

# Nonstationary spatial data: think globally act locally

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# Summary

- NCAR Large Ensemble
- Nonstationary Gaussian fields
- Estimating the covariance
- Emulating climate fields

## Challenges:

Building covariance models for large problems and actually computing the beasts!

# Credits

- SAR: Ashton Wiens (CU), Mitchell Krock (CU), Dorit Hammerling (CSM) William Kleiber (CU)
- Parallel computation: Florian Gerber (CSM)
- Climate Model Experiments: Claudia Tebaldi (PNNL) Stacey Alexeeff (Kaiser)



## PART 1

# Spatial problems in climate science

# Future climate

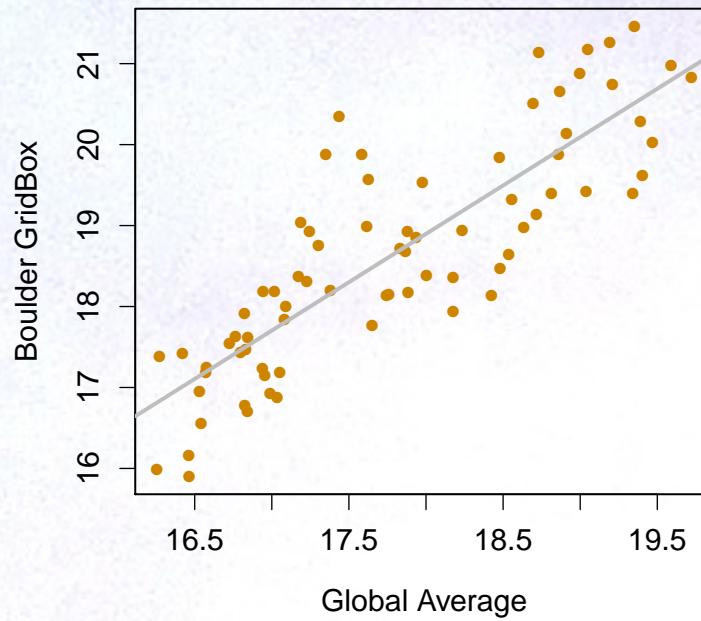
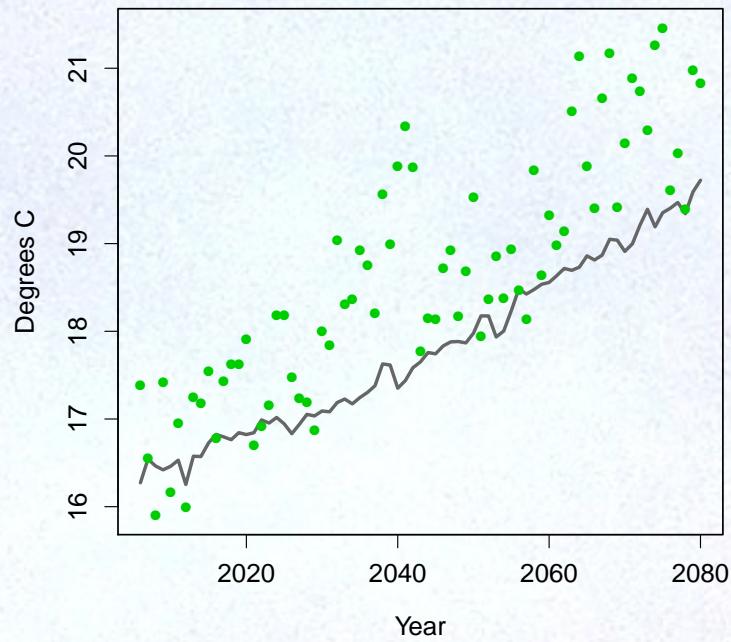
*CESM Large Ensemble (CESM-LENS)* A 30+ member ensemble of CESM simulations that have been designed to study the local effects of climate change

The range of ensemble members characterize some of the uncertainty due to natural variability in the Earth system

