



Royal Netherlands
Meteorological Institute
*Ministry of Infrastructure and the
Environment*



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OESCHGER CENTRE
CLIMATE CHANGE RESEARCH



RECONSTRUCTION OF DAILY AIR TEMPERATURE VARIATIONS GLOBALLY SINCE THE MID 19TH CENTURY



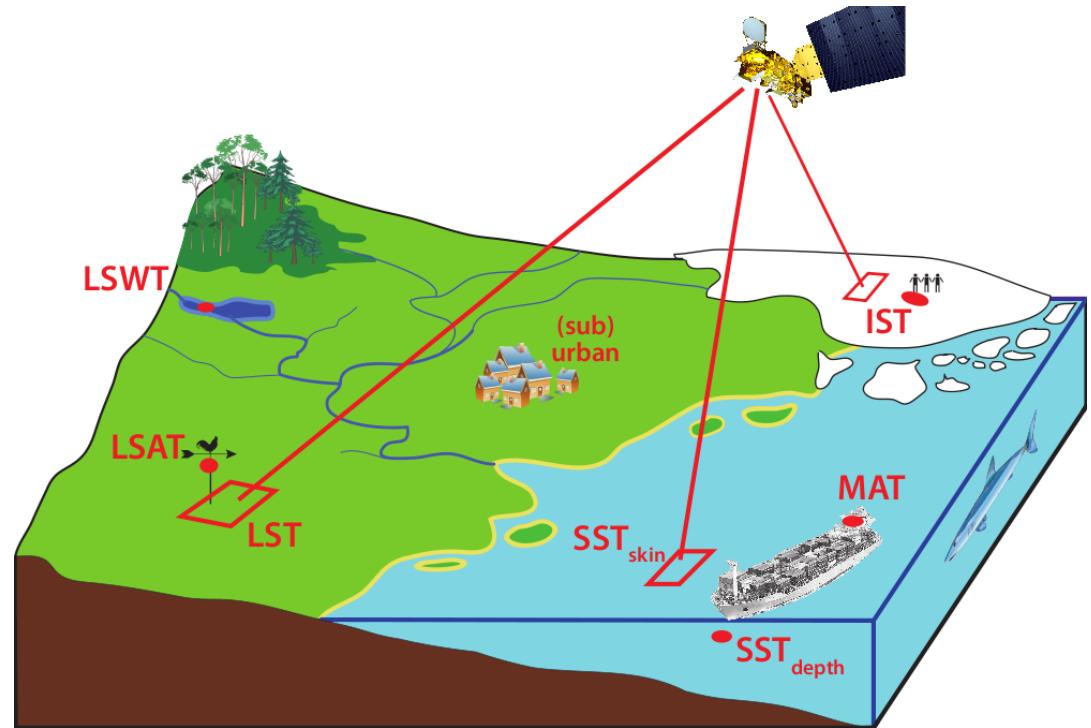
EUSTACE has received funding from the European Union's Horizon 2020 Programme for Research and Innovation, under Grant Agreement no 640171



OVERVIEW

- Brief overview of the EUSTACE project:
 - Aim
 - Tasks
- Observational analysis (one-of-two):
 - Observation model:
 - Modelling biases and uncertainties
 - Air temperature model:
 - Daily local component
 - Climatology component
 - Large-scale component
 - Examples of preliminary results.

UNDERSTAND AND EXPLOIT THE RELATIONSHIP BETWEEN AIR AND SKIN TEMPERATURE



From Merchant et al., 2013 community paper and roadmap:

<http://www.geosci-instrum-method-data-syst.net/2/305/2013/gi-2-305-2013.html>

WP1: Observation integration

- Develop skin-air temperature relationships (over land, sea, ice, lakes).
- Quality control observations
- Develop observation bias/error models. Breakpoint detection.

WP2: Data set construction

- Merge WP1 data products.
- Produce spatio-temporal statistical analyses (global, 1850-present).
- Develop and build system for dataset construction.

WP3: Validation and intercomparison

- Validate WP1 and WP2 products and uncertainty estimates against independent reference data.

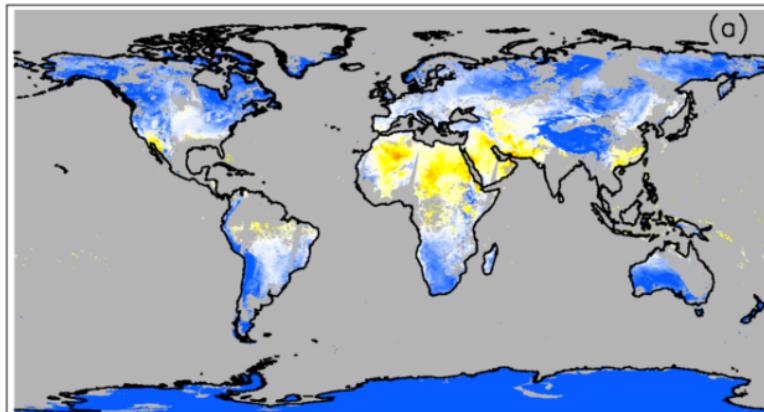
WP4: Outreach and dissemination

WP5: Science leadership

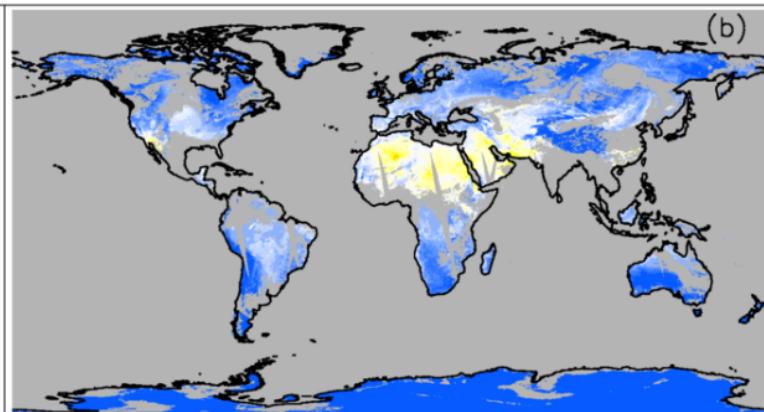
WP6: Project management

EXAMPLE SATELLITE DERIVED 2M AIR TEMPERATURE (1 JULY 2010)

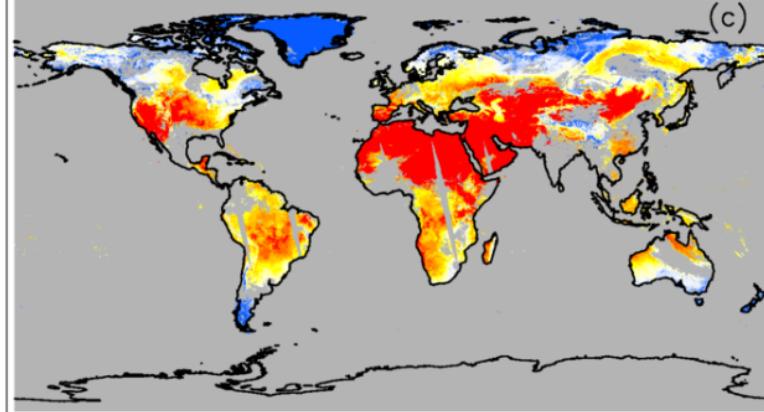
LST Night



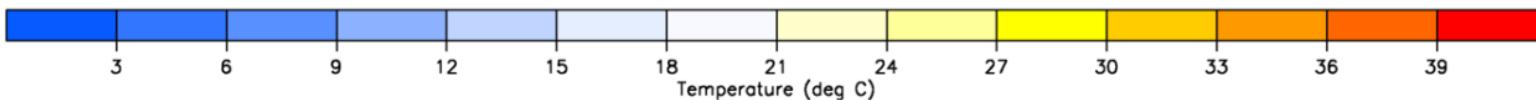
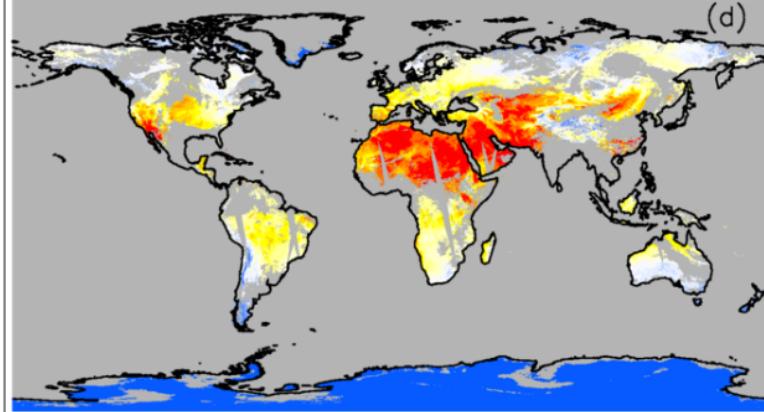
Tmin



