Domain Uncertainty Quantification

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Forward UQ & Inverse UQ

- Key element in (mathematical and numerical) analysis of UQ:

[Uncertain] Data-to-[Uncertain] Response Map

Well-posed Mathematical Model $\simeq$ *Continuous* Data-to-Solution Forward Map

- This talk:

Holomorphic Data-to-Solution Dependence $\Longrightarrow$ Sparsity in gpc representations of responses.

Quantified Holomorphy $\simeq$ *Dimension Independent Convergence Rates* [of gpc, SC, SG, QMC, CS, DNN]

- Parametric Holomorphy crucial in numerical analysis of gpc approximations (SG, SC, MISC,...):
  Babuska, Nobile, Tempone, ... (2002,...), Gunzburger, Webster (2005,...),

Forward UQ & Inverse UQ

- Example 1:
  - Data: $a(x) \in L^\infty(\mathrm{D})$ diffusion coefficient, $\mathrm{D} \subset \mathbb{R}^d$ bounded, Lipschitz, $f \in H^{-1}(\mathrm{D})$ source term.
  - Mathematical (forward) Model: for fixed f, uncertain a, find solution u of

$$\mathcal{D}(u,a) := f + \nabla_x \cdot (a \nabla_x u) = 0 \quad \text{in} \quad H^{-1}(\mathrm{D}) \;, \qquad u|_{\partial \mathrm{D}} = 0 \;.$$

  - Variational Formulation: given D, f and a, find

$$u \in H^1_0(\mathrm{D}) : \qquad (a\nabla_x u, \nabla_x v) = (f, v) \qquad \text{for all} \;\; v \in H^1_0(\mathrm{D}) \;.$$

  - Admissible Data: $\mathcal{A}_{adm} := \{a \in L^\infty(\mathrm{D}) | 0 < a_{min} = \operatorname{ess\,inf}_{x \in \mathrm{D}} a(x)\}$.
  - Solution: $u \in H^1_0(\mathrm{D})$: Existence, Uniqueness *given admissible data* D, f *and* a.
- *Continuous Dependence*: given admissible data a_1, a_2, for *fixed, known* D and f, there holds

$$\|u_1 - u_2\|_{H^1(\mathrm{D})} \leq \frac{C(\mathrm{D})}{a_{min}^2} \|a_1 - a_2\|_{L^\infty(\mathrm{D})} \|f\|_{H^{-1}(\mathrm{D})} \;.$$

- Continuity depends on topology: consider $f \in L^2(\mathrm{D})$, admissible $a \in W^{1,\infty}(\mathrm{D})$.
  Data-to-Solution map $a \mapsto u \in (H^2 \cap H^1_0)(\mathrm{D})$ continuous *provided* D convex.

Forward UQ & Inverse UQ

- Example 1 (cont'd): UQ and Data $\Longrightarrow$ new mathematical questions in 'old' areas.
  - Variational Formulation 2:

$$f + \nabla \cdot q = 0 \ , \qquad \nabla u - a^{-1} q = 0 \qquad \text{in} \quad \mathrm{D} \subset \mathbb{R}^d \ .$$

  - **Conservation Law** ["1st principle"] and **Constitutive Equation** ["empirical", "data driven"].

$$f + \nabla \cdot q = 0 \ , \qquad K(u, q) = 0 \qquad \text{in} \quad \mathrm{D} \ .$$

  - Q1: **characterize admissible** $K(\cdot, \cdot) : H^1_0(\mathrm{D}) \times H(\mathrm{div}; \mathrm{D}) \to L^2(\mathrm{D})^d$ s.t. Fwd Pbm. well-posed.
  - Q2: given D, can we **'learn'** $K(\cdot, \cdot)$ **from data** f for QoI $u \mapsto Q(u)$?

Forward UQ & Inverse UQ

- Example 1 (cont'd):
  ***Analyticity* of Data-to-Solution map** $a \mapsto u$?

  1. $L^\infty(\mathrm{D}) \ni a \mapsto \mathcal{P}[a](\partial_x) := -\nabla_x \cdot a \nabla_x \in \mathcal{L}(H_0^1(\mathrm{D}), H^{-1}(\mathrm{D}))$ is *linear*, thus analytic,
  2. $\mathcal{A}_{adm} \ni a \mapsto \mathcal{P}[a](\partial_x) \in \mathcal{L}_{iso}(H_0^1(\mathrm{D}), H^{-1}(\mathrm{D}))$ is *linear*, thus analytic,
  3. $\mathrm{INV} : \mathcal{L}_{iso}(H_0^1(\mathrm{D}), H^{-1}(\mathrm{D})) \to \mathcal{L}_{iso}(H^{-1}(\mathrm{D}), H_0^1(\mathrm{D})) : \mathcal{P} \mapsto \mathcal{P}^{-1}$ is analytic
  4. $\Longrightarrow$: $\quad \mathcal{A}_{adm} \ni a \mapsto u := (\mathrm{INV} \circ \mathcal{P} \circ a) f \in H_0^1(\mathrm{D})$ analytic.

- ***Holomorphy* of Data-to-Solution map** $a \mapsto u$? By "the same reasoning":

  1. "Complexify": $\mathcal{A}_{adm,\mathbb{C}} := \{a \in L^\infty(\mathrm{D};\mathbb{C}) |\ 0 < a_{min} \leq \Re a \text{ in } \mathrm{D}\}$
  2. Consider $\quad u \in H_0^1(\mathrm{D};\mathbb{C})$, $f \in H^{-1}(\mathrm{D}) \subset H^{-1}(\mathrm{D};\mathbb{C})$.
  3. Complex version of the Lax-Milgram Lemma:

  $$\forall a \in \mathcal{A}_{adm,\mathbb{C}} : \quad \mathcal{P}[a](\partial_x) \in \mathcal{L}_{iso}(H_0^1(\mathrm{D};\mathbb{C}), H^{-1}(\mathrm{D};\mathbb{C}))$$

  4. $\mathrm{INV} : \mathcal{L}_{iso}(H_0^1(\mathrm{D};\mathbb{C}), H^{-1}(\mathrm{D};\mathbb{C})) \to \mathcal{L}_{iso}(H^{-1}(\mathrm{D};\mathbb{C}), H_0^1(\mathrm{D};\mathbb{C})) : \mathcal{P} \mapsto \mathcal{P}^{-1}$ is holomorphic.

Forward UQ: Parametric Holomorphy

- Example 1 (cont'd):
- ***Uncertainty Parametrization*** : parametrize $a \in X \subset \mathcal{A}_{adm}$, e.g. *affine*:

$$X = \{a \in L^\infty(\mathrm{D}) | a(x, \boldsymbol{y}) = \bar{a}(x) + \sum_{j \geq 1} y_j \psi_j(x)\}$$

where

1. $\bar{a} \in L^\infty(\mathrm{D})$, $\bar{a} \geq \bar{a}_{min} > 0$ a.e., $\{\psi_j\}_{j \geq 1} \subset L^\infty(\mathrm{D})$,
2. $\boldsymbol{y} = (y_j)_{j \geq 1} \in U := [-1, 1]^\infty$, i.e. $|y_j| \leq 1$,
3. $b_j := \|\psi_j\|_{L^\infty(\mathrm{D})}$ satisfy $\boldsymbol{b} = (b_j)_{j \geq 1} \in \ell^p(\mathbb{N})$ some $0 < p \leq 1$, $\|\boldsymbol{b}\|_{\ell^1} < \bar{a}_{min}$.

