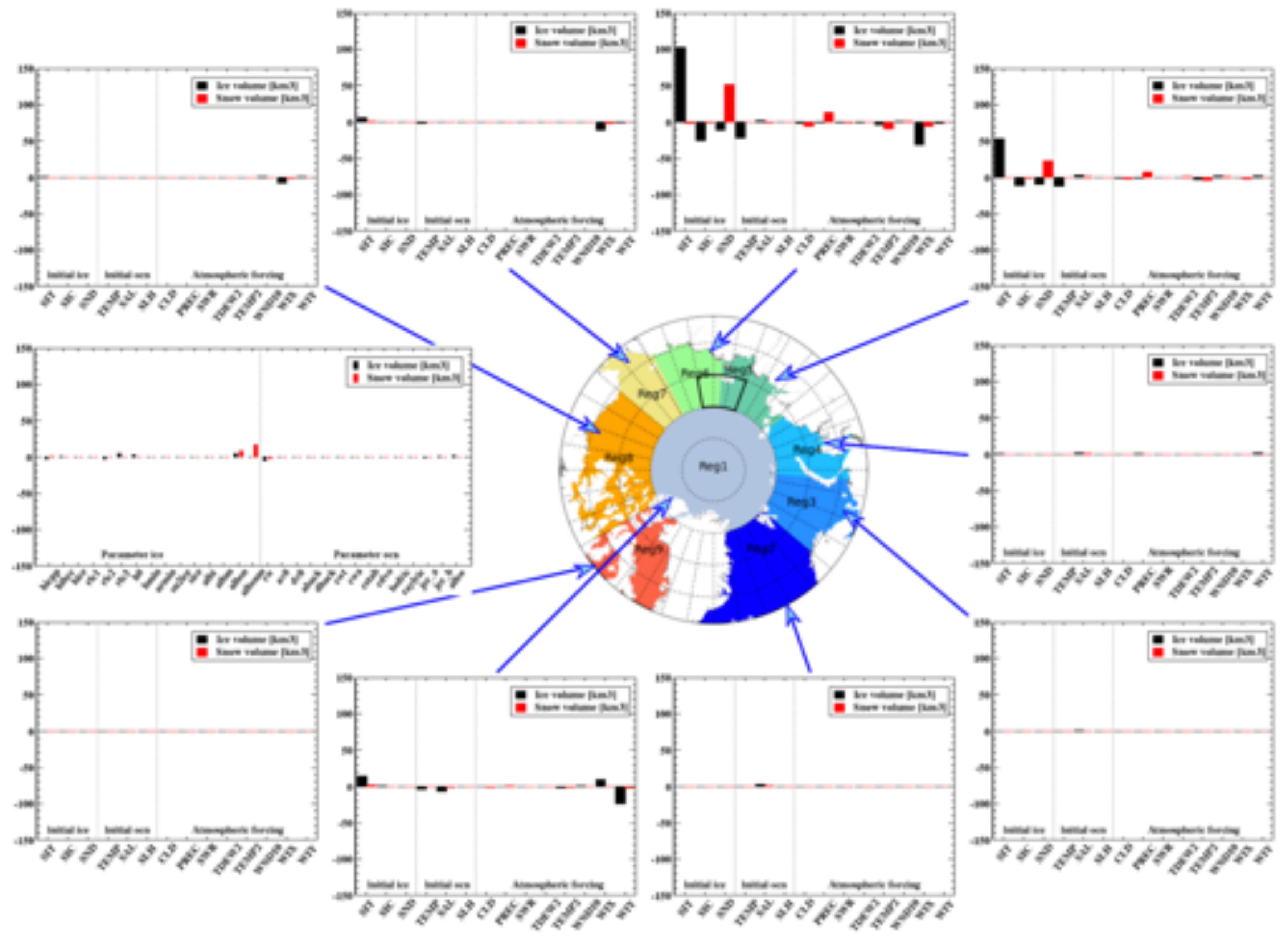
Kaminski et al., The Cryosphere (2015, 2018)

QoI

sensitivities

(information required by Quantity of Interest)



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Kaminski et al., The Cryosphere (2015, 2018)

