

# An explicit link between Gaussian fields and Gaussian Markov random fields; the stochastic partial differential equation approach

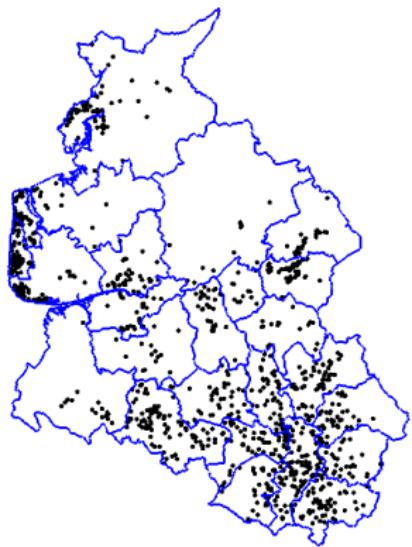
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RSS, London, 16th March 2011

# Computationally efficient spatial models



Leukaemia survival in  
NW England

Spatial random field models

Dense covariance:

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

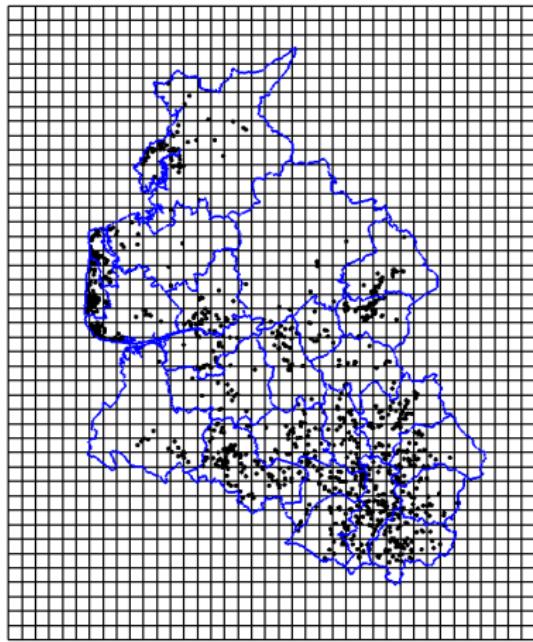
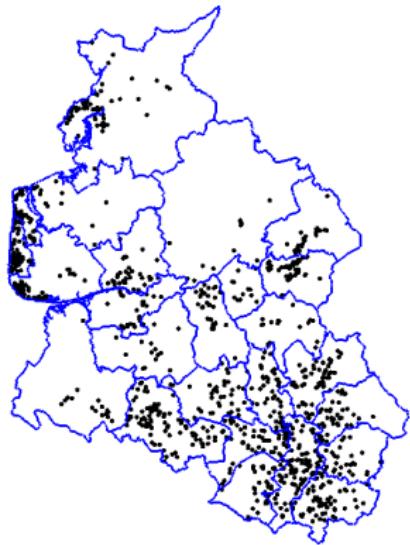
⇒ expensive computations

Sparse precision:

$$\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{Q}^{-1})$$

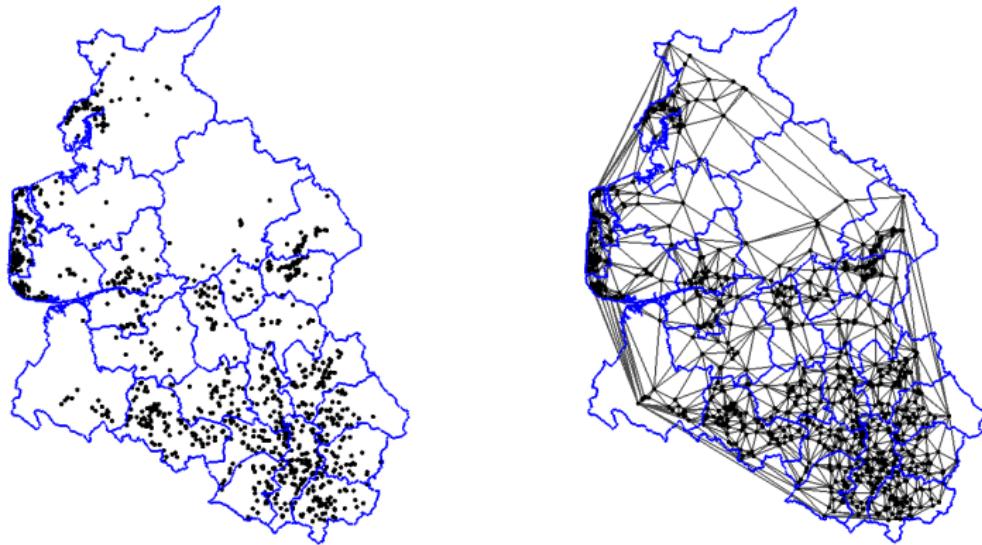
⇒ efficient computations

# Irregular discrete data locations – lattice CAR models



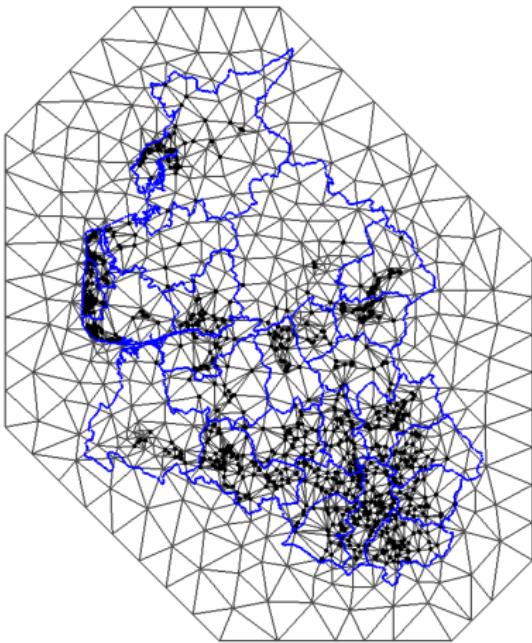
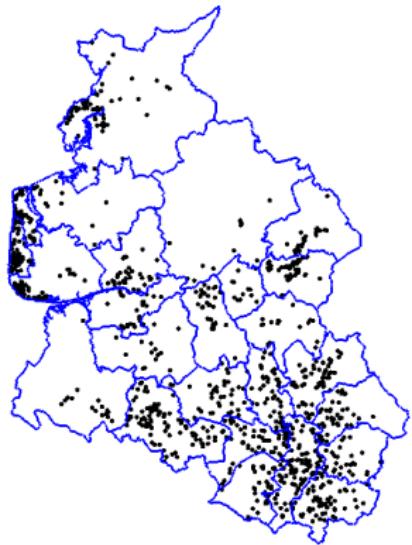
We need models with well-defined continuous interpretation