- Then $X \subset \mathcal{A}_{adm}$: for every $\boldsymbol{y} \in U$ holds $a(x, \boldsymbol{y}) \geq \bar{a}_{min} - \|\boldsymbol{b}\|_{\ell^1(\mathbb{N})} =: a_{min} > 0$.
- For $\boldsymbol{y} \in U$ and $z_k \in \mathbb{C}$, denote $\boldsymbol{z}^{(k)} := (y_1, ..., y_{k-1}, z_k, y_{k+1}, ...)$. Then

$$\forall f \in H^{-1}(\mathrm{D}) : \quad \mathcal{D}_{\rho_k} \ni z_k \mapsto u(\boldsymbol{z}^{(k)}) := (\mathrm{INV} \circ \mathcal{P}[a(\boldsymbol{z}^{(k)})])f \quad \text{is holomorphic from } \mathcal{D}_{\rho_k} \text{ to } H_0^1(\mathrm{D}; \mathbb{C}),$$

- $\mathcal{D}_r := \{z \in \mathbb{C} | |z| \leq r\}$ and $\rho_k \sim 1/b_k$,
- Restriction to $y_k \in [-1, 1]$ yields 'real-valued', parametric solution u.

Forward UQ: $(\boldsymbol{b},\varepsilon)$-Holomorphy of Parametric Solution Maps

Holomorphy Domains: **Disc** $\mathcal{D}_s$ of radius $s>1$ or **Bernstein Ellipse** $\mathcal{E}_s$ of semiaxis-sum $s>1$:

$$\mathcal{D}_s := \{w \in \mathbb{C} : \ |w| \le s\} \ , \ \ \mathcal{E}_s := \left\{ \frac{w+w^{-1}}{2} : w \in \mathbb{C} \ , \ \ 1 \le |w| \le s \right\} \subset \mathbb{C} \ .$$

Definition:

A parametric mapping $U \ni \boldsymbol{y} \mapsto u(\boldsymbol{y}) \in X$ satisfies the $(\boldsymbol{b},\varepsilon)$-*holomorphy assumption* in the Banach space X for positive sequence $\boldsymbol{b} = (b_j)_{j\ge1} \in \ell^p(\mathbb{N})$ some $0<p<1$ and for some $\varepsilon>0$,

if for any sequence $\boldsymbol{\rho} := (\rho_j)_{j\ge1}$ that is $(\boldsymbol{b},\varepsilon)$-*admissible*, i.e.

$$\sum_{j=1}^{\infty} (\rho_j - 1) b_j \le \varepsilon, \tag{1}$$

$\boldsymbol{y} \mapsto u(\boldsymbol{y}) \in X$ admits a complex extension $\boldsymbol{z} \mapsto u(\boldsymbol{z}) \in X_{\mathbb{C}}$ that is holomorphic w.ro to each z_j on cylinder $\mathcal{O}_{\boldsymbol{\rho}} := \bigotimes_{j\ge1} \mathcal{O}_{\rho_j}$, $\mathcal{O}_{\rho_j} \subset \mathbb{C}$ open set containing $\mathcal{E}_{\rho_j}$, and

$$\sup_{\boldsymbol{z}\in\mathcal{E}_{\boldsymbol{\rho}}} \|u(\boldsymbol{z})\|_X \le C(\boldsymbol{b},\varepsilon) \ . \tag{2}$$

Forward UQ: Parametric Holomorphy

- Example 1 (cont'd):

Proposition [$(\boldsymbol{b},\varepsilon)$-holomorphy of affine-parametric diffusion problem]
The Data-to-Solution map $\mathcal{A}_{adm} \ni a \mapsto u$ of the diffusion problem
with affine uncertainty parametrization is $(\boldsymbol{b},\varepsilon)$-holomorphic.

- *verbatim same proof* gives $(\boldsymbol{b},\varepsilon)$-holomorphy for

$$a(x,\boldsymbol{y}) = \begin{cases} \exp\left(\bar{a}(x) + \sum_{j\geq 1} y_j\psi_j(x)\right) \ , \\ \left(\bar{a}(x) + \sum_{j\geq 1} y_j\psi_j(x)\right)^k \ , \\ \ldots \\ g\left(\bar{a}(x) + \sum_{j\geq 1} y_j\psi_j(x)\right) \ , \quad \zeta \to g(\zeta) \text{ holom. on } \Re\zeta \in [a_{min},\infty) \ , \end{cases}$$

for anisotropic coefficients (matrix-valued $\bar{a}$, ψ_j).

Forward UQ: Parametric Holomorphy

- **Example 2**: Linear, Affine-Parametric Operator Equation

$$\text{Given } f \in \mathcal{Y}' , \quad \text{for every } \boldsymbol{y} \in U \text{ find } u(\boldsymbol{y}) \in \mathcal{X} : \quad A(\boldsymbol{y})\, u(\boldsymbol{y}) = f \;.$$

Here

$$A(\boldsymbol{y}) = A_0 + \sum_{j\geq 1} y_j\, A_j \in \mathcal{L}(\mathcal{X};\mathcal{Y}') \;, \quad \forall \boldsymbol{y} := (y_j)_{j\geq 1} \in U := [-1,1]^\infty \;.$$

- Assumptions:

$$\sum_{j\geq 1} \|A_j\|_{\mathcal{L}(\mathcal{X},\mathcal{Y}')} \text{ ``small'' } , \quad \textbf{Sparsity}\text{: } \exists 0 < p < 1 : \qquad \sum_{j\geq 1} \|A_j\|^p_{\mathcal{L}(\mathcal{X},\mathcal{Y}')} < \infty \;.$$

- Uncertainty parametrisation by Karhúnen-Loeve expansion: $a(x, \boldsymbol{y}) = \bar{a}(x) + \sum_{j\geq 1} y_j \psi_j(x)$

$$A(\boldsymbol{y}) = -\nabla_x \cdot a(x,\boldsymbol{y})\nabla_x = \underbrace{-\nabla_x \cdot \bar{a}(x)\nabla_x}_{A_0} - \sum_{j\geq 1} y_j \underbrace{\nabla_x \cdot \psi_j(x)\nabla_x}_{-A_j} , \quad \mathcal{X} = \mathcal{Y} = H^1_0(D) \;.$$

- Parametric solution map $U \ni \boldsymbol{y} \mapsto u(\boldsymbol{y}) \in \mathcal{X}$ is $(\boldsymbol{b}, \varepsilon)$-holomorphic.