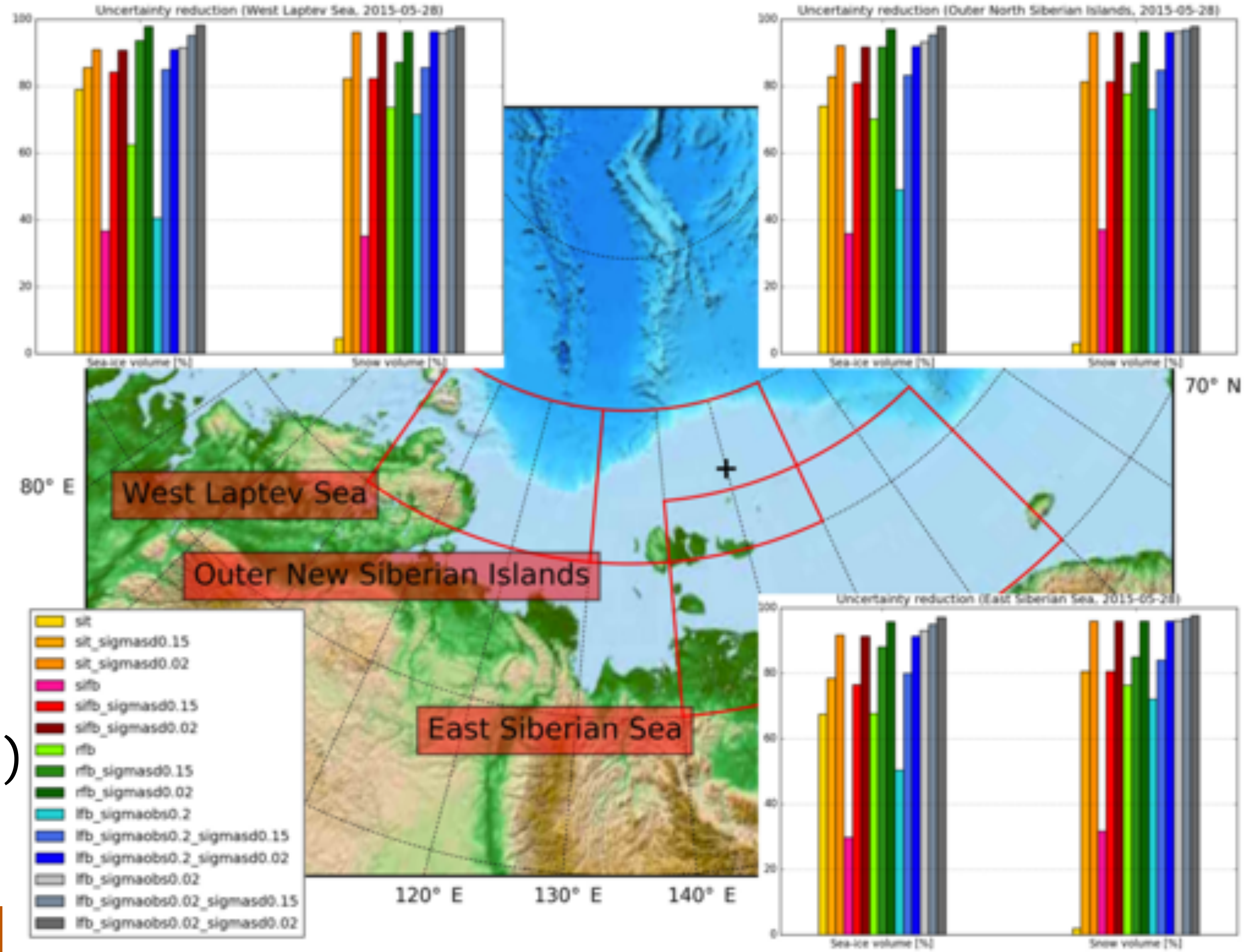
Uncertainty Reduction:

Projects observation uncertainties onto QoI uncertainties

A simplified statement on how to evaluate posterior error covariance by means of inverse Hessian

Find data-informed subspaces

Find data complementarity vs. redundancy (not just “a lot of data”)



Conclusions

Adjoint & Hessian-based UQ and observing system design offers:

- Dynamics-based assessment of existing or hypothetical obs. systems
- Links observational assets to a QoI that is …
  - … unobservable or unobserved,
  - … a different type of quantity/variable than measured quantity,
  - … spatially and/or temporally non-collocated
  - … a forecast, a parameter, …
- Quantifies the degree to which information required by QoI is transmitted by the information ”transmitted” by the observation
- Quantifies observational complementarity vs. redundancy
- Accounts for high-dimensional, multi-variable uncertainty spaces

Conclusions

Adjoint & Hessian-based UQ and observing system design offers:

