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Adaptive multi-index collocation for quantifying uncertainty in an aerospace nozzle

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Explore and predict with confidence

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Nozzle Aero-Thermal-Structural Design

Inspired by the X-47B aircraft

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Application

- Unmanned combat vehicle aircraft demonstrator, capable of carrier take-off and landing
- Complex nozzle shape integrated into aft end of vehicle
- Advanced materials and significant heat environment and thermal management issues
- Nozzle weight is a substantial portion of the overall propulsion system weight
- Uncertainties in all areas of multi-physics problem
- Complex multi-physics analysis and design problem

Top image: Northrop Grumman X-47B UCAS Data-sheet, 2015
Bottom image Ferguson et al, Virginia Tech X-47 A/B student presentation, 2015

Multidisciplinary analysis (MDA)

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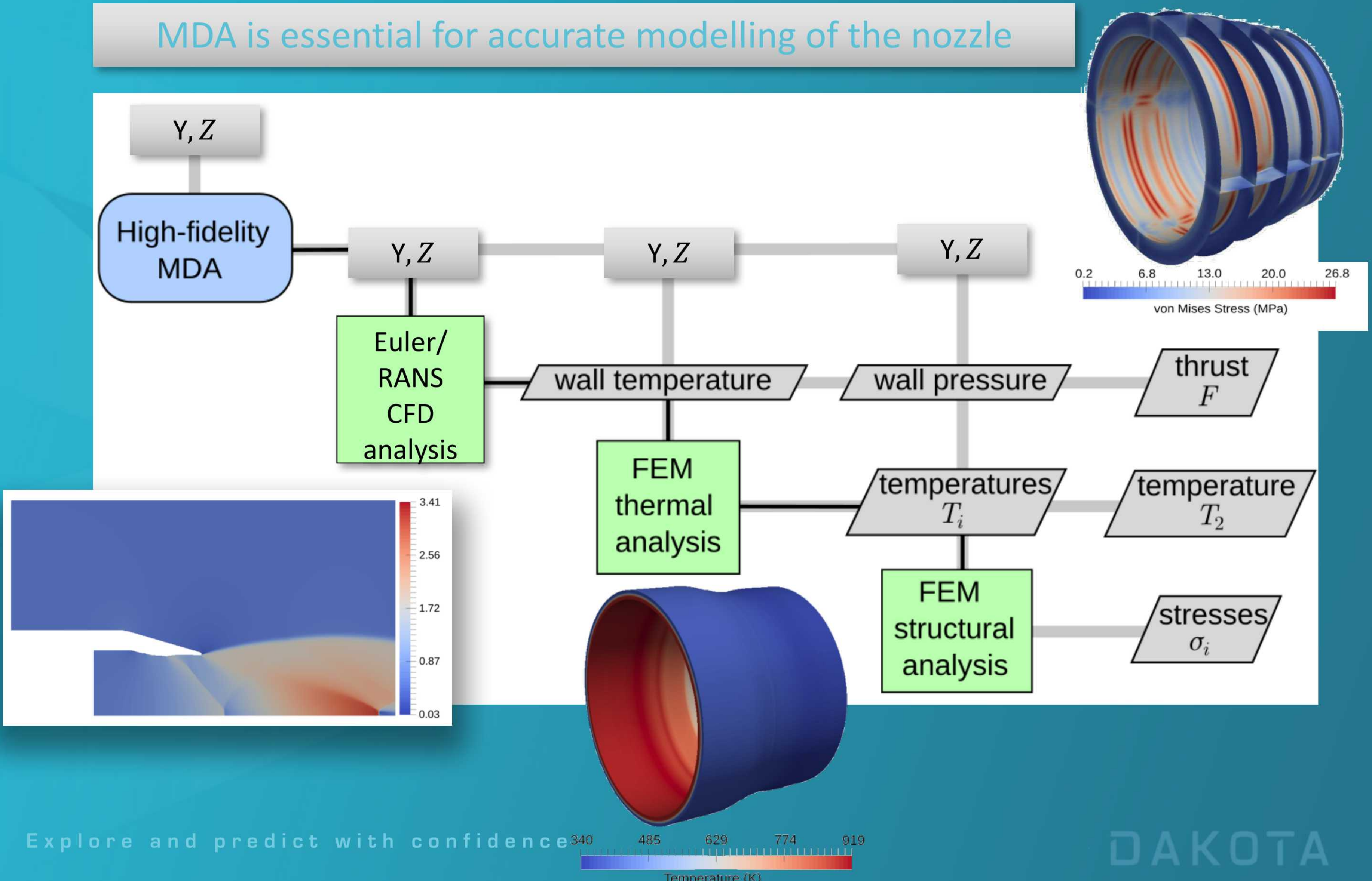
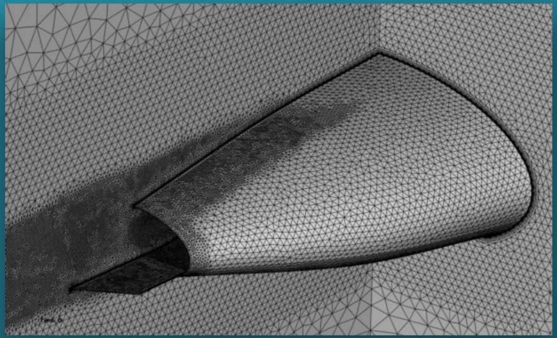
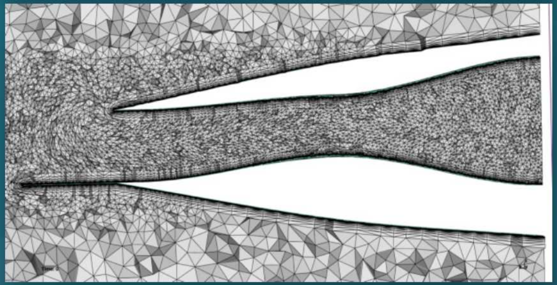
MDA is essential for accurate modelling of the nozzle



Aero Analysis

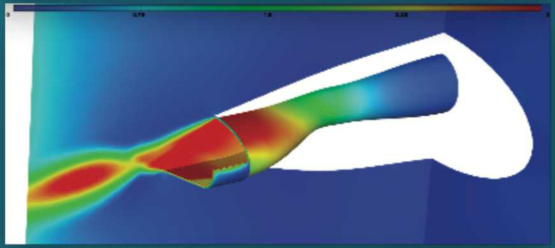


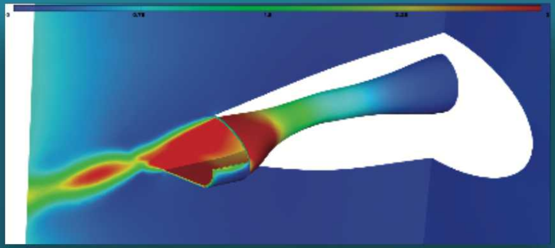


3D RANS CFD computation

Steady analysis: engine transients do not impact problem formulation sufficiently to justify cost of unsteady analysis (AFRL visit)

Model is fully automated and robust with respect to nozzle shape perturbations





Fluid-Structure Interface

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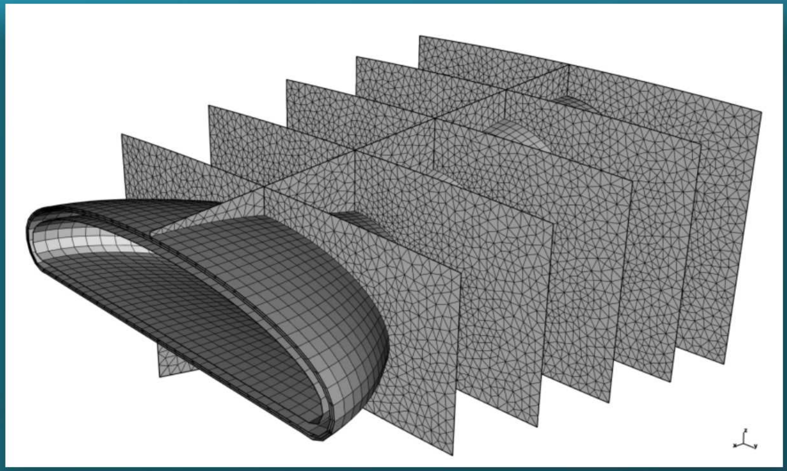
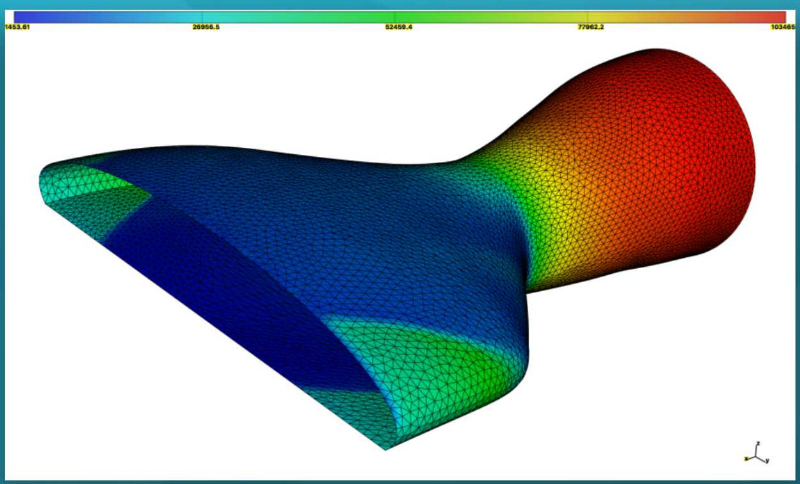
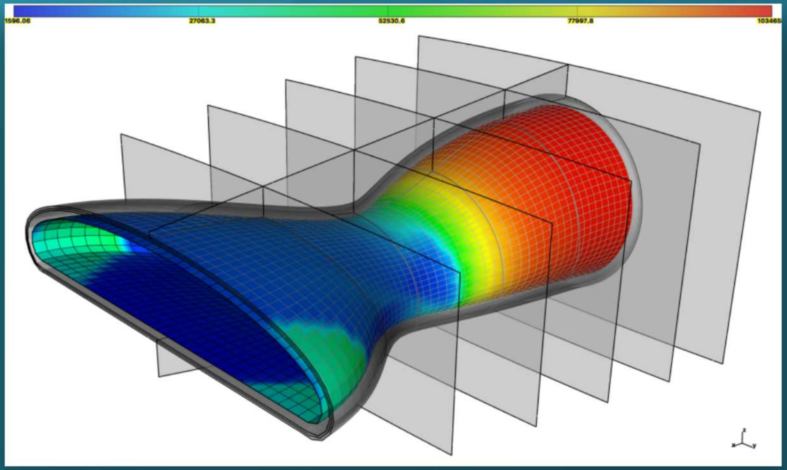
The wall pressure and temperature computed using the aero analysis are interpolated onto the structural mesh



Mesh for the thermo-structural analysis



CFD mesh / pressure



Interpolated pressure onto structural mesh

Thermo-structural Analysis

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Thermal analysis : wall layers + air gap

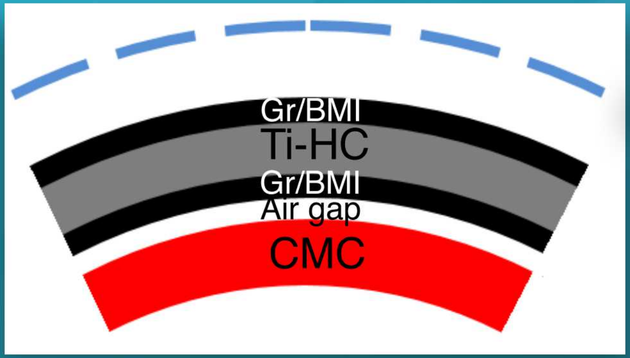
Conduction & convection modeled

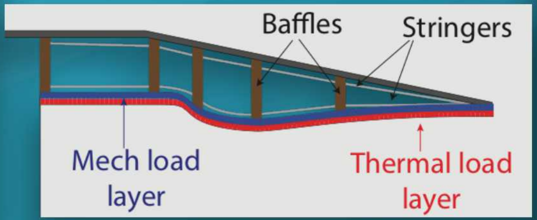
BC: prescribed temperature on inner surface of innermost layer; convection on outer surface of outermost layer