# Irregular discrete data locations – triangular graph



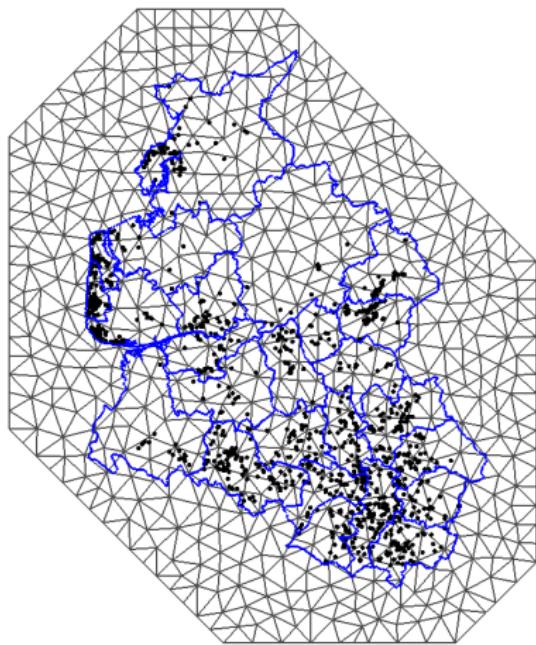
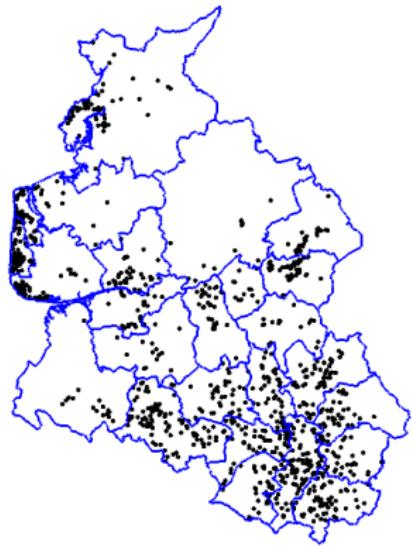
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# Irregular discrete data locations – refined triangulation



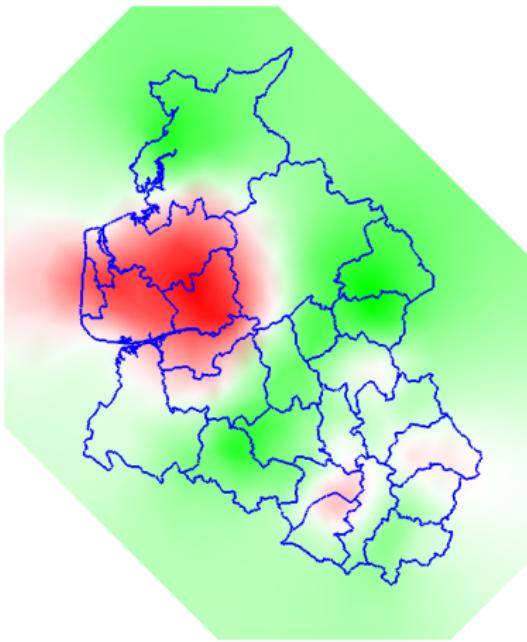
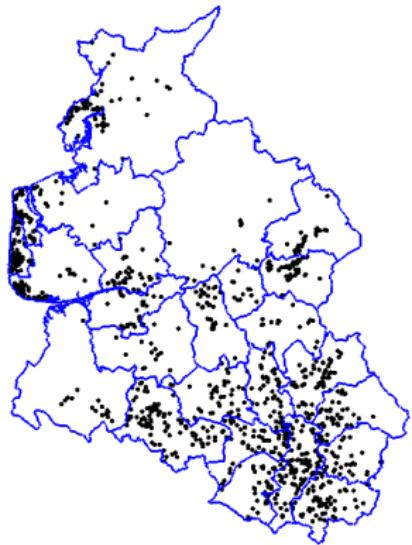
We need models with well-defined continuous interpretation

# Irregular discrete data locations – smooth triangulation



We need models with well-defined continuous interpretation

# Irregular discrete data locations – continuous space



We need models with well-defined continuous interpretation

# Conditional autoregression models on lattices

GMRF

Covariance

$$\text{CAR}(2) \propto \kappa \|\mathbf{u}\| K_1(\kappa \|\mathbf{u}\|) \quad \text{Whittle (1954)}$$

$$\text{CAR}(1) \quad \frac{1}{2\pi} K_0(\kappa \|\mathbf{u}\|) \quad \text{Besag (1981)}$$

$$\text{ICAR}(1) \quad -\frac{1}{2\pi} \log(\|\mathbf{u}\|) \quad \text{Besag \& Mondal (2005)}$$



# Matérn covariances (Bertil Matérn)

## The Matérn covariance family

$$\text{Cov}(x(\mathbf{0}), x(\mathbf{u})) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} (\kappa \|\mathbf{u}\|)^\nu K_\nu(\kappa \|\mathbf{u}\|), \quad \mathbf{u} \in \mathbb{R}^d$$

Scale  $\kappa > 0$ , smoothness  $\nu > 0$ , variance  $\sigma^2 > 0$

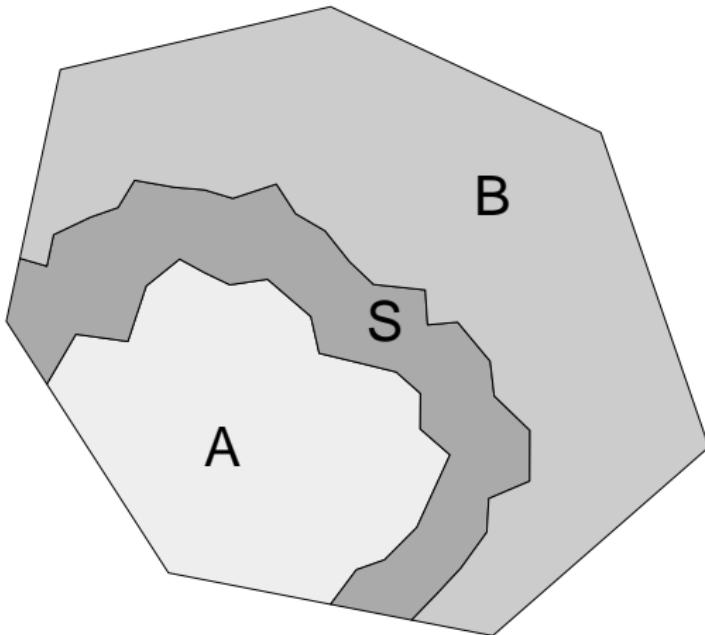
Are any other discrete domain Markov fields close to Matérn fields?

Are any Matérn fields continuous domain Markov fields?



# The continuous domain Markov property

$S$  is a separating set for  $A$  and  $B$ :  $x(A) \perp x(B) | x(S)$



# Identifying a Markov field by its spectrum

Spectral representation:  $x(\mathbf{u}) = \int_{\mathbb{R}^d} \exp(i\mathbf{u} \cdot \mathbf{k}) \hat{x}(\mathbf{k}) d\mathbf{k}$

Spectrum:  $S_x(\mathbf{k}) = E(|\hat{x}(\mathbf{k})|^2)$

Rozanov (1977)

$x(\mathbf{u})$  is Markov  $\iff S_x(\mathbf{k}) \propto P(\mathbf{k})^{-1}$

where  $P(\mathbf{k})$  is a non-negative symmetric polynomial



What is the spectrum of a Matérn field?