Further Examples for $(\boldsymbol{b}, \varepsilon)$ - Holomorphy

- Parabolic PDEs with uncertain coefficients (Cohen, DeVore & CS 2011,2012):

$$-\nabla \cdot (a(x,\boldsymbol{y})\nabla u) = f \quad \text{in} \quad \mathrm{D}\,, \quad u|_{\partial \mathrm{D}} = 0\,, \quad a(x,\boldsymbol{y}) = a_0(x) + \sum_{j\geq 1} y_j a_j(x)\;.$$

- Linear Elliptic Multiscale PDEs (V.H. Hoang & CS 2013):

$$-\nabla \cdot (a(x, x/\varepsilon; \boldsymbol{y})\nabla u) = f \;\text{ in } \mathrm{D}\,, \quad u|_{\partial \mathrm{D}} = 0\;.$$

- Nonlinear, affine-parametric initial value ODEs (Hansen, Schillings & CS):

$$\frac{dX}{dt} = f_0(t,X) + \sum_{j\geq 1} y_j f_j(t,X)\;, \quad X(0,\boldsymbol{y}) = X_0(\boldsymbol{y})\;.$$

- 2nd order, linear scalar elliptic and parabolic PDEs in random domains
(Chkifa, Cohen & CS 2013), (Nobile, Tempone etal 2014), (Hiptmair, Scarabosio, Schillings & CS 2015):

$$-\Delta u - k^2 u = f \;\text{ in }\; \mathrm{D}_{\boldsymbol{y}} = \Phi_{\boldsymbol{y}}(\mathrm{D}_0) \iff -\nabla \cdot (A(x,\boldsymbol{y})\nabla u) - k^2 u = \tilde{f}(\boldsymbol{y}) \;\text{ in }\; \mathrm{D}_0\;.$$

Implications of $(\boldsymbol{b}, \varepsilon)$ holomorphy for numerical analysis?

Holmorphy and gpc Approximation

Equip $U = [-1,1]^\infty$ with probability measure, Bochner spaces $L^2(U,X)$, $L^\infty(U,X)$.

- gpc Expansions of $U \ni \boldsymbol{y} \mapsto u(\boldsymbol{y})$:

$$u(\boldsymbol{y}) = \sum_{\boldsymbol{\nu}\in\mathcal{F}} u_{\boldsymbol{\nu}} P_{\boldsymbol{\nu}}(\boldsymbol{y}) = \sum_{\boldsymbol{\nu}\in\mathcal{F}} v_{\boldsymbol{\nu}} L_{\boldsymbol{\nu}}(\boldsymbol{y}) \quad P_{\boldsymbol{\nu}}(\boldsymbol{y}) := \prod_{j\geq 1} P_{\nu_j}(y_j)$$

  – P_n Legendre polynomial of degree n on $[-1,1]$, classical normalization $\|P_n\|_{L^\infty([-1,1])} = |P_n(1)| = 1$,
  – L_n "probabilistic" Legendre polynomial, normalized in $L^2([-1,1], \frac{dt}{2})$,
  – $\mathcal{F} = \{\boldsymbol{\nu} \in \mathbb{N}_0^{\mathbb{N}} \mid |\boldsymbol{\nu}| < \infty\}$ countable index set for gpc coefficients.

- Taylor gpc expansion:

$$u(\boldsymbol{y}) = \sum_{\boldsymbol{\nu}\in\mathcal{F}} t_{\boldsymbol{\nu}} \boldsymbol{y}^{\boldsymbol{\nu}} \;, \quad t_{\boldsymbol{\nu}} := \frac{1}{\boldsymbol{\nu}!}(\partial_{\boldsymbol{y}} u)(\boldsymbol{0}) \quad \text{"parameter sensitivities"}$$

Holmorphy and gpc Approximation

Theorem [gpc approximation rates for $(\boldsymbol{b},\varepsilon)$-holom. maps]
Assume solution map $\{\boldsymbol{y} \mapsto u(\boldsymbol{y})\} \in L^2(U,X)$ is $(\boldsymbol{b},\varepsilon)$-holomorphic for $\boldsymbol{b} \in \ell^p$, some $0 < p < 1$ and some $\varepsilon > 0$.
Then,

1. sequences $(\|u_{\boldsymbol{\nu}}\|_X)_{\boldsymbol{\nu}\in\mathcal{F}}$ and $(\|v_{\boldsymbol{\nu}}\|_X)_{\boldsymbol{\nu}\in\mathcal{F}}$ of Legendre coefficients belong to $\ell^p_m(\mathcal{F})$.
2. gpc series conv. unconditionally in $L^\infty(U,X)$.
3. There exist sequences $(\Lambda_n^2)_{n\geq 1}$ and $(\Lambda_n^\infty)_{n\geq 1}$, of nested downward closed subsets of $\mathcal{F}$ and a constant C such that, with $\#(\Lambda_n^2) = \#(\Lambda_n^\infty) = n$,
$$\|u - \sum_{\boldsymbol{\nu}\in\Lambda_n^\infty} v_{\boldsymbol{\nu}} L_{\boldsymbol{\nu}}\|_{L^\infty(U,X)} \leq C(n+1)^{-s}, \quad s = \frac{1}{p} - 1,$$
and
$$\|u - \sum_{\boldsymbol{\nu}\in\Lambda_n^2} v_{\boldsymbol{\nu}} L_{\boldsymbol{\nu}}\|_{L^2(U,X)} \leq C(n+1)^{-r}, \quad r = \frac{1}{p} - \frac{1}{2}.$$
Here, $\Lambda \subset \mathcal{F}$ is *downward closed* if and only if $\boldsymbol{\nu} \in \Lambda \quad \text{and} \quad \boldsymbol{\mu} \leq \boldsymbol{\nu} \Rightarrow \boldsymbol{\mu} \in \Lambda$.

Holmorphy and Stochastic Collocation

- Univariate Points: $\boldsymbol{z} := (z_j)_{j\geq 1}$ sequence of pairwise distinct points in $[-1,1]$,
- $\Lambda \subset \mathcal{F}$ finite, arbitrary. *Sparse Grid in* U: $\Gamma_\Lambda := \{\boldsymbol{z_\nu} : \boldsymbol{\nu} \in \Lambda\}$ where $\boldsymbol{z_\nu} := (z_{\nu_j})_{j\geq 1}$
- If $\Lambda \subset \mathcal{F}$ is downward closed, Γ_Λ is unisolvent for X_Λ. $I_\Lambda u \in X_\Lambda := X \otimes \mathbb{P}_\Lambda$ unique and well-defined.

Theorem [Stochastic Collocation Convergence Rates for $(\boldsymbol{b},\varepsilon)$-holomorphic $u : U \to X$]

Assume

- gpc series of $u : U \to X$ converges unconditionally in $L^\infty(U,X)$ to $\boldsymbol{y} \mapsto u(\boldsymbol{y})$,
- $\boldsymbol{y} \mapsto u(\boldsymbol{y})$ is $(\boldsymbol{b},\varepsilon)$-holomorphic for $\boldsymbol{b} \in \ell^p$ with some $0 < p < 1$ and some $\varepsilon > 0$,
- Assume in addition that $\boldsymbol{y} \mapsto u(\boldsymbol{y})$ is continuous from U equipped with the product topology to X,
- Lebesgue constants of the n-sections of the sequence $\boldsymbol{z} := (z_j)_{j\geq 1}$ of pairwise distinct points in $[-1,1]$ constituting Γ_Λ are bounded polynomially as $(1+n)^\theta$ for some $\theta \geq 0$.