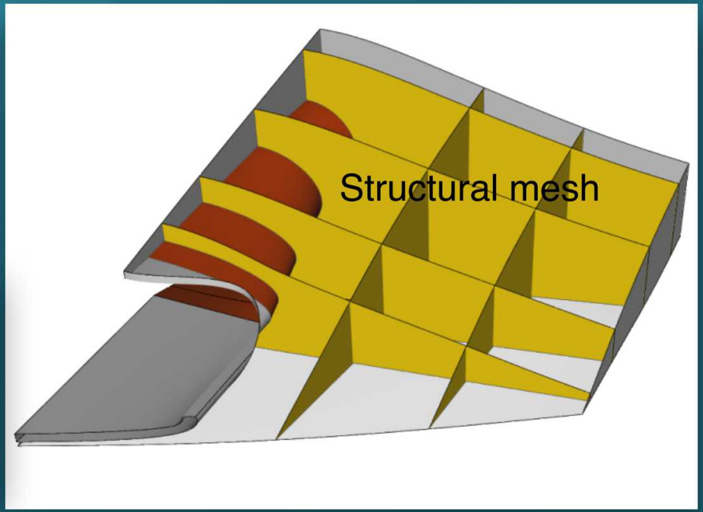
Structural analysis: wall layers, stringers, baffles

Material failure criterion (e.g. maximum strain) available for composite materials

Pressure and temperature-induced forces in load layers, only temperature-induced forces in thermal layer







Multifidelity Modeling

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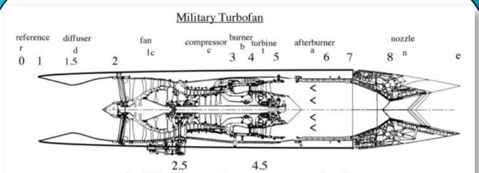
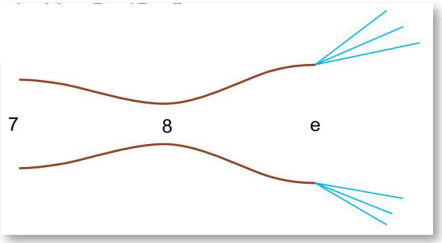
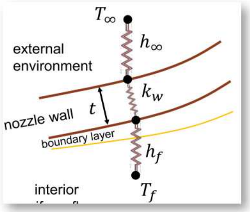


1-D engine model



Ideal and non-ideal nozzle aero

Analytic or

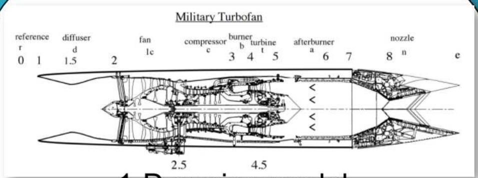


1-D Heat Transfer

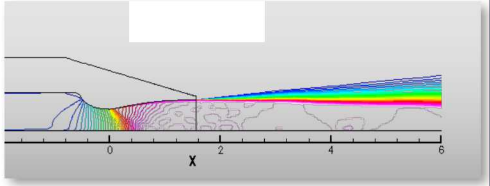
$$\sigma(x) = P(x)\frac{D(x)}{2t(x)}$$

Simplified hoop stresses

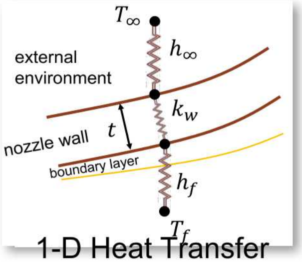
LOW FIDELITY



1-D engine model



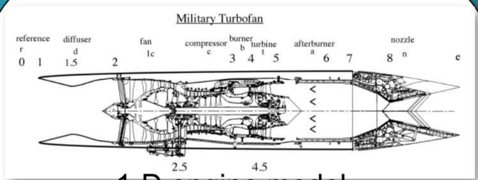
2D Axisymmetric Euler/RANS aero



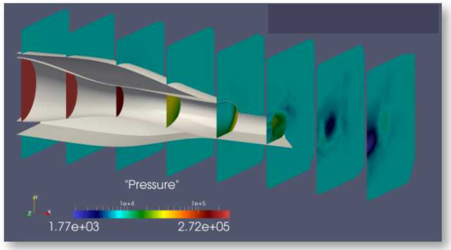
1-D Heat Transfer

Coarse FEM structural model

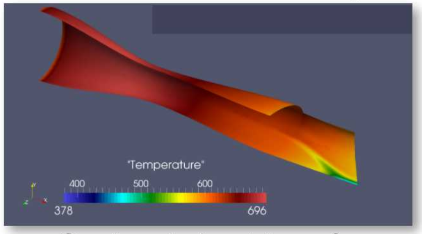
MEDIUM FIDELITY



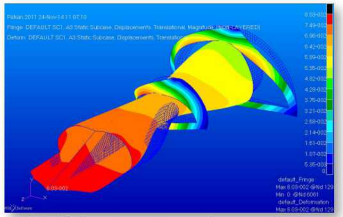
1-D engine model



3D Euler/RANS nozzle aerodynamics



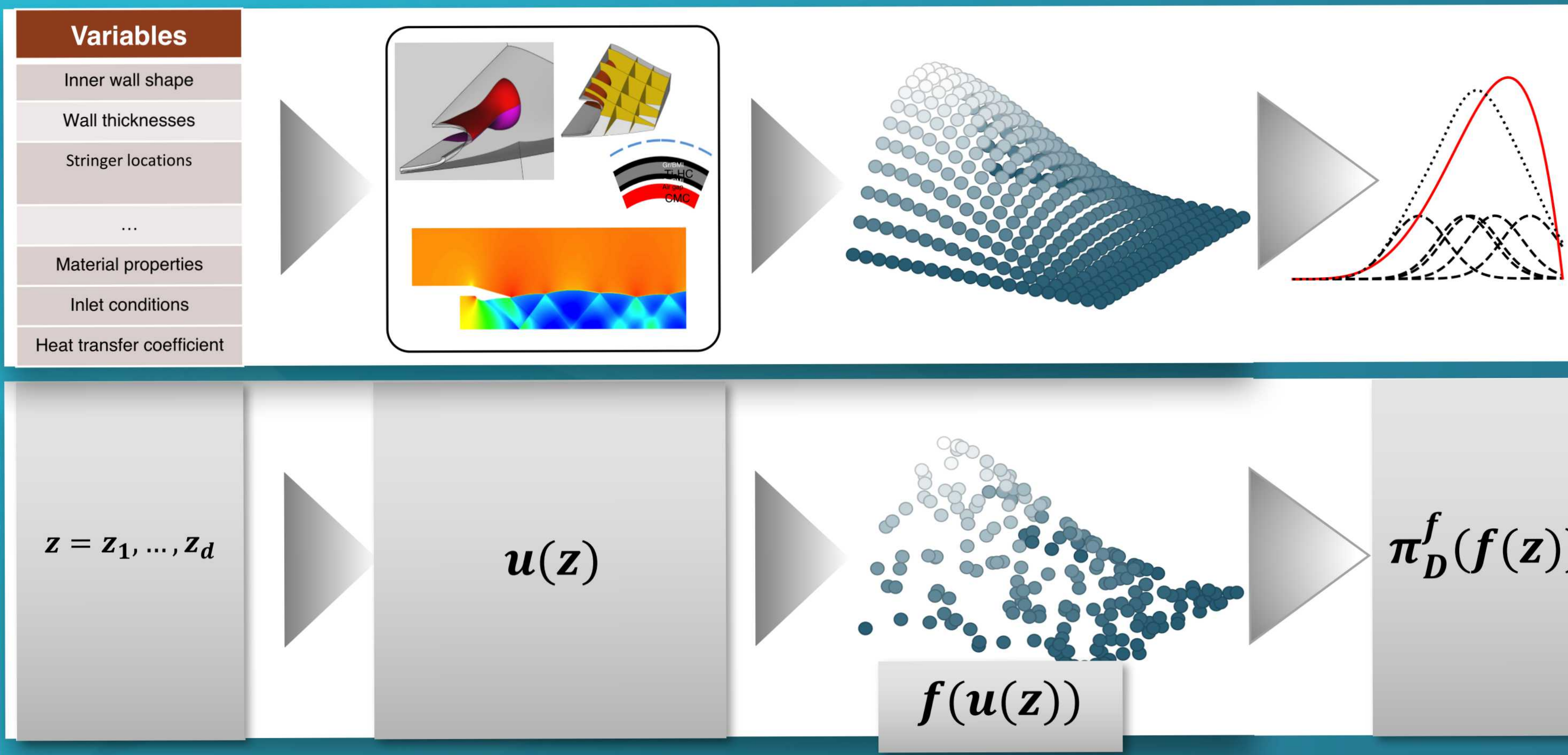
Conjugate heat transfer



FEM structural model

HIGH FIDELITY

Forward UQ



Must compute statistics from limited number of samples (simulations)
Computational cost is amplified as number of uncertainties increases

Convergence of densities

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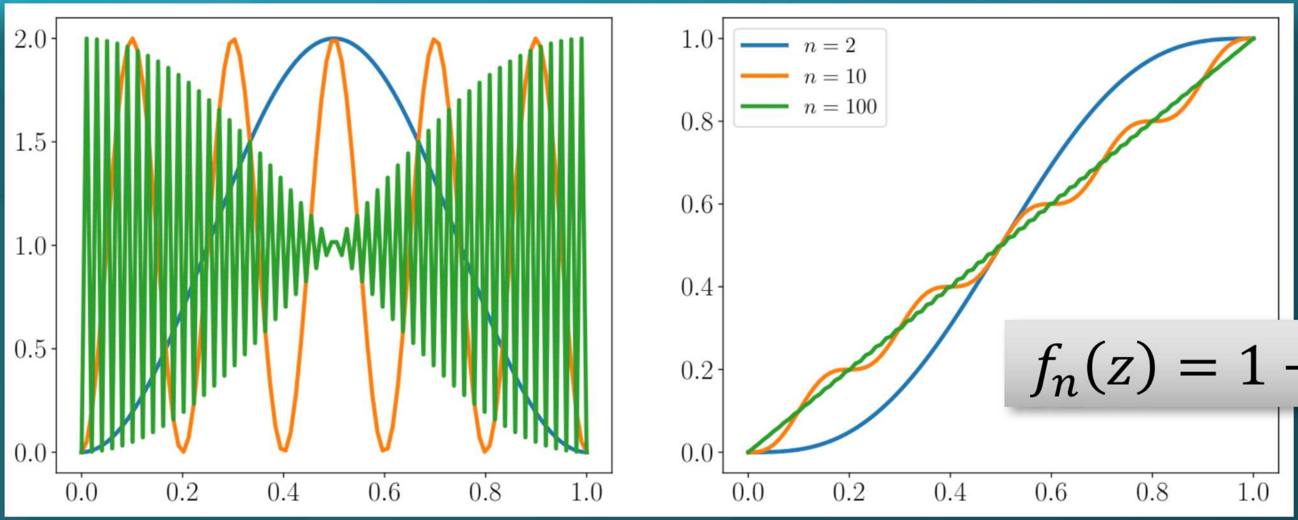
Most literature focuses on convergence of statistics of sequences of random variables



$$f_n(z) = 1 - \cos(n\pi z)$$

But convergence in distribution does not imply convergence almost surely.

