

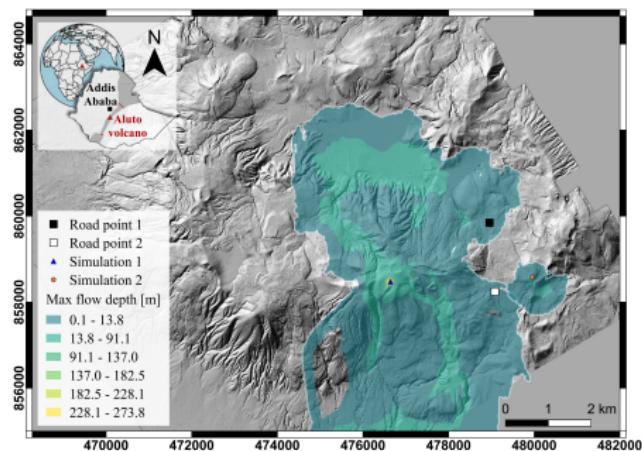
Two recent advance in UQ with Gaussian process models: the zGP and the PPLE

Elaine Spiller, Marquette University

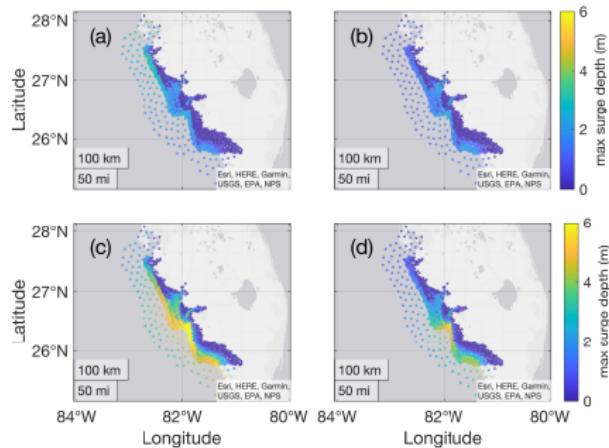
November 30, 2023

The zero problem for geophysical flows

Volcanoes:
pyroclastic density currents



Hurricanes:
storm surge



High-dimensional multi-physics systems

According to a US DOE report (Brown *et al*, 2008):

The issue of coupling models of different events at different scales and governed by different physical laws is largely wide open and represents an enormously challenging area for future research.

Another DOE report details the computational challenges of a host of multi-physics models (Keyes *et al*, 2013), including:

Fluid-structure problems, subsurface hydrology, fission reactor operation, ultra-fast DNA sequencing, fusion, climate modeling, and geo-dynamics

Process/physical models: systems of ODEs or PDEs

$$\frac{du}{dt} = h(t, u(t), \text{parameters})$$

u – state of the system
 $u(0) = u_o$ – initial conditions, IC
parameters $\in \mathbb{R}^N$
boundary conditions, BC

For UQ, we'd like the mapping

$$f : \text{IC, BC, parameters} \longrightarrow u \text{ or } F(u)$$

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Computer model : inputs \longrightarrow outputs

GP emulators – statistical surrogate

Our quantity of interest:

$$E[Y] = \int f(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} \quad \text{where } Y = f(\mathbf{X}) \text{ and } \mathbf{X} \sim p$$

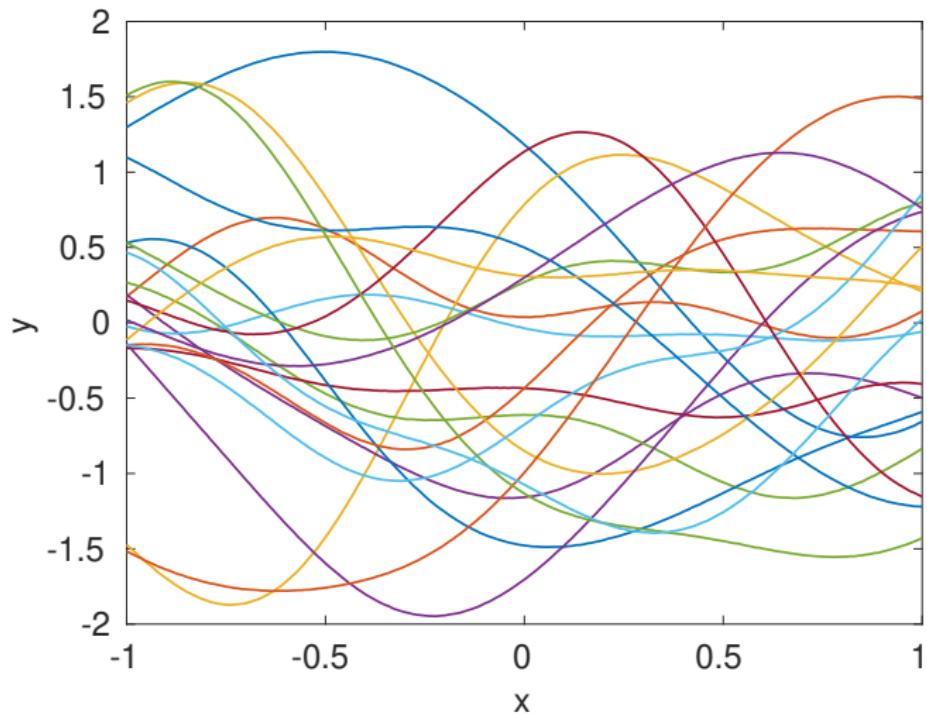
Goal: We want to **predict**, with **uncertainty**, simulator output $f(\cdot)$ at untested inputs.

Strategy: View computer model output as a single realization of a random process – Gaussian Process (GP)

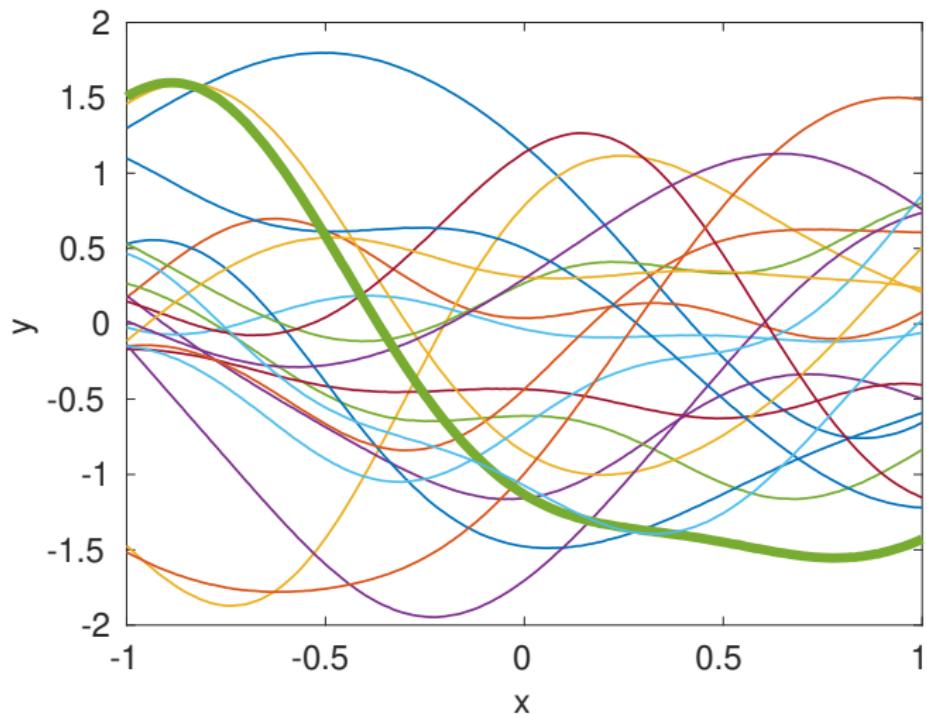
(Sacks, Welch, Mitchell, Wynn (1989); Sacks, Schiller, Welch (1989); Welch *et al* (1992))

(Santner, Williams, Notz (2018); Gramacy (2020))

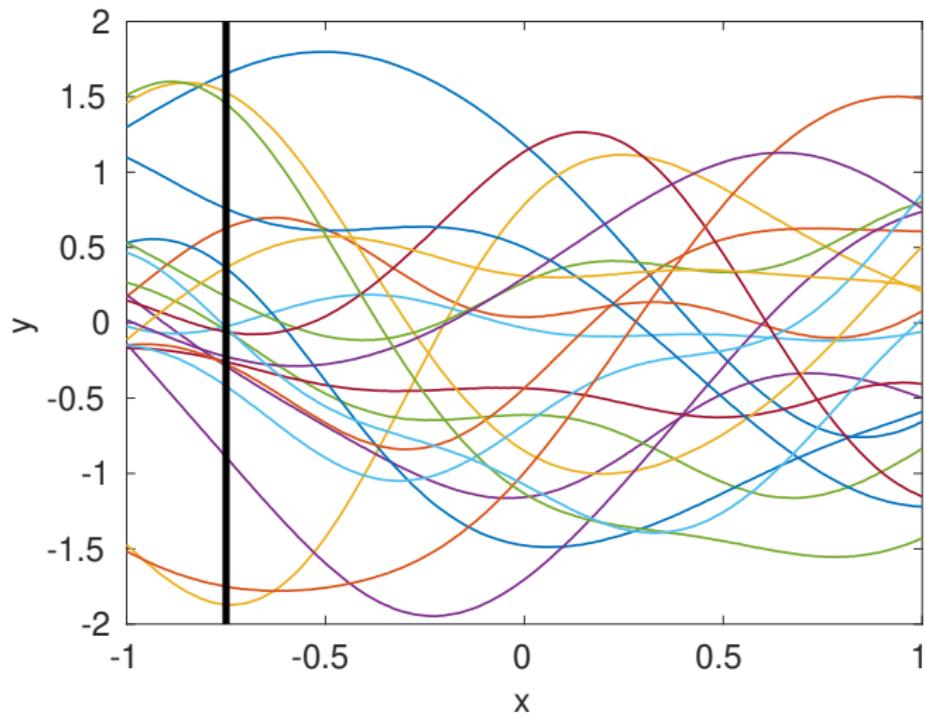
Random functions



Random functions



Random functions

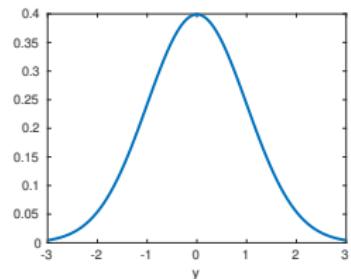


Random functions

Assume computer model is a realization of a random function

$$y(\mathbf{x}) = \mu + Z(\mathbf{x})$$

where



$$E[Z(\mathbf{x})] = 0$$

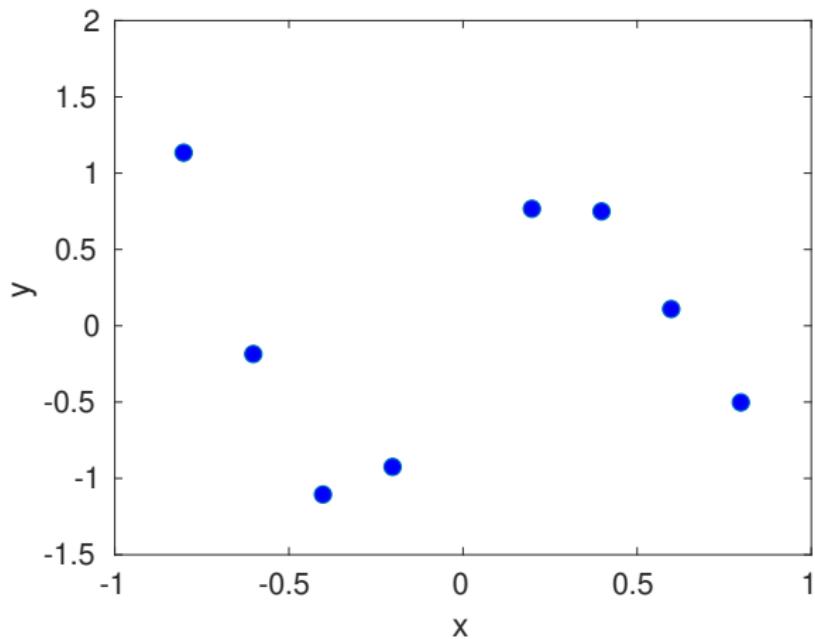
$$\text{Var}[Z(\mathbf{x})] = \sigma^2$$

$$Z(\mathbf{x}) \sim N(0, \sigma^2)$$

$$\text{Corr}(Z(\mathbf{x}), Z(\mathbf{x}')) = \prod_{i=1}^d c(x_i, {x'_i}; \gamma_i)$$