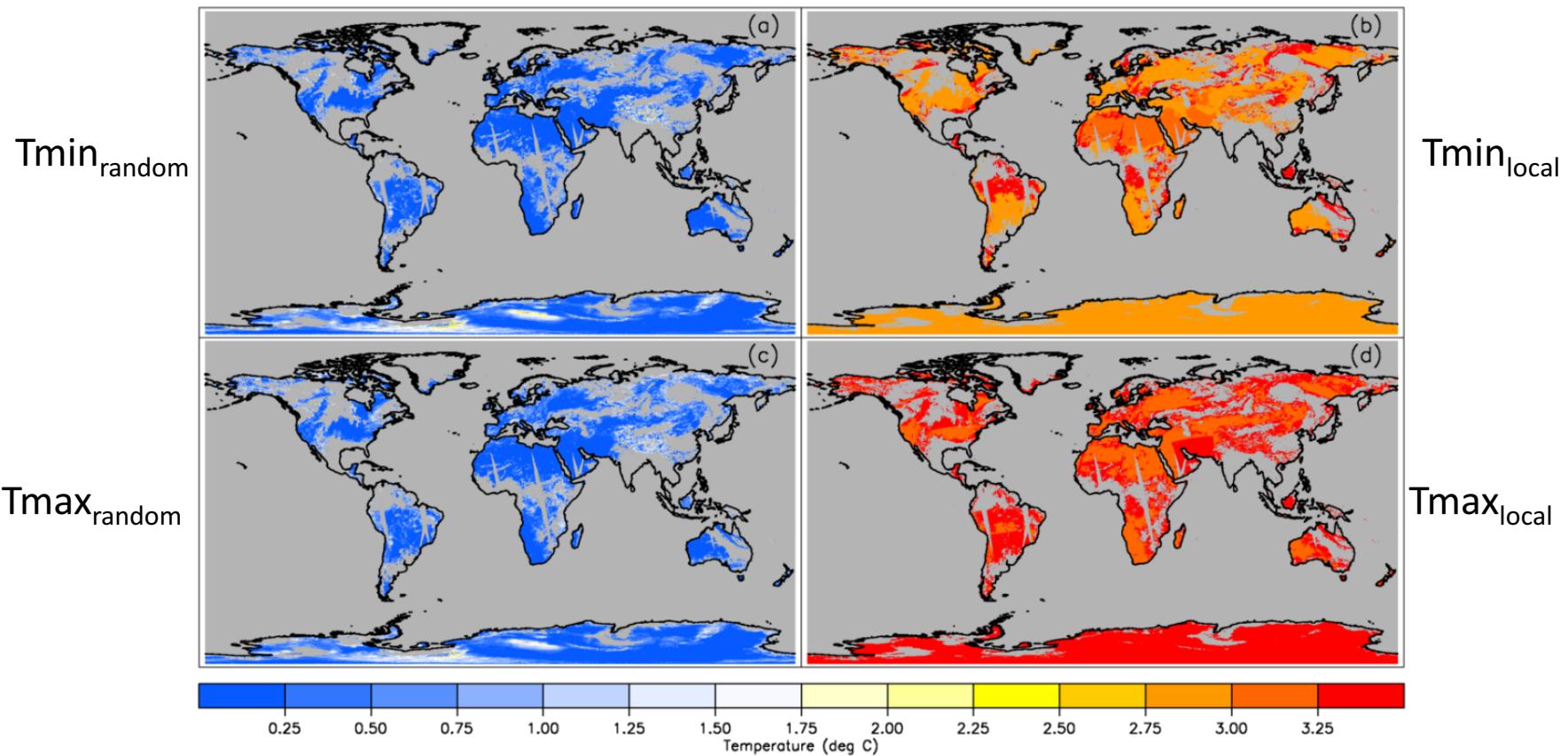
LST Day



Tmax



EXAMPLE UNCERTAINTY FIELDS (1 JULY 2010)



SOURCES OF OBSERVATIONAL UNCERTAINTY

- **Satellite observations over land, sea, ice:**
 - **Structural errors:** brightness temperature calibration, conversion to air temperature, observed surface related.
 - **Correlated errors:** atmospheric corrections, surface emissivity errors.
 - **Uncorrelated errors:** sensor noise, geolocation.
- **In situ observations from weather stations, ships, buoys.**
 - **Structural errors:** observing platform specific biases, instrumentation changes calibration, station siting changes.
 - **Uncorrelated errors:** observational noise, local representivity.

AN EMPIRICAL LAND SURFACE TEMPERATURE – AIR TEMPERATURE RELATIONSHIP

- Build multiple linear regression model using weather stations and satellite Land Surface Temperature observations, together with other explanatory variables.

$$T_{\max} = \alpha_0 + \alpha_1 \cdot LST_{\text{day}} + \alpha_2 \cdot LST_{\text{ngt}} + \alpha_3 \cdot FVC + \alpha_4 \cdot DEM + \alpha_5 \cdot SZA_{\text{noon}} + \alpha_6 \cdot Snow + \varepsilon_{T\max}$$

$$T_{\min} = \beta_0 + \beta_1 \cdot LST_{\text{day}} + \beta_2 \cdot LST_{\text{ngt}} + \beta_3 \cdot FVC + \beta_4 \cdot DEM + \beta_5 \cdot SZA_{\text{noon}} + \beta_6 \cdot Snow + \varepsilon_{T\min}$$

Air Temperature

Satellite observed
LST (day/night)

Vegetation
fraction

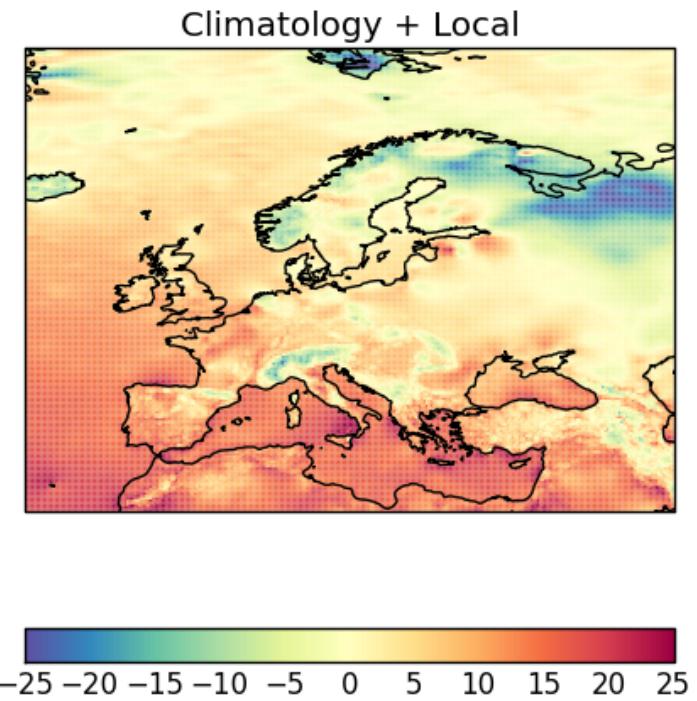
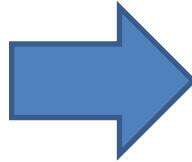
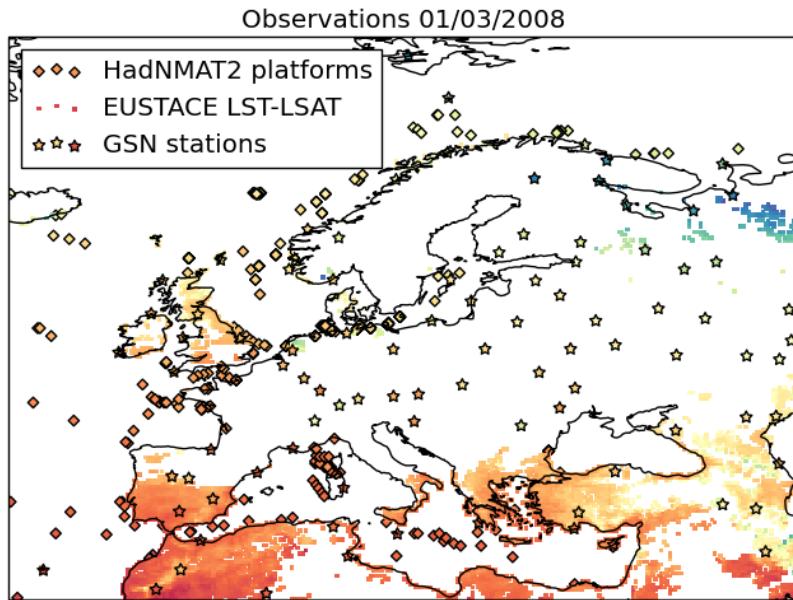
Elevation

Solar Zenith
angle at noon

Error

ANALYSIS SYSTEM AIM

Construct a **spatially and temporally complete** analysis of global air temperatures from 1850 to present with **validated uncertainty estimates**, constructed from **satellite and in situ data sources**.