Convergence of densities

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Theorem 1 [BJW18]

Let $f_M(\mathbf{z})$ be sequence of approximations s.t. $f_M(\mathbf{z}) \to f$ *as* $M \to \infty$

$$\forall \delta > 0, \exists\, M^\star \text{ s.t. } M > M^\star \Rightarrow \|f_M(\mathbf{z}) - f(\mathbf{z})\|_{L^\infty(\Gamma)} < \delta$$

Then for any $\epsilon > 0, \exists\, \mathrm{M}^\star$ s.t. $\mathrm{M} > \mathrm{M}^\star$ implies

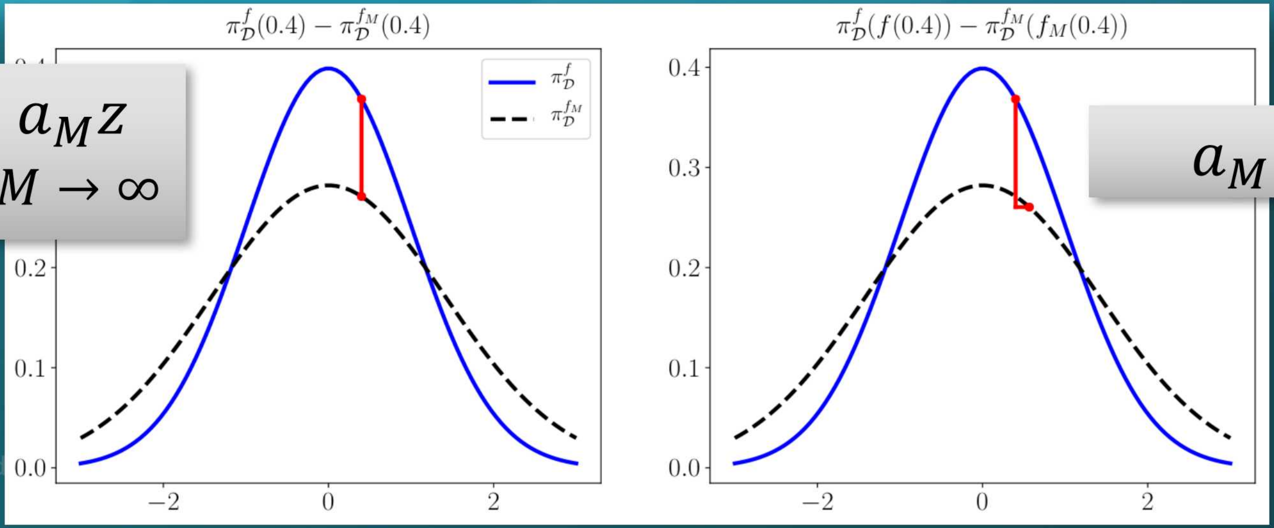
Approximate π converges when evaluated at the true function value $\mathbf{y}=f(\mathbf{z})$

$$\left\|\pi_{\mathcal{D}}^{f}(\mathbf{y}) - \pi_{\mathcal{D}}^{f_M}(\mathbf{y})\right\|_{L^\infty(\mathcal{D})} < \epsilon$$

Approximate π converges when evaluated at the approximation of the function value $f_M(\mathbf{z})$

$$\left\|\pi_{\mathcal{D}}^{f}(f(\mathbf{z})) - \pi_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} < \epsilon$$

$$f_M(\mathbf{z}) = a_M z$$
$$a_M \to 1 \text{ as } M \to \infty$$



$$a_M = 1.2$$

Convergence of densities

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Assumption 1

Let $\pi(\boldsymbol{z})$ *be chosen such that* $\sup_{y \in \mathcal{D}} \pi_{\mathcal{D}}^{f}(\boldsymbol{y}) \leq B_1, B_1 > 0$ *and* $\pi_{\mathcal{D}}^{f}$ *is continuous on* $\mathcal{D}$ *except on a set* $A \subset \mathcal{D}$ *of zero* $\mu_{\mathcal{D}}$ *measure*

Definition 1

A sequence of functions is asymptotically uniformly equicontinuous (a.u.e.c.) if

$$\forall \epsilon > 0, \exists \delta(\epsilon)\ s.t.\ |y - x| < \delta(\epsilon), M > M(\epsilon) \Rightarrow |f_M(x) - f_M(y)| < \epsilon$$

Assumption 2

Let f_M *be an sequence of approximations to* f, $\exists B_2 > 0$ *s.t for any* M $\sup_{y \in \mathcal{D}} \pi_{\mathcal{D}}^{f_M}(\boldsymbol{y}) \leq B_2$. *Moreover for any* $\delta > 0\ \exists \mathcal{D}_\delta \subset \mathcal{D}$ *s.t* $A \subset \mathcal{D}_\delta$ *and* $\mu_{\mathcal{D}}(\mathcal{D}_\delta) < \delta$ *the sequence* $\pi_{\mathcal{D}}^{f_M}$ *is a.u.e.c. on* $\mathcal{D} \backslash \mathcal{D}_\delta$.

Convergence of densities

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Proof: Choose

$$\delta = \frac{\epsilon}{2(B_1 + B_2)}$$

$$\left\|\pi_{\mathcal{D}}^{f}(\mathbf{y}) - \pi_{\mathcal{D}}^{f_M}(\mathbf{y})\right\|_{L^\infty(\mathcal{D})} \leq \left\|\pi_{\mathcal{D}}^{f}(\mathbf{y}) - \pi_{\mathcal{D}}^{f_M}(\mathbf{y})\right\|_{L^\infty(\mathcal{D}_\delta)} + \left\|\pi_{\mathcal{D}}^{f}(\mathbf{y}) - \pi_{\mathcal{D}}^{f_M}(\mathbf{y})\right\|_{L^\infty(\mathcal{D}\setminus\mathcal{D}_\delta)}$$

- By choice of $\boldsymbol{\delta}$ first term bounded by $\epsilon/2$
- By Theorem 1 in [Swe86] $\pi_{\mathcal{D}}^{f_M} \to \pi_{\mathcal{D}}^{f}$ uniformly on $\mathcal{D}\setminus\mathcal{D}_\delta$ thus second term can be bounded by $\epsilon/2$ by choosing M sufficiently large

$$\left\|\pi_{\mathcal{D}}^{f}(f(\mathbf{z})) - \pi_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} \leq \left\|\pi_{\mathcal{D}}^{f}(f(\mathbf{z})) - \pi_{\mathcal{D}}^{f}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} + \left\|\pi_{\mathcal{D}}^{f}(f_M(\mathbf{z})) - \pi_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)}$$

- By $\forall\delta > 0, \exists\, M^\star\ s.t.\ M > M^\star \Rightarrow \|f_M(\mathbf{z}) - f(\mathbf{z})\|_{L^\infty(\Gamma)} < \delta$ and Assumption 1 there exists δ such that first term bounded by $\epsilon/2$
- The norm $\|\quad\|_{L^\infty(\Gamma)}$ is equivalent to $\|\quad\|_{L^\infty(\mathcal{D})}$ since the arguments to the densities are identical so by the second argument in top box second term can also be bounded by $\epsilon/2$

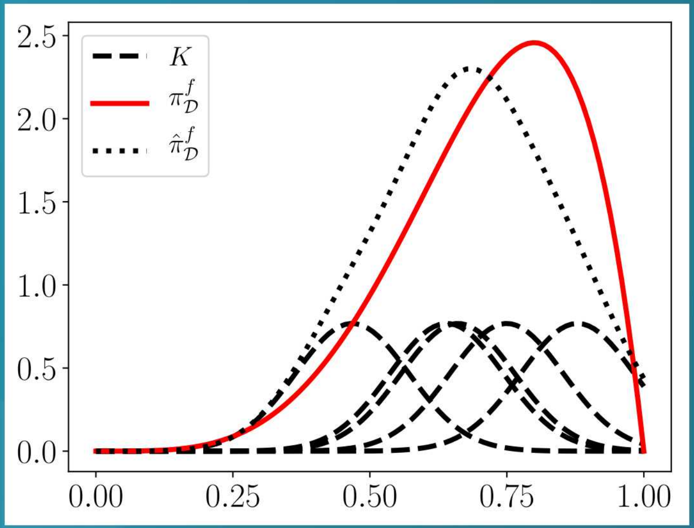
Convergence of densities using KDE and sparse grids

Kernel Density Estimation constructed with M_π samples (satisfies Assumption 1)

$$\hat{\pi}_D^f(\mathbf{y}) = \frac{1}{M_\pi h_{M_\pi}^d} \sum_{i=1}^{M_\pi} K\left(\frac{\mathbf{y}-\mathbf{y}_i}{h_{M_\pi}}\right)$$

If π_D^f has continuous s derivatives and K(y) is a s-th order kernel then

$$\left\|\pi_D^f(\mathbf{y}) - \hat{\pi}_D^f(\mathbf{y})\right\|_{L^\infty(\Gamma)} < C\left(\frac{\log M_\pi}{M_\pi}\right)^{s/(2s+d)}$$



Theorem 2 [BJW18]: Under assumptions of Theorem 1

$$\left\|\pi_D^f(f(\mathbf{z})) - \hat{\pi}_D^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} \le C\left(\left(\frac{\log M_\pi}{M_\pi}\right)^{s/(2s+d)} + \|f_M(\mathbf{z}) - f(\mathbf{z})\|_{L^\infty(\Gamma)}\right)$$

Convergence of densities using KDE and sparse grids

Proof:

$$\left\|\pi_{\mathcal{D}}^{f}(f(\mathbf{z})) - \hat{\pi}_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} \leq \left\|\pi_{\mathcal{D}}^{f}(f(\mathbf{z})) - \hat{\pi}_{\mathcal{D}}^{f}(f(\mathbf{z}))\right\|_{L^\infty(\Gamma)} + \left\|\hat{\pi}_{\mathcal{D}}^{f}(f(\mathbf{z})) - \hat{\pi}_{\mathcal{D}}^{f_M}(f(\mathbf{z}))\right\|_{L^\infty(\Gamma)} + \left\|\hat{\pi}_{\mathcal{D}}^{f_M}(f(\mathbf{z})) - \hat{\pi}_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)}$$

By Lipschitz continuity of K

$$\left\|\hat{\pi}_{\mathcal{D}}^{f}(f(\mathbf{z})) - \hat{\pi}_{\mathcal{D}}^{f_M}(f(\mathbf{z}))\right\|_{L^\infty(\Gamma)}, \left\|\hat{\pi}_{\mathcal{D}}^{f}(f(\mathbf{z})) - \hat{\pi}_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} \leq C\|f_M(\mathbf{z}) - f(\mathbf{z})\|_{L^\infty(\Gamma)}$$

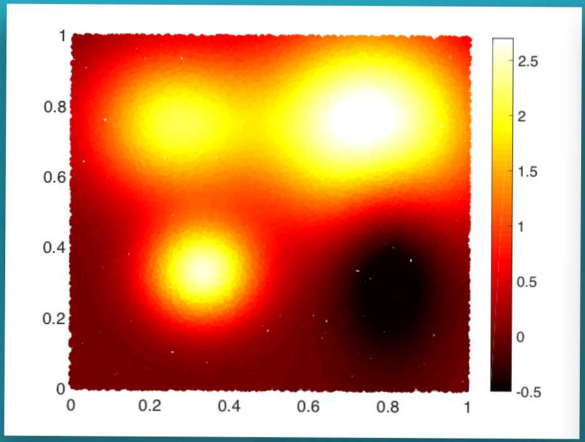
Corrollary 1 [BJW18]*: Given that the isotropic level l sparse grid with Clenshaw-Curtis abscissa satisfies*