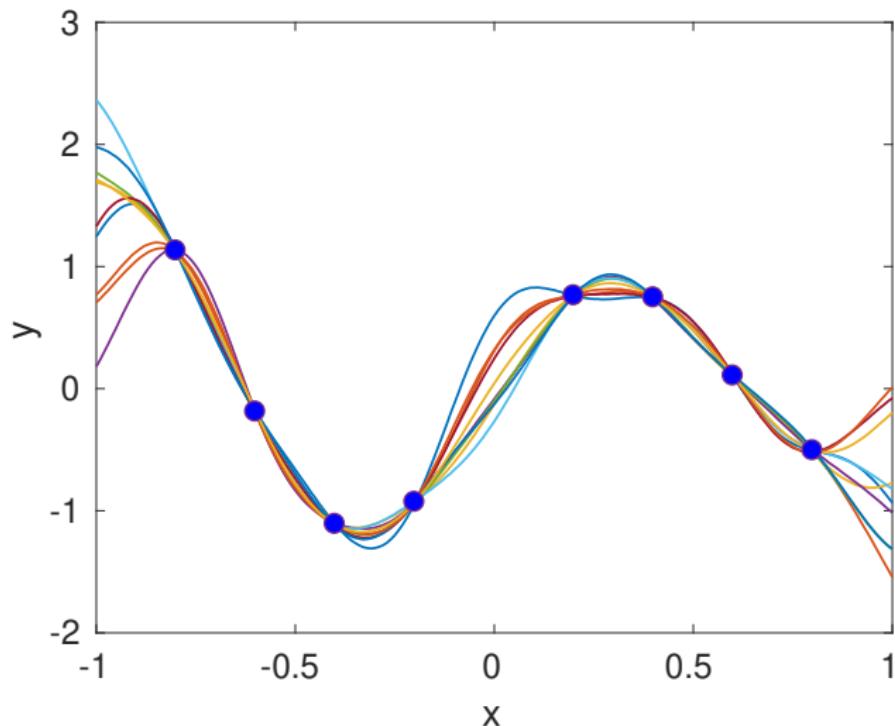
For m design points, correlation matrix $\boldsymbol{\Sigma} = \sigma^2 \mathbf{R}$

Computer model runs



Only consider GP to go through simulator runs

Conditional GPs



Fitting a GP

- Have simulator runs $\mathbf{y}^M = f(\mathbf{x})$ at $\mathbf{x} \in \mathcal{D}$

Vector of responses follows multivariate normal

$$\mathbf{y}^M \sim MVN(\mu(\mathbf{x}), \boldsymbol{\Sigma})$$

- Need to estimate μ, σ^2, γ
- MLE, or MAP w/reference prior

$$L(\mu, \sigma^2, \gamma \mid \mathbf{y}^M) = \frac{1}{|2\pi\boldsymbol{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\mathbf{y}^M - \mu)^T \boldsymbol{\Sigma}^{-1} (\mathbf{y}^M - \mu)}$$

(Gu, Wang, Berger (2018); Gu, Palomo, Berger (2019))

GP fit, plug-in estimates

W/estimates of μ , σ^2 , γ , consider an untested input, \mathbf{x}^*

GP predictive mean:

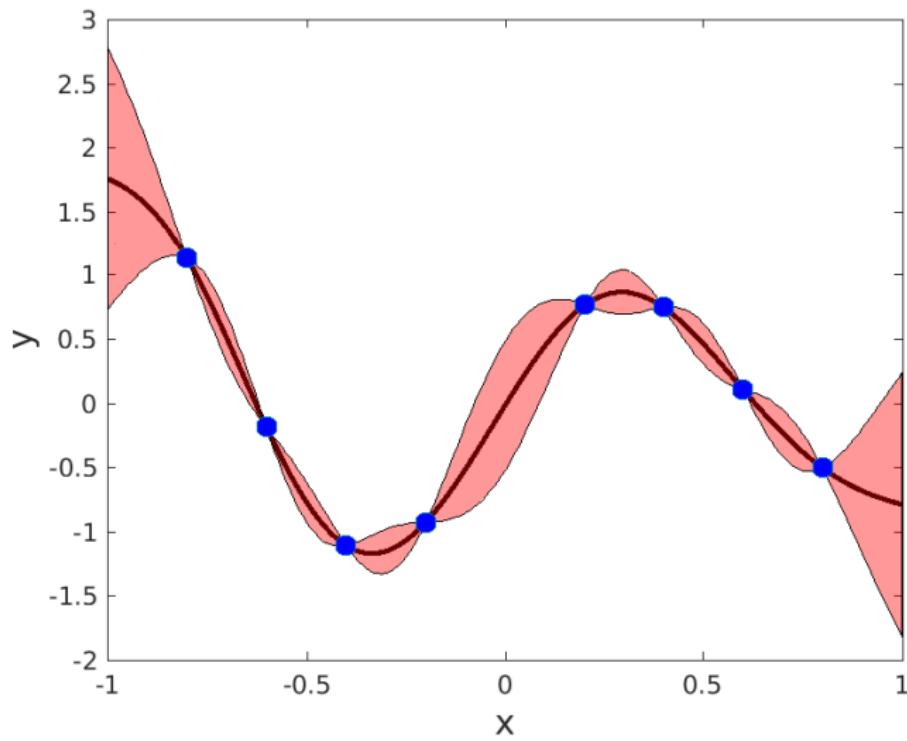
$$\hat{y}(\mathbf{x}^*) = \mu + \mathbf{r}^T \mathbf{R}^{-1} (\mathbf{y}^M - \mu)$$

GP standard error:

$$s^2(\mathbf{x}^*) = \sigma^2 \left(1 - \mathbf{r}^T \mathbf{R}^{-1} \mathbf{r} + \frac{(1 - \mathbf{1}^T \mathbf{R}^{-1} \mathbf{r})^2}{\mathbf{1}^T \mathbf{R}^{-1} \mathbf{1}} \right)$$

\mathbf{r} is an m -vector of correlations between \mathbf{x}^* and each of the m design points.

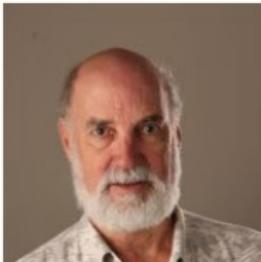
Predictive emulator with uncertainty



Part I

Zero-censored Gaussian Process (zGP) w/
Robert Wolpert, Pablo Tierz & Taylor Asher

With a little help from...

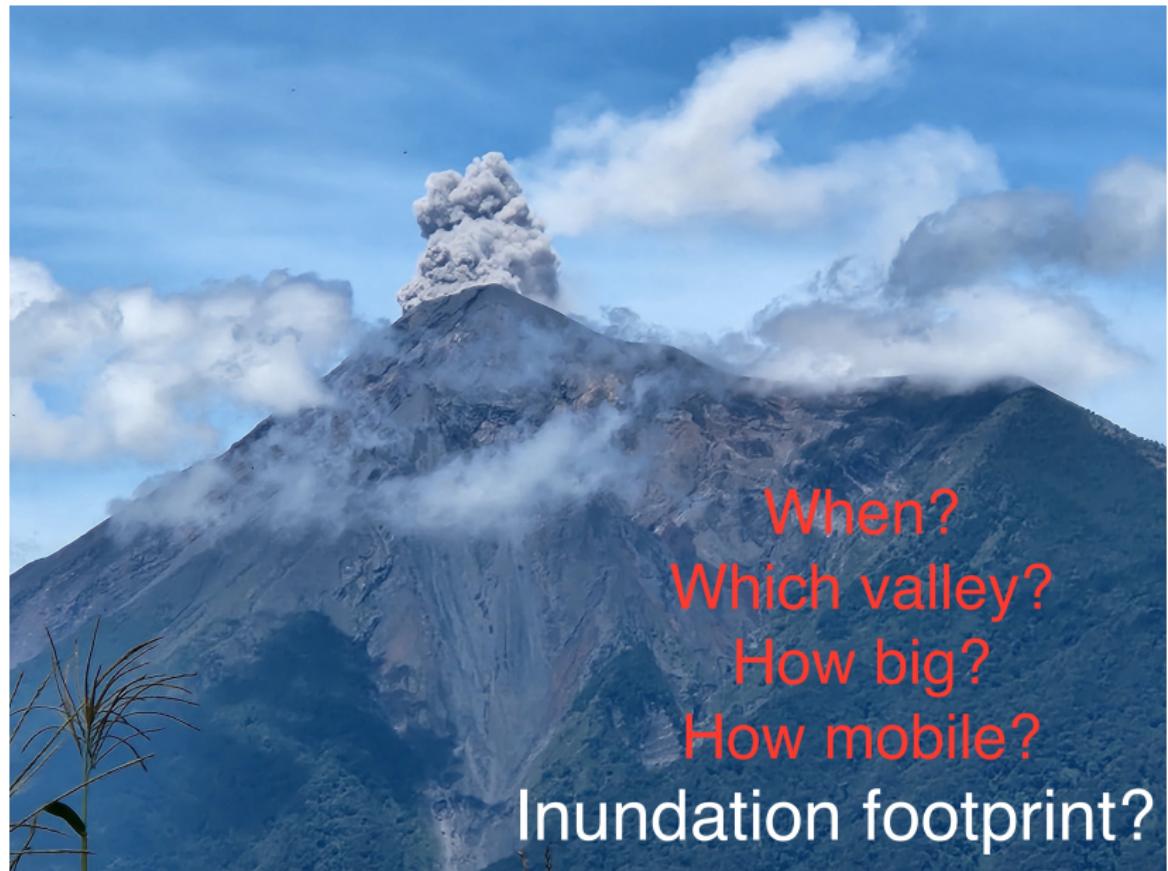


Mount Pelée, Martinique – 30,000 fatalities

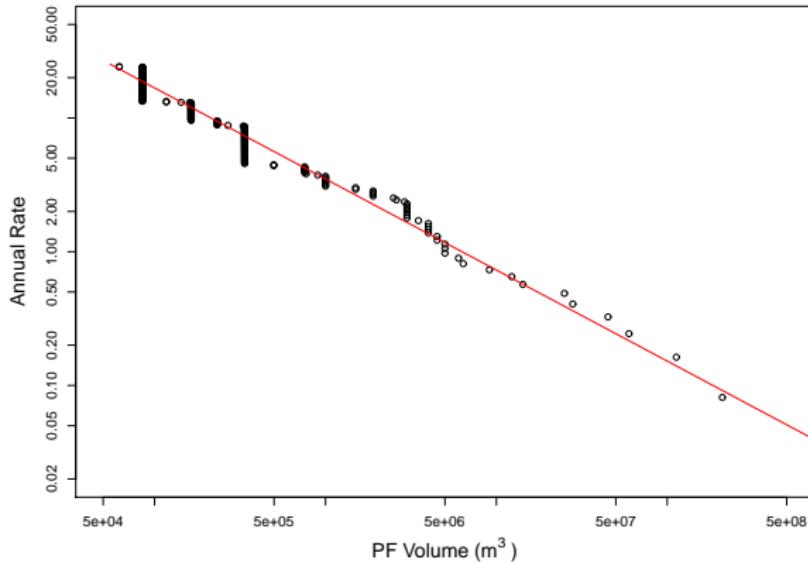
“One hundred years ago, government officials in Martinique made the mistake of assuming that, despite signs to the contrary, Mount Pelée would behave in 1902 as it had in 1851 – when a rain of ash from what they considered a benign volcano surprised, but did not harm those living under its shadow.” (Cristina Reed, *Geotimes* 2002)



Volcán de Fuego



Volcanic flows at Montserrat



$$p(V | \alpha_V) = \frac{\alpha_V}{\epsilon} \left(\frac{V}{\epsilon} \right)^{-(\alpha_V + 1)} \mathbf{1}_{V > \epsilon}$$

Rare Events

Pareto model is much more likely to observe future volumes that far exceed those in the recent history...

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non-heavy tailed:

$$P(V_{11} > 10 \max(v_1, \dots, v_{10})) = 1/200,000$$

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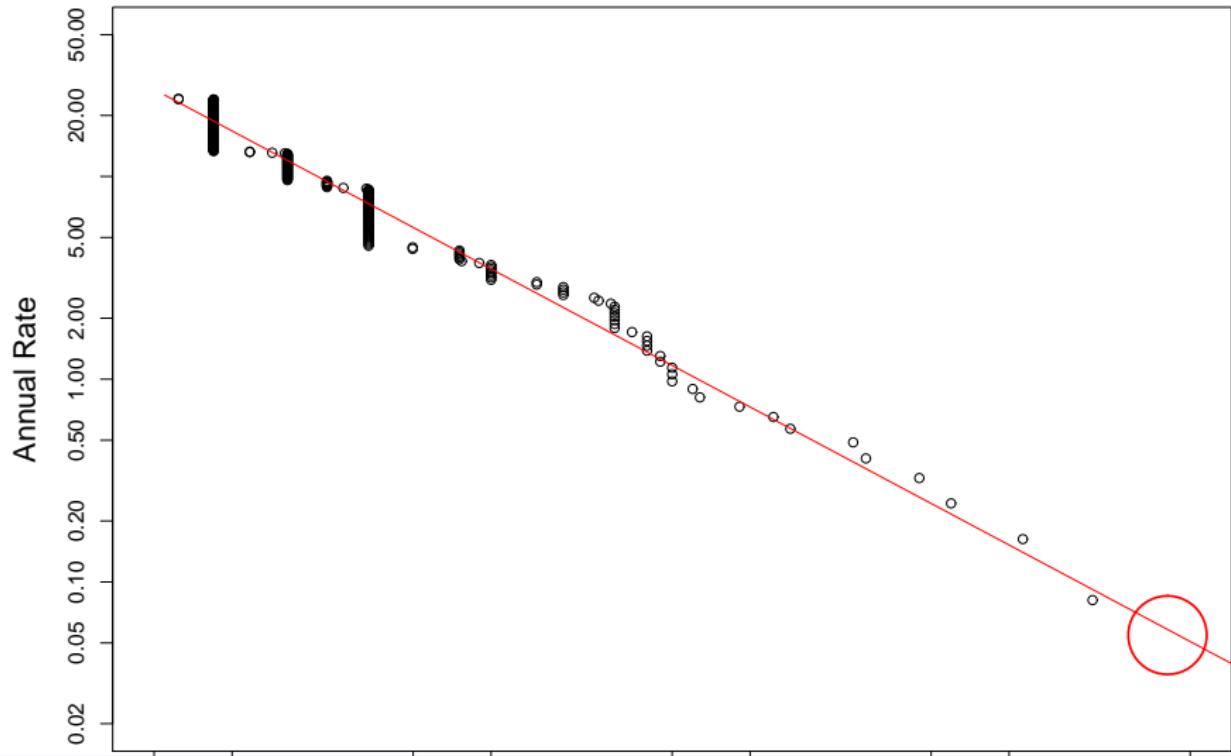
non-heavy tailed:

