

SSRF Covariance Models

Covariance

Covariance Models Based on Local Interaction (Spartan) Functionals

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#### Outline





SSRF Covariance Models

**Environmental Applications** 

- Need for flexible positive-definite kernel functions [Genton, 2002]
- Faster interpolation and simulation methods for "big data"

#### Motivation



Groundwater monitoring

sparsely monitored

Groundwater level estimation in

## Response to environmental threats Radioactivity monitoring and emergency warning system [Dubois et al., 2011]





Motivation

# **Applications in Mineral Reserves Estimation**

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#### Coal reserves & quality

Modeling of complex geological structures: Interpolation and simulation



#### Estimated lower calorific value (kcal/kg) — Amyndeo Mine (Western Macedonia)



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#### Fluctuation-Gradient-Curvature (FGC) SSRF

 $f[\phi(\mathbf{s})] = \frac{e^{-\mathcal{H}[\phi(\mathbf{s})]}}{Z}, \ \mathcal{H}[\phi(\mathbf{s})]:$  energy functional,

 $\mathcal{H}_{\rm fgc}[\phi(\mathbf{s})] = \frac{1}{2\eta_0\xi^d} \int_{\mathcal{D}} d\mathbf{s} \left\{ [\phi(\mathbf{s})]^2 + \eta_1 \, \xi^2 \, [\nabla\phi(\mathbf{s})]^2 + \xi^4 \, \left[ \nabla^2 \phi(\mathbf{s}) \right]^2 \right\}$ 

SSRF Covariance Gibbs probability density function (PDF) Models

Local interaction models

 $\eta_0$ : scale,  $\eta_1$ : stiffness,  $\xi$ : characteristic length;  $k_c$ : spectral cutoff

• FGC energy functional - for simplicity assume  $\mathbb{E}[\phi(\mathbf{s})] = 0$ 

• Correlation (covariance) function:  $G(\mathbf{r}) = \mathbb{E} \left[ \phi(\mathbf{s} + \mathbf{r}) \phi(\mathbf{s}) \right]$ 

Properties: Gaussian, zero-mean, stationary, isotropic SRF



# FGC-SSRF Covariance & Spectral Density

#### SSRF Covariance Models

• Covariance:  $G(\mathbf{r}) = \mathbb{E} [\phi(\mathbf{s}) \phi(\mathbf{s} + \mathbf{r})]$ . Fourier transform pair:

$$ilde{G}(\mathbf{k}) = \int d\mathbf{r} \; e^{-\jmath \mathbf{k} \cdot \mathbf{r}} \; G(\mathbf{r}),$$

SSRF Covariance Functions

$$G(\mathbf{r}) = rac{1}{(2 \pi)^d} \int d\mathbf{k} \; e^{\jmath \mathbf{k} \cdot \mathbf{r}} \; ilde{G}(\mathbf{k}).$$

Covariance spectral density:

$$\tilde{G}(k) = \frac{\mathbb{1}_{k_c \ge \kappa}(\kappa) \eta_0 \xi^d}{1 + \eta_1 \kappa^2 \xi^2 + \kappa^4 \xi^4}, \ \kappa = \|\mathbf{k}\|, \ \mathbb{1}_B(\cdot) : \text{indicator function}$$

Permissibility conditions (Bochner's theorem) Hristopulos [2003]:

For any  $k_c$ :  $\eta_0 > 0, \xi > 0, \eta_1 > -2$ 

For finite  $k_c$ :  $\eta_1 < -2$ , if  $k_c \xi < \sqrt{rac{|\eta_1| - \Delta}{2}}$  $\Delta = \sqrt{\eta_1^2 - 4}$ 

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# **Covariance Spectral Density**

**FGC-SSRF** Coefficients



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Functions







## Covariance functions



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#### Spectral Representation of Covariance **Functions**

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#### Spectral Representation (Inverse Hankel transform)

 For isotropic covariance functions the following holds: [Schoenberg, 1938] d/2 . Z 11 11X 1.

$$G(\mathbf{r}) = \frac{\eta_0 \,\xi^d \,\|\mathbf{r}\|}{(2\pi \|\mathbf{r}\|)^{d/2}} \int_0^{\kappa_c} d\kappa \frac{\kappa^{d/2} J_{d/2-1}(\kappa \|\mathbf{r}\|)}{1 + \eta_1(\kappa\xi)^2 + (\kappa\xi)^4}$$