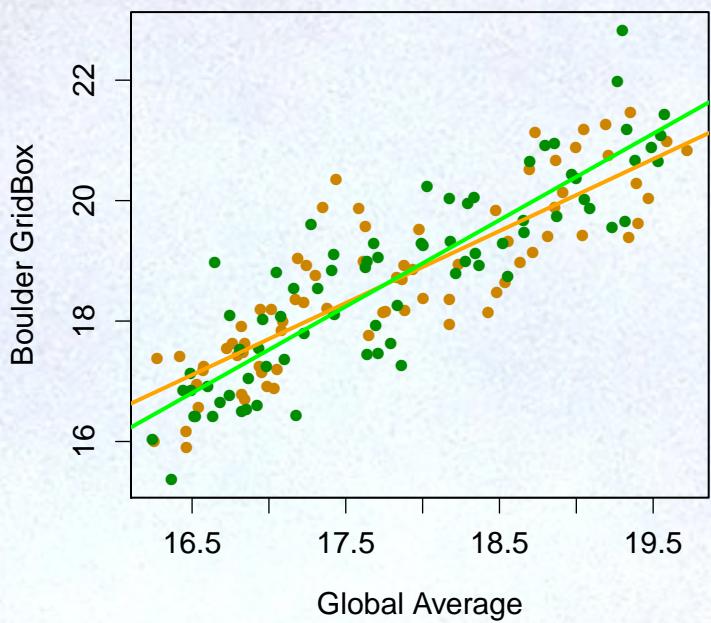
- $\approx 1^\circ$  spatial resolution – about 55K locations
- Simulation period 1920 - 2080
- Using RCP 8.5 after 2005

# Simulated JJA Temperature

Grid box around Boulder/Denver – average summer temperature.