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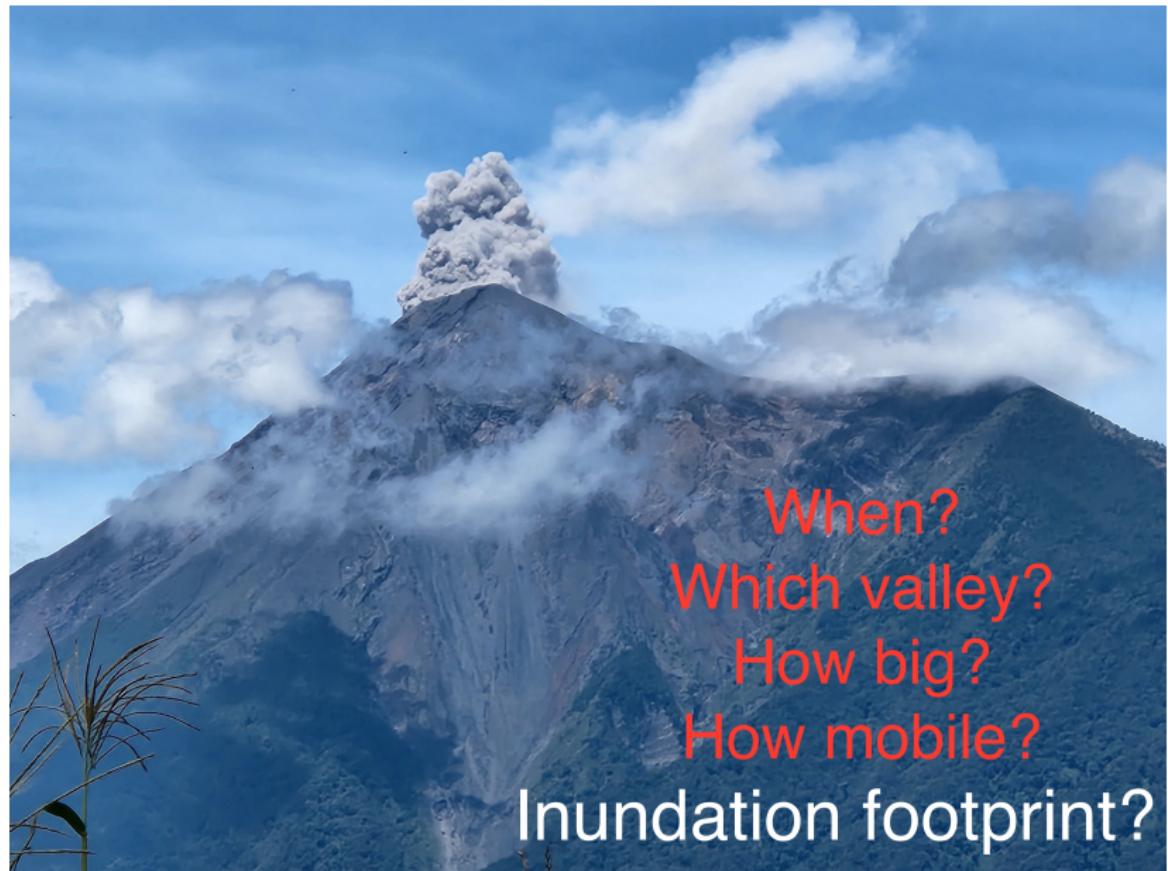
heavy tailed:

$$P(V_{11} > 10 \max(v_1, \dots, v_{10})) = 1/100$$

What happens at larger-than-recorded volumes?



Volcán de Fuego



When?
Which valley?
How big?
How mobile?
Inundation footprint?

Physical model of flow mass

Assume: flow layer thin relative to lateral extension

continuity

$$\frac{\partial h}{\partial t} + \frac{\partial hu_x}{\partial x} + \frac{\partial hu_y}{\partial y} = e_s$$

x momentum

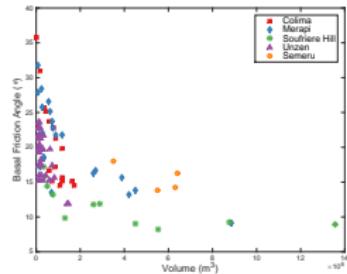
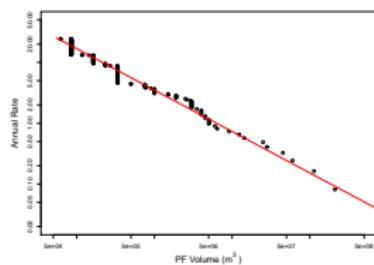
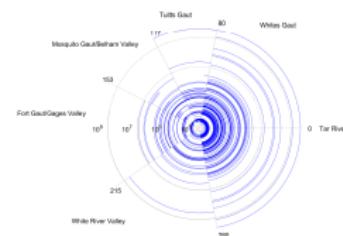
$$\frac{\partial hu_x}{\partial t} + \frac{\partial (hu_x^2 + k_{ap}g_z h^2/2)}{\partial x} + \frac{\partial hu_y u_x}{\partial y} =$$

$$g_x h + u_x e_s - \frac{u_x}{\sqrt{u_x^2 + u_y^2}} \left(g_z + \frac{u_x^2}{\kappa_x} \right) h \tan(\phi_{bed}) - \text{sgn}(\partial u_x y) h k_{ap} \frac{\partial h g_z}{\partial y} \sin(\phi_{int})$$

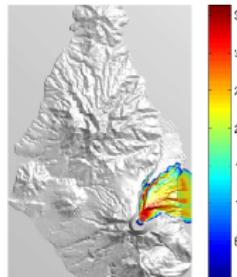
- ① Gravitational driving force
- ② Coulomb friction at the base – ϕ_{bed}
- ③ Intergranular Coulomb force – ϕ_{int}
due to velocity gradients normal to flow direction

(see Savage; Bursik; Pitman)

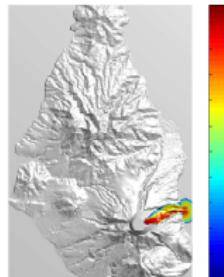
Data + physical models



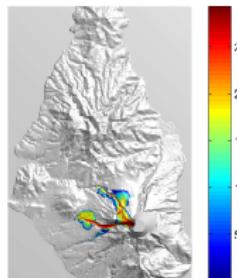
$\log V = 6.3751$, Orientation = 60°



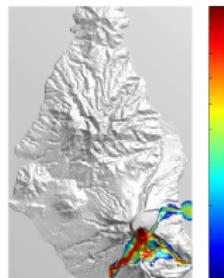
$\log V = 5.5779$, Orientation = 16°



$\log V = 6.0987$, Orientation = 166°



$\log V = 6.6456$, Orientation = 286°

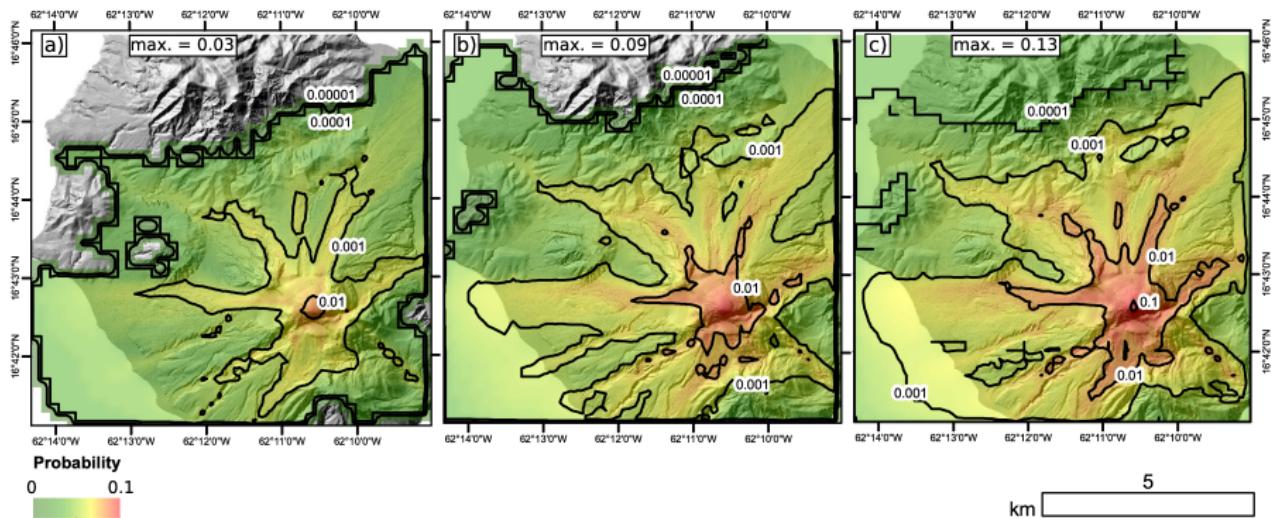


Montserrat: PDC probabilistic hazard forecast maps

Left: $t = 1$ year,

Middle $t = 5$ years,

Right: $t = 20$ years



(S, Wolpert, Ogburn, et al 2020)

What we'd like to do: hazard assessment inundation probabilities:

$$\Pr[h \geq h_{\text{crit}}] = \int \mathbf{1}_{h(x) \geq h_{\text{crit}}} \underbrace{p(x \mid \theta)}_{\text{aleatory}} \underbrace{\pi(\theta)}_{\text{epistemic}} d\theta dx$$

inundation as function of one parameter (e.g. volume):

$$h(x_i) \quad x_i = \text{input of interest , } \quad x^{-i} \text{ other inputs}$$

$$h(x_i) = \int h(x) p(x^{-i} \mid \theta) \pi(\theta) d\theta dx^{-i}$$

Monte Carlo is not feasible as each evaluation of $h(\cdot)$ is 1-10 hours.

How we can do what we'd like to do

inundation probabilities:

$$\Pr[h \geq h_{\text{crit}}] \approx \int \mathbf{1}_{\hat{h}(x) \geq h_{\text{crit}}} \underbrace{p(x \mid \theta)}_{\text{aleatory}} \underbrace{\pi(\theta)}_{\text{epistemic}} d\theta dx$$