COMMENTS ON SCALE

**Output resolution = 0.25 degree latitude/longitude grid
= 1,036,800 output locations per day**

Number of days > 60,000

Three variables: maximum, minimum and mean temperatures

Ensemble output – small number of samples of whole dataset to sample uncertainty in analysis.

Full space-time statistical model solve requires big computing (this is also being investigated in the project in a second analysis approach).

The approach discussed today takes a different route, splitting the problem into smaller, solvable chunks. Many similarities in modelling.

OBSERVATION MODEL

Air temperature measurement are considered to be subject to a variety of error sources with different correlation structures:

$$y^i = T(\mathbf{s}^i, t^i) + \mathbf{J}_\beta^i \boldsymbol{\beta} + \varepsilon_c(\mathbf{s}^i, t^i) + \varepsilon_u^i$$

y^i = Air temperature observation i

$\mathbf{J}_\beta^i \boldsymbol{\beta}$ = Linear model for systematic errors

$\varepsilon_c(\mathbf{s}^i, t^i)$ = Locally correlated error

ε_u^i = Uncorrelated error

PROCESS MODEL

Daily mean air temperatures are decomposed into variability at different scales:

$$T(\mathbf{s}, t) = T^{\text{clim}}(\mathbf{s}, t) + T^{\text{large}}(\mathbf{s}, t) + T^{\text{local}}(\mathbf{s}, t)$$

$T(\mathbf{s}, t)$ = Temperature at space/time location (\mathbf{s}, t)

$T^{\text{clim}}(\mathbf{s}, t)$ = Climatological temperature

$T^{\text{large}}(\mathbf{s}, t)$ = Large spatial/temporal scale component

$T^{\text{local}}(\mathbf{s}, t)$ = Daily, short scale component

MODEL COMPONENT:

DAILY LOCAL ANALYSIS

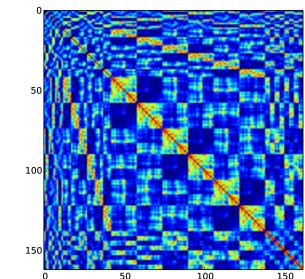
Independent, daily analyses of a spatial smooth temperature field.

Use SPDE approach (Lindgren et al 2011):

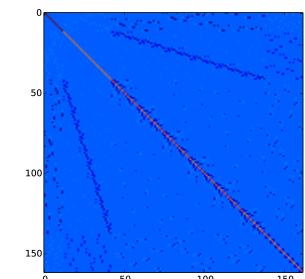
- Describes smooth function as weighted sum of local basis functions.
- Smoothness - Gaussian Markov Random Field prior weights. Smoothness controlled by parameters of the prior precision matrix.
- Objective of estimation is to learn the probability density function of the coefficients conditioned on the data.

FROM COVARIANCE FUNCTIONS TO SPDE MODELS

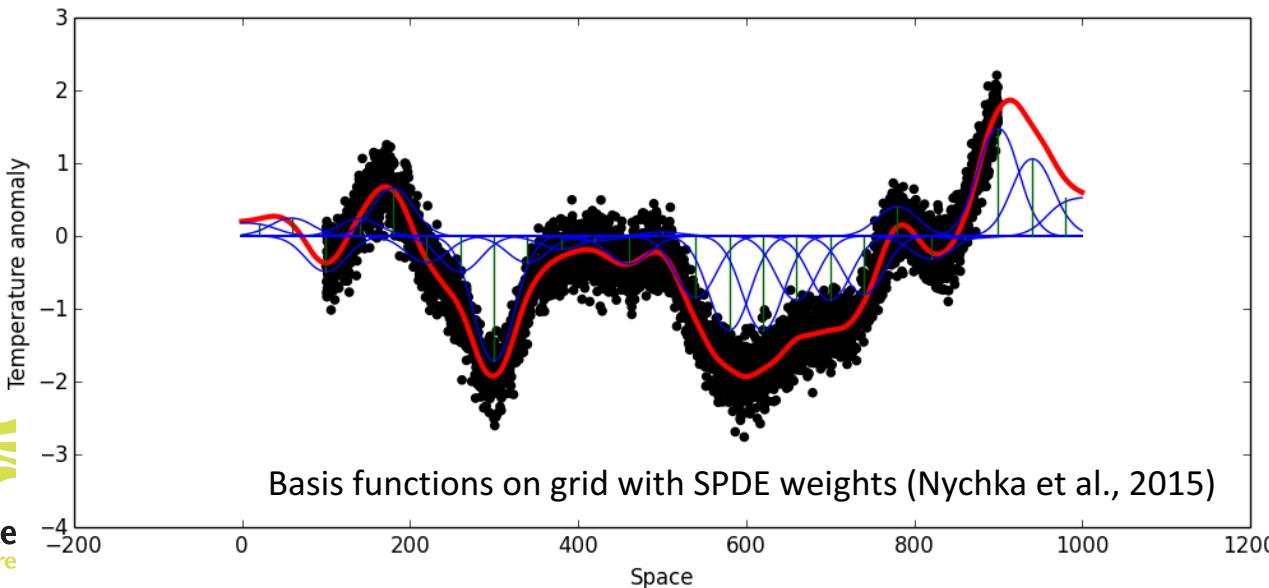
- Traditional Kriging is not feasible for data volumes in EUSTACE.
 - (Requires solutions to linear systems involving big, dense covariance matrices)
- Lindgren et al. (2011) result allows much more efficient computation.
 - (Can directly compute *sparse* inverse covariance matrices corresponding to Matérn covariance functions)