•  $J_{d/2-1}(||\mathbf{r}||)$ : Bessel function of the first kind of order d/2 - 1

• For  $k_c \to \infty$  (limit of infinite UV cutoff) the spectral integral exists for *d* < 3



#### SSRF Covariance function d = 1

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#### Unlimited band, $k_{ m c} ightarrow \infty$ [Hristopulos and Elogne, 2007]

$$\begin{split} G(h) &= \frac{\eta_0}{4} e^{-h\beta_2} \left[ \frac{\cos(h\beta_1)}{\beta_2} + \frac{\sin(h\beta_1)}{\beta_1} \right], \quad |\eta_1| < 2\\ G(h) &= \eta_0 \frac{(1+h)}{4 e^h}, \quad \eta_1 = 2\\ G(h) &= \frac{\eta_0}{2 \Delta} \left( \frac{e^{-h\omega_1}}{\omega_1} - \frac{e^{-h\omega_2}}{\omega_2} \right), \quad \eta_1 > 2 \end{split}$$

#### • $h = |r|/\xi$ : normalized lag

• 
$$\beta_{1,2} = \left(\frac{|2\mp\eta_1|}{4}\right)^{1/2}, \quad \omega_{1,2} = \left(\frac{|\eta_1\mp\Delta|}{2}\right)^{1/2}, \quad \Delta = |\eta_1^2 - 4|^{\frac{1}{2}}$$



#### SSRF Covariance function d = 1

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# SSRF Covariance function d = 2

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#### Unlimited band, $k_{\rm c} \rightarrow \infty$ [Hristopulos, 2013]

$$G(h) = \frac{\eta_0 \Im [K_0(hz_+)]}{\pi \sqrt{4 - \eta_1^2}}, \quad |\eta_1| < 2$$
$$G(h) = \left(\frac{\eta_0 h}{4\pi}\right) K_{-1}(h), \quad \eta_1 = 2$$
$$G(h) = \frac{\eta_0 [K_0(hz_+) - K_0(hz_-)]}{2\pi \sqrt{\eta_1^2 - 4}}, \quad \eta_1 > 2$$

•  $h = \|\mathbf{r}\|/\xi$ , ः Imaginary part

$$z_{\pm} = \sqrt{-t_{\pm}^*}, \quad t_{\pm}^* = \left(-\eta_1 \pm \sqrt{\eta_1^2 - 4}\right)/2$$

•  $K_{\nu}(z)$ : modified Bessel function of the second kind and order  $\nu$ 



#### SSRF Covariance function d = 2







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## SSRF Covariance function d = 3

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Unlimited band,  $k_c \rightarrow \infty$  [Hristopulos and Elogne, 2007]

 $G(h) = \eta_0 \, rac{e^{-heta_2}}{\Delta} \left[ rac{\sin{(heta_1)}}{h} 
ight], \quad |\eta_1| < 2$  $G(h) = rac{\eta_0}{4} e^{-h}, \quad \eta_1 = 2$  $G(h) = rac{1}{2\Delta}\left(rac{e^{-h\omega_1}-e^{-h\omega_2}}{h}
ight), \quad \eta_1 > 2$ 



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#### SSRF Covariance function d = 3







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# FGC-SSRF Realizations d = 1



 $\eta_1 = -1.999$  $\eta_1 = -1$ Five SRF states for n, =-1.999 Five SRF states for n, =-1 State 1 5 0 5 SSRF Covariance C O C Functions Covariance 400 300 300 20

400

500



#### FGC-SSRF Realizations d = 1

SSRF Covariance Models





## FGC-SSRF Length Scales

#### SSRF Covariance Models

FGC-SSRF covariance functions have non-linear dependence of correlation scales on model parameters [*Hristopulos and Žukovič, 2011*]





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### FGC-SSRF Length Scales

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FGC-SSRF covariance functions have non-linear dependence of correlation scales on model parameters [*Hristopulos and Žukovič, 2011*]





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# Karhunen-Loève Expansions of SSRFs

#### SSRF Covariance

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#### Karhunen-Loève Theorem

A second-order φ(s) with continuous covariance covariance G(s, s') can be expanded on a closed and bounded domain D as:

$$\psi(\mathbf{s}) = m_{\mathrm{x}}(\mathbf{s}) + \sum_{m=1}^{\infty} \sqrt{\lambda_m} c_m \psi_m(\mathbf{s}).$$

The convergence is uniform on  $\mathcal{D}$ .