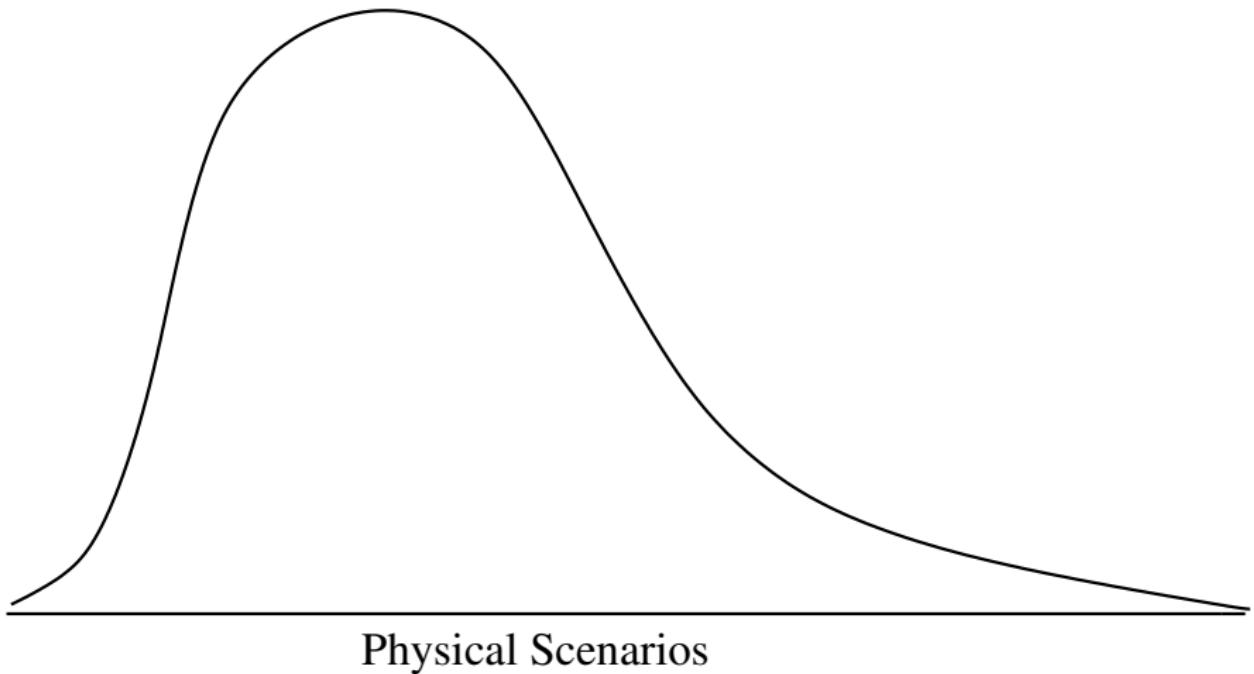
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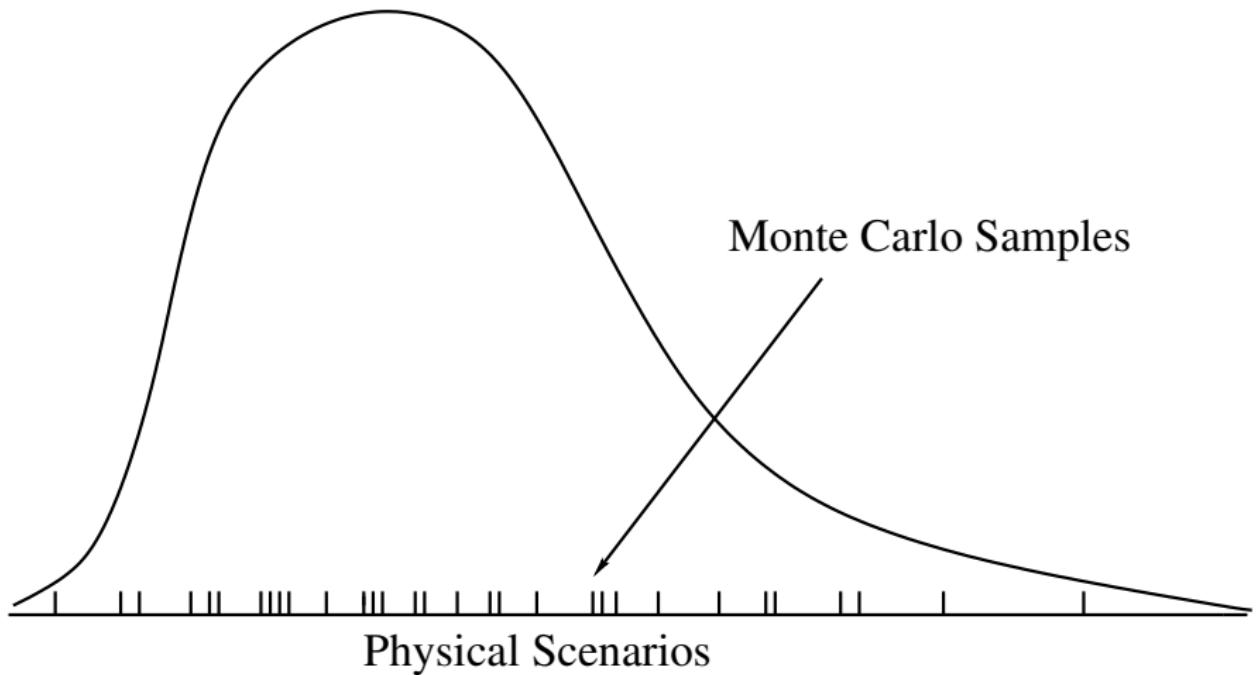
$$h(x_i) \approx \int \hat{h}(x) p(x^{-i} \mid \theta) \pi(\theta) d\theta dx^{-i}$$

Key: \hat{h} is a cheap approximation of h

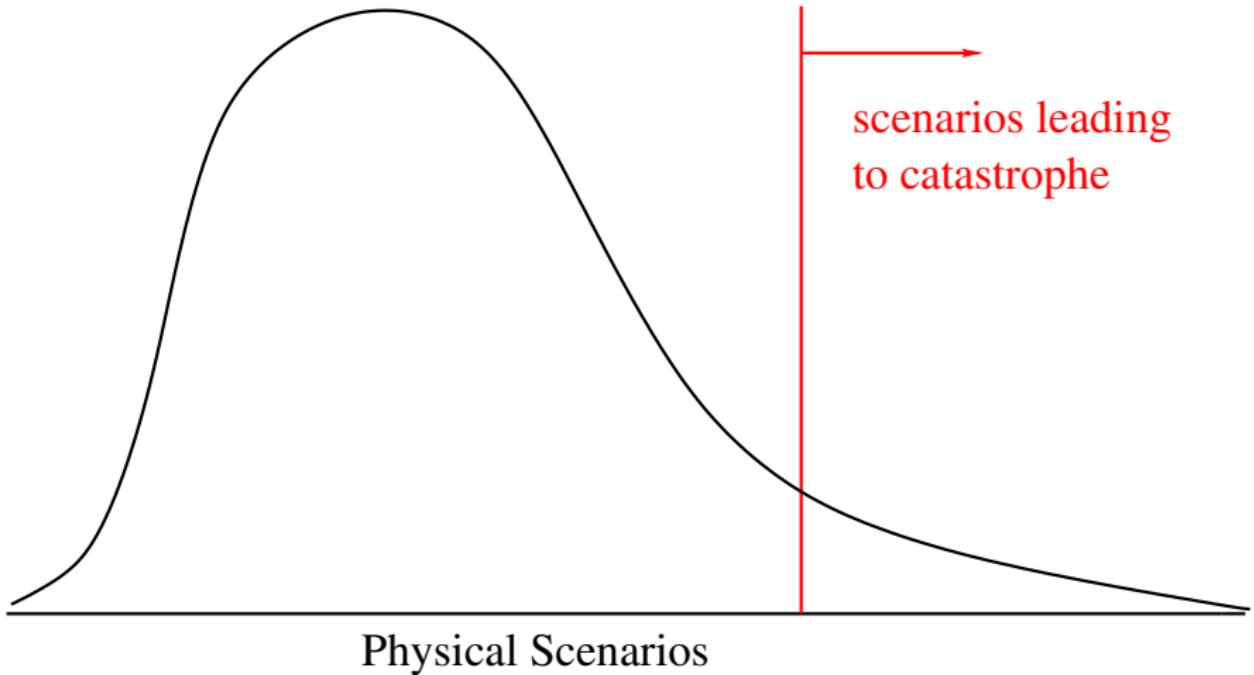
Cartoon $p(\text{physical scenario})$



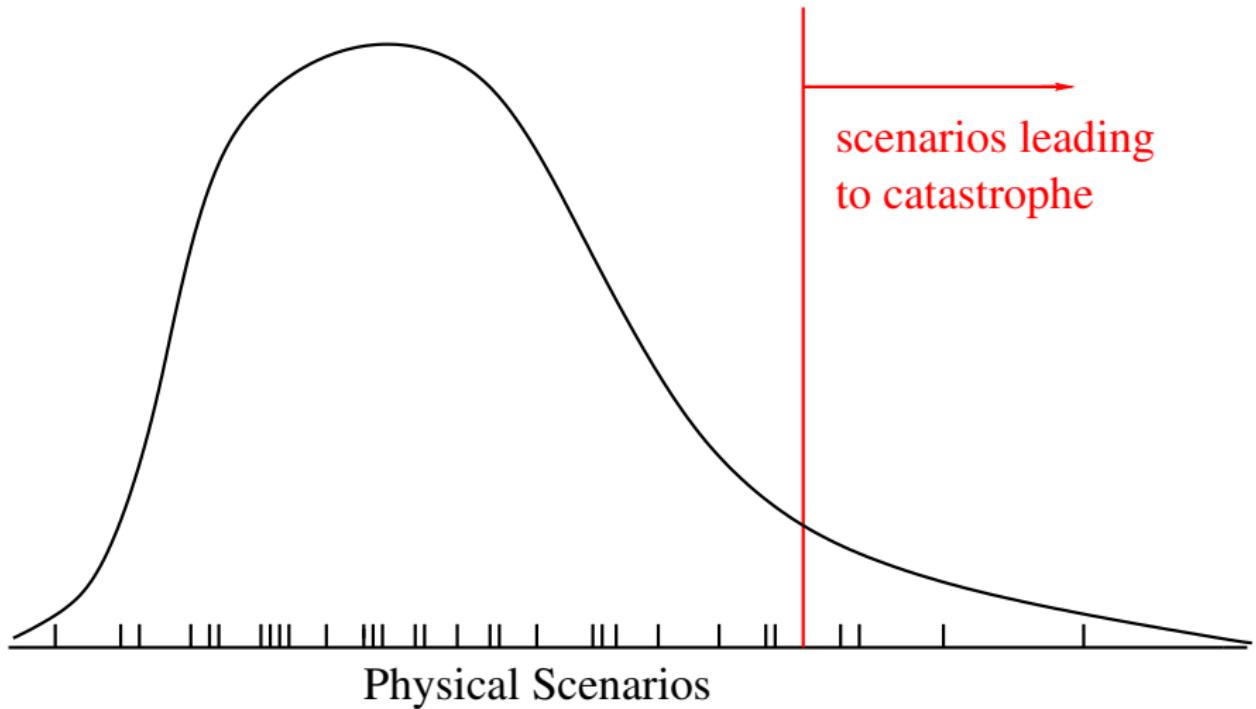
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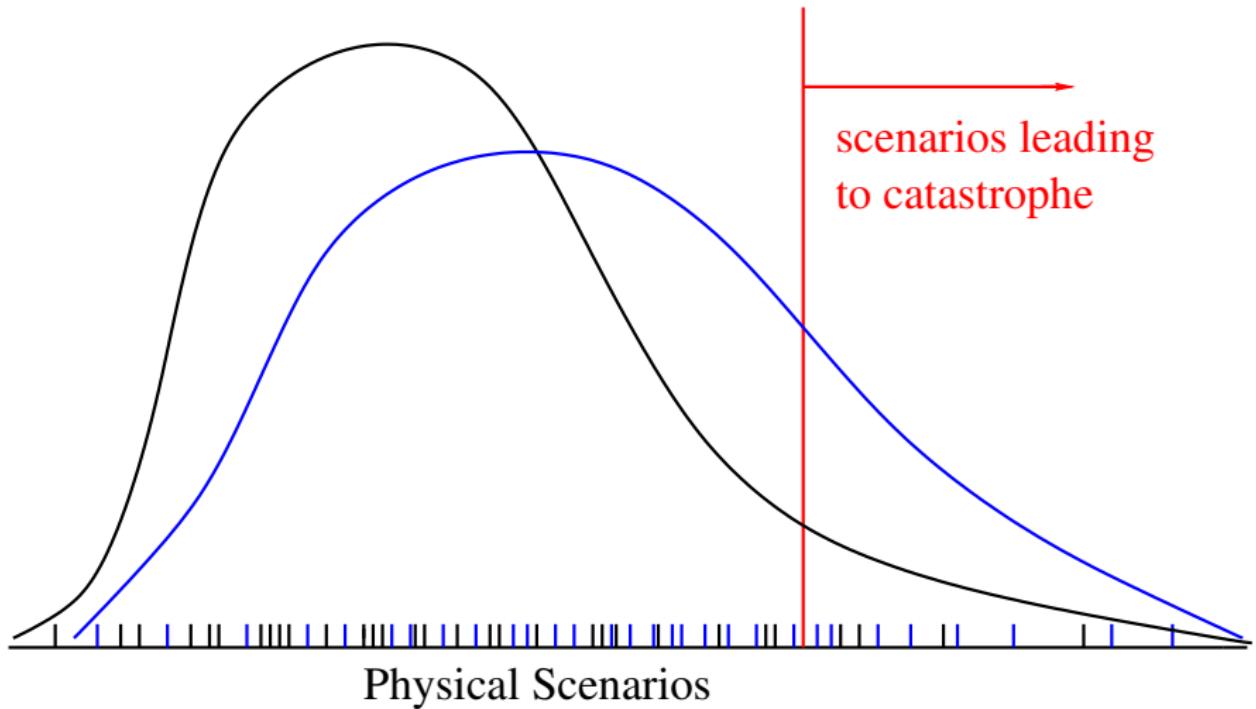
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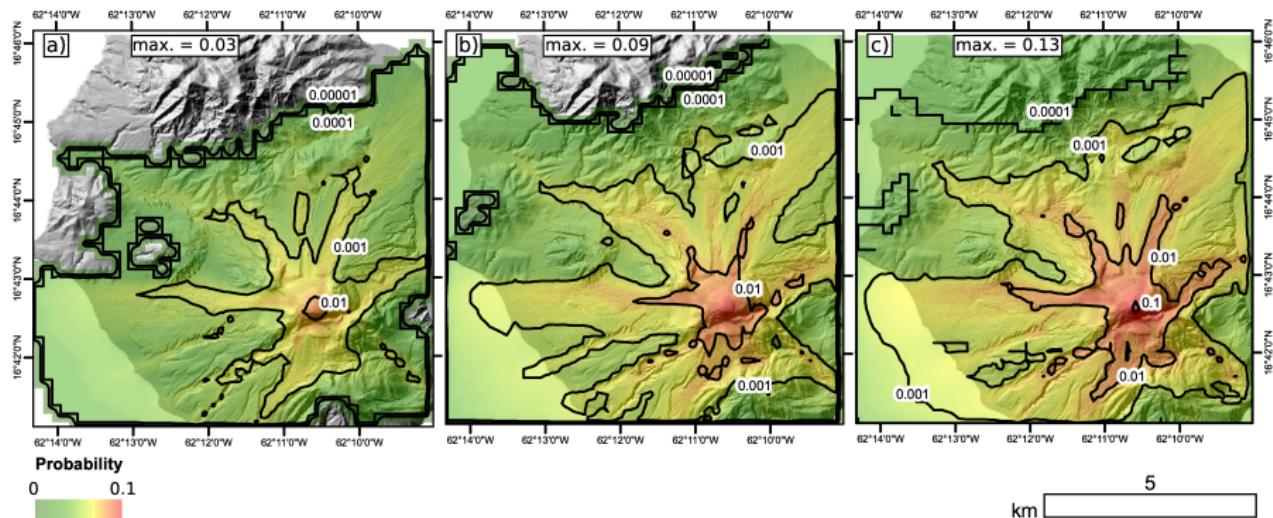