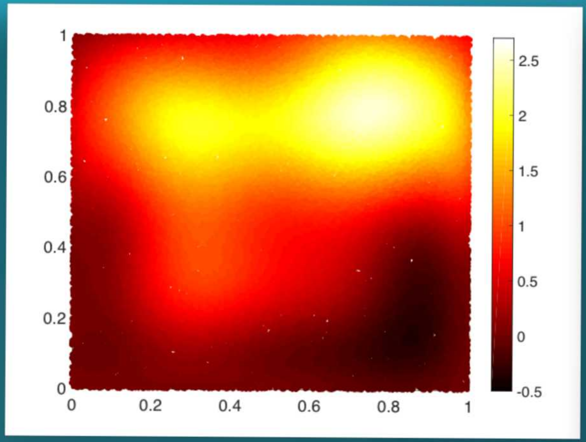
$$\|f_M(\mathbf{z}) - f(\mathbf{z})\|_{L^\infty(\Gamma)} \leq C_1(\sigma)M_l^{-\mu_1},\ \mu_1 = \frac{\sigma}{1 + \log 2d}$$

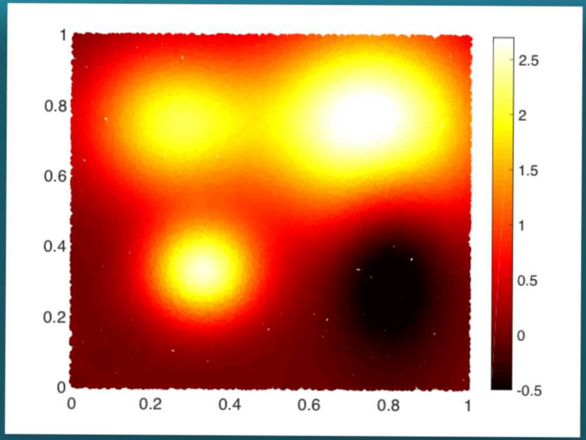
Then

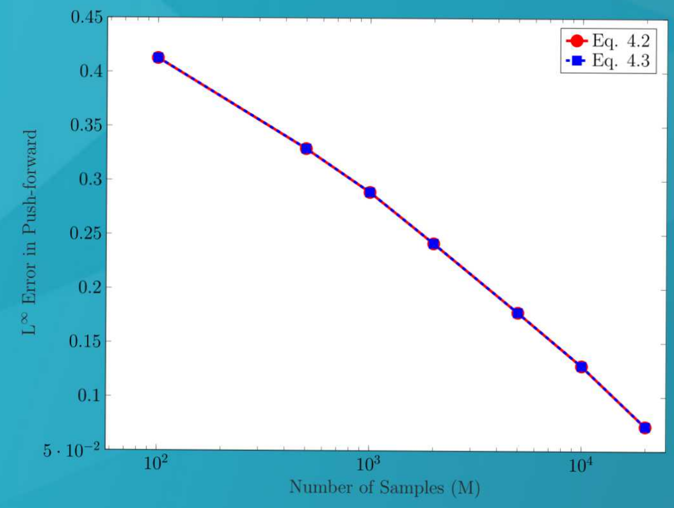
$$\left\|\pi_{\mathcal{D}}^{f}(f(\mathbf{z})) - \hat{\pi}_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} \leq C\left(\left(\frac{\log M}{M}\right)^{s/(2s+d)} + C_1(\sigma)M_l^{-\mu_1}\right)$$

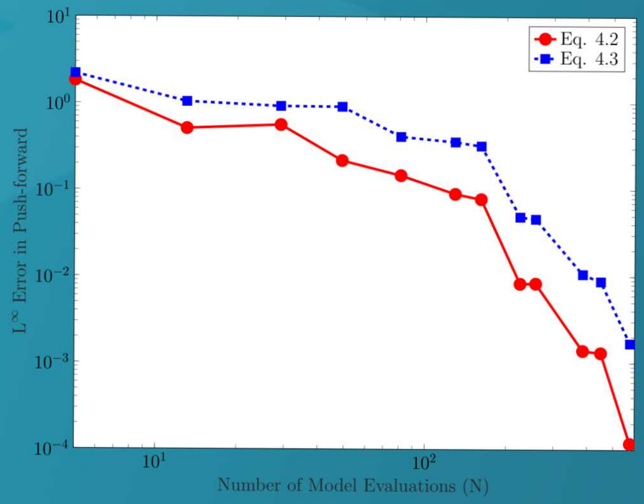
Convergence of densities











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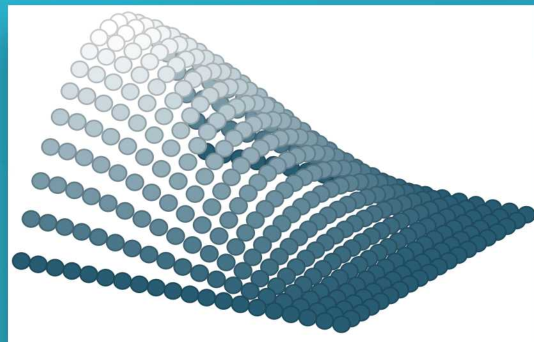
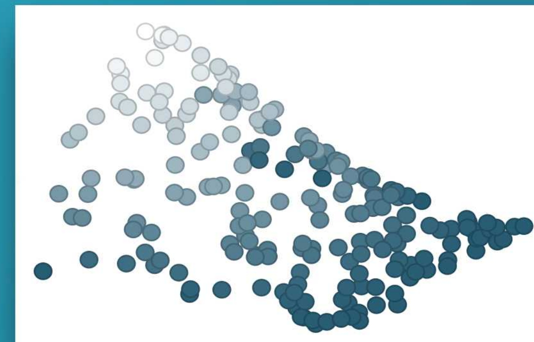
Multivariate Approximation





Let $f = Q(u(x,t,z))$ be a functional of the solution of a PDE $u(x,t,z)$

The error in the approximation of f is bounded by

$$\|f - f_{\alpha,\beta}\|_{L^p_w} \leq \underbrace{\|f - f_{\alpha}\|}_{\text{(I)}}{}_{L^p_w} + \underbrace{\|f_{\alpha} - f_{\alpha,\beta}\|}_{\text{(II)}}{}_{L^p_w}$$

α: multi-index specifying PDE discretization

β: multi–index specifying sampling discretization

w: PDF of variables **Z**

To minimize simulation cost we should balance physical error (I) with stochastic error (II). I.e. only sample highest fidelity model when stochastic error is smaller than deterministic error

Multilevel Monte Carlo Quadrature

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Monte Carlo Quadrature using an approximate model f_α

We can approximate the expectation of a function f by

$$E_{M(\beta)}[f_\alpha] \approx \hat{Q}_{\alpha,\beta} = \frac{1}{M(\beta)} \sum_{i=1}^{M(\beta)} f_\alpha(\mathbf{z}_i), \qquad V[\hat{Q}_{\alpha,\beta}] = \frac{V[f_\alpha]}{M(\beta)}$$

The mean squared error in the approximation

$$E\left[\left(\hat{Q}_{\alpha,\beta} - E[Q]\right)^2\right] = V[\hat{Q}_{\alpha,\beta}] + \left(E[\hat{Q}_{\alpha,\beta}] - E[Q]\right)^2$$

Multilevel Monte Carlo: reduce computational cost by balancing physical and deterministic errors

Use converging sequence of functions f_α to reduce variance of estimator

$$E[f] \approx \hat{Q}_{\alpha,\beta}^{ML} = \sum_{\alpha=0}^{L} \frac{1}{M_\alpha} \sum_{i=1}^{M_\alpha} \left((f_\alpha(\mathbf{z}_i) - f_{\alpha-1}(\mathbf{z}_i)\right) = \sum_{\alpha=1}^{L} \hat{Y}_\alpha,$$

$$f_0 = 0$$

Allocate samples across function levels to achieve accuracy ϵ

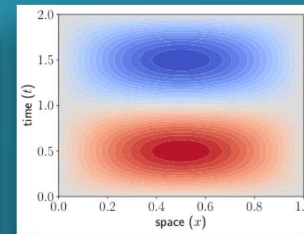
$$C\left(\hat{Q}^{ML}\right) = \textstyle\sum_{\alpha=1}^{L} C_\alpha M_\alpha$$

$$\sum_{\alpha=0}^{L} M_\alpha^{-1} V[Y_\alpha] = \epsilon^2/2$$

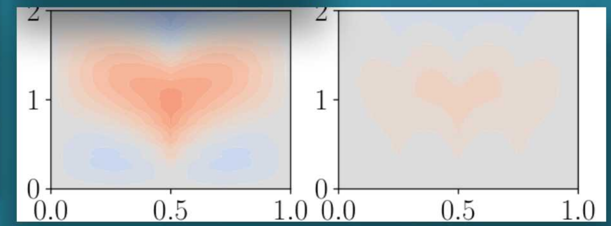
constraints

$$M_\alpha = \frac{2}{\epsilon^2}\left[\sum_{\alpha=0}^{L} (V[Y_\alpha]C_\alpha)^{1/2}\right]\sqrt{\frac{(V[Y_\alpha])}{C_\alpha}}$$

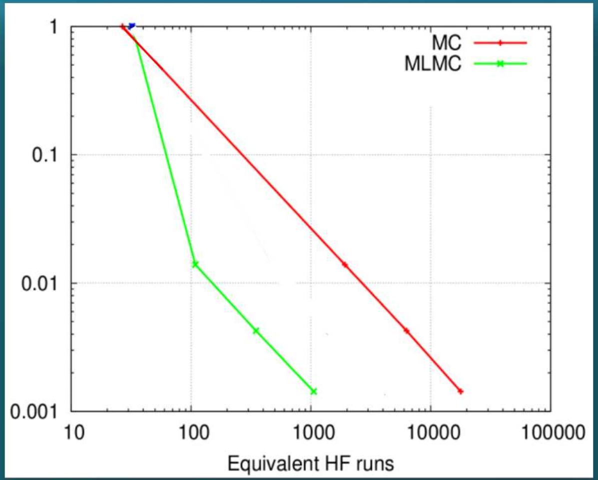
solution



Exact solution(left) discrepancies (below)



Discrepancy between model predictions decays as mesh resolution increases



MC and MLMC applied to an early version of the nozzle model

Multilevel collocation

Approximate PDE solution(functional) using a sequence of FEM models with increasing mesh refinement [TJWG15]

Let $F_{M(\beta)}$ be a sequence of interpolation operators

$$f_{\alpha,\beta}(z) = F_{M(\beta)}[f_\alpha](z)$$

Let $f_\alpha = f(u_\alpha(x,z))$ be a sequence of functions which are functionals of PDE FEM solutions with decreasing mesh size h_α

The multilevel approximation is

$$f^L_{\alpha,\beta}(z) = \sum_{l=0}^{L} F_{M(\beta_l)}[f_{\alpha_l} - f_{\alpha_{l-1}}](z)$$