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# The Whittle-Matérn connection

Whittle (1954, 1963)

Matérn fields on  $\mathbb{R}^d$  are stationary solutions to the SPDE

$$(\kappa^2 - \Delta)^{\alpha/2} x(\mathbf{u}) = \mathcal{W}(\mathbf{u}), \quad \alpha = \nu + d/2$$

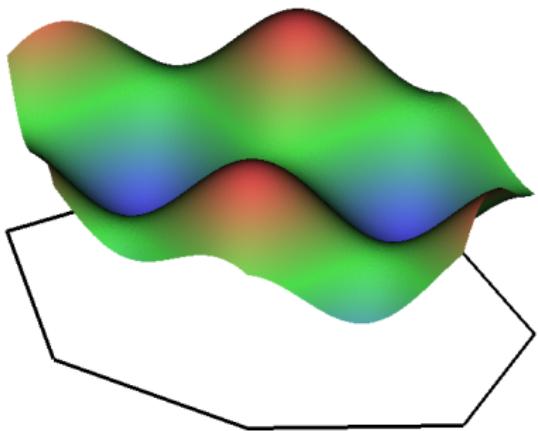
The spectrum is  $S_x(\mathbf{k}) = (2\pi)^{-d}(\kappa^2 + \|\mathbf{k}\|^2)^{-\alpha}$

Therefore Matérn fields are Markov when  $\nu + d/2$  is an integer.

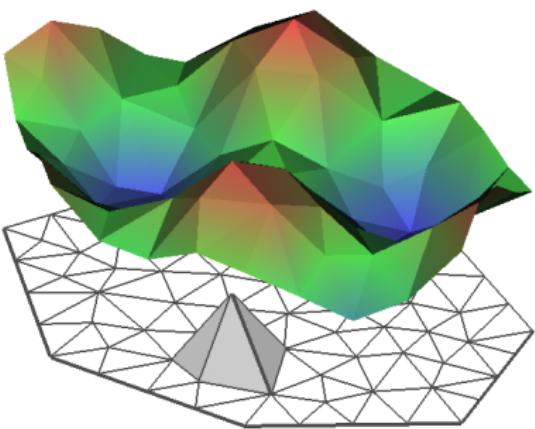
Laplacian:  $\Delta = \sum_{i=1}^d \frac{\partial^2}{\partial u_i^2}$

# Piecewise linear representations

$$x(\mathbf{u}) = \cos(u_1) + \sin(u_2)$$



$$x(\mathbf{u}) = \sum_k \psi_k(\mathbf{u}) x_k$$



## Guiding principle

Attack the SPDE with local finite dimensional representations instead of covariances or kernels (subsets of Green's functions)!

# The best piecewise linear approximation $\sum_k \psi_k(\mathbf{u}) x_k$

Projection of the SPDE: Linear systems of equations ( $\alpha = 2$ )

$$\sum_j (\kappa^2 \underbrace{\langle \psi_i, \psi_j \rangle}_{\mathbf{C}_{ij}} + \underbrace{\langle \psi_i, -\Delta \psi_j \rangle}_{\mathbf{G}_{ij}}) x_j \stackrel{D}{=} \langle \psi_i, \mathcal{W} \rangle \quad \text{jointly for all } i.$$

$\mathbf{C}$  and  $\mathbf{G}$  are as sparse as the triangulation neighbourhood

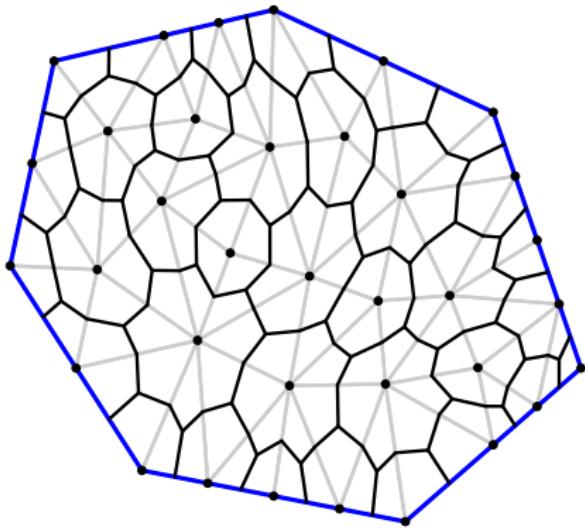
Constructing the precision matrices

$\mathbf{K} = \kappa^2 \mathbf{C} + \mathbf{G}$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3, 4, \dots$
$\mathbf{K}_x$	$\mathcal{N}(\mathbf{0}, \mathbf{K})$	$\mathcal{N}(\mathbf{0}, \mathbf{C})$	$\mathcal{N}(\mathbf{0}, \mathbf{CQ}_{x,\alpha-2}^{-1}\mathbf{C})$
$\mathbf{Q}_{x,\alpha}$	$\mathbf{K}$	$\mathbf{K}^T \mathbf{C}^{-1} \mathbf{K}$	$\mathbf{K}^T \mathbf{C}^{-1} \mathbf{Q}_{x,\alpha-2} \mathbf{C}^{-1} \mathbf{K}$

# Markov approximation

$\mathbf{C}^{-1}$  is dense, which leads to non-Markov models!

The diagonal matrix  $\tilde{\mathbf{C}}$ ,  $\tilde{\mathbf{C}}_{i,i} = \langle \psi_i, 1 \rangle$  = the local cell area, gives a sparse precision with the total energy preserved.



# Lattice on $\mathbb{R}^2$ , node distance $h$ , regular triangulation

Order  $\alpha = 1$ : generalised covariance  $\frac{1}{2\pi} K_0(\kappa \|\mathbf{u}\|)$

$$\kappa^2 h^2 \begin{bmatrix} 1 \\ -1 \end{bmatrix} + \begin{bmatrix} 1 & -1 & -1 \\ -1 & 4 & -1 \\ -1 & -1 & 1 \end{bmatrix}$$

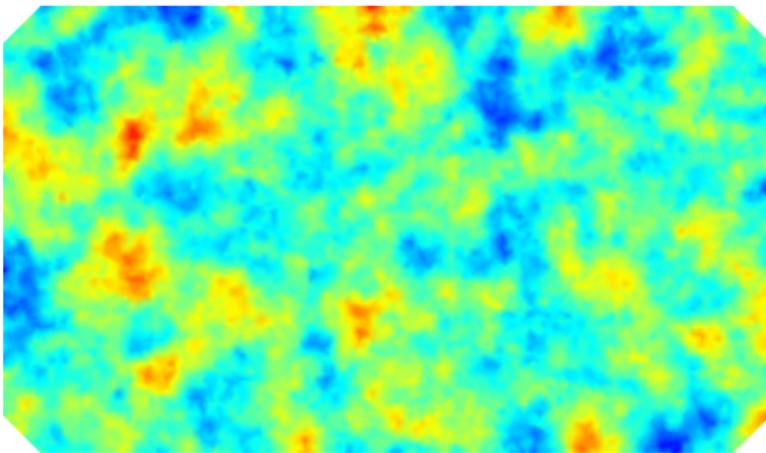
Order  $\alpha = 2$ : covariance  $\frac{1}{4\pi\kappa^2} \kappa \|\mathbf{u}\| K_1(\kappa \|\mathbf{u}\|)$

$$\kappa^4 h^2 \begin{bmatrix} 1 \\ -1 \end{bmatrix} + 2\kappa^2 \begin{bmatrix} 1 & -1 & -1 \\ -1 & 4 & -1 \\ -1 & -1 & 1 \end{bmatrix} + \frac{1}{h^2} \begin{bmatrix} 1 & 2 & -8 & 2 & 1 \\ 1 & -8 & 20 & -8 & 1 \\ 2 & -8 & 2 & 2 & 1 \end{bmatrix}$$

# Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

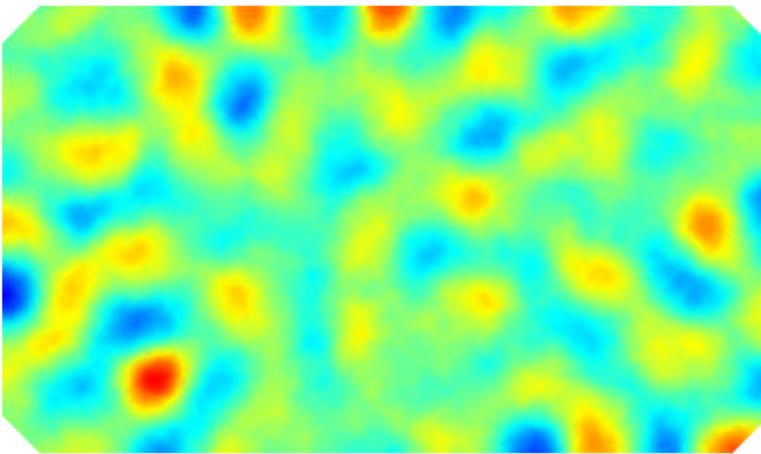
$$(\kappa^2 - \Delta)^{\alpha/2}(\tau x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



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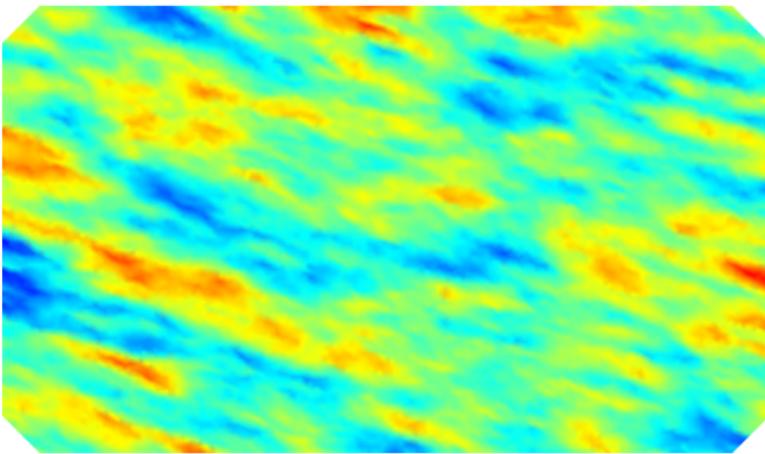
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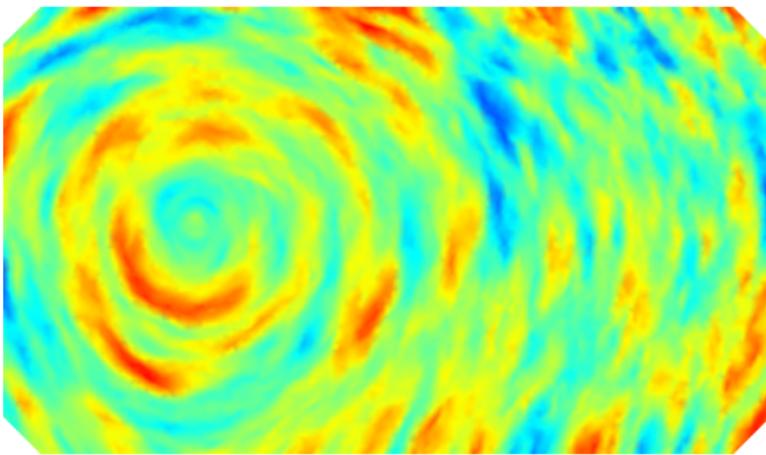
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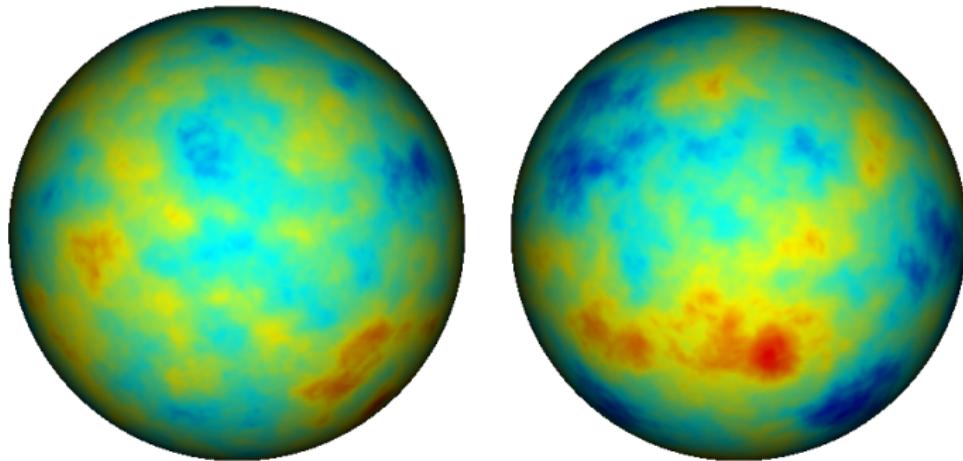
$$(\kappa_{\mathbf{u}}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u}} - \nabla \cdot \mathbf{M}_{\mathbf{u}} \nabla)^{\alpha/2} (\tau_{\mathbf{u}} x(\mathbf{u})) = \mathcal{W}(\mathbf{u}), \quad \mathbf{u} \in \mathbb{R}^d$$