PDC probabilistic hazard forecast maps

Left: $t = 1$ year,

Middle $t = 5$ years,

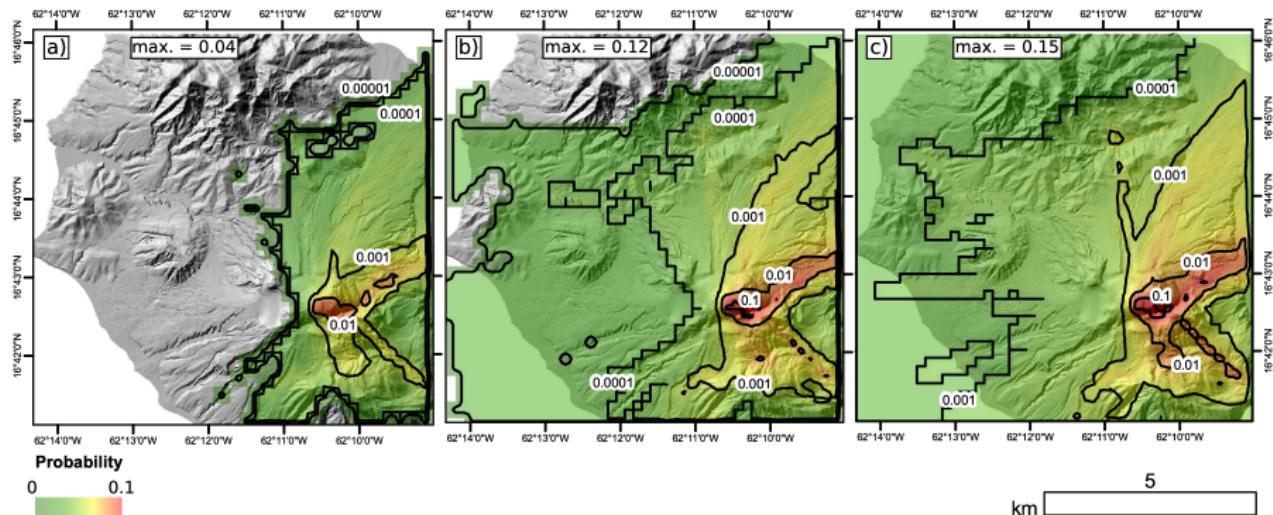
Right: $t = 20$ years



(S, Wolpert, Ogburn, et al 2020)

Probabilistic hazard forecast maps

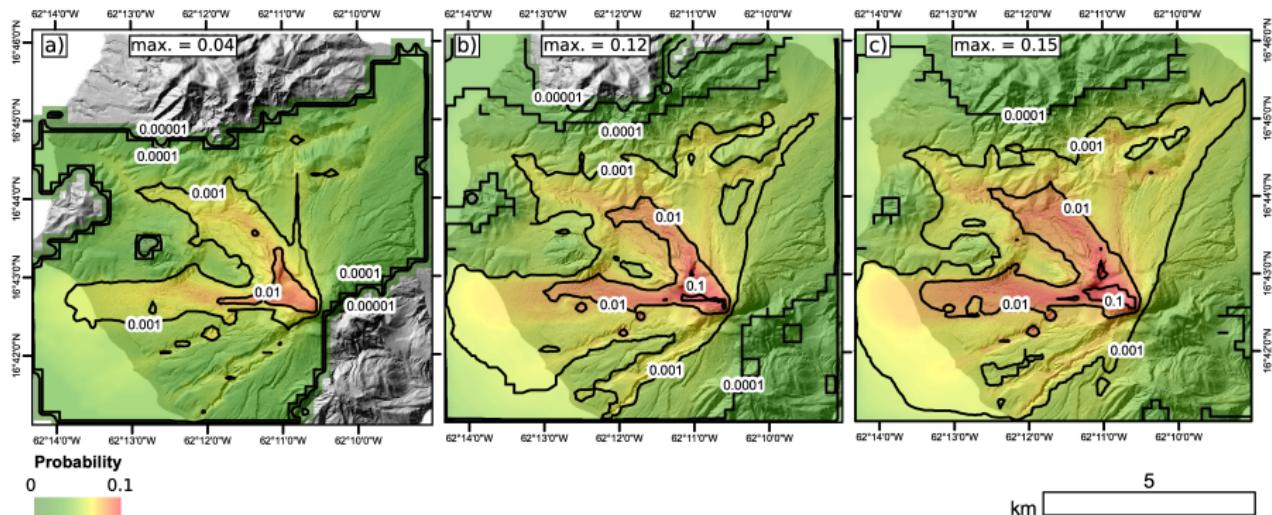
Left: $t = 1$ year, Middle $t = 5$ years, Right: $t = 20$ years



(S, Wolpert, Ogburn, et al 2020)

Probabilistic hazard forecast maps

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A hundred step random walk

- Flip a coin 100 times:
heads, step right; tails, step left; X is final position

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- $P(X \geq 70) = ??$

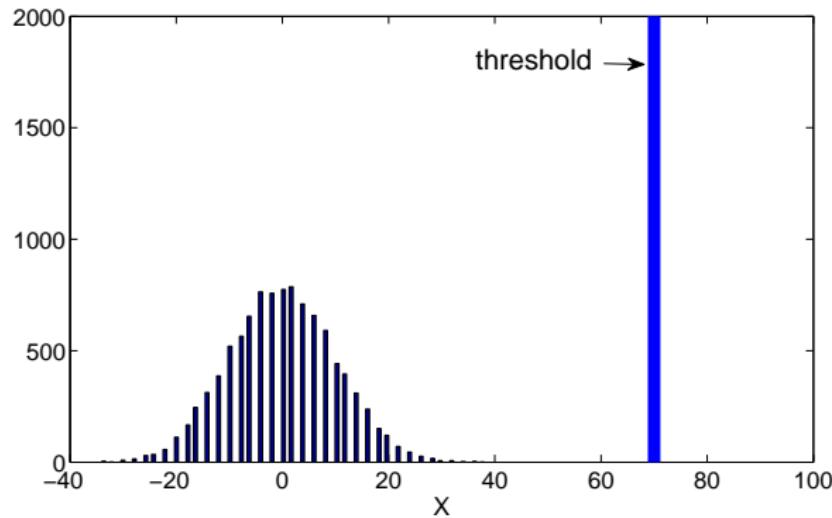
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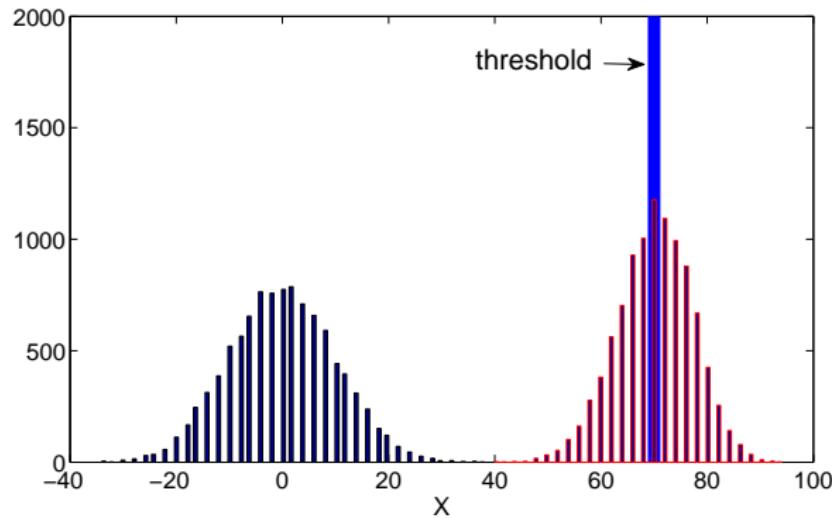
Standard Monte Carlo: $P(X \geq 70) = 0$



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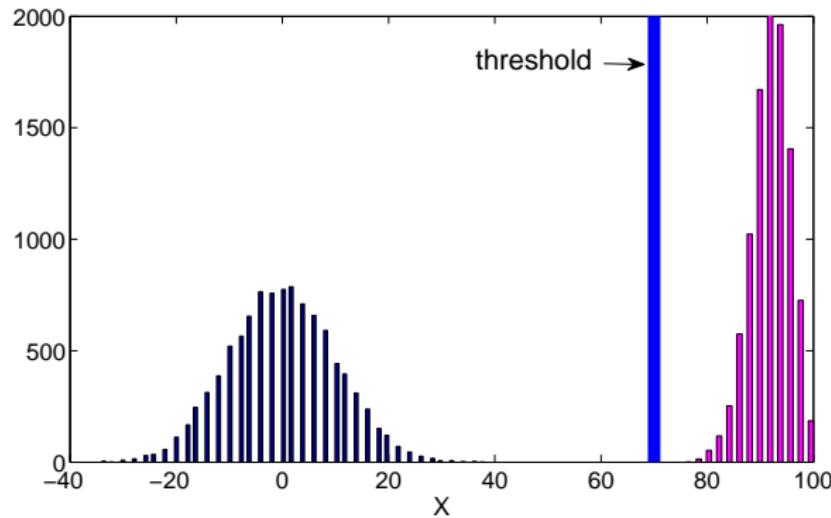
MC w/importance sampling: $P(X \geq 70) = 2.5 \times 10^{-13}$



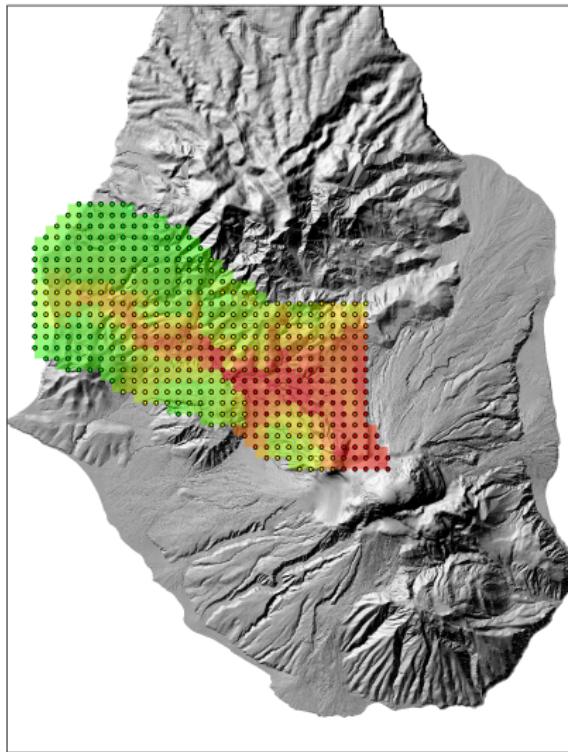
A hundred step random walk

- Flip a coin 100 times:
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MC w/bad importance sampling: $P(X \geq 70) = 2.9 \times 10^{-16}$



Sampling strategy for whole map?