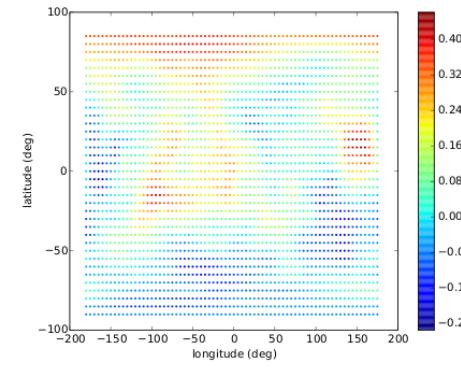
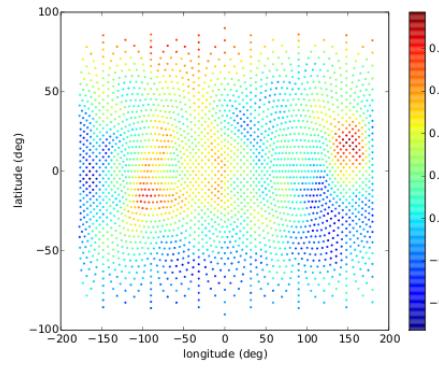
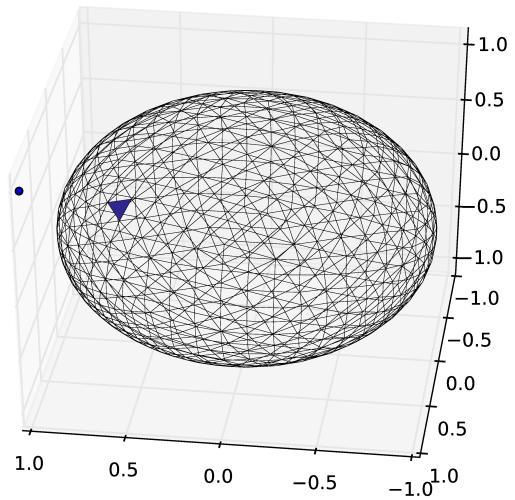
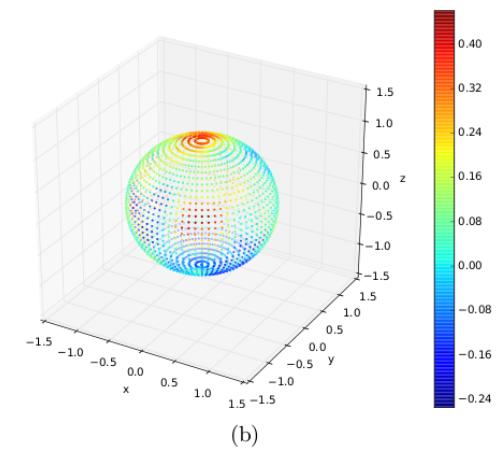
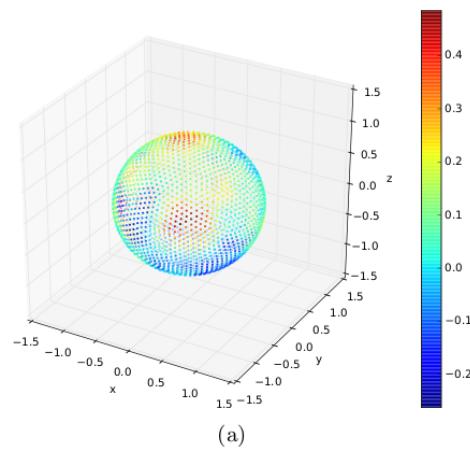
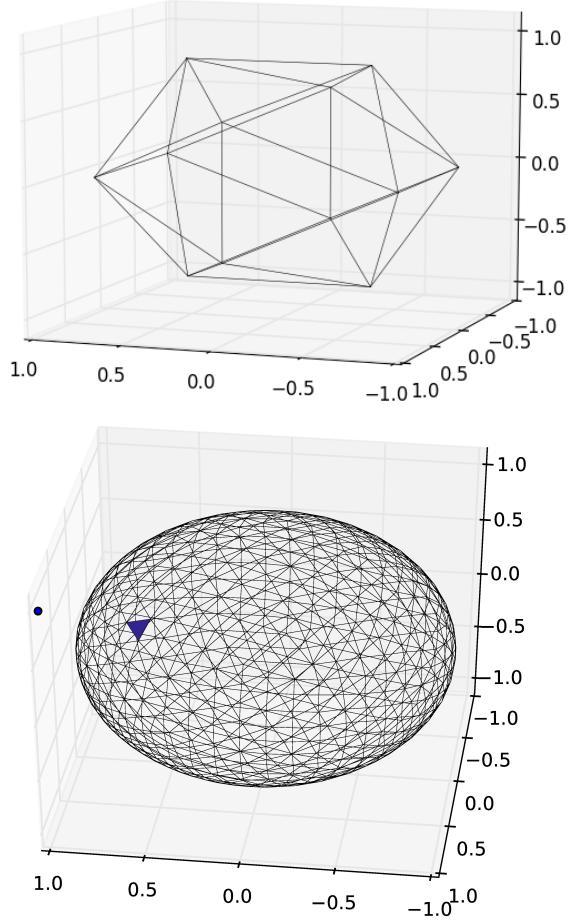
Dense covariance matrix



Sparse inverse covariance matrix
(lots of zeros)



RANDOM PROCESSES ON SPHERES



ESTIMATION THROUGH CONDITIONAL GAUSSIANS

Model:

Construct a design matrix \mathbf{J} to form a linear observation equation as:

$$\mathbf{y} = \mathbf{Ju} + \boldsymbol{\varepsilon}_y$$

Observations are subject to Gaussian measurement error: $p(\boldsymbol{\varepsilon}_y) = \mathcal{N}(\mathbf{0}, \mathbf{Q}_{\boldsymbol{\varepsilon}}^{-1})$

Latent variables \mathbf{u} have Gaussian prior distribution: $p(\mathbf{u}) = \mathcal{N}(\boldsymbol{\mu}_u, \mathbf{Q}_u^{-1})$

Estimation:

Compute the distribution of \mathbf{u} conditioned on the observations:

$$p(\mathbf{u} | \mathbf{y}, \boldsymbol{\theta} = \hat{\boldsymbol{\theta}}) = \mathcal{N}(\boldsymbol{\mu}_{u|\mathbf{y}}, \mathbf{Q}_{u|\mathbf{y}}^{-1})$$

$$\boldsymbol{\mu}_{u|\mathbf{y}} = \boldsymbol{\mu}_u + \mathbf{Q}_{u|\mathbf{y}}^{-1} \mathbf{J}^T \mathbf{Q}_{\boldsymbol{\varepsilon}} (\mathbf{y} - \mathbf{Ju})$$

$$\mathbf{Q}_{u|\mathbf{y}} = \mathbf{Q}_u + \mathbf{J}^T \mathbf{Q}_{\boldsymbol{\varepsilon}} \mathbf{J}$$

JOINT ESTIMATION OF BIASES

$$\mathbf{y} = \mathbf{J}_u \mathbf{u} + \mathbf{J}_\beta \boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

The design matrix \mathbf{J}_β describes the structure of systematic errors.
The unknown vector $\boldsymbol{\beta}$ controls the magnitude of systematic error

Append observation bias variables $\boldsymbol{\beta}$ onto model variable vector \mathbf{u} and estimate jointly.

Joint prior: $p(\mathbf{u}, \boldsymbol{\beta}) = \mathcal{N}(\boldsymbol{\mu}_{u,\beta}, \mathbf{Q}_{u,\beta}^{-1})$

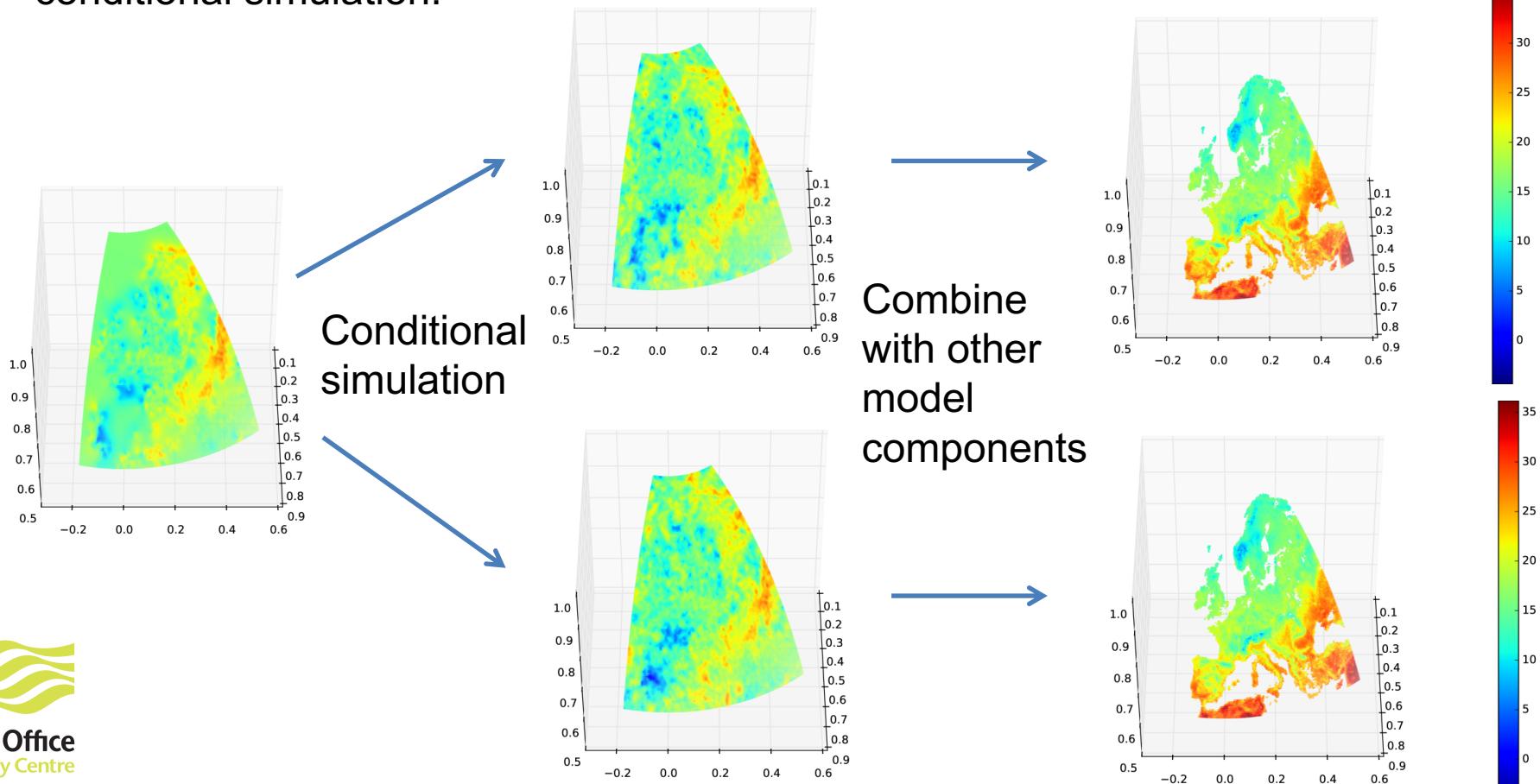
$$\boldsymbol{\mu}_{u,\beta} = \begin{pmatrix} \boldsymbol{\mu}_u \\ \boldsymbol{\mu}_\beta \end{pmatrix}$$

$$\mathbf{Q}_{u,\beta} = \begin{pmatrix} \mathbf{Q}_u & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_\beta \end{pmatrix}$$

ENSEMBLE GENERATION

Aim to produce a dataset that can be used to undertake scientific analysis, including assessment of uncertainty.