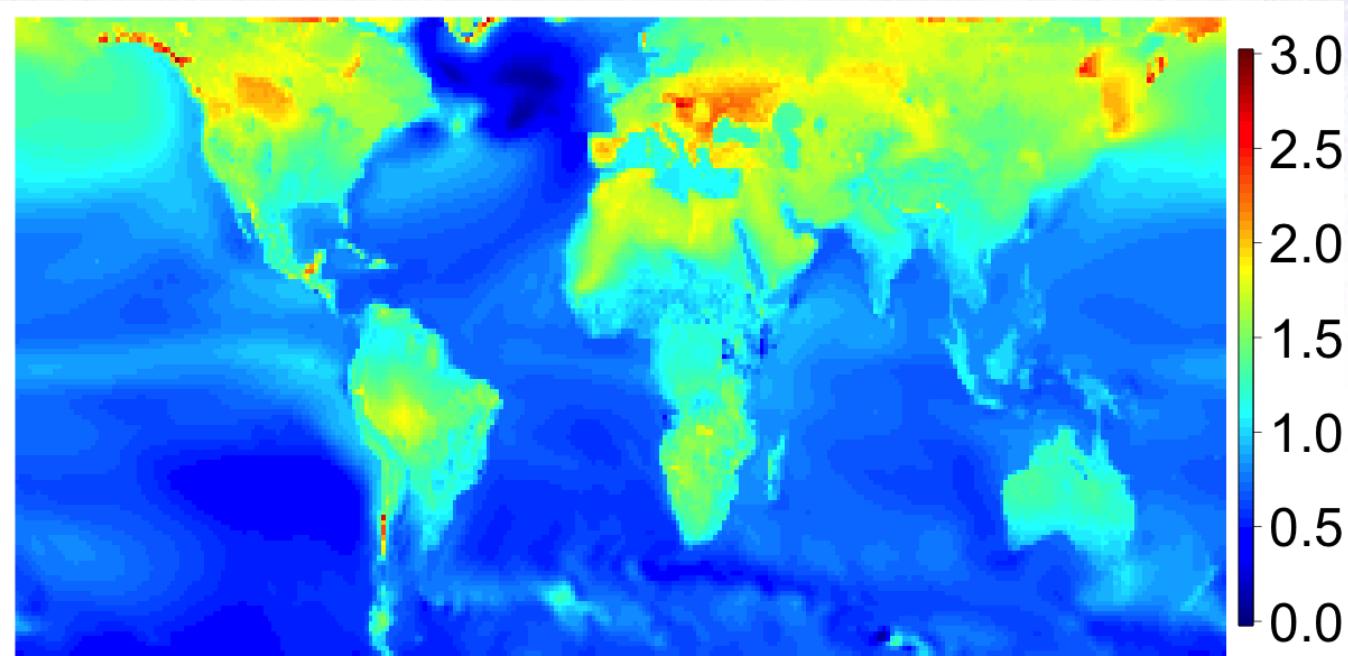
# First and second ensemble member



*We have 30 of these and at 50K+ grid boxes – and this is just surface temperature!*

# Mean scaling pattern

*OLS slopes across 30 CESM-LENS members for JJA*

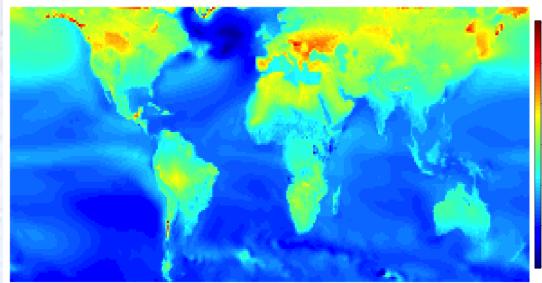


E. g. value of 2.5 means: a  $1^\circ$  global increase implies  $2.5^\circ$  increase locally.

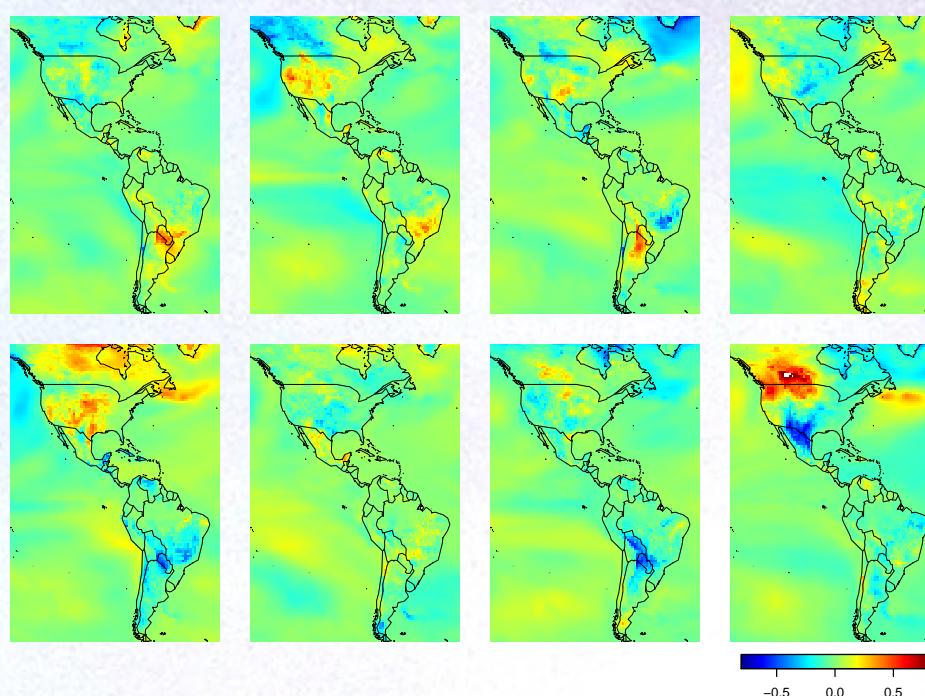
*This allows us to determine the local temperature change based on a simpler model for the global average temperature*

# Individual patterns

Ensemble mean



First 8 out of 30 centered ensemble members



*Goal:* Simulate additional fields efficiently that match the spatial dependence in this 30 member ensemble.

*Build a statistical emulator of this part of the model.*

# PART 2

# Nonstationary Gaussian Processes

# Gaussian process models

$u(s)$  value of the field at location  $s$ .