Then exists $C > 0$ and nested sequence of downward closed sets $(\Lambda_n)_{n\geq 1}$ with $\#(\Lambda_n) = n$ such that

$$\|u - I_{\Lambda_n} u\|_{L^\infty(U,X)} \leq C(n+1)^{-s}, \quad s = \frac{1}{p} - 1.$$

Holmorphy and Smolyak Quadrature

For $\boldsymbol{\nu} \in \mathcal{F}$ define $I_{\boldsymbol{\nu}} := \bigotimes_{j\in\mathbb{N}} I_{\nu_j}$, $Q_{\boldsymbol{\nu}} := \bigotimes_{j\in\mathbb{N}} Q_{\nu_j}$, and *$\boldsymbol{\nu}$-increments*

$$\Delta_{\boldsymbol{\nu}}^{I} := \bigotimes_{j\in\mathbb{N}} (I_{\nu_j} - I_{\nu_j - 1}) = \sum_{\{\boldsymbol{e}\in\{0,1\}^{\mathbb{N}} : \boldsymbol{\nu}-\boldsymbol{e}\in\mathcal{F}\}} (-1)^{|\boldsymbol{e}|} I_{\boldsymbol{\nu}-\boldsymbol{e}}, \tag{3a}$$

$$\Delta_{\boldsymbol{\nu}}^{Q} := \bigotimes_{j\in\mathbb{N}} (Q_{\nu_j} - Q_{\nu_j - 1}) = \sum_{\{\boldsymbol{e}\in\{0,1\}^{\mathbb{N}} : \boldsymbol{\nu}-\boldsymbol{e}\in\mathcal{F}\}} (-1)^{|\boldsymbol{e}|} Q_{\boldsymbol{\nu}-\boldsymbol{e}} \ . \tag{3b}$$

For $\emptyset \neq \Lambda \subseteq \mathcal{F}$, downward closed with $|\Lambda| < \infty$

$$I_\Lambda := \sum_{\boldsymbol{\nu}\in\Lambda} \Delta_{\boldsymbol{\nu}}^{I} = \sum_{\boldsymbol{\nu}\in\Lambda} \left(\sum_{\{\boldsymbol{e}\in\{0,1\}^{\mathbb{N}} : \boldsymbol{\nu}+\boldsymbol{e}\in\Lambda\}} (-1)^{|\boldsymbol{e}|} \right) I_{\boldsymbol{\nu}}, \tag{4a}$$

$$Q_\Lambda := \sum_{\boldsymbol{\nu}\in\Lambda} \Delta_{\boldsymbol{\nu}}^{I} = \sum_{\boldsymbol{\nu}\in\Lambda} \left(\sum_{\{\boldsymbol{e}\in\{0,1\}^{\mathbb{N}} : \boldsymbol{\nu}+\boldsymbol{e}\in\Lambda\}} (-1)^{|\boldsymbol{e}|} \right) Q_{\boldsymbol{\nu}}, \tag{4b}$$

$$I_\emptyset := 0,\ Q_\emptyset := 0 \qquad \text{and} \qquad I_{\mathcal{F}} := \mathrm{Id},\ Q_{\mathcal{F}} := \int_U \cdot \ \mathrm{d}\mu(\boldsymbol{y}).$$

For every $f \in C^0(U, X)$ and for every index set $\Lambda \subseteq \mathcal{F}$ that is downward closed and finite,

$$Q_\Lambda f = \int_U I_\Lambda f(\boldsymbol{y}) \ \mathrm{d}\mu(\boldsymbol{y}) \ . \tag{5}$$

Holmorphy and Smolyak Quadrature

Theorem [Smolyak Convergence Rates for $(\boldsymbol{b}, \varepsilon)$-Holomorphic integrands (J. Zech & CS 2017)]

Let X be a Banach space, $U = [-1,1]^\infty$ and let μ be the uniform product probability measure on U. Assume $u : U \to X$ is strongly μ measurable and $(\boldsymbol{b}, \varepsilon)$-holomorphic with $\boldsymbol{b} \in \ell^p(\mathbb{N})$ for some $0 < p < 1$.
Then ex. $C > 0$ and, for every $N \in \mathbb{N}$ exists a dc set $\Lambda_N \subset \mathcal{F}$ with $|\Lambda_N| \leq N$, such that

$$\left\| \int_U u(\boldsymbol{y}) d\mu(\boldsymbol{y}) - Q_{\Lambda_N} u \right\|_X \leq C N^{-\left(\frac{2}{p}-1\right)} .$$

Remarks:

1. Proof is constructive: novel algorithm to locate Λ_N in work $\leq C N^{1+\varepsilon}$.
2. Also for integration w.r. to μ against densities $\varrho(\boldsymbol{y})$ which are $(\boldsymbol{b}, \varepsilon)$-holomorphic.
3. Analogous results for quadrature against gaussian measure γ (Zech & CS in preparation 2018).

Multilevel Stochastic Collocation under $(\boldsymbol{b},\varepsilon)$-Holomorphy

Theorem [J. Zech, D. Düng & ChS (2018)]

Assume

- discretization in X and X^{s} a linear [regularity] subspace of X, such that for every $n \in \mathbb{N}_0$ there exists a space $X_n \subseteq X$ of dimension at most n and a linear mapping $\Pi_n : X^{\mathrm{s}} \to X_n$ such that $\Pi_0 = 0$ and for all $v \in X^{\mathrm{s}}$

$$\|v - \Pi_n v\|_X \leq C(\alpha, X^{\mathrm{s}})(n+1)^{-\alpha}\|v\|_{X^{\mathrm{s}}}.$$

- that $p_0 \in (0,1)$, $p_1 \in [p_0, 1]$, $q \in [1,2]$ and that $u : U \to X^{\mathrm{s}}$ be $(\boldsymbol{b}_0, \varepsilon_0, X)$-holomorphic and $(\boldsymbol{b}_1, \varepsilon_1, X^{\mathrm{s}})$-holomorphic, with $\boldsymbol{b}_0 \in \ell^{p_0}(\mathbb{N})$, $\boldsymbol{b}_1 \in \ell^{p_1}(\mathbb{N})$. Additionally, assume X (but not X^{s}) to be a Hilbert space.

Then, for every $N \in \mathbb{N}$ there exists a gpc work-allocation $\mathbf{w}_N = (w_{N;\boldsymbol{\nu}})_{\boldsymbol{\nu}\in\mathcal{F}} \in \mathfrak{W}^{\mathcal{F}}$ from admissible work-measures $\mathfrak{W}$, with $|\mathbf{w}_N| \leq N$ such that

$$\|u(\boldsymbol{y}) - \sum_{\boldsymbol{\nu}\in\mathcal{F}} L_{\boldsymbol{\nu}}(\boldsymbol{y})\Pi_{w_{N;\boldsymbol{\nu}}} u_{\boldsymbol{\nu}}\|_{L^{q^*}(U,X)} \leq C \begin{cases} N^{-r(p_0,p_1,q,\alpha)/q^*} & \text{if } q^* < \infty \\ N^{-r(p_0,p_1,q,\alpha)} & \text{if } q^* = \infty \end{cases},$$

$$r(p_0,p_1,q,\alpha) := \begin{cases} \alpha q & \text{if } p_1 \leq \frac{q}{\alpha q+1}, \\ \beta(\frac{q}{p_0} - 1) & \text{if } p_1 > \frac{q}{\alpha q+1}, \end{cases} \quad \text{with} \quad \beta := \frac{\alpha}{\alpha + p_0^{-1} - p_1^{-1}}.$$