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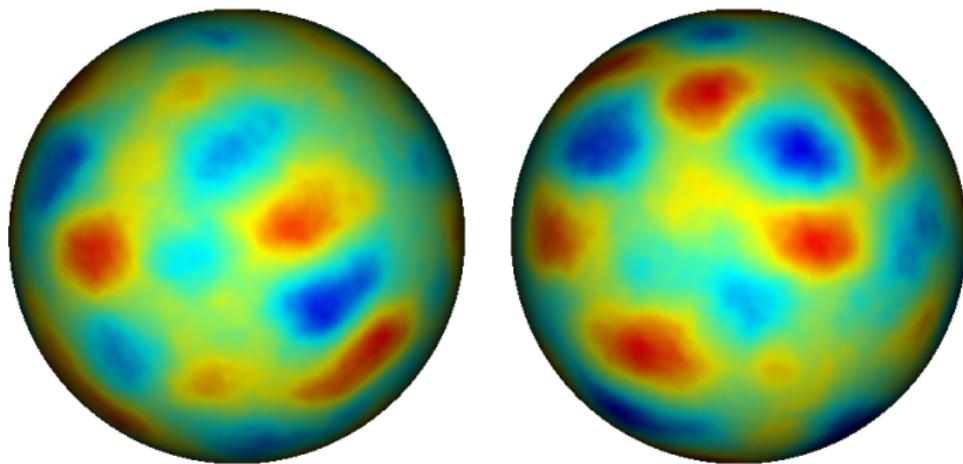
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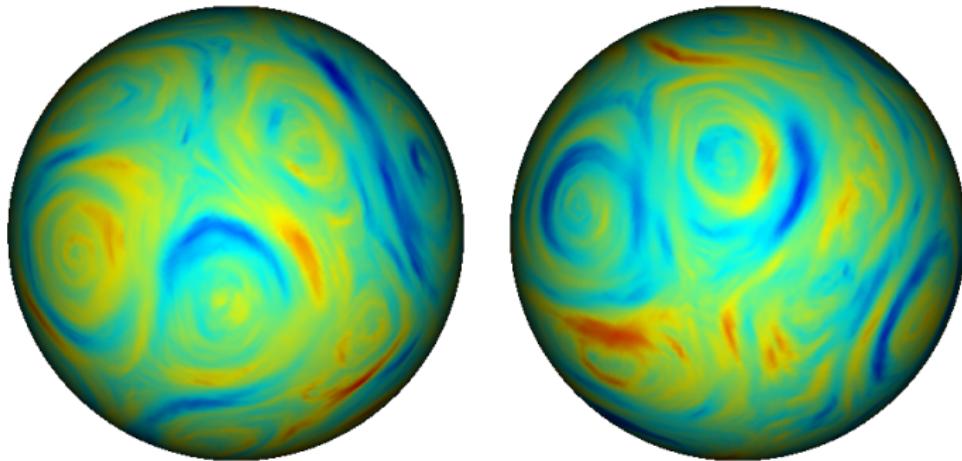
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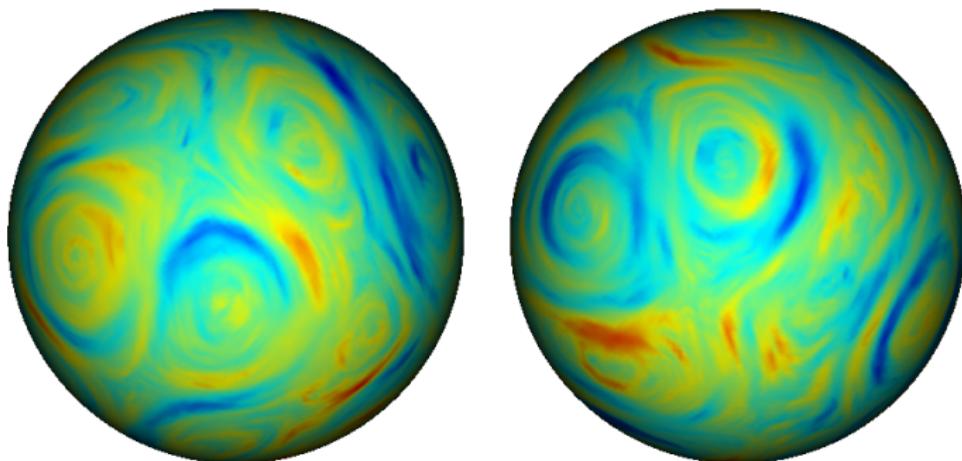
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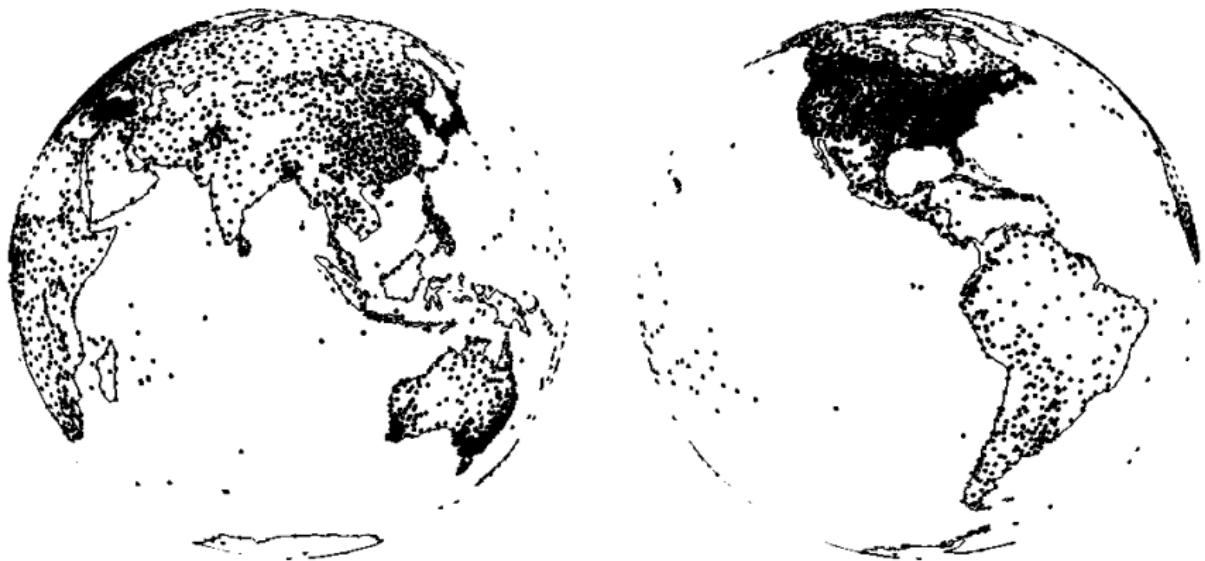
# Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, **non-separable spatio-temporal**, and **multivariate** fields on manifolds.

$$\left( \frac{\partial}{\partial t} + \kappa_{\mathbf{u},t}^2 + \nabla \cdot \mathbf{m}_{\mathbf{u},t} - \nabla \cdot \mathbf{M}_{\mathbf{u},t} \nabla \right) (\tau_{\mathbf{u},t} x(\mathbf{u}, t)) = \mathcal{E}(\mathbf{u}, t), \quad (\mathbf{u}, t) \in \Omega \times \mathbb{R}$$



# Large spatial problems: covariances are impractical



Data points  $n \approx 2500 \cdot 20$  Kriging locations  $m \approx 15000 \cdot 20$

Estimation: time  $\mathcal{O}(n^3)$ , storage  $\mathcal{O}(n^2) \sim 20\text{Gbytes}$

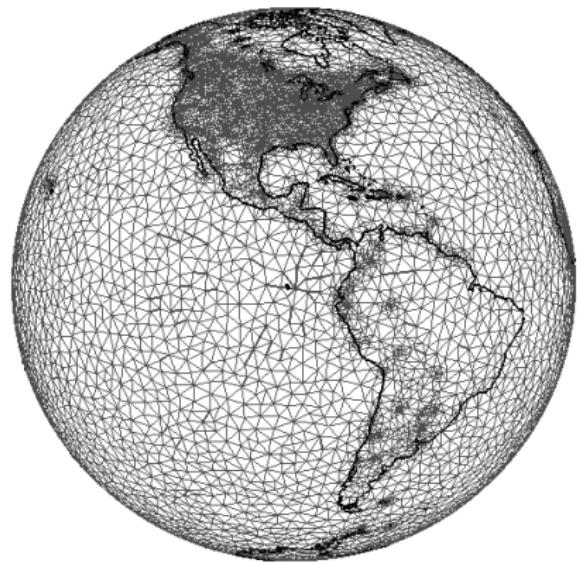
Kriging: time  $\mathcal{O}(mn + n^3)$ , storage  $\mathcal{O}(mn + n^2) \sim 130\text{Gbytes}$

This is *not* a “huge” data set.