- $E[u(s)] = 0$  and  $C(s_1, s_2) = E[u(s_1)u(s_2)]$
- A covariance that is stationary and isotropic:

$$C(s_1, s_2) = \sigma^2 \mathcal{M}(\kappa ||s_1 - s_2||).$$

– a strong assumption, note two covariance parameters  $\sigma$  and  $\kappa$ .

- Anisotropy:  $A$  a linear transformation :

$$C(s_1, s_2) = \sigma^2 \mathcal{M}(||A(s_1 - s_2)||).$$

$A$  is a linear rotation and scaling of the coordinates

# Nonstationary covariance functions

- Convolution model (Higdon, Fuentes)

Represent the process first, then figure out the covariance function

$$u(s) = \int_{\mathbb{R}^2} \Psi(s, s^*) dW(s^*)$$

$dW(u)$  a two dimensional standard, white noise process.

The covariance function:

$$C(s_1, s_2) = \int_{\mathbb{R}^2} \Psi(s_1, s^*) \Psi(s_2, s^*) ds^*$$

- $\Psi$  can be the Green's function for a stochastic PDE
  - a connection to INLA

## 2-D exponential kernel example:

$$\Psi(s, s^*) = \sigma(s) e^{-\kappa(s) \|s - s^*\|}$$

$$C(s_1, s_2) = \sigma(s_1)\sigma(s_2) \int e^{-\kappa(s)\|s_1 - s^*\|} e^{-\kappa(s^*)\|s_2 - s^*\|} ds^*$$

- If  $\theta(s) \equiv \theta$  in 2-d this gives a Matérn with smoothness  $\nu = 1.0$
- $C$  is positive definite because it is built from the process description.
- For unequal  $\kappa$  no simple closed form for this covariance.  
–direct use of covariance is not feasible for large problems

*Anisotropy:*

$\textcolor{magenta}{A}$  = diagonal  $\times$  rotation .

$$\psi(s, u) = \sigma e^{-||\textcolor{magenta}{A}(s-u)||}$$

*Nonstationarity:*  $A(s)$  varies in space.

$$\psi(s, s^*) = \sigma(s) e^{-||\textcolor{magenta}{A}(s)(s-s^*)||}$$



# Our approach

- Represent the process in terms of a differential operator
- Discretize the problem to give sparse matrices.

# Stochastic partial differential equations

Let  $\Psi$  can be the Green's function for a stochastic PDE with operator  $\mathcal{L}$ . I.e.

$$u(s) = \int_{\mathbb{R}^2} \Psi(s, u) dW(u)$$

is equivalent to

$$\mathcal{L}(u(s)) = dW(s)$$

An SPDE model ( Lindgren and Rue) for  $u$  ( $\alpha = 2$ )

$$(\kappa^2 - \nabla \cdot \nabla)u(s) = dW(s)$$

$$\Delta u = \frac{\partial^2}{\partial s_1^2}u + \frac{\partial^2}{\partial s_2^2}u \equiv \nabla \cdot \nabla u$$

This gives a process that is Matérn, range  $\kappa$  and smoothness 1.



# Discretizing

$u_{i,j}$  now the process on a unit lattice

$\frac{\partial^2}{\partial s_1^2}u + \frac{\partial^2}{\partial s_2^2}u$  is approximated by differences

$$\frac{\partial^2}{\partial s_1^2}u \approx (u_{i+1,j} - u_{i,j}) - (u_{i,j} - u_{i-1,j}) = u_{i+1,j} - 2u_{i,j} + u_{i-1,j}$$

The full discretization of the SPDE

$$(\kappa^2 - \Delta)u(s) = dW(s)$$

$$\kappa^2 u(s) - \frac{\partial^2}{\partial s_1^2}u(s) - \frac{\partial^2}{\partial s_2^2}u(s) = dW(s)$$

$$\kappa^2 u_{i,j} - (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) - (u_{i,j+1} - 2u_{i,j} + u_{i,j-1}) = e_{i,j}$$

$$\kappa^2 u_{i,j} + 4u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = e_{i,j}$$

$$[\kappa^2 + 4]u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} = e_{i,j}$$