2 The  $\lambda_m$  and  $\psi_m(\mathbf{s})$  are respectively, *eigenvalues and eigenfunctions* of the covariance operator, that satisfy the Fredholm integral equation

$$\int_{\mathcal{D}} d\mathbf{s}' G(\mathbf{s}, \mathbf{s}') \, \psi_m(\mathbf{s}') = \lambda_m \, \psi_m(\mathbf{s}').$$

**③** The *c<sub>m</sub>* are *zero-mean*, *uncorrelated random variables*, i.e,  $\mathbb{E}[c_m] = 0$  and  $\mathbb{E}[c_m c_n] = \delta_{n,m}$ , ∀*n*, *m* ∈ ℕ.



#### Karhunen-Loève Expansions of SSRFs

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Simulations on Square Domain

- Square lattice 100  $\times$  100, Modes used: 100  $\times$  100 wave-vectors
- Pinned boundaries (no fluctuations)
- SSRF eigenvalues

$$\lambda_m = \frac{\eta_0 \xi^2}{1 + \eta_1 \xi^2 \|\mathbf{k}_m\|^2 + \xi^4 \|\mathbf{k}_m\|^4}, \ \mathbf{k}_m = \left(\frac{2\pi n_{m,1}}{L}, \frac{2\pi n_{m,2}}{L}\right)^T$$

SSRF K-L eigenfunctions

0.26

0.24

0.22

0.2

0.18 © 0.16 0.14

$$\psi_m(s_1, s_2) = \frac{1}{L} \sin(k_{m,1} s_1) \sin(k_{m,2} s_2)$$



## Karhunen-Loève Expansions of SSRFs



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# Karhunen-Loève Expansions of SSRFs

SRRF Variance Evolution versus number of ordered eigenvalues



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KL Expansions

Covariance Kernel Fast interpolatio





- η<sub>1</sub>=-1.5

η\_=0

– η<sub>1</sub>=1.5

η,=-15



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# SSRF Inverse Covariance Kernel with Ultraviolet Cutoff

• Spectral integral of  $\tilde{\mathbb{J}}_{\mathcal{S}}(\|\mathbf{k}\|) = (\eta_0 \xi^d)^{-1} \left[1 + \eta_1(\xi \|\mathbf{k}\|)^2 + c_2(\xi \|\mathbf{k}\|)^4\right]$ ,

$$\mathbb{J}_{\mathcal{S}}(\mathbf{r};\boldsymbol{\theta}) = \frac{\|\mathbf{r}\|}{(2\pi\|\mathbf{r}\|)^{d/2}} \int_0^{k_c} d\|\mathbf{k}\| \|\mathbf{k}\|^{d/2} J_{d/2-1}(\|\mathbf{k}\|\|\mathbf{r}\|) \, \tilde{\mathbb{J}}_{\mathcal{S}}(\|\mathbf{k}\|;\boldsymbol{\theta})$$

Lommel functions

$$z^{2} \frac{d^{2}w(z)}{dz^{2}} + z \frac{dw(z)}{dz} + (z^{2} - \nu^{2}) w(z) = z^{\mu+1}$$

 $S_{\mu,\nu}(z) = z^{\mu-1} \left[ 1 - \frac{(\mu-1)^2 - \nu^2}{z^2} + \frac{[(\mu-1)^2 - \nu^2][(\mu-3)^2 - \nu^2]}{z^4} - \dots \right]$ 

• If  $\mu - \nu = 2l + 1$  the following Lommel series terminates after l + 1 terms

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# SSRF Inverse Covariance Kernel with Ultraviolet Cutoff

following tripartite sum, where  $u_c = k_c \xi$ ,  $z = k_c ||\mathbf{r}||$ , and  $\nu = d/2 - 1$ 