- different probabilities correspond to different thresholds
- a good sampling strategy targeting one region will result in a poor strategy for others
- need surrogate that can faithfully model the threshold at each map point

How we can do what we'd like to do

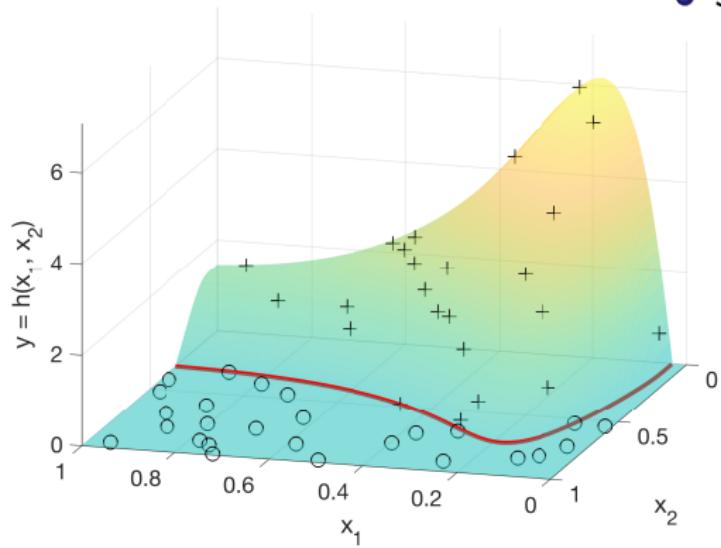
inundation probabilities:

$$\Pr[h \geq h_{\text{crit}}] \approx \int \mathbf{1}_{\hat{h}(x) \geq h_{\text{crit}}} \underbrace{p(x | \theta)}_{\text{aleatory}} \underbrace{\pi(\theta)}_{\text{epistemic}} d\theta dx$$

- \hat{h} is a cheap approximation of h
- can easily explore/update models of aleatoric and/or epistemic uncertainty for UQed probabilistic hazard analysis/forecasts
- \hat{h} is a faithful approximation of h near inundation boundaries

The zero problem

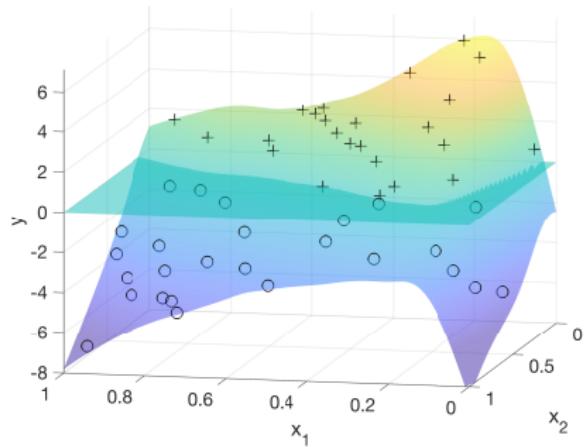
- GPs have full support
- Different number of zeros at each map point
- Strong non-stationarity
 - ▶ zero-boundaries vary for different map points
 - ▶ strategies that partition the input space (Gramacy, Lee (2008); Pope *et al.* (2019)) or fit mixtures of input-region specific kernels Volodina, Williamson (2020)) are map point specific



The zero-censored Gaussian process (zGP)

Model flow depth as max of zero & a latent Gaussian process

Impute “negative” responses for zero-output responses $\{\mathbf{x}_j\}$ ($j \in J_0$)

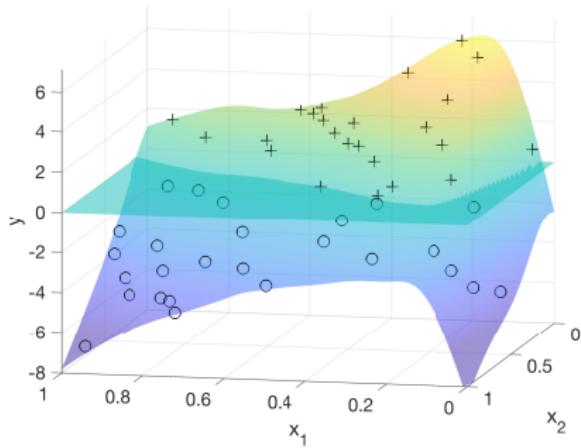


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Substitution sampling



0. Begin with negative sample of all responses to \mathbf{x}_j ($j \in J_0$).
1. Fit GP to positive-output runs $\{\mathbf{x}_j\}$ ($j \in J_+$) to estimate μ, γ .
2. Condition GP on all but one negative response $\{\mathbf{x}_j\}$ ($j \in J_0 \setminus i$).
3. Sample \mathbf{x}_i from 2.
4. Repeat 2-3 for all ($j \in J_0$).
5. Repeat 2-4 N times, average negative imputed runs.

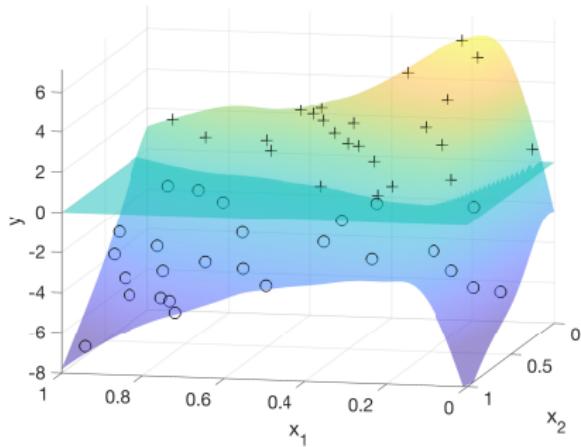
(S, Wolpert, Tierz, Asher (2023))

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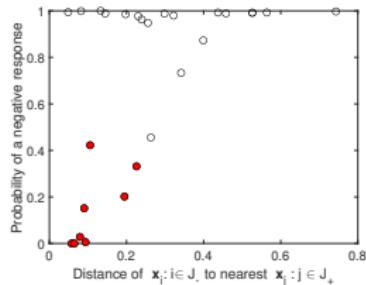


0. Begin with negative sample of all responses to \mathbf{x}_j ($j \in J_0$).
1. Fit GP to $+$ runs & “close” zeros $\{\mathbf{x}_j\}$ ($j \in J_+ \cup J_0^*$) to estimate μ, γ .
2. Condition GP on all but one negative response $\{\mathbf{x}_j\}$ ($j \in J_0 \setminus i$).
3. Sample \mathbf{x}_i from 2.
4. Repeat 1-3 for all ($j \in J_0$).
5. Repeat 1-4 N times, average negative imputed runs.

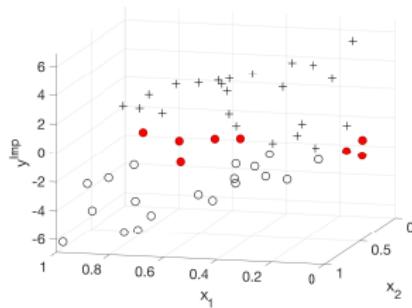
(S, Wolpert, Tierz, Asher (2023))

Including nearby zeros

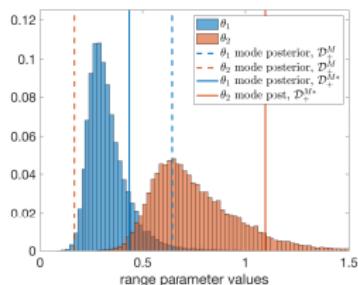
(a)



(b)



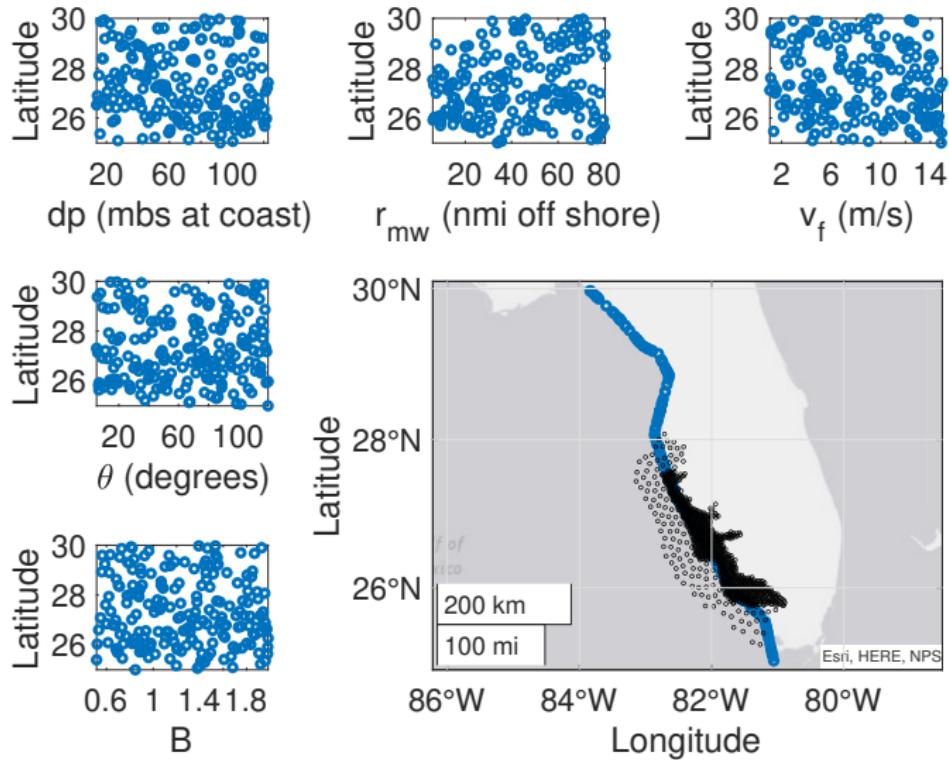
(c)



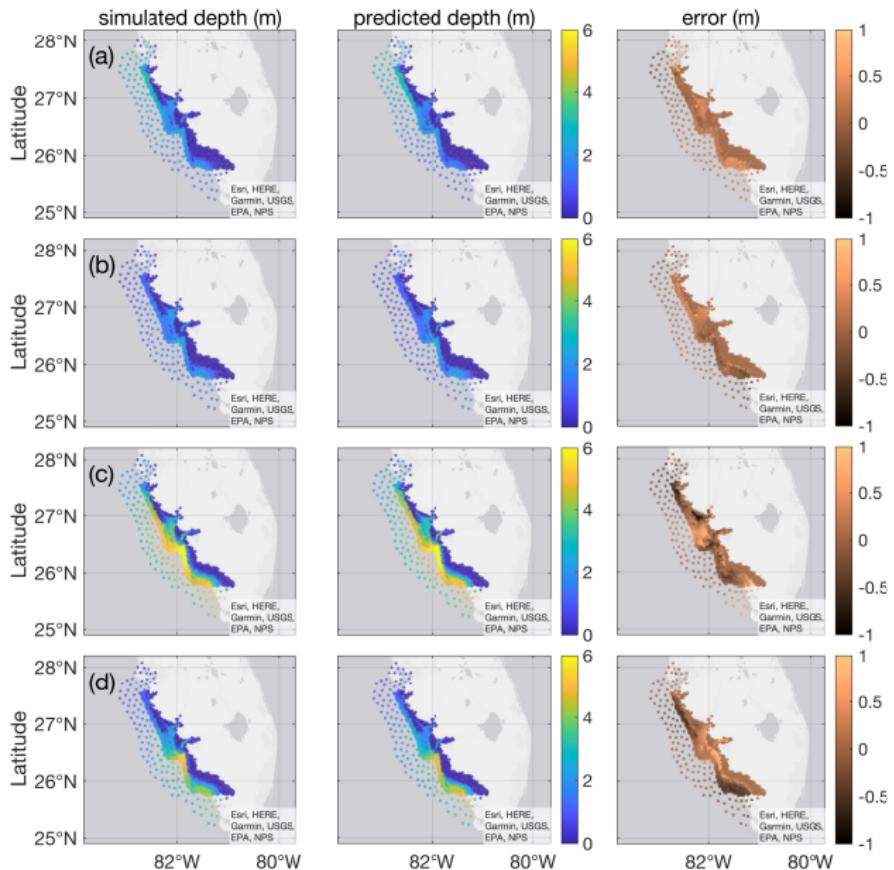
- (a) $\text{Prob}(\text{negative response})$ vs distance to nearest $x_j, j \in J_+$
- (b) Imputed negative responses included in estimating μ, γ
- (c) Estimated range parameters (solid MAP fit to $j \in J_+$, dashed MAP fit to $j \in J_+ \cup J_0^*$, histograms MAP estimates)

(RobustGaSP MAP estimates – Gu, Wang, Beger (2018); Gu, Paloma, Berger (2019))

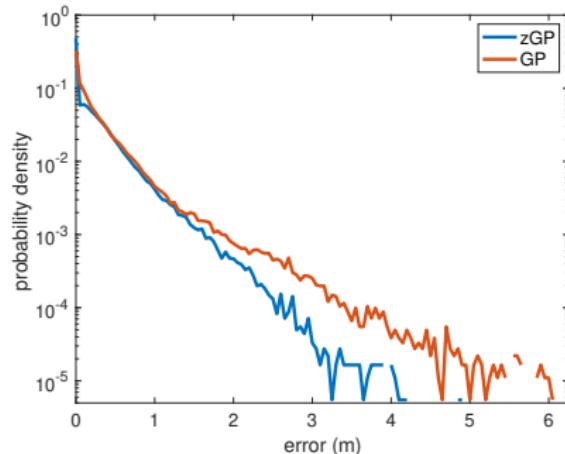
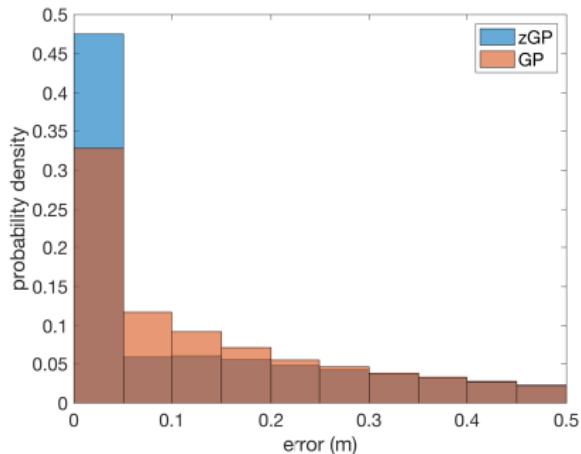
Estimating storm surge with zGP: Design