To this end, multiple realisations of the dataset will be produced through conditional simulation.



SINGLE VARIABLE ANALYSIS

MODEL:

MEAN/MAX/MIN TEMPERATURE

Strategy for solution:

Decompose the space-time temperature field into components with defined structure in space/time:

$$T(\mathbf{s}, t) = T^{\text{clim}}(\mathbf{s}, t) + T^{\text{large}}(\mathbf{s}, t) + T^{\text{local}}(\mathbf{s}, t)$$

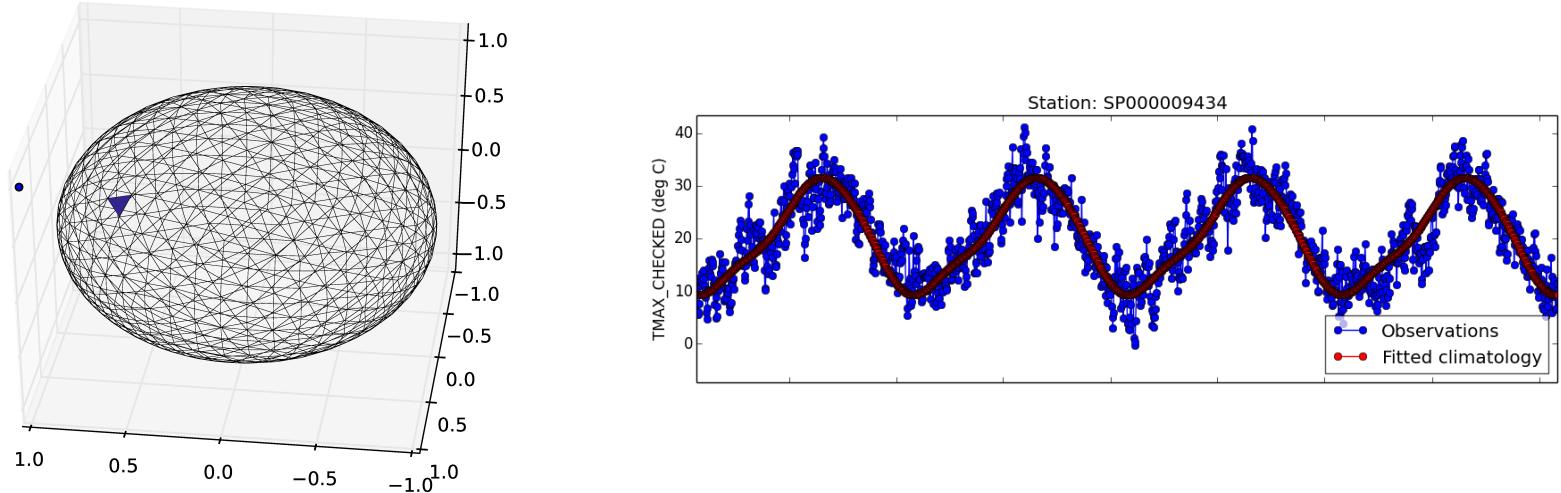
Append bias variables onto model components and estimate jointly.

Solve each component conditioned on the expected value of other components.

Refine solutions by iteratively re-estimating each component.

CLIMATOLOGY

Climatology = Covariates (e.g. altitude, latitude) + Seasonal component



Seasonal component constructed as Fourier series in time.

Fourier series coefficients varying smoothly spatially.

Spatial fields of coefficients are constructed as a weighted sum of spatial basis functions. The weights are modelled as latent variables with GMRF priors.

COMPONENT: CLIMATOLOGY

The climatology model is comprised of a covariate model and a seasonal model:

$$T^{\text{clim}}(\mathbf{s}, t) = T^{\text{covariate}}(\mathbf{s}, t) + T^{\text{seasonal}}(\mathbf{s}, t)$$

The covariate model is a linear model for explanatory variables affecting mean temperatures (e.g. function of latitude, distance from coast):

$$T^{\text{covariate}}(\mathbf{s}, t) = \sum_{k=1}^K f_k^{\text{covariate}}(\mathbf{s}, t) w_k$$

With a Gaussian prior on the coefficients:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \mathbf{Q}_{\mathbf{w}}^{-1})$$

COMPONENT: CLIMATOLOGY

The seasonal model looks like a fourier series in time, with spatially varying coefficients:

$$T^{\text{seasonal}}(\mathbf{s}, t) = \sum_{l=1}^L \left[\sin(2\pi lt) \sum_{m=1}^M f_m(\mathbf{s}) u_{l,m} + \cos(2\pi lt) \sum_{m=1}^M f_m(\mathbf{s}) v_{l,m} \right]$$

where:

$f_m(\mathbf{s})$ = Locally supported spatial basis function

$u_{l,m}$ = Coefficient for sine components(l, m)

$v_{l,m}$ = Coefficient for cosine components(l, m)

Coefficients for each harmonic are constrained vary smoothly through SPDE prior precision.

$$p(\mathbf{u}_l) = \mathcal{N}(\mathbf{0}, \mathbf{Q}_{\mathbf{u}_l}^{-1})$$

$$p(\mathbf{v}_l) = \mathcal{N}(\mathbf{0}, \mathbf{Q}_{\mathbf{v}_l}^{-1})$$

CLIMATOLOGY COMPONENT

And the joint prior is built up in blocks (L harmonics plus the covariate block):

$$p(\boldsymbol{u}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{u}}, \boldsymbol{Q}_{\boldsymbol{u}}^{-1})$$

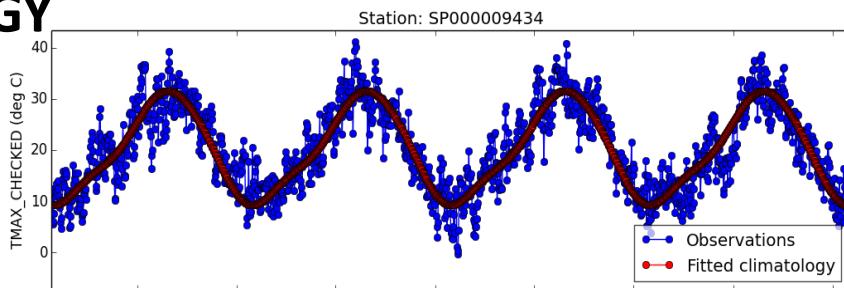
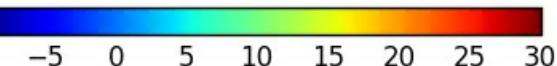
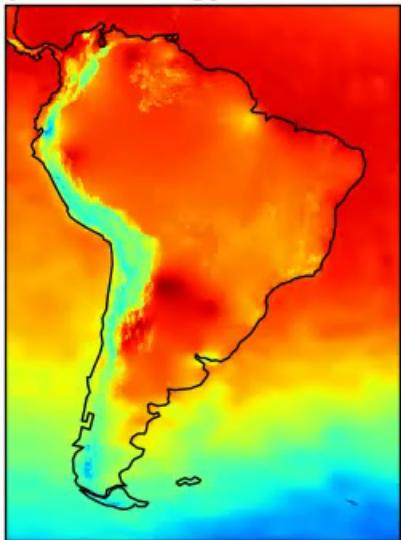
$$\boldsymbol{\mu}_{\boldsymbol{u}} = \mathbf{0}$$

$$\boldsymbol{Q}_{\boldsymbol{u}} = \begin{bmatrix} \boldsymbol{Q}_{u_1} & & & \\ & \boldsymbol{Q}_{v_1} & & \\ & & \ddots & \\ & & & \boldsymbol{Q}_{u_L} \\ & & & & \boldsymbol{Q}_{v_L} \\ & & & & & \boldsymbol{Q}_w \end{bmatrix}$$