$(\boldsymbol{b},\varepsilon)$-Holomorhpy and DNNs

Consider parametric solution map $U \ni \boldsymbol{y} \to u(\boldsymbol{y}) \in X$, and QoI $G \in X'$:

$$\textbf{Response Surface:} \qquad f : U \to \mathbb{R} : \boldsymbol{y} \mapsto f(\boldsymbol{y}) := (G \circ u)(\boldsymbol{y}) \ .$$

Proposition[Zech and CS 2017]:
Let u be $(\boldsymbol{b},\varepsilon)$-holomorphic for some $\boldsymbol{b} \in \ell^p$, $p \in (0,1)$, $t_{\boldsymbol{\nu}} \in X$ Taylor gpc coefficient. Then

$$(\|t_{\boldsymbol{\nu}}\|_X)_{\boldsymbol{\nu}\in\mathcal{F}} \in \ell^p(\mathcal{F}).$$

There exists a constant $C > 0$ as well as a sequence of nested, finite and downward closed index sets $\Lambda_N \subset \mathcal{F}$ such that $|\Lambda_N| \leq N$ for all $N \in \mathbb{N}$ and, for $f_{\boldsymbol{\nu}} := G(t_{\boldsymbol{\nu}})$,

1. $\sum_{\boldsymbol{\nu}\notin\Lambda_N} |f_{\boldsymbol{\nu}}| \leq CN^{1-1/p}$, 2. $\sup_{\boldsymbol{\nu}\in\Lambda_N} |\boldsymbol{\nu}|_1 \leq C(1+\log(N))$.

$(\boldsymbol{b}, \varepsilon)$-Holomorhpy and DNNs: Definition of DNNs

Consider deep *feedforward NNs* (FFNNs for short):

- NNs consist of layers of computational nodes and define a function $\tilde{f} : \mathbb{R}^n \to \mathbb{R} : \boldsymbol{x} \mapsto f(\boldsymbol{x})$.
- L number of hidden layers in the NN, “depth” of NN, N_ℓ the number of compute nodes in layer ℓ.
- $N = \sum_{\ell=1}^{L} N_\ell$ is total number of nodes in the NN; “number of degrees of freedom” or *size* of the NN.
- $\boldsymbol{x} = (x_1, ..., x_n) \in \mathbb{R}^n$ will denote the input of the DNN, z_j^ℓ denotes the output of unit j in layer $\ell + 1$, b_j^ℓ denotes the “bias” of unit j in layer ℓ.

$(\boldsymbol{b}, \varepsilon)$-Holomorhpy and DNNs: Definition of DNNs

Deep FFNN $\boldsymbol{x} \mapsto f(\boldsymbol{x})$ characterized by:

1. *input layer*

$$z_j^1 := \sigma\left(\sum_{i=1}^{d} w_{i,j}^0 x_i + b_j^1\right) \ , \quad j \in \{1, \dots, N_1\} \ ,$$

2. $L-1$ "hidden layers":

$$z_j^{\ell+1} := \sigma\left(\sum_{i=1}^{N_\ell} w_{i,j}^\ell z_i^\ell + b_j^{\ell+1}\right) \ , \quad \ell \in \{1, \dots, L-1\}, \ \ j \in \{1, \dots, N_{\ell+1}\} \ ,$$

3. *output layer*

$$f(\boldsymbol{x}) := \sum_{i=1}^{N_L} w_{i,1}^L z_i^L + b_1^{L+1} \ .$$

$\sigma(\cdot)$ *activation function*: **"Rectifier Linear Unit"** (ReLU) $\sigma(x) = \max\{0, x\}$.

$(\boldsymbol{b}, \varepsilon)$-Holomorhpy and DNNs: Expression Theorem for DNN surrogates

Theorem [Zech & CS (2017)]
Assume $f : U \to \mathbb{R}$ be $(\boldsymbol{b}, \varepsilon)$-holomorphic for some $\boldsymbol{b} \in \ell^p(\mathbb{N})$, with some $p \in (0, 1)$.
Then for every $N \in \mathbb{N}$ there exists FFNN ReLU network $\tilde{f}(y_1, \ldots, y_N)$ with

1. N input units
2. size bounded by $C(1 + N \log(N) \log\log(N))$, and
3. depth is bounded by $C(1 + \log(N) \log\log(N))$ (not so deep...)

which satisfies the uniform [“worst case”] bounds

$$\sup_{\boldsymbol{y} \in U} |f(\boldsymbol{y}) - \tilde{f}(y_1, \ldots, y_N)| \le C N^{1-1/p} \ .$$

Quasi Monte-Carlo Integration for $(\boldsymbol{b}, \varepsilon)$-holomorhpic integrands

- Consider *general* s-variate integrand $F \in C^0([0,1]^s)$. Approximate s-dimensional integral

$$I_s(F) := \int_{[0,1]^s} F(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} \tag{6}$$

where $F(\boldsymbol{y}) = G(u_s^h(\boldsymbol{y} - \frac{\mathbf{1}}{\mathbf{2}}))$ by

- N-point QMC quadrature: **equal-weight quadrature** rule

$$Q_{N,s}(F) := \frac{1}{N} \sum_{n=0}^{N-1} F(\boldsymbol{y}_n)\ , \tag{7}$$

with N points $\boldsymbol{y}_0, \ldots, \boldsymbol{y}_{N-1} \in [0,1]^s$ from suitable digital net in $[0,1]^s$.

Quasi Monte-Carlo Integration for $(\boldsymbol{b}, \varepsilon)$-holomorphic integrands

Theorem (SLHoQMC) [Dick, LeGia, CS (SIAM JUQ 2016)]
Let $s \geq 1$ and $N = b^m$ for $m \geq 1$ and prime b. Let $\boldsymbol{\beta} = (\beta_j)_{j\geq 1}$ be a sequence of positive numbers s.t.

$$\exists\, 0 < p < 1 : \quad \sum_{j=1}^{\infty} \beta_j^p < \infty \,.$$

Define $\boldsymbol{\beta}_{\{1:s\}} = (\beta_j)_{1\leq j\leq s}$ and

$$\alpha \;:=\; \lfloor 1/p \rfloor + 1 \,.$$

Assume that the integrand function $F : U \to \mathbb{R}$ is $(\boldsymbol{\beta}, \varepsilon)$-holomorphic.

Then, an interlaced polynomial lattice rule of order $\alpha \geq 1$ with N points can be constructed using a fast component-by-component algorithm, with **cost** $\mathcal{O}(\alpha\, s\, N \log N + \alpha^2\, s^2 N)$ **operations**, such that

$$|I_s(F) - Q_{N,s}(F)| \;\leq\; C_{\alpha,\boldsymbol{\beta},b,p}\, N^{-1/p} \,,$$

where $C_{\alpha,\boldsymbol{\beta},b,p} < \infty$ is independent of s and N.

Combined Error Bound

Corollary (SL HoQMC PG)

1. Approximate $I(G(u(\cdot)))$ by dimension-truncation and interlaced polynomial lattice rule of

   order $\alpha = \lfloor 1/p \rfloor + 1$, with$N = b^m$ points in s dimensions,

   with PG discretization in D with subspace $\mathcal{X}^h$ with $M_h = \dim(\mathcal{X}^h)$ DoF, cost $\mathcal{O}(M_h)$.