# Practical triangulation based GMRFs



Data points  $n \approx 2500 \cdot 20$



Basis functions  $m \approx 15000 \cdot 20$

Estimation+Kriging: time  $\mathcal{O}(m^{3/2})$ , storage  $\mathcal{O}(m + n) \sim 50\text{Mbytes}$

# Global temperature analysis

- ▶ <http://www.ncdc.noaa.gov/ghcn/ghcn.html>
- ▶ Monthly average temperatures
- ▶ On average 2500 locations per year
- ▶ Covariate data (elevation, land use, etc.) for 7000 stations

## Model for yearly mean temperatures

Observations :  $\text{temperature} \sim \text{elevation} + \text{climate} + \text{anomaly}$

Climate :  $\mu_{\mathbf{u}}, \tau_{\mathbf{u}}, \kappa_{\mathbf{u}}^2 = \sum_k \psi_k(\mathbf{u}) \theta_k$

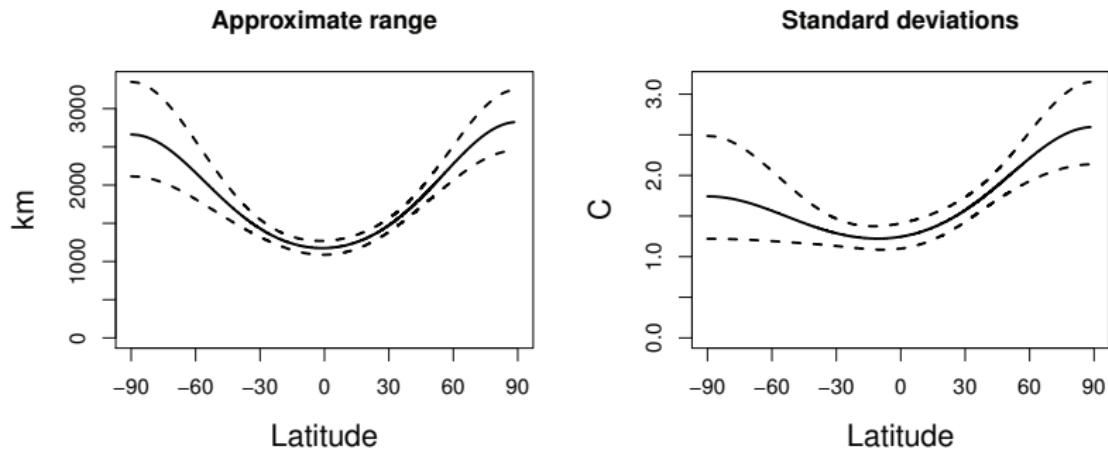
Anomaly :  $(\kappa_{\mathbf{u}}^2 - \Delta) (\tau_{\mathbf{u}} x_t(\mathbf{u})) = \mathcal{W}(\mathbf{u})$

Weather :  $\mu(\mathbf{u}) + x_t(\mathbf{u})$

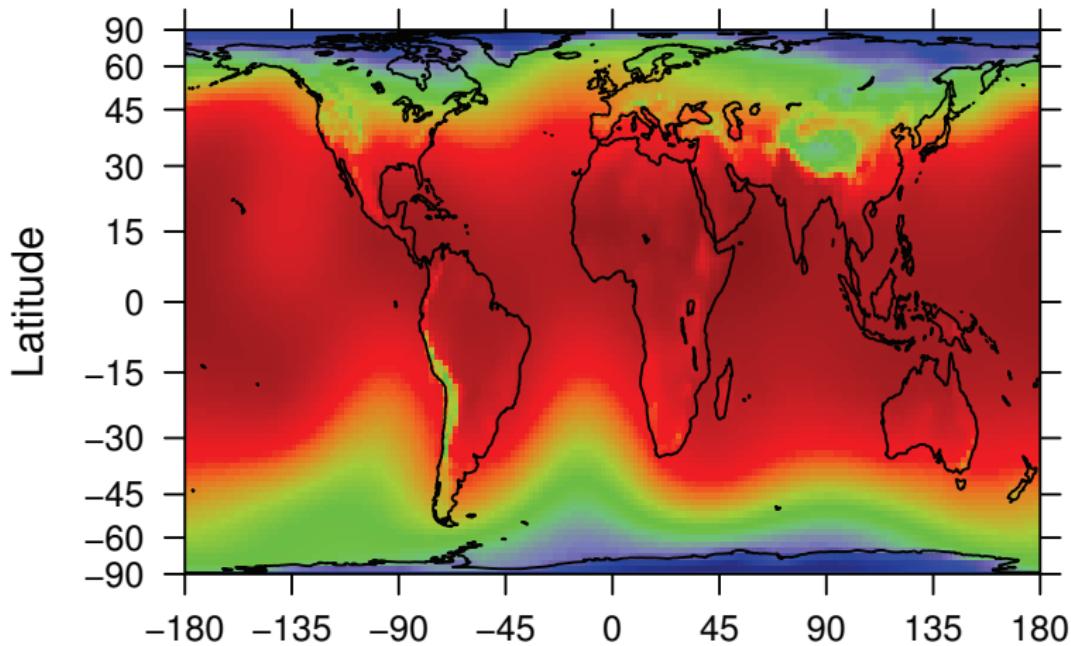
# Code outline for Bayesian inference with R-INLA

```
mesh = inla.mesh(loc=station.locations, ## optional  
                  cutoff=10/earth.radius,  
                  refine=list(max.edge=500/earth.radius))  
  
...  
  
spde = inla.spde(mesh, model="matern", ...  
                  param=list(basis.T=B.tau, ...))  
  
...  
  
formula = temperature ~ elevation + climate.mu +  
          f(anomaly, model=spde,  
             replicate=year)  
  
...  
  
result = inla(formula, data, family="gaussian", ...)
```

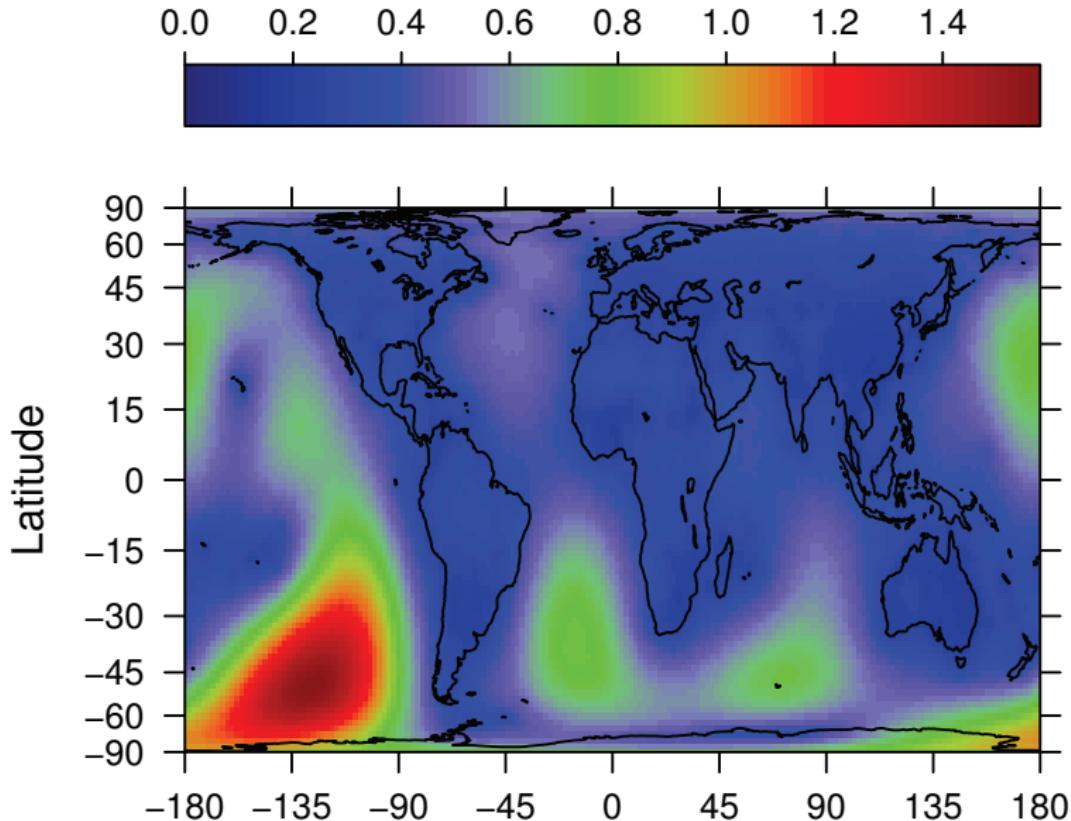
# Estimated climate covariance properties 1970-1989