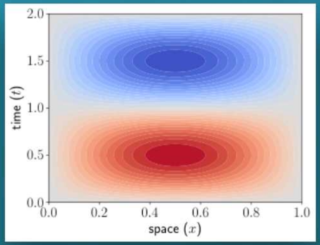
Use most accurate interpolation on coarsest mesh level and least accurate interpolation on finest level

$$M(\beta_0) \le M(\beta_1) \le \cdots \le M(\beta_L)$$

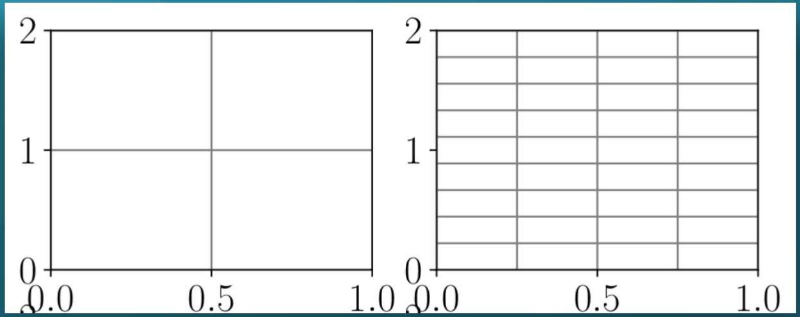
and

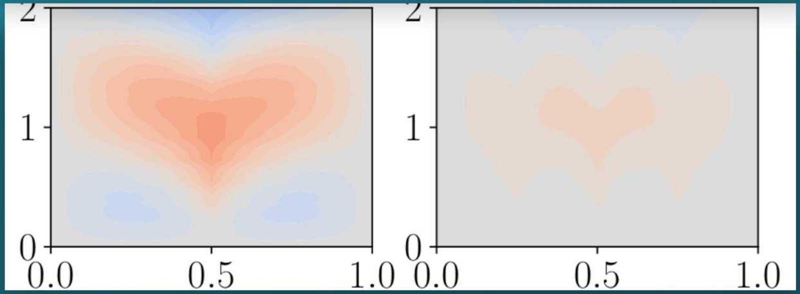
$$h_{\alpha_0} \ge h_{\alpha_1} \ge \cdots \ge h_L$$

Bi-level scheme first proposed by [NE12]



Effectiveness of method depends of rate of discrepancy decay vs approximation error decay





Multilevel collocation

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Approximate a functional of the exact PDE solution using a sequence of models with increasing mesh refinement

The error in the approximation is given by

$$\left\|f - f_{\alpha,\beta}\right\|_{L^p_w} \leq \|f - f_\alpha\|_{L^p_w} + \left\|f_\alpha - f_{\alpha,\beta}\right\|_{L^p_w}$$

Assume

$$\left\|g - g_\beta\right\|_{L^p_w} \leq C_I \sigma_\alpha \zeta(g),$$

$$\zeta(f_\alpha) \leq C_\zeta h_0^\beta, \zeta(f_\alpha - f_{\alpha-1}) \leq C_\zeta h_\alpha^\beta$$

and

$$\|f - f_\alpha\|_{L^p_w} \leq C_s h_L^\kappa$$

Then if we choose interpolation operators such that

$$\sigma_{L-\alpha} \leq C_s \left((L+1) C_I C_\zeta\right)^{-1} h_L^\kappa h_\alpha^{-\beta}$$

$$\left\|f_\alpha - f_{\alpha,\beta}\right\|_{L^p_w} \leq \sum_{\alpha=0}^{L} C_I C_\zeta \sigma_{L-\alpha} h_L^\kappa = C_s h_L^\kappa$$

Then

$$\left\|f - f_{\alpha,\beta}\right\|_{L^p_w} \leq 2 C_s h_L^\kappa$$

Single fidelity cost is $C_\epsilon \leq \epsilon^{-\frac{1}{\mu}-\frac{\gamma}{\kappa}}$

Theorem 3 [TJWG15]: The following holds for sparse grids using a Lagrange basis

$$\sigma_\alpha = M(\alpha)^{-\mu(d)}$$

Assume $\exists \gamma$ such that the cost $C_\alpha \leq C_c h_\alpha^{-\gamma}$.

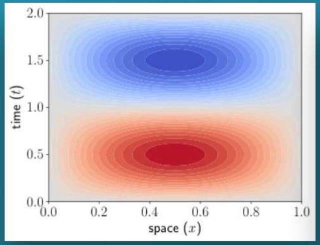
For multigrid solver $\gamma = D$

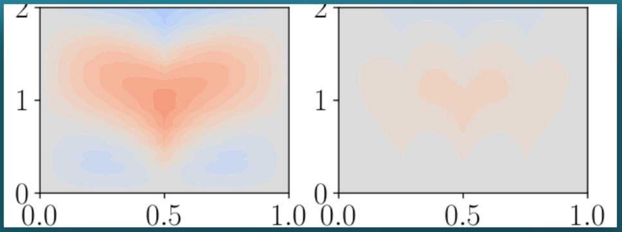
Assume $\kappa \geq \min(\beta, \mu\gamma)$ then $\exists$ a level L such that

$$\left\|f - f_{\alpha,\beta}\right\|_{L^p_w} \leq \epsilon,$$

for any $\epsilon \leq e^{-1}$ and

$$C_\epsilon = \sum_{\alpha=0}^{L} M(L-\alpha) C_\alpha \lesssim \begin{cases} \epsilon^{-\frac{1}{\mu}}, & \beta > \mu\gamma \\ \epsilon^{-\frac{1}{\mu}} |\log \epsilon|^{1+\frac{1}{\mu}}, & \beta = \mu\gamma \\ \epsilon^{-\frac{1}{\mu}-\frac{\gamma}{\kappa}+\frac{\beta}{\kappa\mu}}, & \beta < \mu\gamma \end{cases}$$





Effectiveness of method depends of rate of discrepancy decay vs approximation error decay

Convergence of densities

Theorem 4 [BJWPreprint]*:* Under assumptions of Theorem 1 there exists a M such that the error in the multi-level sparse grid approximation satisfies

$$\left\|\pi_{\mathcal{D}}^{f}(f(\mathbf{z})) - \pi_{\mathcal{D}}^{f_M}(f_M(\mathbf{z}))\right\|_{L^\infty(\Gamma)} \leq 2C\left(\left(\frac{\log M_\pi}{M_\pi}\right)^{s/(2s+d)}\right)$$

Which can be computed with cost

$$C_\epsilon = \sum_{\alpha=0}^{L} M(L-\alpha)C_\alpha \lesssim \begin{cases} \epsilon^{-\frac{1}{\mu}}, & \beta > \mu\gamma \\ \epsilon^{-\frac{1}{\mu}}|\log \epsilon|^{1+\frac{1}{\mu}}, & \beta = \mu\gamma \\ \epsilon^{-\frac{1}{\mu}-\frac{\gamma}{\kappa}+\frac{\beta}{\kappa\mu}}, & \beta < \mu\gamma \end{cases}$$

Where we have chosen $\epsilon = \left(\frac{\log M_\pi}{M_\pi}\right)^{s/(2s+d)}$

Proof: Direct application of Corrolary 1 and modification of Theorem 3 to use L^∞ norm

Tensor product interpolation

DAKOTA

Univariate interpolation

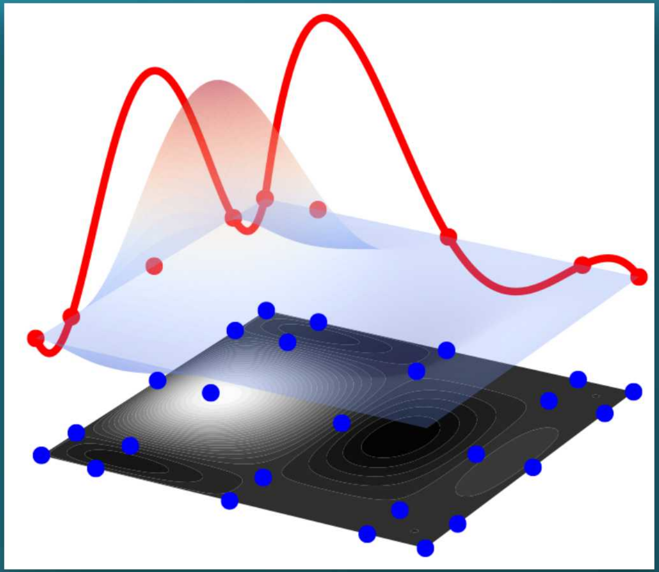
Define set of 1D samples

$$\mathcal{Z}^k_{m(\beta_k)} = \left(z_k^{(1)}, \cdots z_k^{(m(\beta_k))}\right)$$

$$z_k^{(j)} = \cos\left(\frac{(j-1)\pi}{m(\beta_k)}\right), m(1) = 1, m(l) = 2^{l-1} + 1$$

And univariate basis functions

$$\phi_{\beta_k,i}(z_k) = \prod_{n=1,n\neq k}^{m(k)} \frac{(z_k - z_k^{(n)})}{(z_k^{(i)} - z_k^{(n)})}$$



Multivariate interpolation

Interpolant is tensor product of 1D interpolants

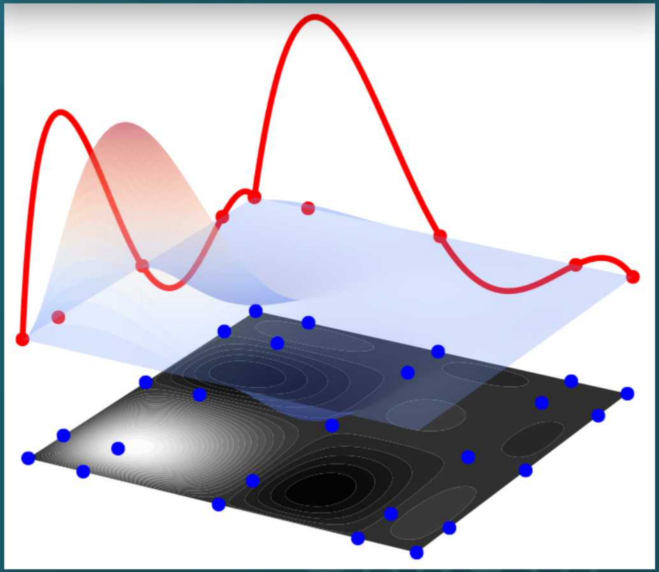
$$f_{\boldsymbol{\alpha},\boldsymbol{\beta}} = \sum_{\boldsymbol{i}\in\mathcal{J}} f_{\boldsymbol{\alpha}}(\boldsymbol{z}^{(\boldsymbol{i})})\, \phi_{\boldsymbol{\beta},\boldsymbol{i}}(\boldsymbol{z}), \qquad \phi_{\boldsymbol{\beta},\boldsymbol{i}}(\boldsymbol{z}) = \prod_{k=1}^{d} \phi_{\beta_k,i_k}(z_k)$$

$$\mathcal{J} = \{\, \boldsymbol{i} \mid i_k \le m(\beta_k), k = 1, \dots, d \,\}$$

Requires evaluating function on a tensor product grid

$$\mathcal{Z}_\beta = \bigotimes_{k=1}^{d} \mathcal{Z}^k_{m(\beta_k)}, \qquad M(\boldsymbol{\beta}) = \prod_{k=1}^{d} m(\beta_k)$$

$$\mathcal{Z}_\beta = \{\boldsymbol{z}^{(\boldsymbol{i})}\}_{\boldsymbol{i}\in\mathcal{J}}, \qquad \boldsymbol{z}^{(\boldsymbol{i})} = (z_1^{(i_1)}, \dots, z_d^{(i_d)})^{\boldsymbol{T}}$$



Sparse grid interpolation

Combination Technique [Smo63,BNR00]