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 $\mathbb{J}_{S}(z;\theta) = \sum_{l=0,1,2} \frac{g_{l}(\theta)}{z^{2\nu+2l+1}} \left[ (2\nu+2l)J_{\nu}(z) S_{\nu+2l,\nu-1}(z) - J_{\nu-1}(z) S_{\nu+2l+1,\nu}(z) \right]$ 

In d  $\geq$  2, the SSRF inverse covariance kernel  $\mathbb{J}_{S}(z; \theta)$  is given by means of the

$$g_0(\theta) = \frac{k_c^d}{(2\pi)^{d/2} \eta_0 \, \xi^d}, \ g_1(\theta) = \eta_1 \, u_c^2 \, g_0(\theta), \ g_2(\theta) = u_c^4 \, g_0(\theta),$$

The above equations define a positive semidefinite kernel function for  $\eta_1 > -2$ . In particular, the value at the origin is

$$\mathbb{J}_{\mathcal{S}}(0;\theta) = \frac{g_0(\theta)}{2^{\nu+1}\,\Gamma(\nu+2)} \left[1 + \eta_1\,u_c^2\,\left(\frac{\nu+1}{\nu+2}\right) + u_c^4\,\left(\frac{\nu+1}{\nu+3}\right)\right],$$

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# SSRF Inverse Covariance Kernel with Ultraviolet Cutoff

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# SSRF Inverse Covariance Kernel with Ultraviolet Cutoff





### Fast optimal interpolation

SSRF Covariance Models

#### Theorem

Let  $\mathbf{X}_s = (X_1, ..., X_N)^T$  a vector of measurements at  $\mathbf{s}_n$ , n = 1, ..., N, and  $X_p = X_{N+1}$  the SSRF value at unmeasured location  $\mathbf{s}_{N+1}$ . Assume that the data are samples of the SSRF with the energy functional

$$\mathcal{H}_{ ext{fgc}}[\mathbf{X}_{s;
ho}; oldsymbol{ heta}] = rac{1}{2} \, \mathbf{X}_{s;
ho}^{ au} \, \mathbf{J}(oldsymbol{ heta}) \, \mathbf{X}_{s;
ho} \, \mathbf{J}(oldsymbol{ heta}) \, \mathbf{J}($$

where  $\mathbf{X}_{s;p} = (X_1, \dots, X_N, X_p)^T$ , and  $\mathbf{J}(\theta)$  is the inverse covariance (precision) matrix. The mode estimate  $\hat{X}_p$  which maximizes the joint pdf is given by

$$\hat{X}_{\rho} = -\frac{\mathbf{J}_{\rho;s}^{T}(\boldsymbol{\theta}) \, \mathbf{X}_{s}}{J_{\rho;\rho}(\boldsymbol{\theta})} = -\sum_{i=1}^{N} \frac{J_{\rho,i}(\boldsymbol{\theta}) \, X_{i}}{J_{\rho;\rho}(\boldsymbol{\theta})}.$$
(1)

eferences

Fast interpolation



#### Grid Approximation of Continuum SSRF

On a grid with lattice step  $a \to 0$ :  $\delta(\mathbf{s}_i - \mathbf{s}_j) \to \delta_{i,j} / \mathbf{v}_c, \mathbf{v}_c = a^d$ .

 $\mathbb{J}_{\mathcal{S}}(\mathbf{r}_{\mathbf{n}};\boldsymbol{\theta}) = c_0 \left[ 1 - \eta_1 \left( \sum_{i=1}^d \frac{\xi^2}{a_i^2} \mathrm{D}_{\mathbf{n},i}^2 \right) + \left( \sum_{i=1}^d \sum_{j=1}^d \frac{\xi^4}{a_i^2 a_j^2} \mathrm{D}_{\mathbf{n},i}^2 \mathrm{D}_{\mathbf{n},j}^2 \right) \right] \delta(\mathbf{r}_{\mathbf{n}}).$ 

 $\delta_{\mathbf{n},i}[f(\mathbf{r}_n)] = f\left(\mathbf{r}_n + \frac{a_i}{2}\,\hat{\mathbf{e}}_i\right) - f\left(\mathbf{r}_n - \frac{a_i}{2}\,\hat{\mathbf{e}}_i\right), \ i = 1, \dots, d.$ 