# Empirical Climate 1970–1989 (C)

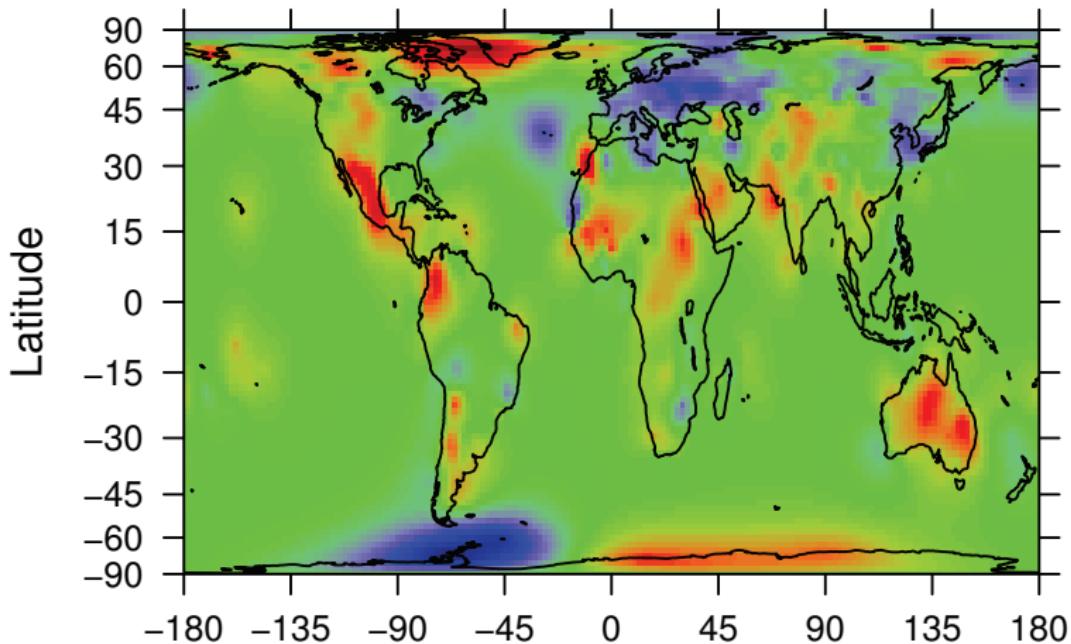


# Std dev for Climate 1970–1989 (C)

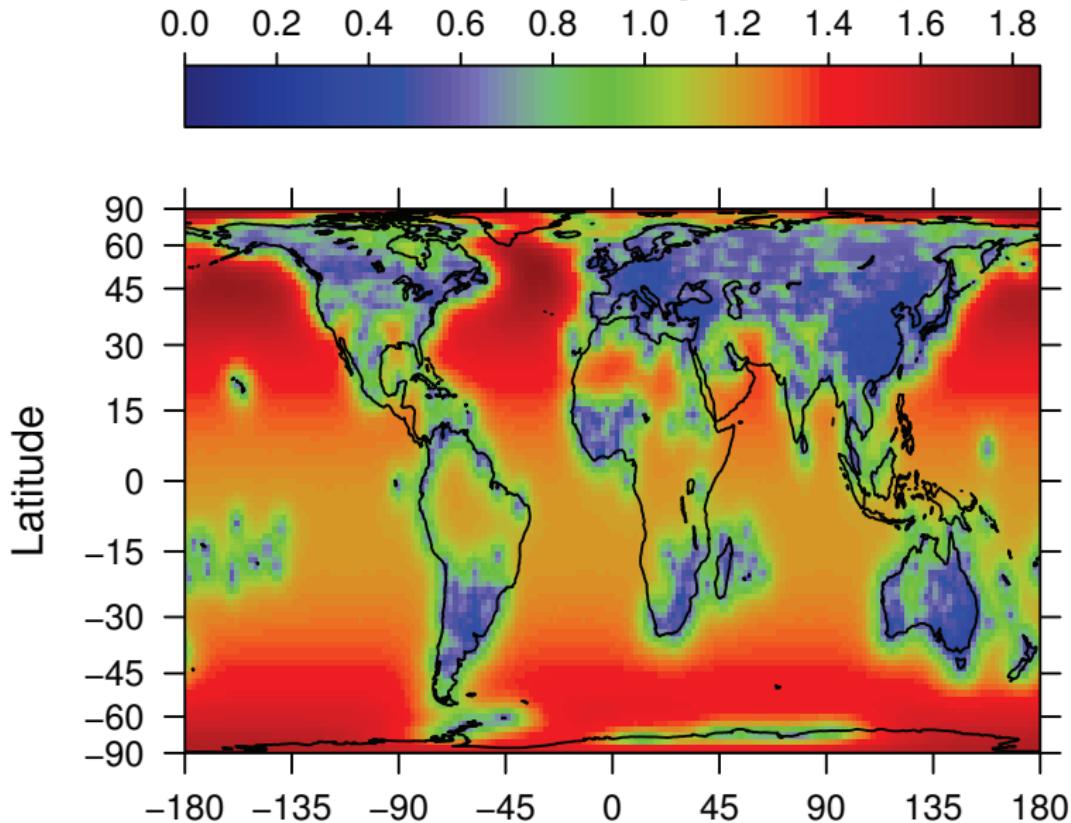


# Empirical Anomaly 1980 (C)

-2.0 -1.5 -1.0 -0.5 0.0 0.5 1.0 1.5 2.0



# Std dev for Anomaly 1980 (C)



# Conclusion

## SPDE/GMRF

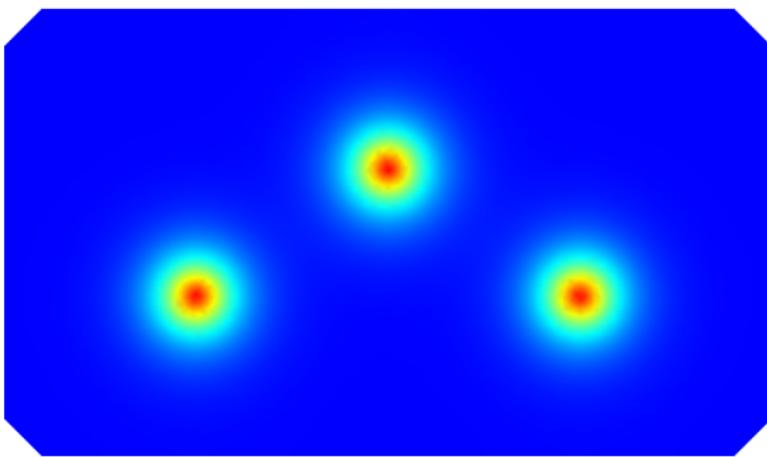
The connection allows for consistent local specifications of general spatio-temporal models that allow efficient practical computations.