Interpolant is tensor product of 1D interpolants

$$f_L = \sum_{\beta \in I_L} c_\beta f_\beta$$

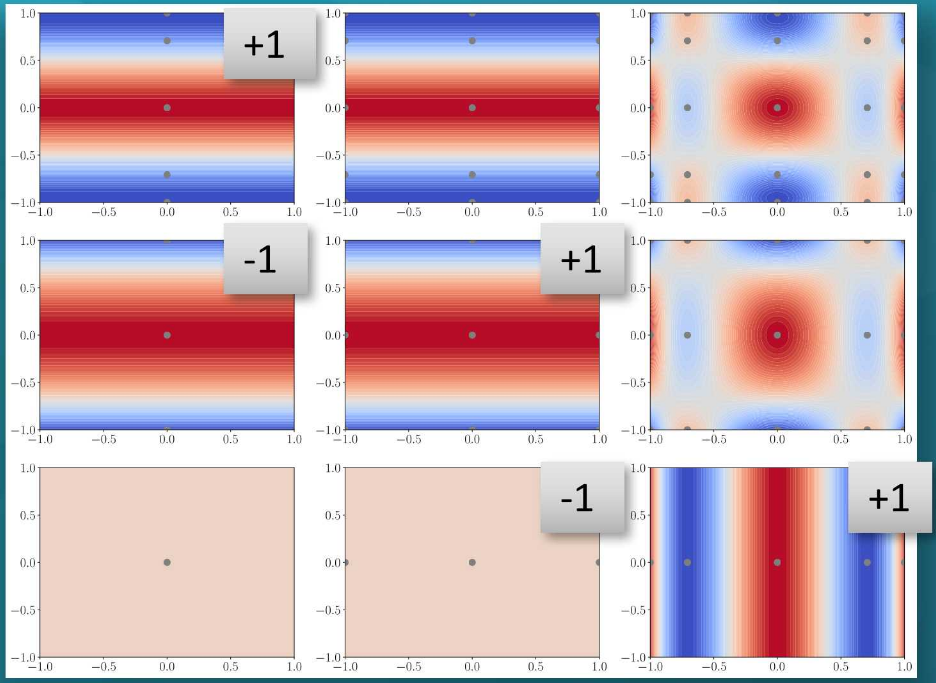
The isotropic index set is given by

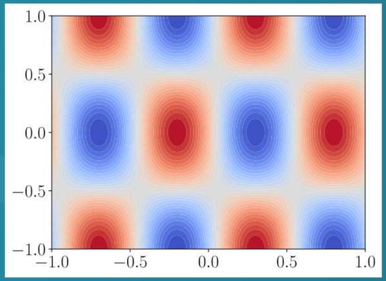
$$I_L = \{ \boldsymbol{\beta} \mid L - d + 1 \leq \|\boldsymbol{\beta}\|_1 \leq L \}$$

Building the interpolant requires evaluating the functions f_α on the union of samples of all tensor product grids

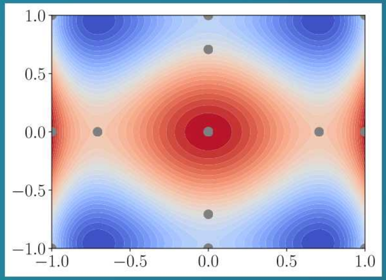
$$\mathcal{Z}_{I_L} = \bigcup_{\beta \in I_L} \mathcal{Z}_\beta , \qquad M(I_L) = card(\mathcal{Z}_{I_L})$$

s is number of model discretization parameters





$f(\mathbf{z}) = \cos(2\pi z_1)\cos(\pi z_2)$

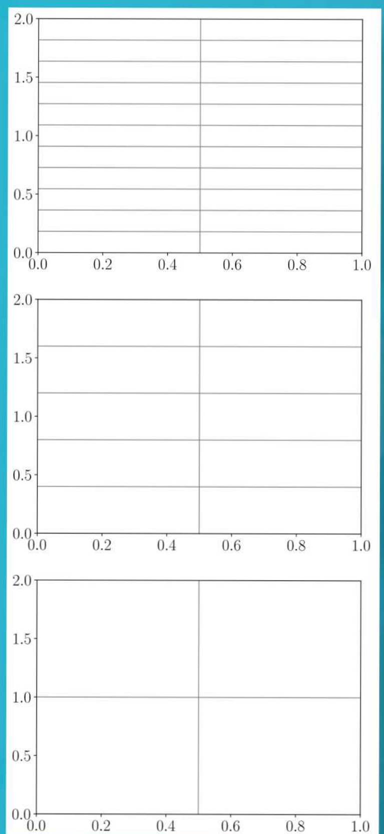


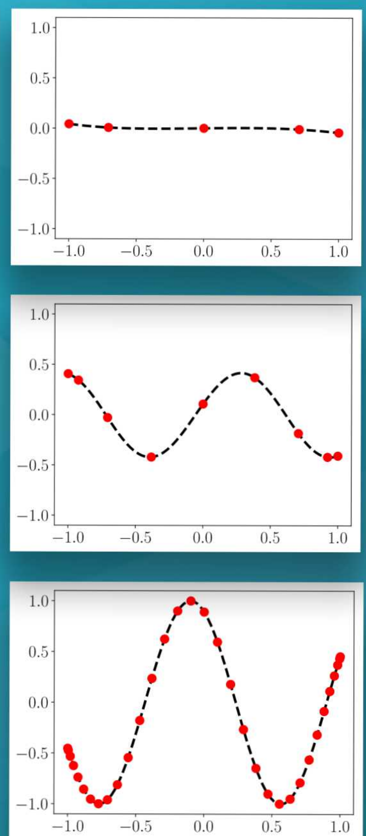
$f_2(\mathbf{z})$

Multilevel collocation

DAKOTA

Construct a separate sparse grid for each discrepancy

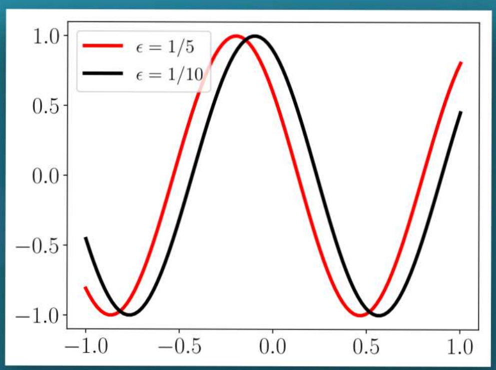




$$F_{M(2)}\,[f_2 - f_1](\mathbf{z})$$

$$F_{M(1)}\,[f_1 - f_0](\mathbf{z})$$

$$F_{M(0)}\,[f_0](\mathbf{z})$$



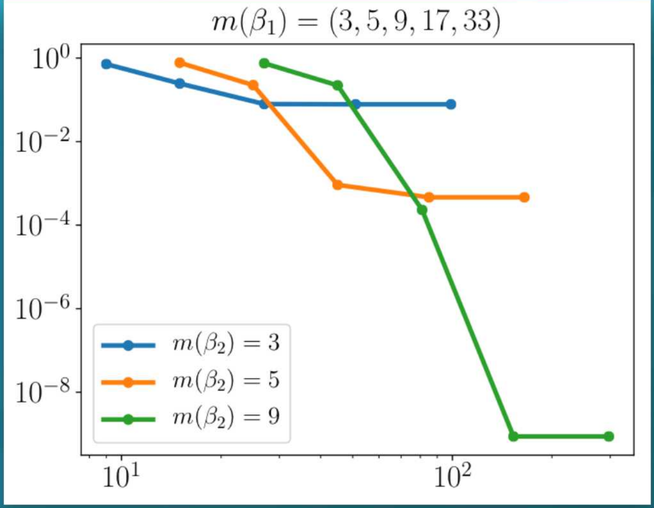
$$f_\alpha(\mathbf{z}) = \cos\big(2\pi\big(z_1 + \epsilon(\alpha)\big)\big)$$

$$\epsilon(0) = \frac{1}{5}, \epsilon(1) = \frac{1}{10}\epsilon(1) = \frac{1}{100}$$

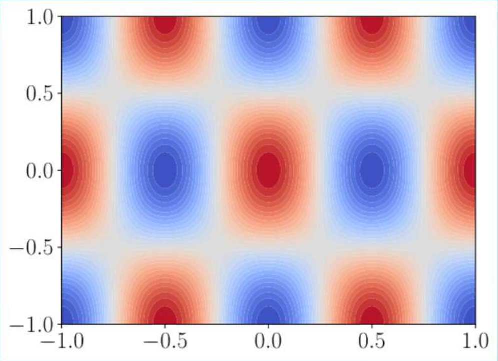
Stochastic discretization

Even for a specified deterministic error it is not clear a priori how which refinement is most efficient (refine z_1 or z_2)

Adaptive sparse grids are great for solving this problem



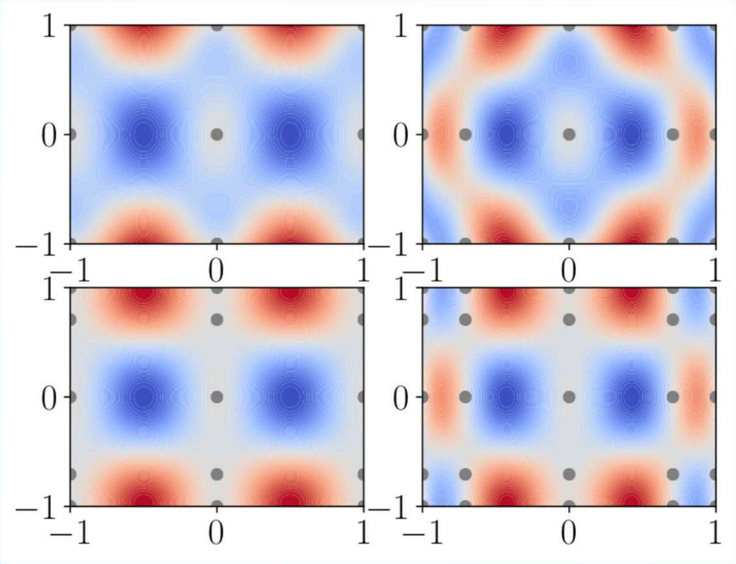
Convergence of interpolant with increasing number of samples



Exact function $f(\mathbf{z}) = \sin(2\pi z_1)\sin(\pi z_2)$

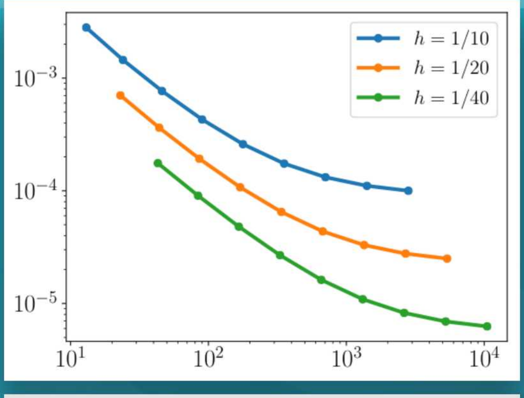
z_1 refinement

z_2 refinement



Discrepancy between exact and interpolated

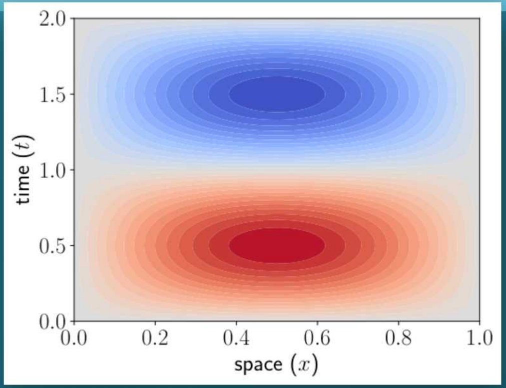
Deterministic discretization



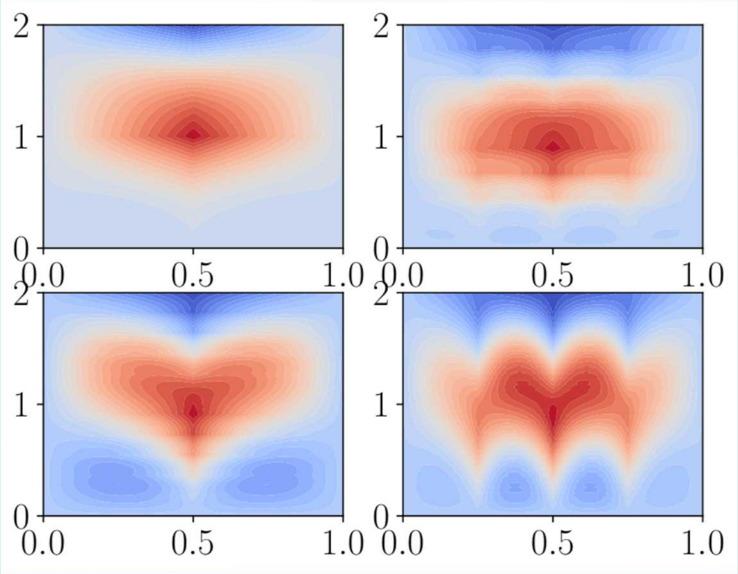
Convergence of solution with increasing number of time steps