MODEL COMPONENT: CLIMATOLOGY

$$T^{\text{clim}}(\mathbf{s}, t) = T^{\text{covariate}}(\mathbf{s}, t) + T^{\text{seasonal}}(\mathbf{s}, t)$$

Daily Climatology Demo (deg C)



Seasonal component	
Local Harmonic	Temporally harmonic, spatially local basis functions.
Local Offset	Temporally constant, spatially local basis functions.
Covariate component	
Grand mean	Constant offset for whole globe.
Harmonics of latitude	Accounts for temperature variation with latitude. Spatially harmonic.
Altitude	Spatially local variation in mean temperature with altitude.
Distance from water	Coastal effect for large water bodies.
Climatological surface type	Indicators of surface type (e.g. water, ice, vegetation)

COMPONENT: LARGE SCALE

Nonlinear model: products of spatial and temporal components:

$$\begin{aligned} T^{\text{large}}(\mathbf{s}, t) &= f(\mathbf{u}^{\text{large}}) \\ &= \sum_{d=1}^D g_d^{\text{large}}(\mathbf{s}) \circ h_d^{\text{large}}(t) \end{aligned}$$

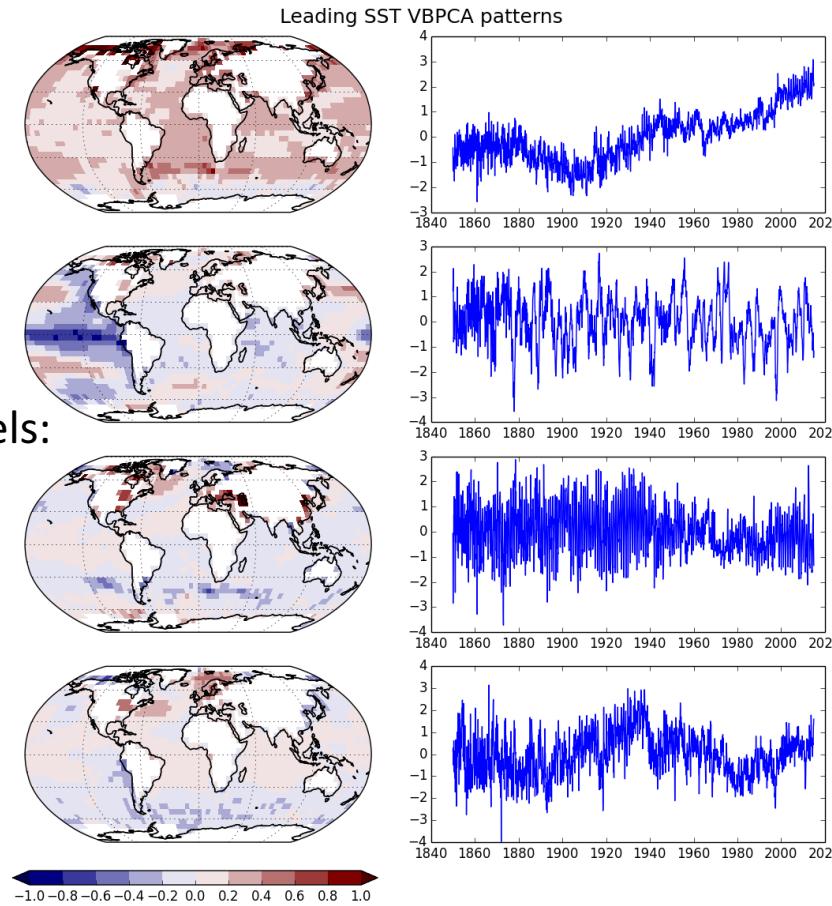
Spatial and temporal functions formed as SPDE models:

$$\begin{aligned} g_d^{\text{large}}(\mathbf{s}) &= \mathbf{A}_d^w(\mathbf{s}) \mathbf{w}_d \\ h_d^{\text{large}}(t) &= \mathbf{A}_d^x(t) \mathbf{x}_d \end{aligned}$$

With Gaussian priors on the latent variables:

$$p(\mathbf{w}_d) = \mathcal{N}(\mathbf{0}, \mathbf{Q}_d^{w^{-1}})$$

$$p(\mathbf{x}_d) = \mathcal{N}(\mathbf{0}, \mathbf{Q}_d^{x^{-1}})$$



MODEL COMPONENT:

LARGE SCALE ANALYSIS

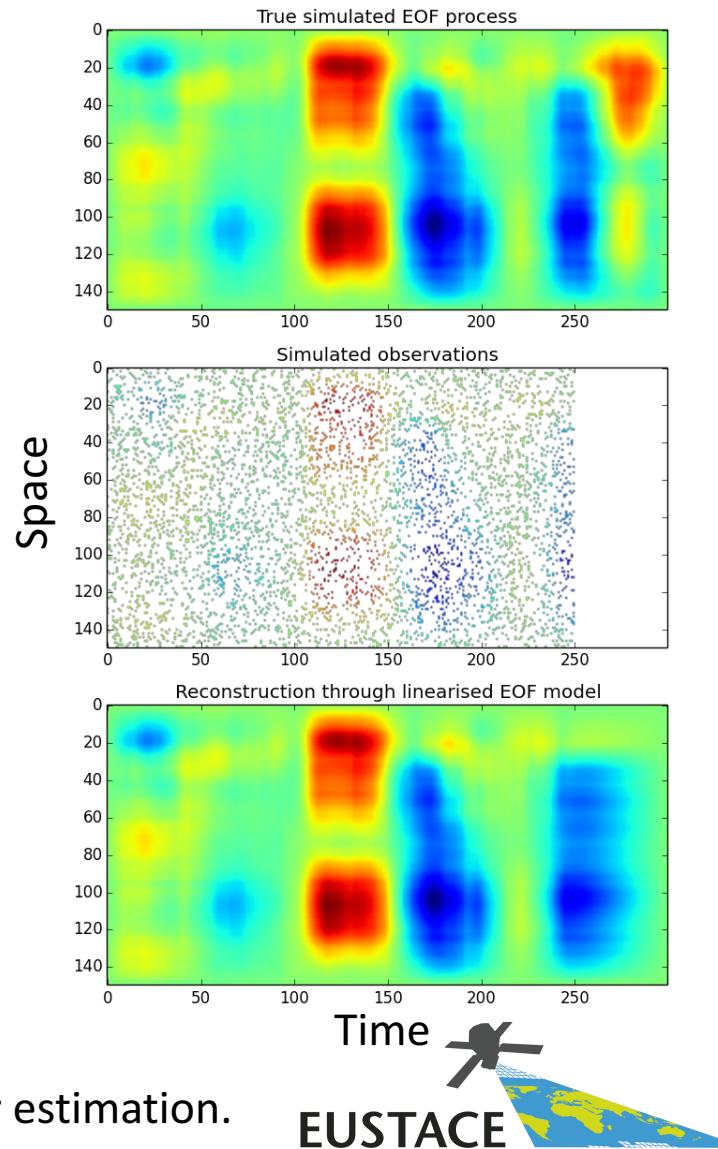
Nonlinear model: products of spatial and temporal components:

$$\begin{aligned} T^{\text{large}}(\mathbf{s}, t) &= f(\mathbf{u}^{\text{large}}) \\ &= \sum_{d=1}^D g_d^{\text{large}}(\mathbf{s}) \circ h_d^{\text{large}}(t) \end{aligned}$$

Form linear approximation through Taylor expansion:

$$\begin{aligned} f(\mathbf{u}^{\text{large}}) &= f(\mathbf{u}^*) + \mathbf{J}(\mathbf{u}^{\text{large}} - \mathbf{u}^*) + \text{H.O.T.} \\ &\approx f(\mathbf{u}^*) - \mathbf{J}\mathbf{u}^* + \mathbf{J}\mathbf{u}^{\text{large}} \end{aligned}$$

$$\mathbf{J} = \left. \frac{\partial f(\mathbf{u}^{\text{large}})}{\partial \mathbf{u}^{\text{large}}} \right|_{\mathbf{u}^{\text{large}}=\mathbf{u}^*}$$