# A Spatial Autoregression (SAR)

Gridded field of  $\mathbf{u}$ :

$$\begin{matrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & u_1 & \cdot & \cdot \\ \cdot & u_2 & u_* & u_3 & \cdot \\ \cdot & \cdot & u_4 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{matrix}$$

SAR weights:

$$\begin{array}{|c|c|c|c|c|} \hline & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & -1 & \cdot & \cdot & \cdot \\ \hline \cdot & -1 & \kappa^2 + 4 & -1 & \cdot & \cdot \\ \hline \cdot & \cdot & -1 & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \end{array}$$

The SAR:

$$(\kappa^2 + 4)u_* - (u_1 + u_2 + u_3 + u_4) = \text{white noise}$$

- $\kappa$  is not exactly equal to the continuous range.
- $B\mathbf{u} = \text{i.i.d.} N(0, 1)$  where  $B$  is a sparse matrix
- Covariance matrix for  $\mathbf{u}$  is  $(B^{-1}B^{-T})$
- A SAR is a CAR with precision  $B^T B$



# Key ideas

$$Bu = \text{i.i.d.} N(0, 1)$$

- Sparsity in  $B$  facilitates computation for large problems
- Coefficients of  $B$  can vary row by row (i.e. lattice point by lattice point) to represent nonstationarity
- $u = B^{-1}e$ , a discretized version of a convolution process.

$$B^{-1} \text{ plays the role of } \Psi \text{ in } u(s) = \int_{\Re^2} \Psi(s, s^*) dW(s^*)$$

- $Bu$ , transforms the field (possibly observations) to white noise

$$B \text{ plays the role of } \mathcal{L} \text{ in } \mathcal{L}u = dW$$



# The Anisotropic Stencil

For a single lattice point ( Flugstadt, et al. )

.	.	.	.	.	.
.	$2H_{12}$		$-H_{22}$		$-2H_{12}$
.	$-H_{11}$	$\kappa^2 + 2H_{11} + 2H_{22}$		$-H_{11}$	.
.	$-2H_{12}$		$-H_{22}$		$2H_{12}$
.	.		.	.	.

- $H = AA^T$
- Key idea is to allow these weights to vary for each lattice point.

# PART 3 Fitting the model

## *Local Likelihoods*

- Estimate  $A$  in local windows for a Matérn smoothness 1.
- Translate this covariance model into the SAR form.

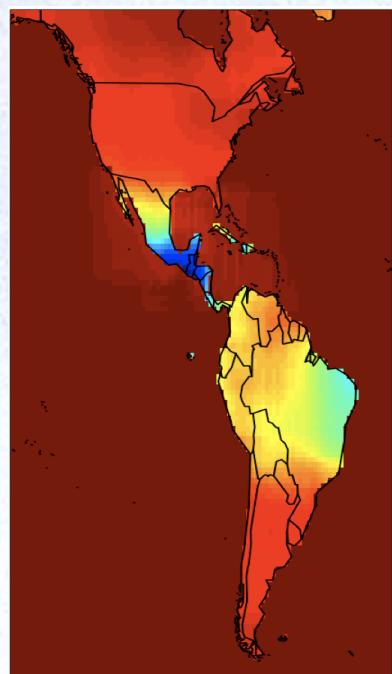
## *What is new?*

- Quantified the accuracy of *local* Matérn estimates based on replicates.
- Established the translation from local covariance estimates into a global SAR model.