Even for a specified stochastic error it is not clear a priori how which refinement is most efficient (time or space)

Adaptive sparse grids are also great for solving this problem



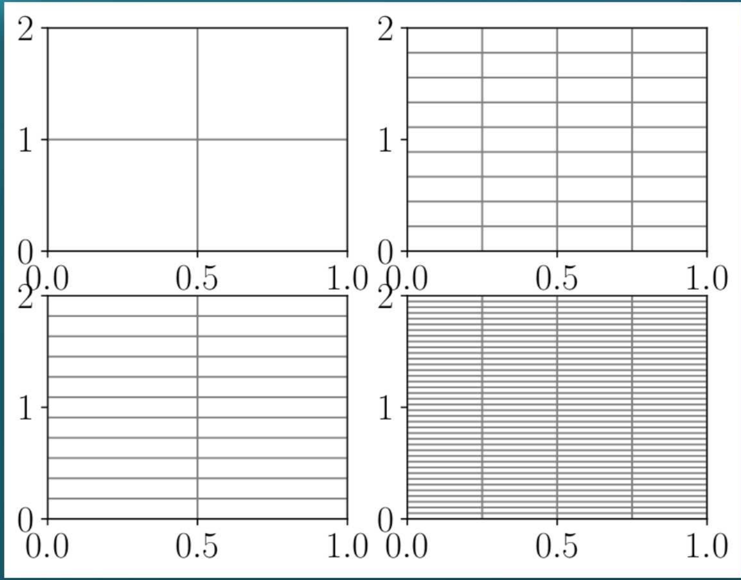
Exact solution $u = \sin(\pi x)\sin(\pi t)$



Discrepancy between exact and FEM solution $u_\alpha - u$

Spatial Refinement

Temporal refinement



Spatial and temporal discretization

Multi-index collocation

DAKOTA

Interpolant is tensor product of 1D interpolants [HANT16]

$$f_L = \sum_{[\alpha,\beta] \in I_L} c_{\alpha,\beta} f_{\alpha,\beta}$$

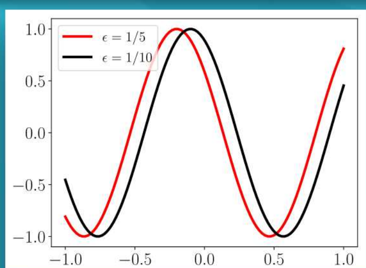
The isotropic index set is given by

$$I_L = \{ [\boldsymbol{\alpha}, \boldsymbol{\beta}] \mid L - (d+s) + 1 \leq \|\boldsymbol{\alpha} + \boldsymbol{\beta}\|_1 \leq L \}$$

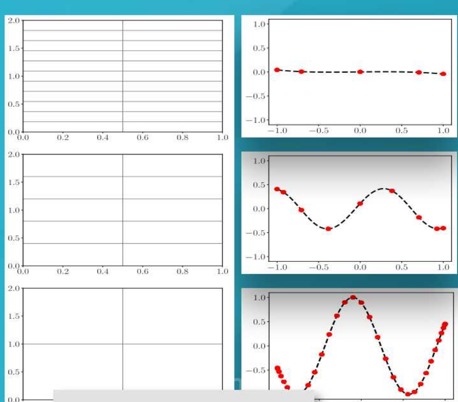
Building the interpolant requires evaluating the functions f_α on the union of samples of all tensor product grids

$$\mathcal{Z}_{\mathrm{B}} = \bigcup_{\beta \in \mathrm{B}} \mathcal{Z}_\beta, \qquad M(\mathbf{B}) = card(\mathcal{Z}_{\mathrm{B}})$$

s is number of model discretization parameters

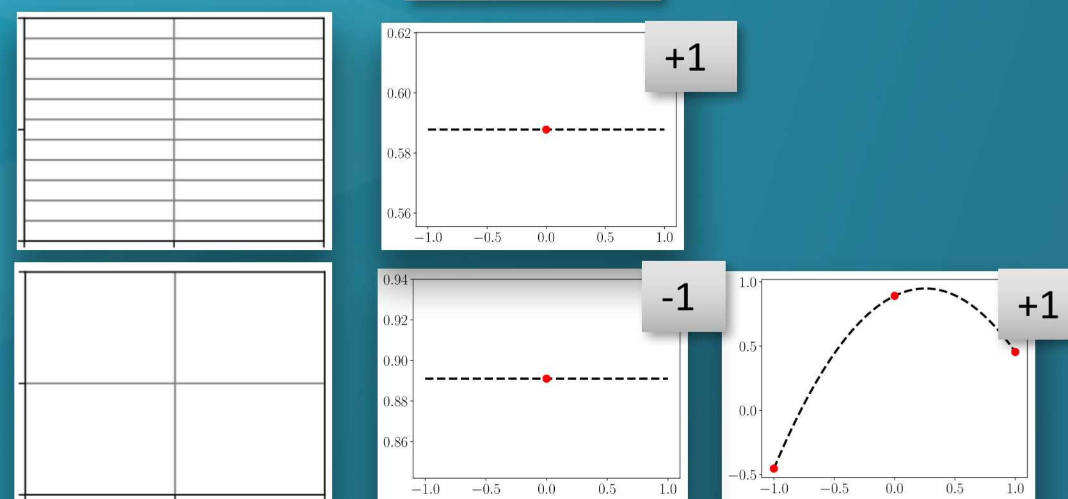


$f_\alpha(\mathbf{z}) = \cos(2\pi(z_1 + \epsilon(\alpha)))$



Multi-level scheme

$[\boldsymbol{\alpha}, \boldsymbol{\beta}]$=[(1), (0)]



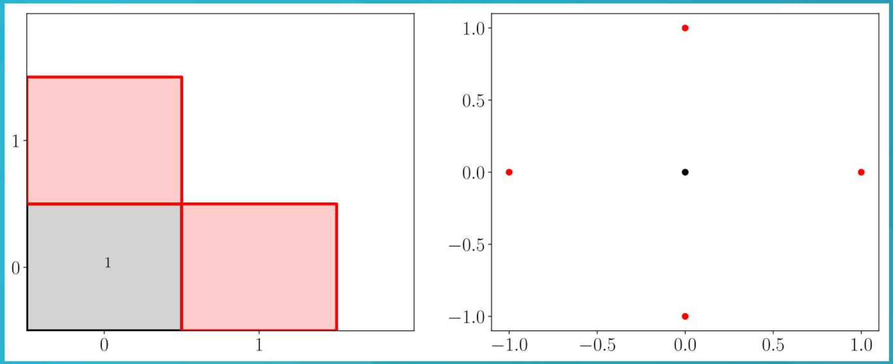
$[\boldsymbol{\alpha}, \boldsymbol{\beta}]$=[(0), (0)]

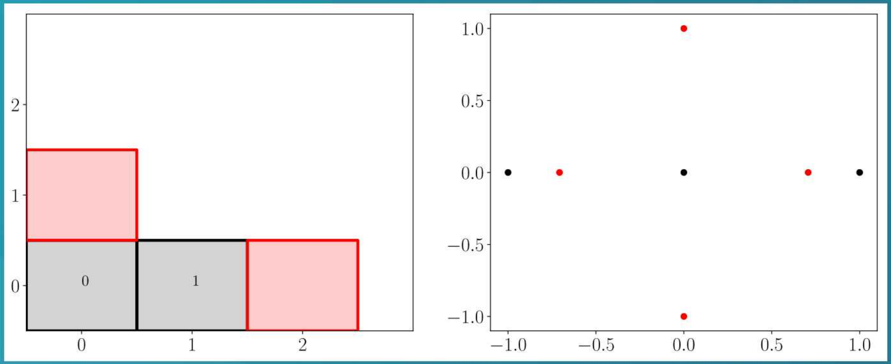
$[\boldsymbol{\alpha}, \boldsymbol{\beta}]$=[(0), (1)]

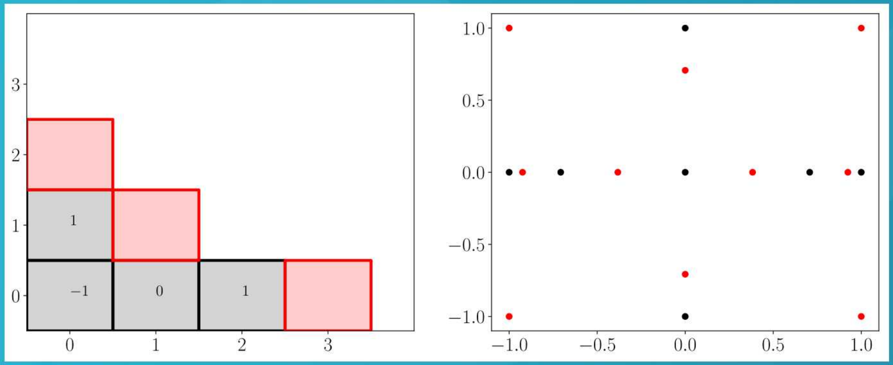
Multi-index scheme

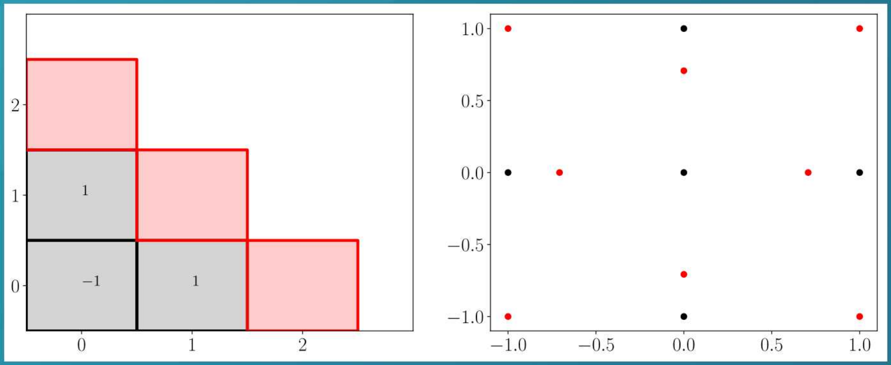
Adaptive refinement

Use adaptive algorithm proposed in [Heg03,GG03], using increment to mean as error indicator









Multi-level scheme

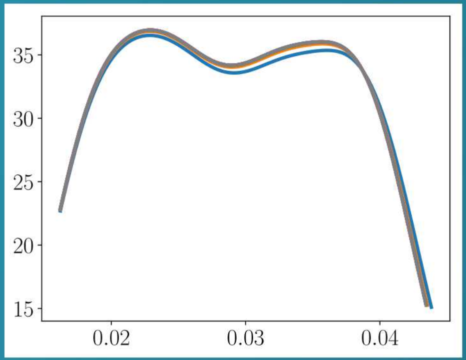
Steady-state advection-diffusion

$$10\nabla u(x) - \nabla \cdot (k(x,z)\nabla u(x)) = 1, \qquad in\ \mathcal{B} = [0,1]$$
$$u(x) = 0, \qquad on\ \partial\mathcal{B}$$