   Then ex. $C > 0$ independent of s, h and N such that with $\tau = t + t'$

   $$|I(G(u)) - Q_{N,s}(G(u_s^h))| \leq C \left((s^{-2(1/p-1)} + N^{-1/p}) \|f\|_{\mathcal{Y}'} \|G(\cdot)\|_{\mathcal{X}'} + h^\tau \|f\|_{\mathcal{Y}'_t} \|G(\cdot)\|_{\mathcal{X}'_{t'}} \right) .$$

2. Cost for evaluation of $Q_{N,s}(G(u_s^h))$ is $\mathcal{O}(sNM_h)$ operations.

3. Cost for CBC construction of (Cools, Kuo, Nuyens 2006) of the interlaced polynomial lattice rule

   $\mathcal{O}(\alpha\, s\, N \log N + \alpha^2 s^2 N)$ operations, $\qquad \mathcal{O}(\alpha\, s\, N)$ memory .

Proof

$$I(G(u)) - Q_{N,s}(G(u_s^h)) = [I(G(u)) - I(G(u_s))] + [I(G(u_s)) - I(G(u_s^h))] + [I(G(u_s^h)) - Q_{N,s}(G(u_s^h))] .$$

$\square$

Shape Holomorphy for NSE

Stationary Navier-Stokes Equation (NSE):

$$-\Delta u + (u \cdot \nabla) u + \nabla p = f \qquad \text{in } \mathrm{D}, \tag{8a}$$

$$\operatorname{div} u = 0 \qquad \text{in } \mathrm{D}, \tag{8b}$$

$$u = 0 \qquad \text{on } \partial \mathrm{D}. \tag{8c}$$

Weak Formulation:

$$\begin{cases} a(u,v) - b(v,p) + t(u,u,v) = F(v), & v \in H_0^1(\mathrm{D})^d, \\ b(u,q) = 0, & q \in L^2_{\#}(\mathrm{D}), \end{cases}$$

where $F(v) := \int_{\mathrm{D}} f \cdot v \, \mathrm{d}x$ and, with $\nabla u \cdot \nabla v = \operatorname{tr}(\nabla u \nabla v^\top)$, $\nabla u := \left(\frac{\partial u_i}{\partial x_j}\right)_{i,j=1,\dots,d}$,

$$a(u,v) := \int_{\mathrm{D}} \nabla u \cdot \nabla v \, \mathrm{d}x \quad \text{and} \quad b(u,v) = \int_{\mathrm{D}} \operatorname{div}(v) p \, \mathrm{d}x,$$

$$t(u,v,w) = \int_{\mathrm{D}} (u \cdot \nabla) v \cdot w \, \mathrm{d}x, \qquad u,v,w \in H_0^1(\mathrm{D})^d \, .$$

$t(\cdot,\cdot,\cdot)$ is continuous on $H_0^1(\mathrm{D})^d \times H_0^1(\mathrm{D})^d \times H_0^1(\mathrm{D})^d$ and antisymmetric in the last two arguments if $\operatorname{div}(u) = 0$.

Shape Holomorphy for NSE: Domain Transformation

- NSE in *nominal domain* $\hat{\mathrm{D}}$ which are satisfied by the pullback of solutions in the *physical domain* D.
- $T : \hat{\mathrm{D}} \to \mathrm{D}$ denotes a bijective bi-Lipschitz map between these Lipschitz domains.
- With $T^{-1} : \mathrm{D} \to \hat{\mathrm{D}}$, $T \in W^{1,\infty}(\hat{\mathrm{D}})^d$ and $T^{-1} \in W^{1,\infty}(\mathrm{D})^d$.
- Assume Jacobian determinant of T positive a.e. in $\hat{\mathrm{D}}$.

Remark: For a Lipschitz domain $\hat{\mathrm{D}} \subseteq \mathbb{R}^d$ and a bijective bi-Lipschitz transformation $T : \mathbb{R}^d \to \mathbb{R}^d$,

$$\mathrm{D} := T(\hat{\mathrm{D}}) \subseteq \mathbb{R}^d \text{ need not be Lipschitz.}$$

We *assume* both $\hat{\mathrm{D}}$ as well as D to be Lipschitz domains.

Shape Holomorphy for NSE: Domain Transformation

Plain pullback transformation:

$$\hat{\varphi}(\hat{x}) = \varphi(x) \quad \text{i.e.} \quad \hat{\varphi} := \varphi \circ T \ .$$

The maps

$$p \in L^2_{\#}(\hat{\mathrm{D}}) \qquad \text{and} \qquad H^1_0(\mathrm{D})^d \ni u \mapsto \hat{u} \in H^1_0(\hat{\mathrm{D}})^d,$$

are isomorphisms: for any constant c, $\hat{c} = c$ and thus

$$\|p - c\|_{L^2(\mathrm{D})} = \|(\hat{p} - c)J^{1/2}\|_{L^2(\hat{\mathrm{D}})}, \quad m_0\|\hat{p}\|_{L^2_{\#}(\hat{\mathrm{D}})} \le \|p\|_{L^2_{\#}(\mathrm{D})} \le M_0\|\hat{p}\|_{L^2_{\#}(\hat{\mathrm{D}})},$$

where $m_0 = m_0(T) := \min_{\hat{x}\in\hat{\mathrm{D}}} J^{1/2}(\hat{x}) > 0$ and $M_0 = M_0(T) := \max_{\hat{x}\in\hat{\mathrm{D}}} J^{1/2}(\hat{x}) < \infty$.

$$\|u\|^2_{H^1_0(\mathrm{D})^d} = \int_{\mathrm{D}} \nabla u \cdot \nabla u \,\mathrm{d}x = \int_{\mathrm{D}} \mathrm{tr}\,(\nabla u \nabla u^\top)\,\mathrm{d}x = \int_{\hat{\mathrm{D}}} \mathrm{tr}(\nabla \hat{u}\, dT^{-1} dT^{-\top} \nabla \hat{u}^\top) J \,\mathrm{d}\hat{x}.$$

$$m_1\|\hat{u}\|_{H^1_0(\hat{\mathrm{D}})} \le \|u\|_{H^1_0(\mathrm{D})} \le M_1\|\hat{u}\|_{H^1_0(\hat{\mathrm{D}})},$$

where $m_1 = m_1(T) := \min_{\hat{x}\in\hat{\mathrm{D}}} J^{1/2}(\hat{x})\|dT(\hat{x})\|^{-1}$ and $M_1 = M_1(T) := \max_{\hat{x}\in\hat{\mathrm{D}}} J^{1/2}(\hat{x})\|dT^{-1}(\hat{x})\|$.
Duality:

$$H^{-1}(\mathrm{D})^d \ni f \mapsto \hat{f} \in H^{-1}(\hat{\mathrm{D}})^d,$$

isomorphism with constants M_1^{-1} and m_1^{-1}.