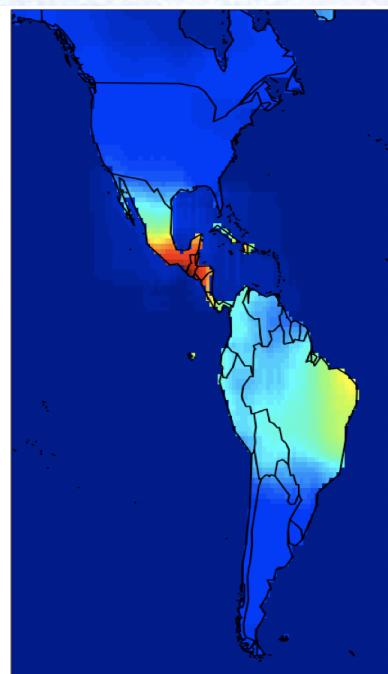
# Climate model patterns

Local Matérn MLEs for the 30 member ensemble patterns

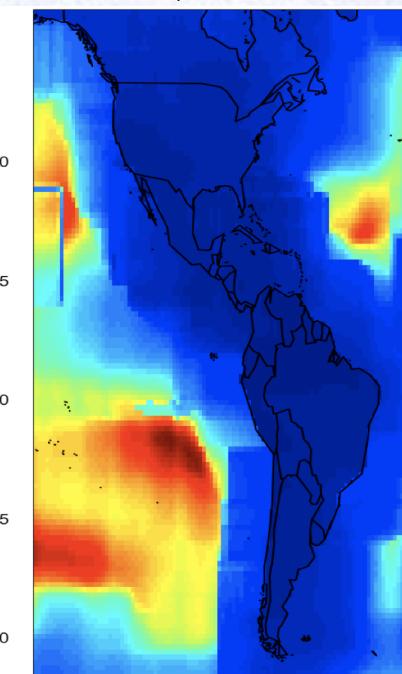
Sill variance



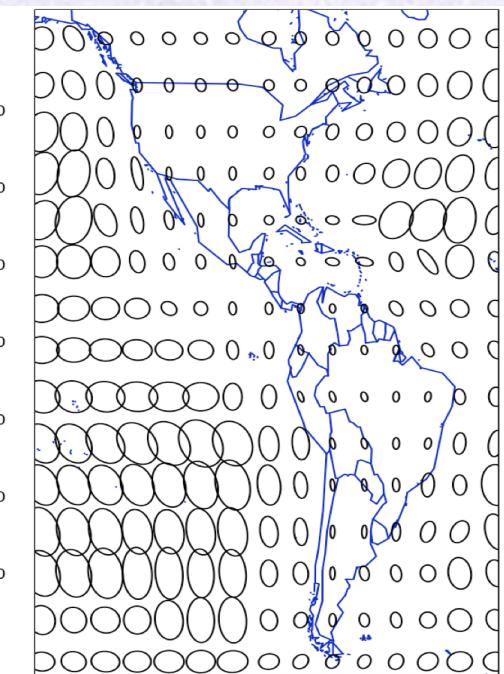
Nugget variance



$1/\sqrt{\kappa_1 \kappa_2}$



Orientation

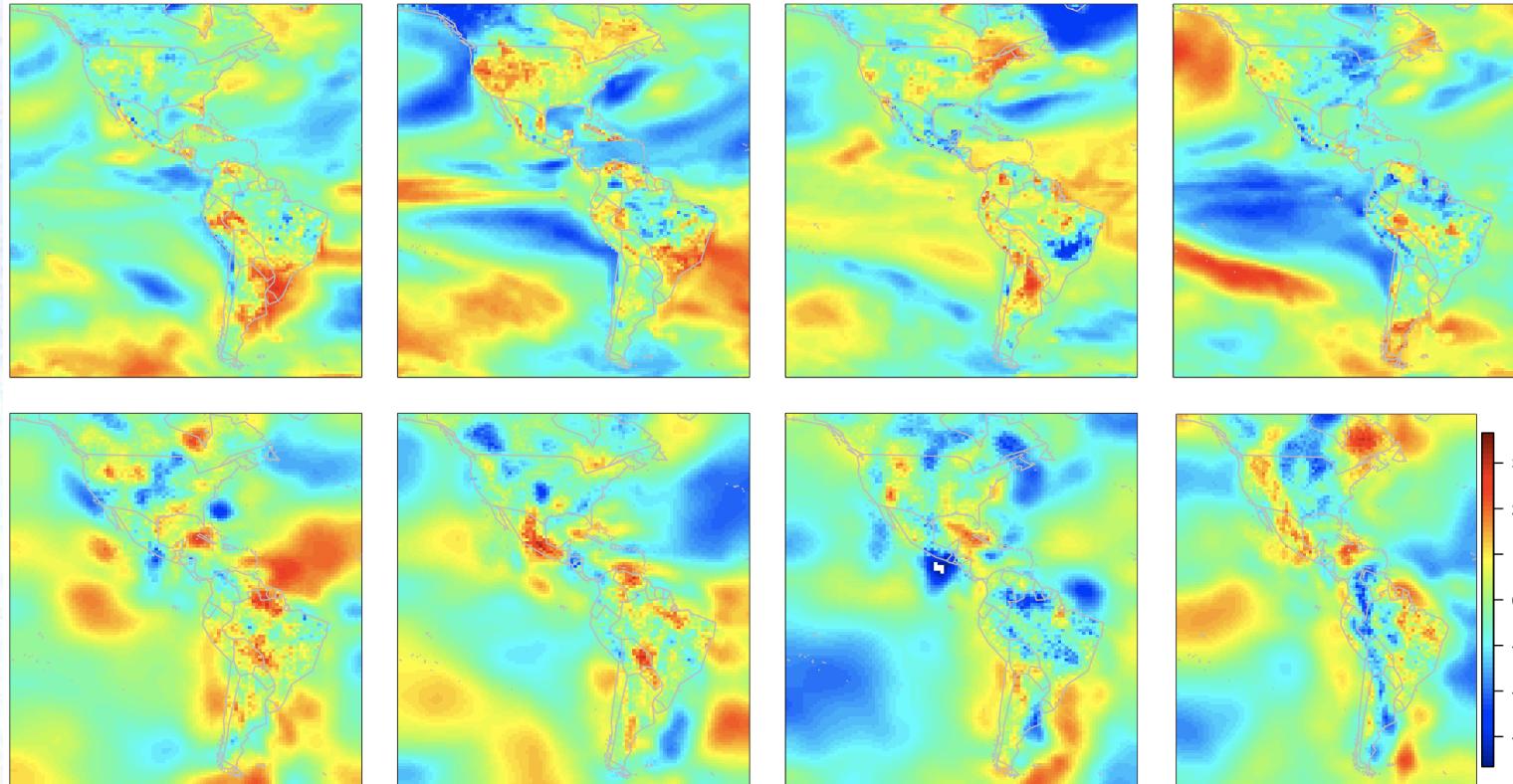


# PART 4

## Simulation and checking

# Some realizations of the process

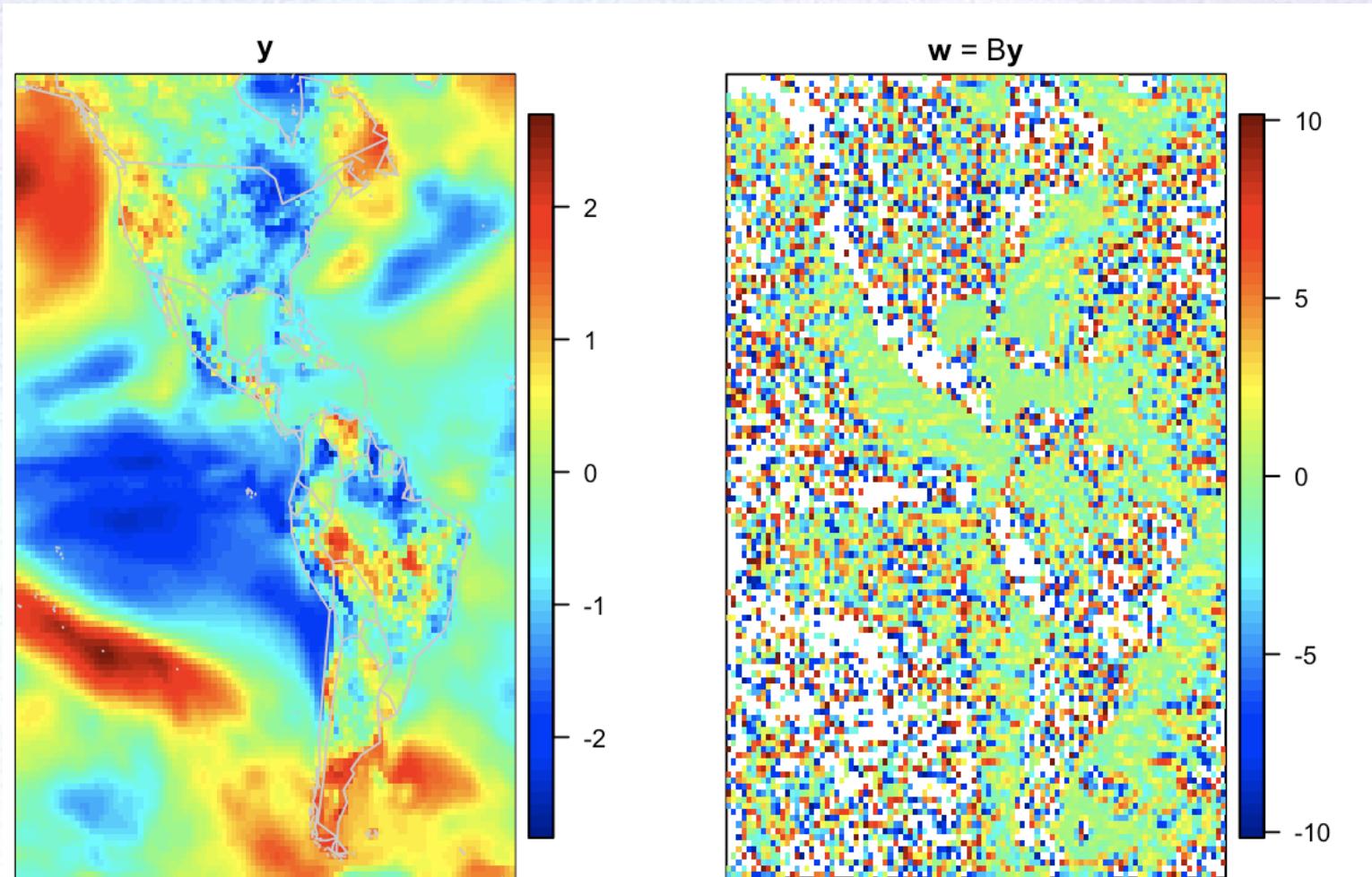
*Top* four ensemble members from LENS climate model experiment.



*Bottom* four realizations from SAR model.

# Transforming to white noise

Applying the  $B$  SAR operator to the first ensemble member