 $\delta_{\mathbf{n}}^{2}[f(\mathbf{r}_{n})] = f(\mathbf{r}_{n} + a_{i} \hat{\mathbf{e}}_{i}) + f(\mathbf{r}_{n} - a_{i} \hat{\mathbf{e}}_{i}) - 2f(\mathbf{r}_{n}).$ 

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### Inverse SSRF Covariance Kernel on Hypercubic Grid

SSRE Covariance Models

$$\mathbb{J}(\mathbf{r_n}; \boldsymbol{\theta}) = c_0 \left[ \delta_{\mathbf{n}, \mathbf{0}} - \eta_1 \, \xi^2 \, S(\mathbf{r_n}) + \xi^4 \, C(\mathbf{r_n}) \right]$$

where the square gradient,  $S(\mathbf{r}_n)$ , and square curvature,  $C(\mathbf{r}_n)$ , are given by

$$S(\mathbf{r_n}) = \sum_{i=1}^{d} D_{\mathbf{n},i}^2, \quad C(\mathbf{r_n}) = \sum_{i=1}^{d} D_{\mathbf{n},i}^4 + \sum_{i=1}^{d} \sum_{j=1}^{d} D_{\mathbf{n},i}^2 D_{\mathbf{n},j}^2,$$

Truncating  $S(\mathbf{r_n})$  and  $C(\mathbf{r_n})$  at order 2p = 12, it follows that

$$S^{(12)}(\mathbf{r_n}) = \sum_{i=1}^d \delta_{\mathbf{n},i}^2 - \frac{\delta_{\mathbf{n},i}^4}{12} + \frac{\delta_{\mathbf{n},i}^6}{90} - \frac{\delta_{\mathbf{n},i}^8}{560} + \frac{\delta_{\mathbf{n},i}^{10}}{3150} - \frac{\delta_{\mathbf{n},i}^{12}}{16632},$$

$$C^{(12)}(\mathbf{r_n}) = \sum_{i=1}^{d} \left( \delta_{\mathbf{n},i}^4 - \frac{\delta_{\mathbf{n},i}^6}{6} + \frac{7 \, \delta_{\mathbf{n},i}^8}{240} - \frac{41 \, \delta_{\mathbf{n},i}^{10}}{7560} + \frac{479 \, \delta_{\mathbf{n},i}^{12}}{453600} \right) + \sum_{i=1}^{d} \sum_{j=1}^{d} \left( \delta_{\mathbf{n},i}^2 \delta_{\mathbf{n},j}^2 - \frac{\delta_{\mathbf{n},i}^2 \, \delta_{\mathbf{n},j}^4}{6} + \frac{\delta_{\mathbf{n},i}^2 \, \delta_{\mathbf{n},j}^{10}}{45} - \frac{\delta_{\mathbf{n},i}^2 \, \delta_{\mathbf{n},j}^8}{1575} + \frac{\delta_{\mathbf{n},i}^4 \, \delta_{\mathbf{n},j}^4}{144} - \frac{\delta_{\mathbf{n},i}^4 \, \delta_{\mathbf{n},j}^6}{540} + \frac{\delta_{\mathbf{n},i}^4 \, \delta_{\mathbf{n},j}^8}{3360} + \frac{\delta_{\mathbf{n},i}^6 \, \delta_{\mathbf{n},j}^6}{8100} \right).$$

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Inverse SSRF	Covariance	Kernel	on
Hypercubic Gr	id		

Table: Central finite differences of orders  $2k, k = 1, \dots, 6$  on hypercubic grid with uniform step a = 1 in each orthogonal direction i = 1, ..., d. FD stands for *finite difference*. The  $f_n$ denotes any lattice function.