Shape Holomorphy for NSE: Pullback of NSE

Define

$$X := H^1_0(\hat{\mathrm{D}})^d \times L^2_{\#}(\hat{\mathrm{D}}) \;.$$

Pullback NSE: Find $(\hat{u},\hat{p}) \in X$ such that for all $(\hat{v},\hat{q}) \in X$:

$$\begin{cases} a_T(\hat{u},\hat{v}) - b_T(\hat{v},\hat{p}) + t_T(\hat{u},\hat{u},\hat{v}) = F_T(\hat{v}), & \hat{v} \in H^1_0(\hat{\mathrm{D}})^d, \\ b_T(\hat{u},\hat{q}) = 0, & \hat{q} \in L^2_{\#}(\hat{\mathrm{D}}). \end{cases}$$

$$a_T(\hat{u},\hat{v}) := \int_{\hat{\mathrm{D}}} \mathrm{tr}(\nabla \hat{u}\, dT^{-1} dT^{-\top} \nabla \hat{v}^\top) J \,\mathrm{d}\hat{x},\; b_T(\hat{v},\hat{p}) := \int_{\hat{\mathrm{D}}} \mathrm{tr}(\nabla \hat{v}\, dT^{-1}) \hat{p} J \,\mathrm{d}\hat{x},\; F_T(\hat{v}) := \int_{\hat{\mathrm{D}}} \hat{f} \cdot \hat{v} J \,\mathrm{d}\hat{x},$$

$$t_T(\hat{u},\hat{v},\hat{w}) := \int_{\hat{\mathrm{D}}} (dT^{-1}\hat{u} \cdot \nabla)\hat{v} \cdot \hat{w} J \,\mathrm{d}\hat{x}.$$

"Usual" argument (due to H. Hopf: Galerkin + Compactness) $\Longrightarrow$ Ex. solution $(\hat{u},\hat{p}) \in X$.

Domain-to-Solution map

$$T \mapsto (\hat{u}_T, \hat{p}_T) \quad \text{well-defined} \;.$$

Shape Holomorphy for NSE: Relation to Shape Derivative

Remark: The differential of domain-to-pullback solution map

$$\mathcal{S} : T \mapsto (\hat{u}_T, \hat{p}_T), \qquad T \in \mathfrak{T}$$

is related to the *material derivative*: If $V = V(x,t)$ is a vector field and T_t the corresponding flow, and if u_Ω is the solution to some given PDE for the domain Ω, define

$$\dot{u}(\Omega, V) = \lim_{t \to 0} \frac{1}{t}\big(u_{T_t(\Omega)} \circ T_t - u_\Omega\big)$$

(limit in a given topology, eg. in strong sense for a Sobolev space $W^{m,p}(\Omega)$).

Then, if $\mathcal{F}_T$ is the Fréchet derivative at T of the map $T \mapsto \hat{u}_T$ for this topology,

$$\dot{u}(\mathrm{D}_T, V) = \mathcal{F}_T(V_0 \circ T) \circ T^{-1}, \quad V_0 = V(\cdot, 0).$$

Shape Holomorphy for NSE: Assumptions

Compactness Assumption:
$\mathfrak{T}$ is compact in $W^{1,\infty}(\hat{\mathrm{D}},\mathbb{R})^d$, $T^{-1} \in W^{1,\infty}(\mathrm{D},\mathbb{R})^d$ for every $T \in \mathfrak{T}$, where $\mathrm{D}_T = T(\hat{\mathrm{D}})$ is Lipschitz.
Analyticity Assumption:
The function f is real-analytic in an open neighborhood of $\overline{\mathrm{D}}_H$, where

$$\mathrm{D}_H = \bigcup_{T\in\mathfrak{T}} T(\hat{\mathrm{D}}) \subseteq \mathbb{R}^d \qquad \text{“Hold-all” domain}$$

Complex valued domain transformations: ε-neighborhood of $\mathfrak{T}$,

$$\mathfrak{T}_\varepsilon := \{\tilde{T} \in W^{1,\infty}(\hat{\mathrm{D}},\mathbb{C})^d \,:\, \exists T \in \mathfrak{T},\ \|\tilde{T} - T\|_{W^{1,\infty}(\hat{\mathrm{D}})^d} < \varepsilon\}\ .$$

Lemma:
Let $T \in W^{1,\infty}(\hat{\mathrm{D}},\mathbb{C})^d$ with $\operatorname{ess\,sup}_{\hat{x}\in\hat{\mathrm{D}}} \det dT(\hat{x}) > 0$. Then

$$F_1 : \begin{cases} W^{1,\infty}(\hat{\mathrm{D}},\mathbb{C})^d \to L^\infty(\hat{\mathrm{D}},\mathbb{C})^d, \\ T \mapsto \det dT, \end{cases} \qquad F_2 : \begin{cases} W^{1,\infty}(\hat{\mathrm{D}},\mathbb{C})^d \to L^\infty(\hat{\mathrm{D}},\mathbb{C})^{d\times d}, \\ T \mapsto dT^{-1}, \end{cases}$$

are locally holomorphic around T with Fréchet derivatives in direction $H \in W^{1,\infty}(\hat{\mathrm{D}},\mathbb{C})^d$ given by

$$dF_1(T)(H) = \operatorname{tr}(\operatorname{Cof}(dT^\top)dH) \qquad \text{and} \qquad dF_2(T)(H) = -dT^{-1}dH\,dT^{-1}.$$

Shape Holomorphy for NSE: Main Result

Theorem:
There exists $\varepsilon = \varepsilon(\hat{\mathrm{D}}, \mathfrak{T}) > 0$ such that the domain-to-solution map $\mathcal{S} : T \mapsto (\hat{u}_T, \hat{p}_T)$, $(\hat{u}_T, \hat{p}_T)$ solving NSE, admits an extension on $\mathfrak{T}_\varepsilon$ which is holomorphic and uniformly bounded as a mapping from $\mathfrak{T}_\varepsilon \subseteq W^{1,\infty}(\hat{\mathrm{D}}, \mathbb{C})^d$ to $X_{\mathbb{C}} := H^1_0(\hat{\mathrm{D}}, \mathbb{C})^d \times L^2_{\#}(\hat{\mathrm{D}}, \mathbb{C})$.
Proof: Derivative $d\mathcal{S}(T)(H)$ of $\mathcal{S}$ at $T \in \mathfrak{T}$ in direction $H \in W^{1,\infty}(\hat{\mathrm{D}}, \mathbb{C})^d$ is unique solution $(\hat{w}, \hat{r}) \in X_{\mathbb{C}}$ of

$$
\begin{aligned}
&a_T(\hat{w}, \hat{v}) - b_T(\hat{v}, \hat{r}) + t_T(\hat{u}_T, \hat{w}, \hat{v}) + t_T(\hat{w}, \hat{u}_T, \hat{v}) = \\
&\quad \int_{\hat{\mathrm{D}}} \mathrm{tr}\left(\nabla \hat{u}_T \left[J(dT^{-1} dH dT^{-1} dT^{-\top} + dT^{-1} dT^{-\top} dH^\top dT^{-\top}) - \mathrm{tr}(\mathrm{Cof}(dT)^\top dH) dT^{-1} dT^{-\top}\right] \nabla \hat{v}^\top\right) \, \mathrm{d}\hat{x} \\
&\quad - \int_{\hat{\mathrm{D}}} \mathrm{tr}\left(\nabla \hat{v} \left[J dT^{-1} dH dT^{-1} - \mathrm{tr}(\mathrm{Cof}(dT)^\top dH) dT^{-1}\right]\right) \hat{p}_T \, \mathrm{d}\hat{x} \\
&\quad + \int_{\hat{\mathrm{D}}} (dT^{-1} dH dT^{-1} J - dT^{-1} \mathrm{tr}(\mathrm{Cof}(dT)^\top dH)(\hat{u}_T \cdot \nabla) \hat{u}_T \cdot \hat{v} \, \mathrm{d}\hat{x} \\
&\quad + \int_{\hat{\mathrm{D}}} (df \circ T) H \cdot \hat{v} J \, \mathrm{d}\hat{x} + \int_{\hat{\mathrm{D}}} \hat{f}_T \cdot \hat{v} \, \mathrm{tr}(\mathrm{Cof}(dT)^\top dH) \, \mathrm{d}\hat{x}, \\
&b_T(\hat{w}, \hat{q}) = \int_{\hat{\mathrm{D}}} \mathrm{tr}\left(\nabla \hat{u}_T \left[J dT^{-1} dH dT^{-1} - \mathrm{tr}(\mathrm{Cof}(dT)^\top dH) dT^{-1}\right]\right) \hat{q} \, \mathrm{d}\hat{x},
\end{aligned}
$$