ANALYSIS PROTOTYPE

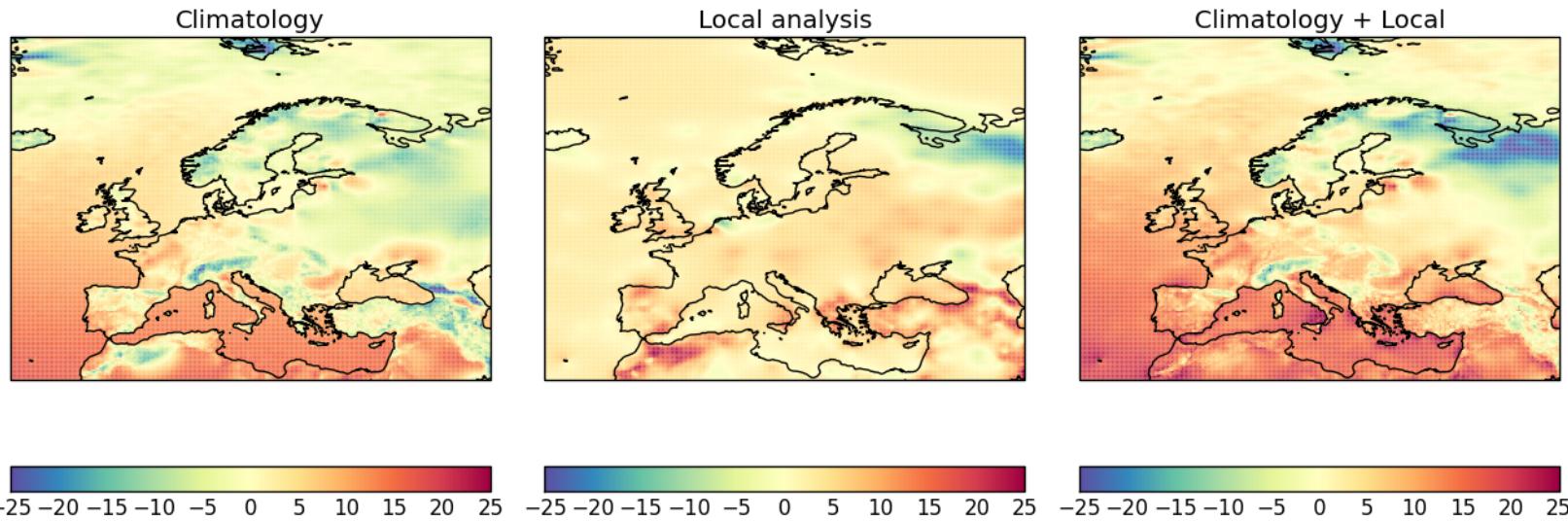
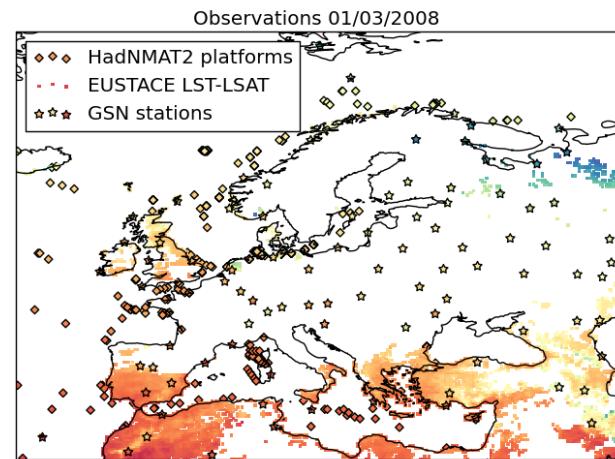
CLIMATOLOGY/LOCAL COMPONENT

Applied to in situ NMAT/SAT & LSAT derived SAT:

- Fitted climatology – spatial SPDE's for coefficients of Fourier components in time.
- Fitted local – daily spatial SPDE.

Climatology used observations in 1961-1990 period.

Currently extending to include all model components.



SUMMARY

- Aim:
 - Produce a globally complete daily temperature analysis with validated uncertainties.
- Approach:
 - Draws heavily on Gaussian latent variable models.
 - Split model into climatology, large-scale and daily local components.
- Extensions:
 - Non-stationary processes (linear model for precision matrix parameters – amplitude and decorrelation range e.g. a function of distance from coast)
 - Diurnal temperature range model (transformed Gaussian model).



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QUESTIONS?



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JOINT ANALYSIS MODEL:

MEAN TEMPERATURE AND DTR

The observation equations for the Joint Analysis are formed as functions of daily mean temperature (τ_m) and diurnal temperature range (τ_r) as:

$$\begin{aligned}y_m^i &= \tau_m(\mathbf{s}^i, t^i) + \beta^i + \varepsilon^i \\y_x^i &= \tau_m(\mathbf{s}^i, t^i) + \frac{1}{2}\tau_r(\mathbf{s}^i, t^i) + \beta^i + \varepsilon^i \\y_n^i &= \tau_m(\mathbf{s}^i, t^i) - \frac{1}{2}\tau_r(\mathbf{s}^i, t^i) + \beta^i + \varepsilon^i\end{aligned}$$

Tmean decomposed as sum of sub-components (as before):

$$\tau_m(\mathbf{s}, t) = \tau_m^{\text{climatology}}(\mathbf{s}, t) + \tau_m^{\text{large}}(\mathbf{s}, t) + \tau_m^{\text{local}}(\mathbf{s}, t)$$

DTR decomposed as product of strictly positive sub-components:

$$\tau_r(\mathbf{s}, t) = \tau_r^{\text{climatology}}(\mathbf{s}, t) \tau_r^{\text{large}}(\mathbf{s}, t) \tau_r^{\text{local}}(\mathbf{s}, t)$$

Each component is formed as a nonlinear transformation of a term that has equivalent form to a component in the mean temperature model:

$$\tau_r^{\text{climatology}}(\mathbf{s}, t) = \exp(\eta_r^{\text{climatology}}(\mathbf{s}, t))$$

$$\tau_r^{\text{large}}(\mathbf{s}, t) = \exp(\eta_r^{\text{large}}(\mathbf{s}, t))$$

$$\tau_r^{\text{local}}(\mathbf{s}, t) = \lambda(\eta_r^{\text{local}}(\mathbf{s}, t))$$

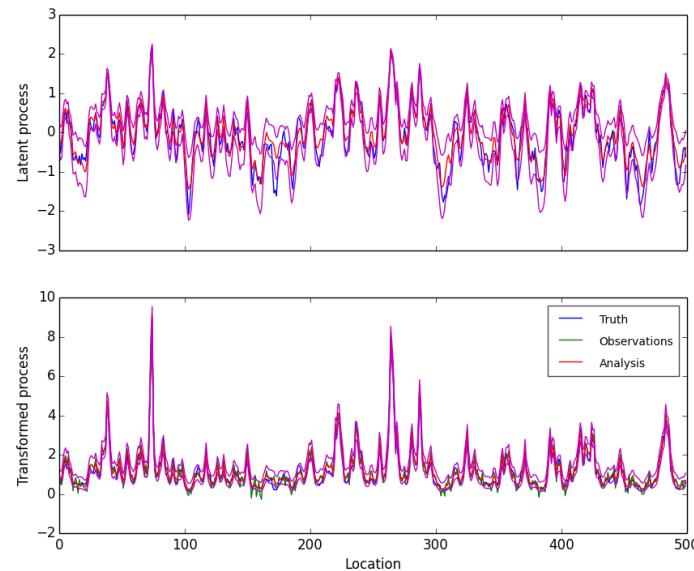
Approximate solution through Taylor expansion of observation equation:

$$\mathbf{y} = \mathbf{f}(\mathbf{u}) + \boldsymbol{\varepsilon}_y$$

$$\begin{aligned}\mathbf{f}(\mathbf{u}) &= \mathbf{f}(\mathbf{u}^*) + \mathbf{J}(\mathbf{u} - \mathbf{u}^*) + \text{H.O.T.} \\ &\approx \mathbf{f}(\mathbf{u}^*) - \mathbf{J}\mathbf{u}^* + \mathbf{J}\mathbf{u}\end{aligned}$$

Can now solve using methods for linear Gaussian model. Iteration is required to refine linearisation set point.

Analysis example (exponential transform)



LINEAR GAUSSIAN MODEL

Parameter estimation:

The prior precision matrix on \mathbf{u} has parameters to be optimised.