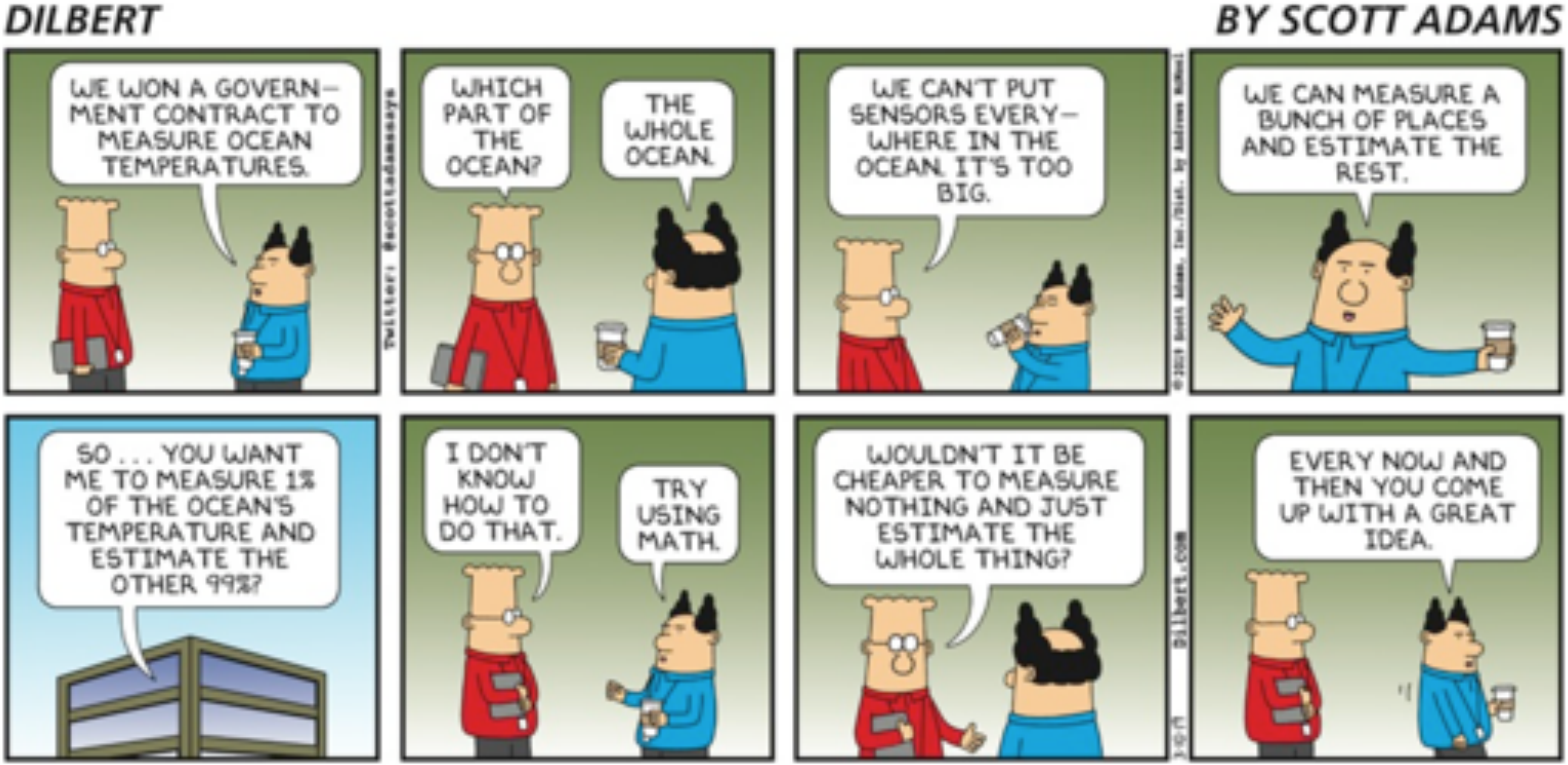
- Framework does not require actual measurement values(!)
  - Can therefore distinguish between hypothetical and effective (noise-masked) proxy potential of observations

Note that…

- These frameworks are still being developed for real-world applications (e.g., ocean / climate models), i.e. ongoing research & development
- These frameworks require:
  - advanced computational algorithms
  - significant computational resources
  - time to fully explore …

Conclusions

- A range of tools available for optimal observing system design
  - Varying degree of sophistication & flexibility
  - Many remain little (or non) explored in real-world applications !
- Given the cost associated with observing system, improving capabilities of quantitative/optimal OSD seems well worth
- No claim is made that OSD will replace human judgement !
  - It is a quantitative tool in a portfolio of decision-making tools
- Ideally a sustained, hand-in-hand iterative process of improving
  - observing systems
  - models (which are required for forecast)
  - DA systems used for calibration, estimation, forecasting, OSD, …


DILBERT
BY SCOTT ADAMS
WE WON A GOVERNMENT CONTRACT TO MEASURE OCEAN TEMPERATURES.
WHICH PART OF THE OCEAN?
THE WHOLE OCEAN.
WE CAN'T PUT SENSORS EVERYWHERE IN THE OCEAN. IT'S TOO BIG.
WE CAN MEASURE A BUNCH OF PLACES AND ESTIMATE THE REST.
SO . . . YOU WANT ME TO MEASURE 1% OF THE OCEAN'S TEMPERATURE AND ESTIMATE THE OTHER 99%?
I DON'T KNOW HOW TO DO THAT.
TRY USING MATH.
WOULDN'T IT BE CHEAPER TO MEASURE NOTHING AND JUST ESTIMATE THE WHOLE THING?
EVERY NOW AND THEN YOU COME UP WITH A GREAT IDEA.

Some useful references

OceanObs'19:

- Fujii et al., Front. Mar. Sci. (2019)
- Heimbach et al., Front. Mar. Sci. (2019)
- Lee et al., Front. Mar. Sci. (2019)
- Moore et al., Front. Mar. Sci. (2019)
- Smith et al., Front. Mar. Sci. (2019)

Others:

- Kaminski et al., The Cryosphere (2015, 2018)
- Atlas & Hoffman, Bull. Amer. Met. Soc. (2014)
- Kalmikov & Heimbach, SIAM J. Sci. Comput. (2014, 2018)
- Alexanderian et al., SIAM J. Sci. Comput. (2016)
- …

Loose, Ph.D. thesis (2019)