for all $(\hat{v}, \hat{q}) \in X_{\mathbb{C}}$. $\square$

Shape Holomorphy for NSE: “Numerical” Consequences

Parametric domain transformations:
Define, for $\mathrm{D} \subseteq \mathbb{R}^d$

$$S(\mathrm{D}) = W^{1,\infty}(\mathrm{D})^d.$$

Uncertainty Parametrization: Assume $\boldsymbol{y} \to T_{\boldsymbol{y}}$ affine (eg. Fourier, spline or wavelet representations).

Let $\overline{T} \in S(\hat{\mathrm{D}})$ be such that $\overline{T}^{-1} \in S(\overline{T}(\hat{\mathrm{D}}))$, and $\psi_j \in S(\hat{\mathrm{D}})$ for every $j \in \mathbb{N}$. Then $\overline{T}$ is bi-Lipschitz and there exists $0 < \kappa_1 \leq \kappa_2 < \infty$ s.t. for each a, b, satisfying $\mathrm{conv}(a, b) \subset \hat{\mathrm{D}}$,

$$\kappa_1 \|a - b\| \leq \|\overline{T}(a) - \overline{T}(b)\| \leq \kappa_2 \|a - b\|. \tag{10}$$

Then

$$T_{\boldsymbol{y}} := \overline{T} + \sum_{j \in \mathbb{N}} y_j \psi_j \qquad \boldsymbol{y} = (y_j)_{j \geq 1} \in U\ . \tag{11}$$

Shape Holomorphy for NSE: Consequences

Assumption:

- For $\boldsymbol{b} = (b_j)_{j\geq 1}$ defined by $b_j := \|\psi_j\|_{S(\hat{\mathrm{D}})}$, $j \in \mathbb{N}$, exists $p \in (0,1)$ with $\boldsymbol{b} \in \ell^p$.
- In addition, $T_{\boldsymbol{y}}$ is invertible with $T_{\boldsymbol{y}}^{-1} \in S(T_{\boldsymbol{y}}(\hat{\mathrm{D}}))$ for all $\boldsymbol{y} \in U$.

Theorem:

1. The map $\boldsymbol{y} \mapsto T_{\boldsymbol{y}}$ is continuous from U equipped with the product topology to $S(\hat{\mathrm{D}})$, and the family

$$\mathfrak{T} := \{T_{\boldsymbol{y}} \,:\, \boldsymbol{y} \in U\} \quad \text{is compact in } S(\hat{\mathrm{D}}) \,.$$

2. The map $\boldsymbol{y} \mapsto T_{\boldsymbol{y}}$ is $(\boldsymbol{b}, \varepsilon)$-holomorphic for any $\varepsilon > 0$.
3. Denote by $(\hat{u}(\boldsymbol{y}), \hat{p}(\boldsymbol{y})) \in X = H_0^1(\hat{\mathrm{D}})^d \times L^2_{\#}(\hat{\mathrm{D}})$ the solution of NSE w.r. to $\{T_{\boldsymbol{y}} : \boldsymbol{y} \in U\}$.
   Then exists $\varepsilon > 0$ such that the parameter-to-solution map

$$U \ni \boldsymbol{z} \mapsto (\hat{u}(\boldsymbol{y}), \hat{p}(\boldsymbol{y})) \in X$$

is $(\boldsymbol{b}, \varepsilon)$-holomorphic.
   In addition this map is continuous from U equipped with the product topology to X.

UQ for Fractional Diffusion

Recall Example 1: linear diffusion problem in D bdd., Lipschitz. Given $f \in H^{-1}(\mathrm{D})$, find $u \in H_0^1(\mathrm{D})$ s.t.

$$f + \mathcal{P}(\boldsymbol{y})u(\boldsymbol{y}) = 0 \quad \text{in} \quad H^{-1}(\mathrm{D}) \; , \quad u(\boldsymbol{y})|_{\partial\mathrm{D}} = 0 \; .$$

Here

$$\mathcal{P}(\boldsymbol{y})u = -\nabla_x \cdot (a(\boldsymbol{y})\nabla u)$$

Affine parametric $a \in \mathcal{A}_{adm}$:

$$a(x, \boldsymbol{y}) = \bar{a}(x) + \sum_{j \geq 1} y_j \psi_j(x)$$

Given $0 < s \leq 1$, $\boldsymbol{y} \in U$, find $u(\boldsymbol{y})$ such that

$$(\mathcal{P}(\boldsymbol{y}))^s u = f \quad \text{in} \quad \mathrm{D} \; , \qquad u|_{\partial\mathrm{D}} = 0 \; .$$

- although $\boldsymbol{y} \to a(\cdot, \boldsymbol{y})$ is affine, $\boldsymbol{y} \to \mathcal{L}(\boldsymbol{y})^s$ is not for $0 < s < 1$.
- however, $\boldsymbol{y} \to \mathcal{L}(\boldsymbol{y})^s$ is (formally) composition of
  1. Affine-parametric function $\boldsymbol{y} \to \mathcal{L}(\boldsymbol{y}) \in \mathcal{L}_{iso}(H_0^1(\mathrm{D}), H^{-1}(\mathrm{D}))$ (which is $(\boldsymbol{b}, \varepsilon)$-holomorphic)
  2. with $\zeta \to \zeta^s$ (which is holomorphic on $\sigma(\mathcal{L}(\boldsymbol{y}))$).

Proposition[Herrmann, CS, Zech (2018)]:
For every $0 < s < 1$, parameter-to-solution map $\boldsymbol{y} \to u(\boldsymbol{y}) \in H_0^s(\mathrm{D})$ is $(\boldsymbol{b}, \varepsilon)$-holomorphic.

Conclusions

- UQ with distributed, uncertain input $\simeq$ infinite-dimensional, holomorphic-parametric operator equations,
- Advection-Diffusion, Helmholtz in random media, random domains, parabolic PDEs,...
- **Sparsity**: expressed in terms of gpc coefficient summability of responses
- implied by $(\boldsymbol{b}, \varepsilon)$-holomorphy
- parametric $(\boldsymbol{b}, \varepsilon)$-holomorphy implies dimension-independent convergence rates of SC, SG, CS, QMC, RB,... with rate determined only by sparsity of the input.
- Uncertainty parametrization: highly non-unique. Choose **parsimonious** and **well-conditioned** representation systems $\{\psi_j\}_{j\geq 1}$.
- DNNs can provide, *in principle*, very compact surrogates to complicated response surfaces from holomorphic forward maps, at moderate depth, in forward and (Bayesian) inverse UQ.

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Thank You.