Optimise the parameters to maximise conditional marginal log likelihood:

$$\begin{aligned}\log p(\mathbf{y} \mid \boldsymbol{\theta}) &= \log \frac{p(\boldsymbol{\theta}, \mathbf{y})}{p(\boldsymbol{\theta})} \\&= \log \frac{p(\boldsymbol{\theta}, \mathbf{y})p(\mathbf{u} \mid \boldsymbol{\theta}, \mathbf{y})}{p(\boldsymbol{\theta})p(\mathbf{u} \mid \boldsymbol{\theta}, \mathbf{y})} \Big|_{\mathbf{u}=\tilde{\mathbf{u}}} \\&= \log \frac{p(\boldsymbol{\theta}, \mathbf{y}, \mathbf{u})}{p(\boldsymbol{\theta})p(\mathbf{u} \mid \boldsymbol{\theta}, \mathbf{y})} \Big|_{\mathbf{u}=\tilde{\mathbf{u}}} \\&= \log \frac{p(\mathbf{y} \mid \boldsymbol{\theta}, \mathbf{u})p(\mathbf{u} \mid \boldsymbol{\theta})}{p(\mathbf{u} \mid \boldsymbol{\theta}, \mathbf{y})} \Big|_{\mathbf{u}=\tilde{\mathbf{u}}} \\&= -\frac{n}{2} \log(2\pi) + \frac{1}{2} \log \det(\mathbf{Q}_{\mathbf{u}}) + \frac{1}{2} \log \det(\mathbf{Q}_{\boldsymbol{\varepsilon}}) - \frac{1}{2} \log \det(\mathbf{Q}_{\mathbf{u}|\mathbf{y}}) \\&\quad - \frac{1}{2} (\tilde{\mathbf{u}} - \boldsymbol{\mu}_{\mathbf{u}})^T \mathbf{Q}_{\mathbf{u}} (\tilde{\mathbf{u}} - \boldsymbol{\mu}_{\mathbf{u}}) - \frac{1}{2} (\mathbf{y} - \mathbf{J}\tilde{\mathbf{u}})^T \mathbf{Q}_{\boldsymbol{\varepsilon}} (\mathbf{y} - \mathbf{J}\tilde{\mathbf{u}}) \\&\quad + \frac{1}{2} (\tilde{\mathbf{u}} - \boldsymbol{\mu}_{\mathbf{u}|\mathbf{y}})^T \mathbf{Q}_{\mathbf{u}|\mathbf{y}} (\tilde{\mathbf{u}} - \boldsymbol{\mu}_{\mathbf{u}|\mathbf{y}})\end{aligned}$$

Will be optimised on subset of data before running the full analysis.

MODEL COMPONENT:

LARGE-SCALE

General form: A sum of D processes. Each defined as a product of a spatial and temporal process.

$$\tau_m^{\text{large}}(\mathbf{s}, t) = \sum_{d=1}^D f_d^{\text{large}}(\mathbf{s}) g_d^{\text{large}}(t)$$

Spherical harmonic option (linear):

$f_d^{\text{large}}(\mathbf{s})$ Spatial spherical harmonic pattern

$g_d^{\text{large}}(t)$ Temporal smooth process to estimate – SPDE approach.

Factor analysis option (nonlinear): :

$f_d^{\text{large}}(\mathbf{s})$ Spatial smooth process to estimate – SPDE approach.

$g_d^{\text{large}}(t)$ Temporal smooth process to estimate – SPDE approach.

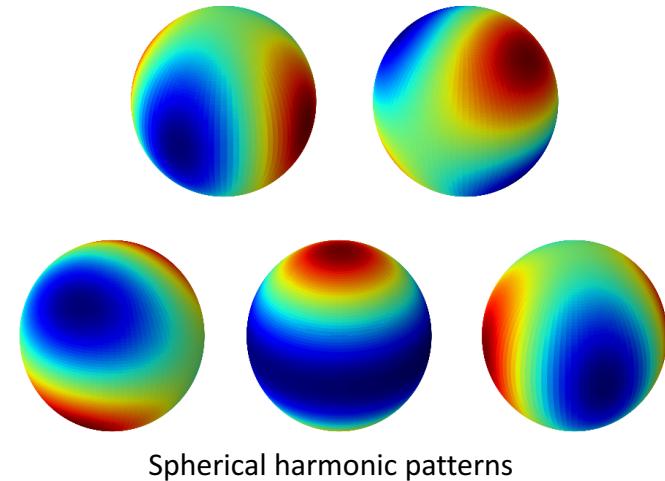
1. SPHERICAL HARMONIC MODEL

The analysis is formed as a weighted sum of spatial spherical harmonics.

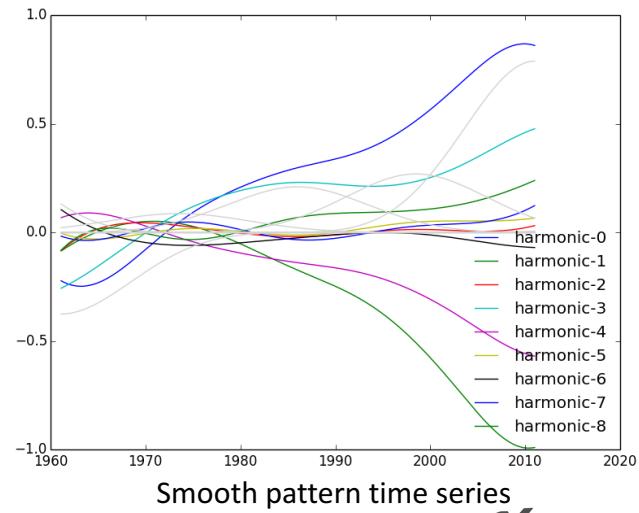
Time series of pattern weights are estimated using the SPDE approach.

A linear model where each basis function is formed as the product of:

- A spherical harmonic spatial pattern.
- A function with local influence in time.



Spherical harmonic patterns



Smooth pattern time series



2. FACTOR ANALYSIS MODEL

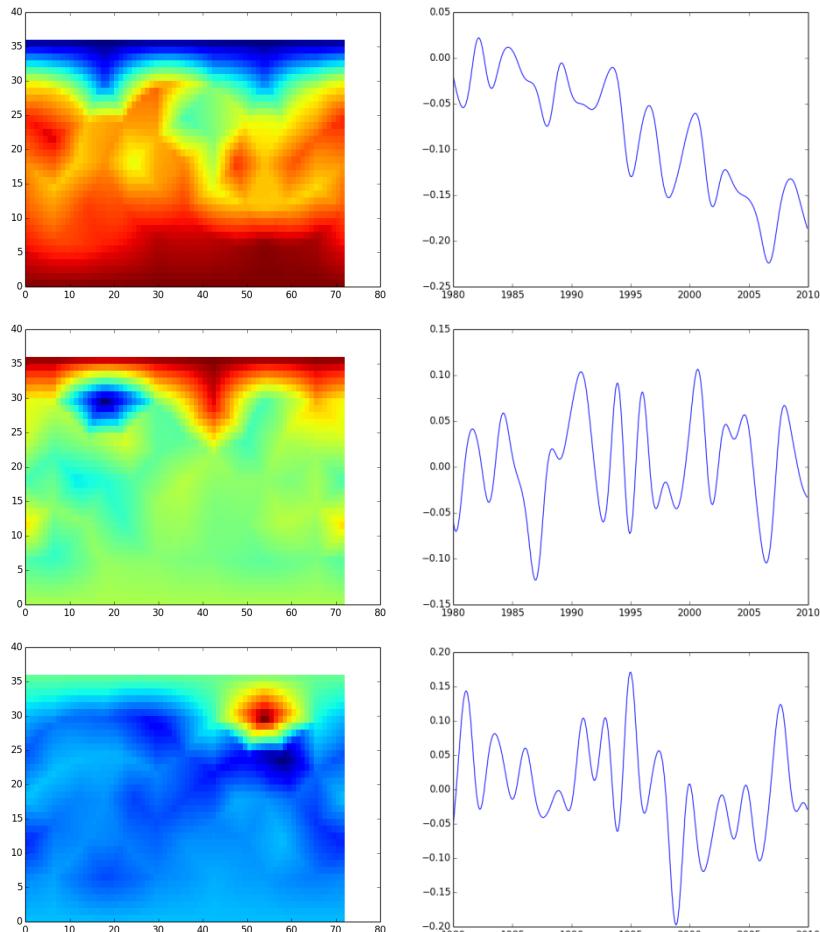
The analysis is formed as a weighted sum of spatial patterns that are now learnt from the data.

Similar to VBPCA but uses SPDEs for both the spatial patterns and time series.

Based on Gaussian Process Factor Analysis (GPFA) (Luttinen & Ilin, 2009). Modified to use SPDEs and include observational errors.

Iterative – flips between estimation of spatial and temporal SPDEs.

Too computationally expensive.



Tests of the prototype SPDE-FA decomposition
applied to global air temperature data
(3 components)