# What is next?

- Combine SAR approximation with basis functions for unequally spaced observations
- Improve approximation adding processes at different scale levels.
- Improve whitening transformation.
- Land verses Ocean ?

.	.	.	.	.
.	$2H_{12}$	$-H_{22}$	$-2H_{12}$	.
.	$-H_{11}$	$\kappa^2 + 2H_{11} + 2H_{22}$	$-H_{11}$	.
.	$-2H_{12}$	$-H_{22}$	$2H_{12}$	.
.	.	.	.	.



## Software

- `fields` R package, Nychka et al. (2000 - present)
- `LatticeKrig` R package, Nychka et al. (2014- present)
- HPC4Stats SAMSI short course August 2017, Nychka, Hammerling and Lenssen.



# Background reading

Nychka, D., Hammerling, D., Krock, M. Wiens, A. (2017). Modeling and emulation of nonstationary Gaussian fields.  
*arXiv:1711.08077*

Kuusela , M and Stein M. (2017). Locally stationary spatio-temporal interpolation of Argo profiling float data  
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Alexeeff, S. E., Nychka, D., Sain, S. R., & Tebaldi, C. (2016). Emulating mean patterns and variability of temperature across and within scenarios in anthropogenic climate change experiments.  
*Climatic Change*, 1-15.

Nychka, D., Bandyopadhyay, S., Hammerling, D., Lindgren, F., & Sain, S. (2015). A multi-resolution Gaussian process model for the analysis of large spatial datasets.  
*Journal of Computational and Graphical Statistics*, 24(2), 579-599.

# Thank you!