- ▶ Unavoidably beyond the traditional computational statistics toolbox
- ▶ Combines standard concepts from different areas in applied mathematics and engineering
- ▶ Detailed knowledge of SPDEs is not needed for practical use
- ▶ Open source software available: <http://www.r-inla.org/>

# Covariances for Beyond classical Matérn models

The approach can in a straightforward way be extended to oscillating, anisotropic, non-stationary, non-separable spatio-temporal, and multivariate fields on manifolds.

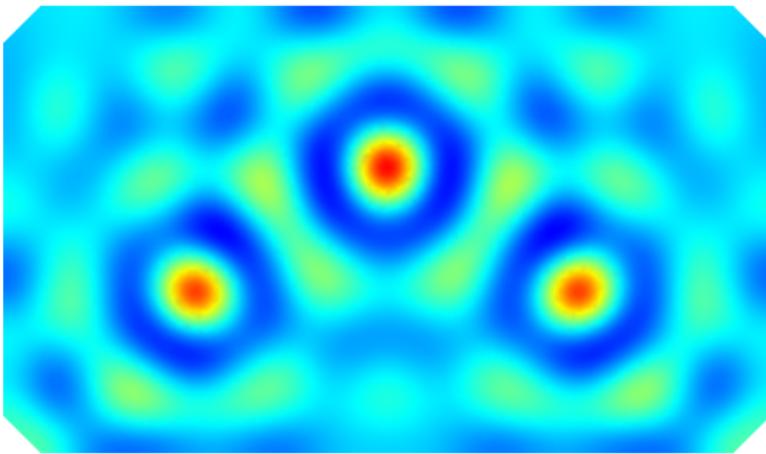
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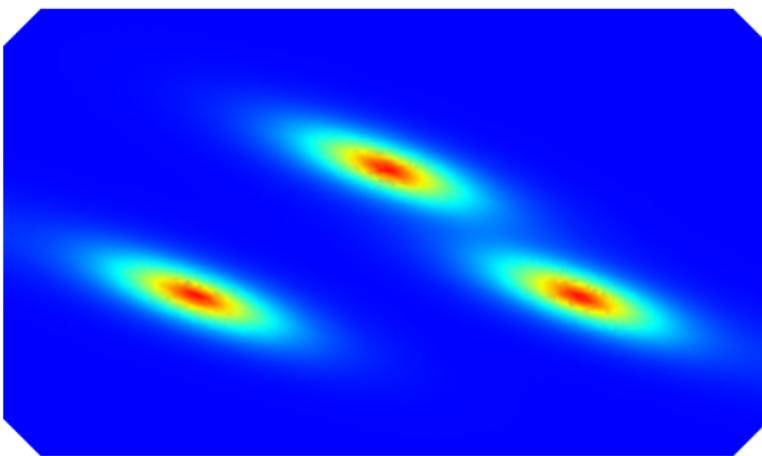
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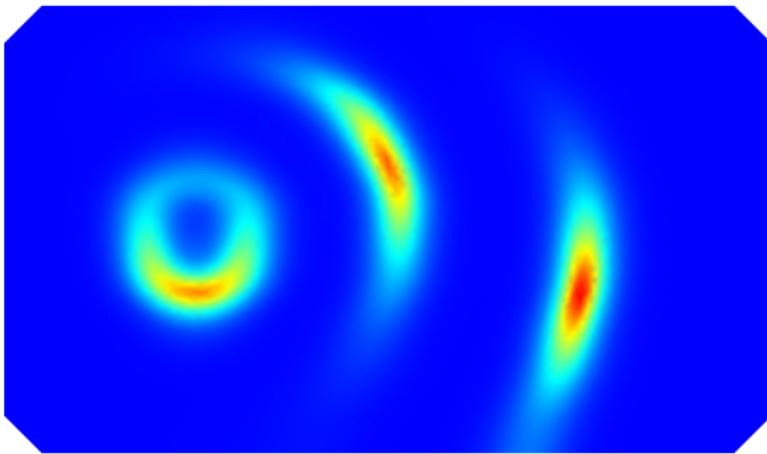
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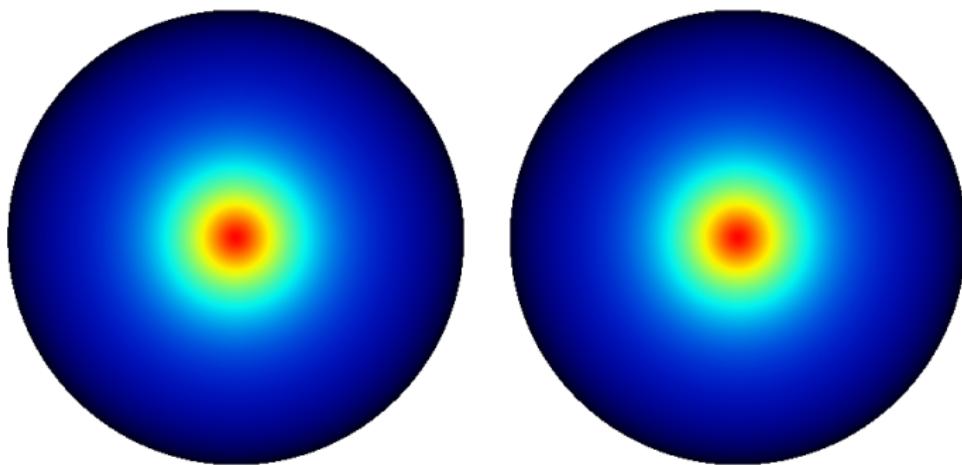
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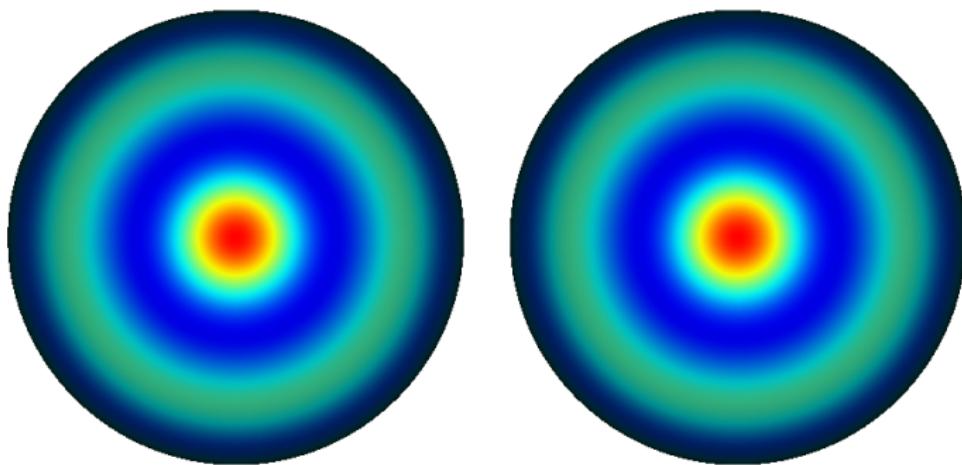
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