FD	Expressions
$\delta^2_{\mathbf{n},i} f_{\mathbf{n}} =$	$f_{\mathbf{n}+\hat{\mathbf{e}}_j} + f_{\mathbf{n}-\hat{\mathbf{e}}_j} - 2f_{\mathbf{n}}$
$\delta_{\mathbf{n},i}^{4} f_{\mathbf{n}} =$	$f_{\mathbf{n}+2\hat{\mathbf{e}}_j} + f_{\mathbf{n}-2\hat{\mathbf{e}}_j} - 4f_{\mathbf{n}+\hat{\mathbf{e}}_j} - 4f_{\mathbf{n}-\hat{\mathbf{e}}_j} + 6f_{\mathbf{n}}$
$\delta_{\mathbf{n},i}^{6} \mathbf{f}_{\mathbf{n}} =$	$f_{n+3\hat{e}_{j}} + f_{n-3\hat{e}_{j}} - 6f_{n+2\hat{e}_{j}} - 6f_{n-2\hat{e}_{j}} + 15f_{n+\hat{e}_{j}} + 15f_{n-\hat{e}_{j}} - 20f_{n-2\hat{e}_{j}}$
$\delta_{\mathbf{n},i}^{8} f_{\mathbf{n}} =$	$f_{n+4\hat{e}_{j}} + f_{n-4\hat{e}_{j}} - 8f_{n+3\hat{e}_{j}} - 8f_{n-3\hat{e}_{j}} + 28f_{n+2\hat{e}_{j}} + 28f_{n-2\hat{e}_{j}} - 56f_{n+\hat{e}_{j}}$
	$-56f_{\mathbf{n}-\hat{\mathbf{e}}_{i}}+70f_{\mathbf{n}}$
$\delta_{\mathbf{n},i}^{10} f_{\mathbf{n}} =$	$f_{n_i+5,n_j} + f_{n_j-5,n_j} - 10f_{n+4\hat{e}_j} - 10f_{n-4\hat{e}_j} + 45f_{n+3\hat{e}_j} + 45f_{n-3\hat{e}_j} - 120f_{n+2\hat{e}_j}$
	$-120f_{n-2\hat{e}_{i}}+210f_{n+\hat{e}_{i}}+210f_{n-\hat{e}_{i}}-252f_{n}$
$\delta_{\mathbf{n},i}^{12} f_{\mathbf{n}} =$	$f_{n_i+6,n_j} + f_{n_i-6,n_j} - 12f_{n_i+5,n_j} - 12f_{n_i-5,n_j} + 66f_{\mathbf{n}+4\hat{\mathbf{e}}_i} + 66f_{\mathbf{n}-4\hat{\mathbf{e}}_i} - 220f_{\mathbf{n}+3\hat{\mathbf{e}}_i}$
	$-220f_{n-3\hat{\mathbf{e}}_{j}} + 495f_{n+2\hat{\mathbf{e}}_{j}} + 495f_{n-2\hat{\mathbf{e}}_{j}} - 792f_{n+\hat{\mathbf{e}}_{j}} - 792f_{n-\hat{\mathbf{e}}_{j}} + 924f_{n}$



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#### Inverse SSRF Covariance Kernel on Hypercubic Grid







### **Conclusions and Future Directions**

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Conclusions

References

- We presented three-parameter, positive-definite, isotropic covariance models based on local interaction "energy" (Spartan) functionals
- SSRF models lead to fast (linear complexity) interpolation on regular grids and on unstructured grids as well [Hristopulos and Elogne, 2009]
- A new family of four-parameter, positive-definite kernels valid in *d* ≥ 2 based on Lommel functions is proposed
- Continuing research involves extensions to: spatial non-homogeneity, space-time correlations, and non-Gaussian dependence



#### Thank you for your attention!

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Ευρωπαϊκή Ένωση

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ΕΠΙΧΕΙΡΗΣΙΑΚΟ ΠΡΟΓΡΑΜΜΑ

ΕΚΠΑΙΔΕΥΣΗ ΚΑΙ ΔΙΑ ΒΙΟΥ ΜΑΘΗΣΗ επέγδυση στην μοιγωνία, της γγώσης

ΥΠΟΥΡΓΕΊΟ ΠΑΙΔΕΊΑΣ & ΟΡΗΣΚΕΥΜΑΤΩΝ, ΠΟΛΙΤΙΣΜΟΥ & ΑΘΛΗΤΙΣΜΟΥ ΕΙΔΙΚΗ ΥΠΗΡΕΣΙΑ ΔΙΑΧΕΙΡΙΣΗΣ

Με τη συνγοηματοδότηση της Ελλάδας και της Ευρωπαϊκής Ένωση

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