Estimating storm surge with zGP+ PCA-GP

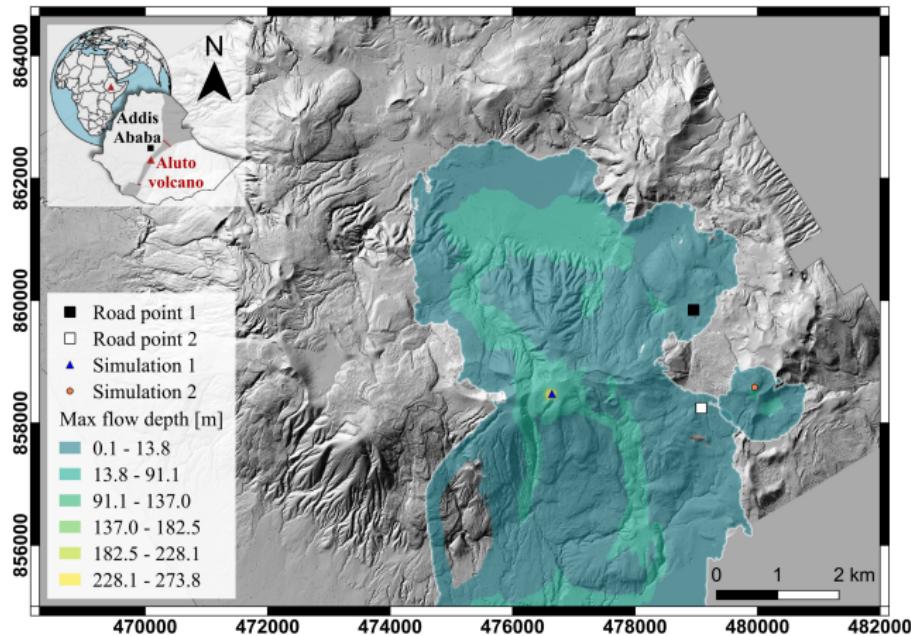


Errors w/zGP+ PCA-GP vs PCA-GP



(S, Wolpert, Tierz, Asher (2023))

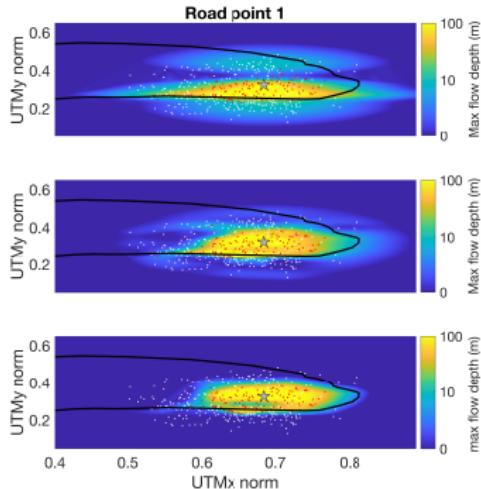
Aluto volcano



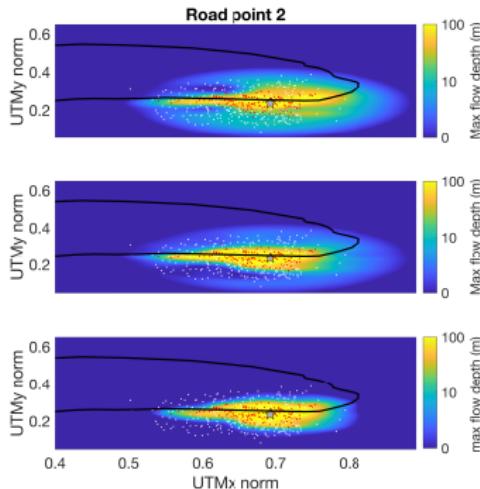
Inputs: vent location (Easting + Northing), volume (vent radius + flux), mobility (basal friction)

Aluto volcano: 3 approaches to the zero problem

Road point 1



Road point 2



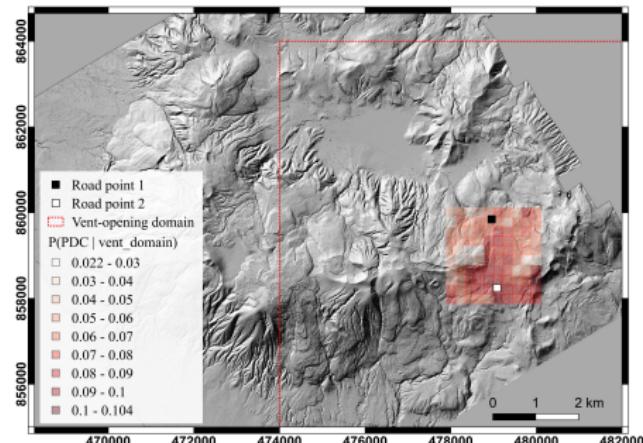
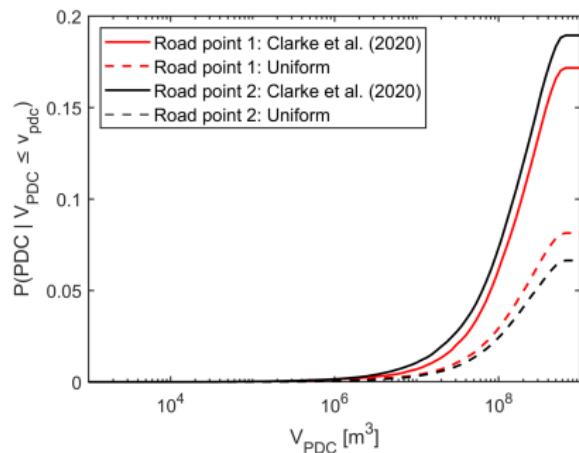
Top: GP fit only to positive output

Middle: GP fit to positive output and “nearest” zeros

Bottom: zGP

(S, Wolpert, Tierz, Asher (2023))

Probabilistic hazard analysis at Aluto using zGP



(S, Wolpert, Tierz, Asher (2023))

Pros and cons of zGP for probabilistic hazard assessment

Pros:

- Pre-processing step, can be done in parallel for each map point
- Naturally handles non-stationarity of semi-binary data
- Easily plugs into existing GP methods for high-dimensional output
(PPE Gu, Berger (2016); PCA-GP Higdon *et. al.* (2008); laGP Gramacy, Apley (2015))

Cons:

- Added computational overhead – challenging for models with very high-dimensional spatial outputs
- Not (directly) exploiting spatial correlations to guide imputation

Part II

Parallel Partial Linked Emulation (PPLE)
w/Tamara Dolski and Sue Minkoff (UTD)

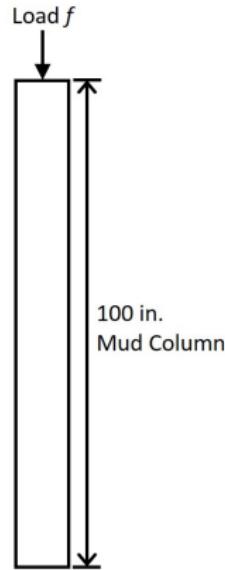
Loose coupling of flow and elastic deformation: subsurface modeling – hydrology (irrigation, filtration) & oil extraction

Flow equation (pressure, p): Darcy's law

$$\rho_0 \frac{\partial(\phi p)}{\partial t}(x, t) = \frac{k}{\mu c} \frac{\partial^2 p}{\partial x^2}(x, t)$$

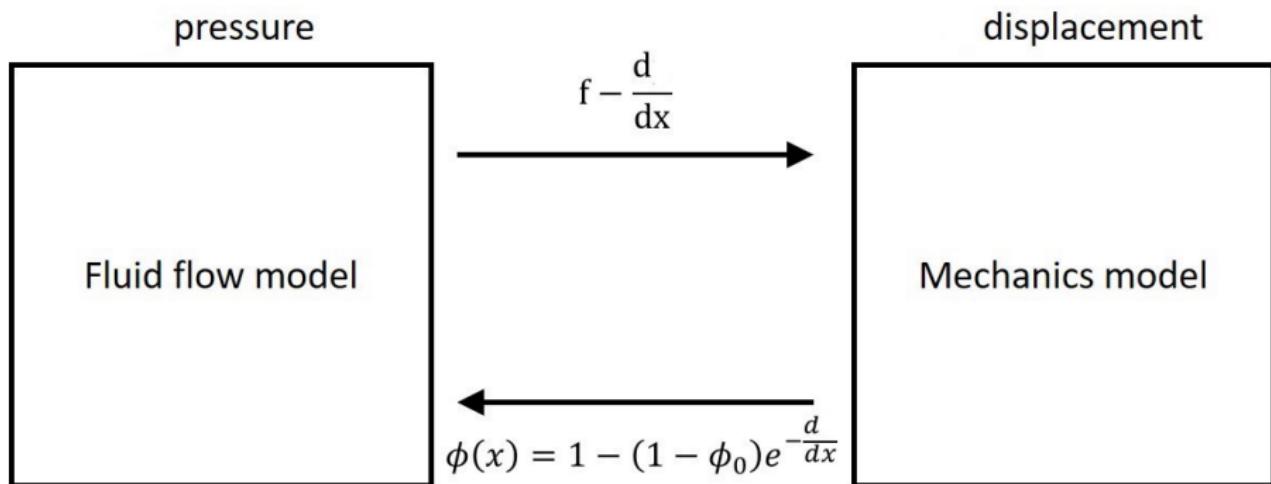
Mechanical deformation equation (displacement, u)

$$-(\lambda + 2\hat{\mu}) \frac{d^2 u}{dx^2} = f - \frac{dp}{dx}$$



Lamé constants λ & $\hat{\mu}$ are nonlinear functions material parameters E & ν

Loosely Coupled Flow and Deformation Models



μ = fluid viscosity

c = fluid compressibility

k = permeability

ϕ_0 = initial porosity

E = Young's modulus

ν = Poisson's ratio

How can we build an emulator for this system?

Challenges for emulating – focus on pressure at one time

- Model outputs of interest are functions of column depth:
 $u(x), p(x), \phi(x)$
- Output from one model is input for the next along with uncertain parameters
- First ignore coupling (porosity, $\phi(x)$), and emulate $p(x)$ for uncertain parameters $\{k, E, \nu, \phi_o\}$
- Parallel partial emulation (PPE) (Gu & Berger (2016))

Parallel Partial Emulation – (Gu and Berger, 2016)

$\hat{y}(\mathbf{x}^*) = \mathbf{w}(\mathbf{x}^*)\mathbf{y}^D$ is the predictive PPE mean at untested \mathbf{x}^* , where

$$\mathbf{w}(\mathbf{x}^*) = \underbrace{\left(\mathbf{h}(\mathbf{x}^*) - \mathbf{r}^T(\mathbf{x}^*)\mathbf{R}^{-1}\mathbf{h}(\mathbf{x}^D) \right)}_{1 \times q} \underbrace{\left(\mathbf{h}^T(\mathbf{x}^D)\mathbf{R}^{-1}\mathbf{h}(\mathbf{x}^D) \right)^{-1}}_{q \times q} \underbrace{\mathbf{h}^T(\mathbf{x}^D)\mathbf{R}^{-1}}_{q \times n}$$
$$+ \underbrace{\mathbf{r}^T(\mathbf{x}^*)\mathbf{R}^{-1}}_{1 \times n}$$

$\mathbf{x}_j^D = \{x_{j1}, \dots, x_{jp}\} \in \mathbb{R}^p$ – p dimensional input space

$\mathbf{x}^D = \{\mathbf{x}_1^D, \dots, \mathbf{x}_n^D\}$ – $n \times p$ input design matrix

$\mathbf{h}(\mathbf{x}^D)$ – $n \times q$ basis design matrix

\mathbf{R} – $n \times n$ design correlation matrix

$\mathbf{r}(\mathbf{x}^*)$ – $n \times 1$ vector of correlations between untested point, \mathbf{x}^* and design

\mathbf{y}^D – $n \times s$ matrix of simulator output

Parallel Partial Emulation – (Gu and Berger, 2016)

PPE predictive mean:

$$\hat{\mathbf{y}}(\mathbf{x}^*) = \mathbf{w}(\mathbf{x}^*)\mathbf{y}^D \quad \text{where}$$

$$\begin{aligned}\mathbf{w}(\mathbf{x}^*) &= \left(\mathbf{h}(\mathbf{x}^*) - \mathbf{r}^T(\mathbf{x}^*)\mathbf{R}^{-1}\mathbf{h}(\mathbf{x}^D) \right) \left(\mathbf{h}^T(\mathbf{x}^D)\mathbf{R}^{-1}\mathbf{h}(\mathbf{x}^D) \right)^{-1} \mathbf{h}^T(\mathbf{x}^D)\mathbf{R}^{-1} \\ &\quad + \mathbf{r}^T(\mathbf{x}^*)\mathbf{R}^{-1}.\end{aligned}$$

Key take aways:

- One set of correlations parameters are shared by s outputs
- Two inverses above only need to be computed once
- Output is treated as independent
- Predictive mean is weighted sum of model output
- PPE mean inherits conservation properties of the simulator
(Gao and Pitman, preprint)

Reorganizing the PPE mean

PPE predictive mean:

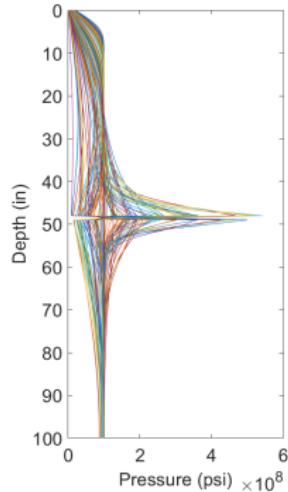
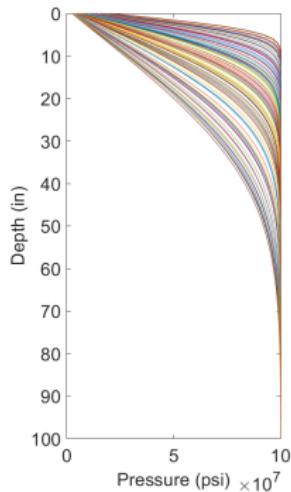
$$\hat{y}(\mathbf{x}^*) = \underbrace{h(\mathbf{x}^*)}_{1 \times q} \underbrace{\hat{\Theta}}_{q \times s} + \underbrace{\mathbf{r}^T(\mathbf{x}^*)}_{1 \times n} \underbrace{\mathbf{R}^{-1}}_{n \times n} \underbrace{(\mathbf{y}^D - h(\mathbf{x}^D) \hat{\Theta})}_{n \times s}, \quad \text{where}$$
$$\hat{\Theta} = \underbrace{\left(\mathbf{h}^T(\mathbf{x}^D) \mathbf{R}^{-1} \mathbf{h}(\mathbf{x}^D) \right)}_{q \times q}^{-1} \underbrace{\mathbf{h}^T(\mathbf{x}^D)}_{q \times n} \underbrace{\mathbf{R}^{-1}}_{n \times n} \underbrace{\mathbf{y}^D}_{n \times s}.$$

Key take aways:

- PPE predictive mean is really just multi-dimensional BLUP
- Each output dimension has its own mean function,
 $\hat{m}_j(\mathbf{x}) = h(\mathbf{x}) \hat{\Theta}_{\cdot j}, j = 1, \dots, s.$
- Likewise, each output dimension has its own variance

Applying PPE to pressure

- 100 LHD over $\{k, E, \nu, \phi_o\}$ (constant permeability)
- 100 LHD over $\{k_{top}, k_{bot}, E, \nu, \phi_o\}$ (two permeabilities)



Avg (over column) RMSE:

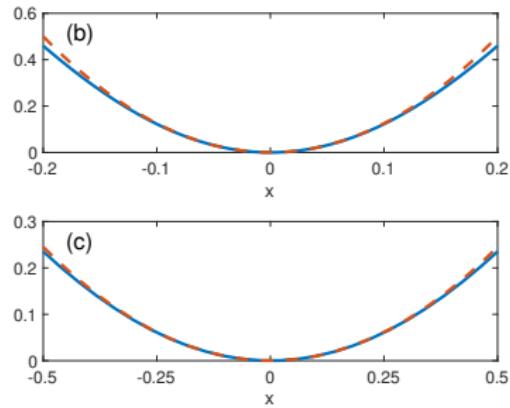
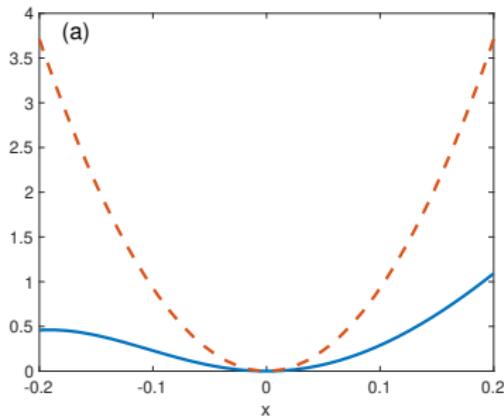
1.4e4 (psi) (one permeability), 2.6e5 (psi) (two permeabilities)

Why emulating $\eta(x) = g(f(x))$ directly is hard

$$\eta(x) \approx L(x) + R(x)$$

$$L(x) = g(f(x^D)) + (x - x^D)g'(f(x^D))f'(x^D)$$

$$R(x) = \frac{1}{2}(x - x^D)^2 \left[(f')^2(\xi_{in})g''(\xi_{out}) + f''(\xi_{in})g'(\xi_{out}) \right]$$



Emulator of composite vs. composite of emulators

Composite emulator (CE) – emulate composite function directly

$$\tilde{\eta} \approx \eta(\mathbf{x}) = g\left(\underbrace{f(\mathbf{x})}_{\text{pressure, } p} \right) \quad \text{porosity, } \phi$$

Linked emulator (LE) (Kyzyurova, Berger, Wolpert, 2018) and (Abdelfatah, Bao, Terejanu, 2018) – consider composite of emulators

- Fit GPs to $g(\cdot)$ and $f(\cdot)$ individually at design/response points $\{\mathbf{w}^D, g(\mathbf{w}^D)\}$ and $\{\mathbf{x}^D, f(\mathbf{x}^D)\}$
- Call those $\tilde{g}(\cdot)$ and $\tilde{f}(\cdot)$ (with GP parameters θ_g and θ_f)
- Consider

$$Y \sim p_\eta\left(\widetilde{g \circ f}(\mathbf{u}) \mid \tilde{g}(\mathbf{w}), \tilde{f}(\mathbf{x}), \theta_g, \theta_f, \mathbf{u}\right)$$

Linked GP emulator

$$Y \sim p_\eta\left(\widetilde{g \circ f}(\mathbf{u}) \mid \tilde{g}(\mathbf{w}), \tilde{f}(\mathbf{x}), \theta_g, \theta_f, \mathbf{u}\right)$$

- Y is not normally distribution, but can find $E[Y]$ and $V[Y]$

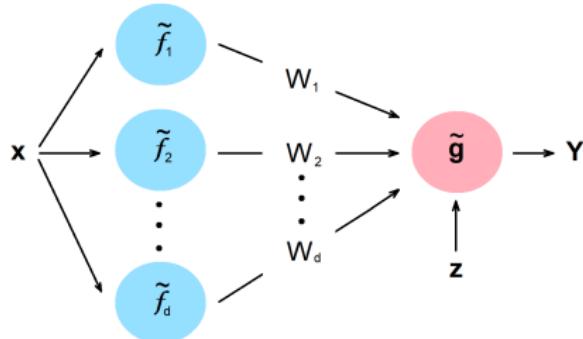
Linked Gaussian Process:

$$\zeta \sim N(E[Y], V[Y])$$

Note:

- Analytic expressions for predictive mean & var (although quite ugly)
- Extension to Matérn (Ming and Guillas, 2021)
- Error bounds between $p_\eta(\cdot \mid \cdot)$ and normal approximation are available (Kyzyurova, 2017)

Parallel Partial Linked GP emulator (PPLE)

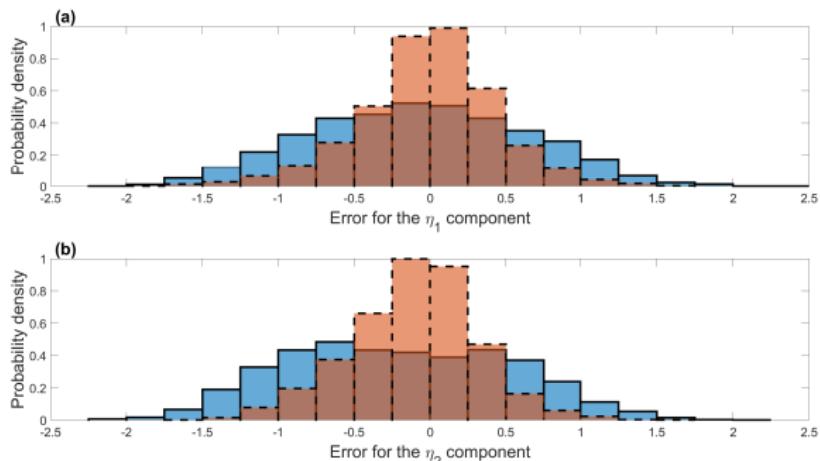


- PPE for “outside” function $\mathbf{g}(\cdot)$
- Linked GP emulator to connect $\tilde{\mathbf{g}}(\cdot)$ and $\tilde{\mathbf{f}}(\cdot)$
- If “inside” function \mathbf{f} is high dimensional
 - ▶ need dimension reduction, i.e., PCA, gKDR (Fukumizu & Leng 2014)
 - ▶ note **no dimension reduction for \mathbf{g}**

Composite trig function example: $\eta(\mathbf{x}, \mathbf{z}) = \mathbf{g}(\mathbf{f}(\mathbf{x}), \mathbf{z})$

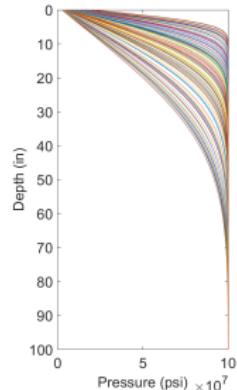
$$\mathbf{f}(\mathbf{x}) = \langle \underbrace{\sin(c_1 x_1) + c_2 x_2^2}_{w_1}, \underbrace{\sin(c_3 x_1 \cos(c_4 \pi x_2))}_{w_2} \rangle$$

$$\mathbf{g}(\mathbf{w}, \mathbf{z}) = \langle \underbrace{\cos(c_5 z_2) \sin(c_6 w_1) + \sin(c_7 z_1) \cos(c_8 w_2),}_{\eta_1(\mathbf{x}, \mathbf{z}) = g_1(\mathbf{w}, \mathbf{z})} \\ \underbrace{\cos(c_9 z_2) \sin(c_{10} w_1) + \sin(c_{11} z_1) \cos(c_{12} w_2)}_{\eta_2(\mathbf{x}, \mathbf{z}) = g_2(\mathbf{w}, \mathbf{z})} \rangle$$

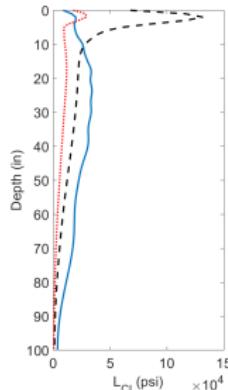
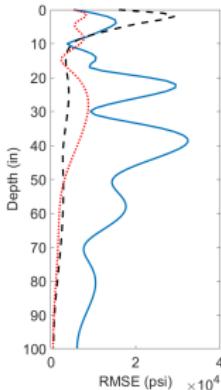


Loosely Coupled Flow and Deformation Models

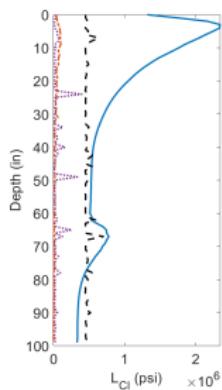
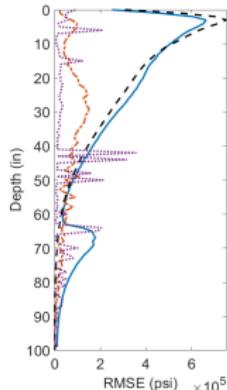
True pressure



PPE methods



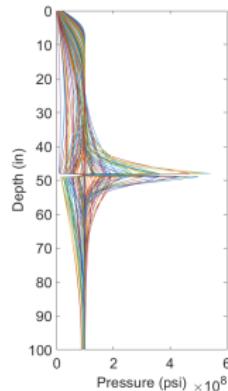
Local GP methods



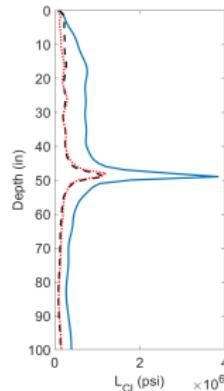
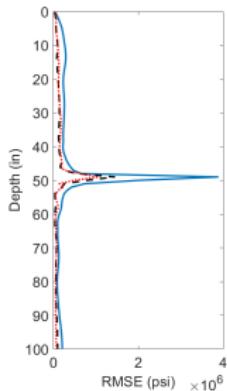
	PPLE PCA	PPLE gKDR	PPCE	LESC	CESC	LE laGP	CE laGP
Timing (s)	2	377	2	143	69	342	135
RMSE (psi)	4.1e3	3.9e3	1.4e4	3.6e4	1.7e5	5.7e4	2.0e5
L_{CI} (psi)	1.7e4	6.5e3	2.1e4	3.9e4	4.7e5	2.7e4	7.9e5
Coverage (%)	97	93	92	93	99	80	94

Loosely Coupled Flow and Deformation Models

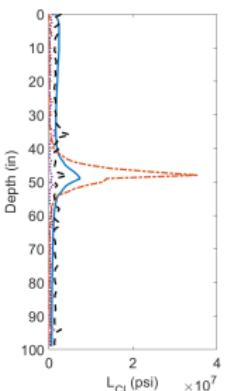
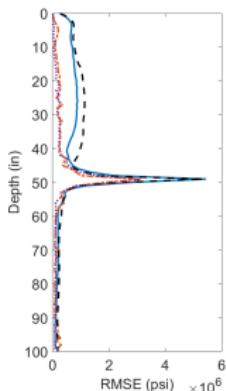
True pressure



PPE methods



Local GP methods



	PPLE PCA	PPLE gKDR	PPCE	LESC	CESC	LE laGP	CE laGP
Timing (s)	2	383	1.8	176	62	291	140
RMSE (psi)	1.2e5	1.1e5	2.6e5	2.4e5	6.6e5	2.6e5	5.6e5
L_{CI} (psi)	2.2e5	2.4e5	6.0e5	4.1e5	1.7e6	1.7e6	1.8e6
Coverage (%)	93	92	94	91	100	86	95

PPLE: wrapping up

- *Gaussian Process Emulation for High-Dimensional Coupled Systems*
Dolski, S, Minkoff (under review)
- Derived analytic expressions for mean and variance of PPLE
- Demonstrated PPLE on pedagogical example and loosely-coupled flow-deformation simulator
- Linked PPEs outperform local GP methods (linked or composite)

Thanks!

Questions? Ideas?

And thanks to the NSF for support under DMS-2053872.