Use KLE of exponential covariance kernel

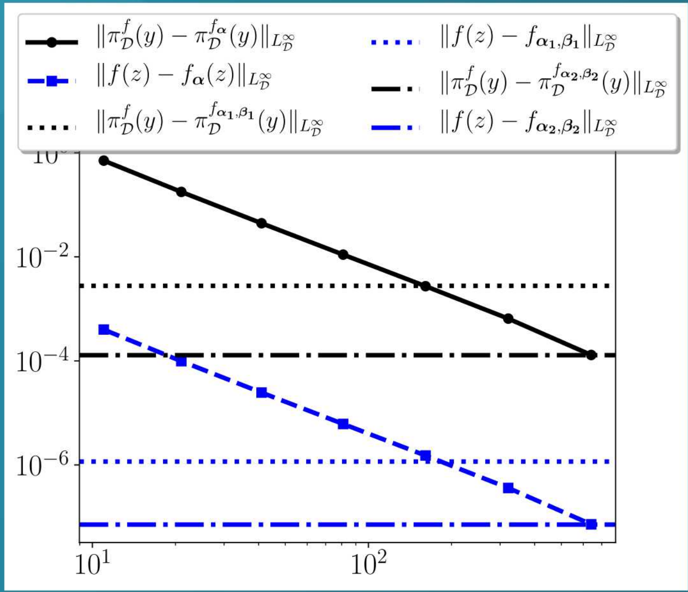
$$\log k(x,z) = 1 + \cos\left(\frac{1+\pi x}{2}\right) + \sum_{i=1}^{d} \lambda_i \phi_i(x) z_i$$

$\lambda_i, \phi_i(x)$ are derived from $C(x_1, x_2) = \exp\left(-\frac{|x_1 - x_2|}{l}\right), l = 1$,d=5



Mesh size: $\Delta x_{\alpha_1} = \Delta x_0 2^{-\alpha_1}$

QoI: $f_\alpha(z) = u(x = 0.5, z)$



We compute error in approximation using ($S = 10{,}000$)

$$\|f - f_M\|_{L^\infty} \approx \max_{s=1,\dots,S} \left|f(Z^{(s)}) - f_N(Z^{(s)})\right|$$

Transient advection-diffusion

$$\frac{du(x,t)}{dt} = -10\nabla \mathrm{u} + \nabla \cdot (k(x,z)\nabla u) + 10, \qquad in\ \mathcal{B} = [0,1]\times[0,T]$$

$$u(x,t) = 0, \qquad on\ \partial\mathcal{B}$$

Use KLE of exponential covariance kernel

$$\log k(\mathrm{x},\mathrm{z}) = \bar{k}(x) + \sum_{i=1}^{d} \lambda_i \phi_i(x) z_i$$

$\lambda_i, \phi_i\,(x)$ are derived from $C(x_1,x_2) = \exp\left(-\frac{|x_1-x_2|}{l}\right), l = 0.1$,d=5

$$\bar{k}(x) = \log\left(\frac{1}{20}\left(2 + \sin\left(\frac{\pi \mathrm{x}}{2}\right)\right)\right), \qquad T = 1$$

Mesh size: $\Delta x_{\alpha_1} = \Delta x_0 2^{-\alpha_1}$

Time-step size: $\Delta t_{\alpha_2} = \left\lfloor \left(\frac{2\mathrm{T}k^{\star}}{\Delta x_{\alpha_1}^2} + 1\right) 2^{\alpha_2} \right\rfloor^{-1}$ (smallest time step must satisfy CFL condition)

QoI: $f_\alpha(z) = u(x = 0.5, \mathrm{t} = \mathrm{T}, z)$

We compute error in approximation using $(S = 10{,}000)$

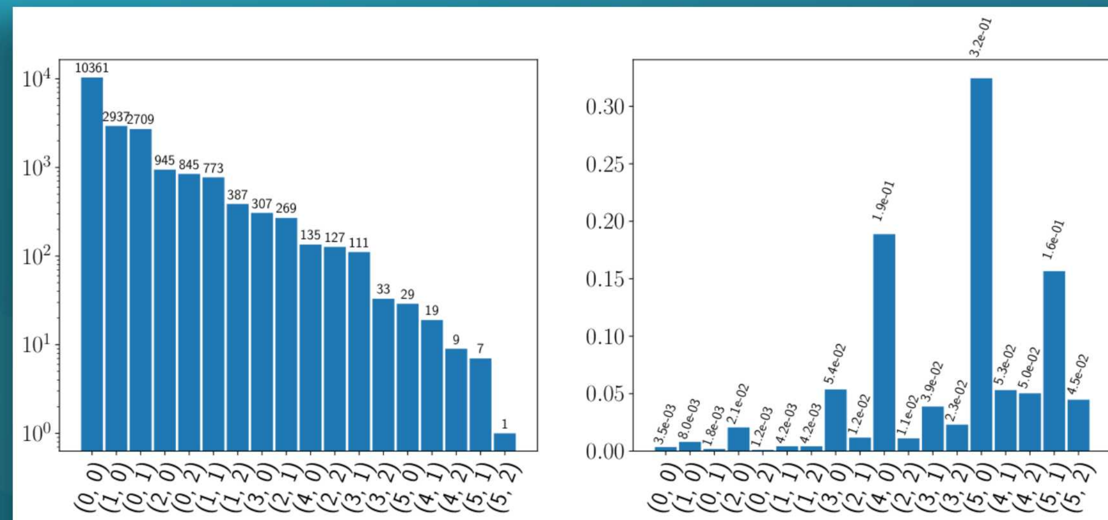
$$\|f - f_N\|_{L^\infty} \approx \max_{\mathrm{s}=1,\ldots,\mathrm{S}} \left| f(Z^{(s)}) - f_N(Z^{(s)}) \right|$$

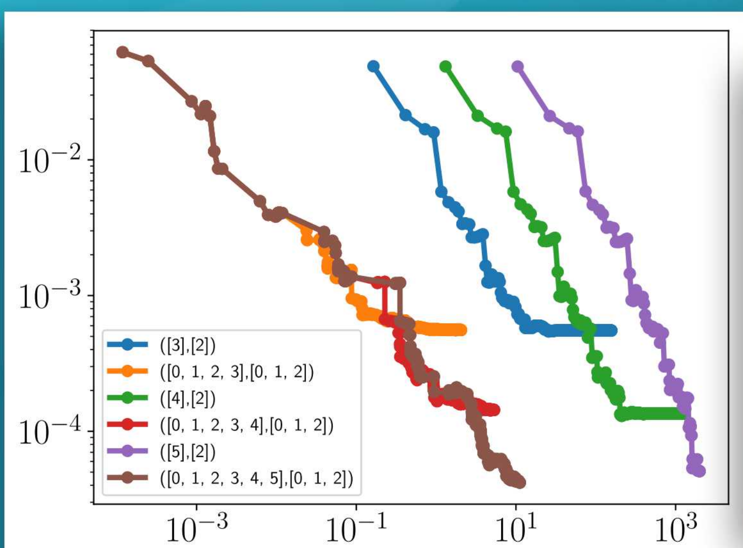
Transient advection-diffusion

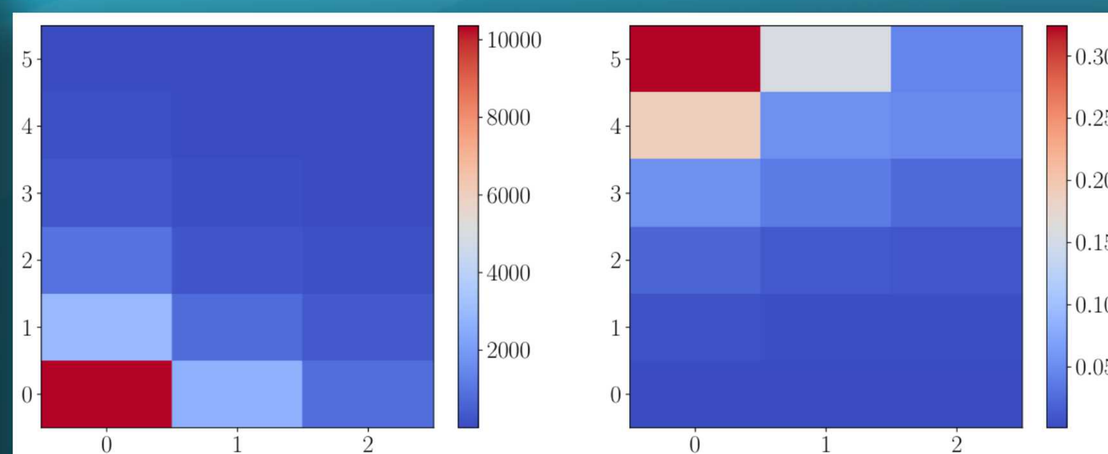
DAKOTA

Transient advection-diffusion model relative costs

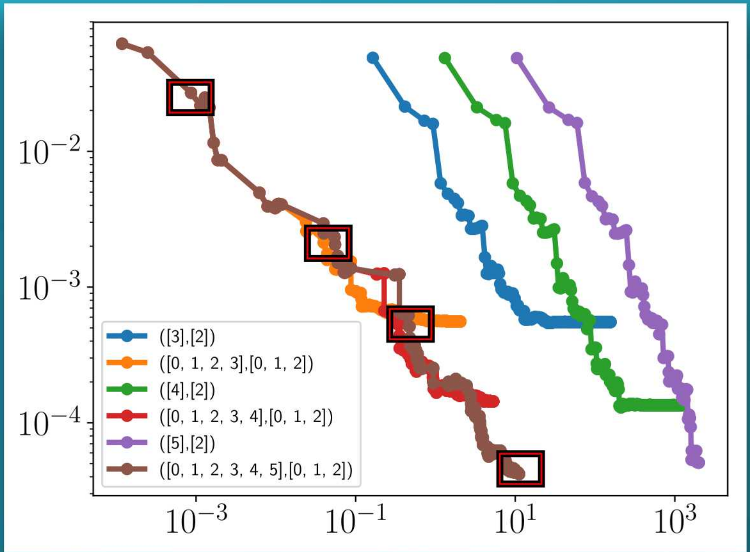
α_1 \ α_2	1	2	2
0	7.6e-06	1.5e-05	3.1e-05
1	6.1e-05	1.2e-04	2.4e-04
2	4.9e-04	9.8e-04	2.0e-03
3	3.9e-03	7.8e-03	1.6e-02
4	3.1e-02	6.2e-02	1.2e-01
5	2.5e-01	5.0e-01	1.0e+00

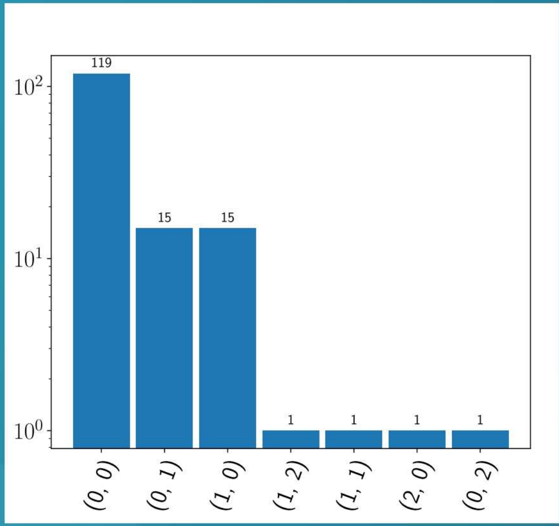


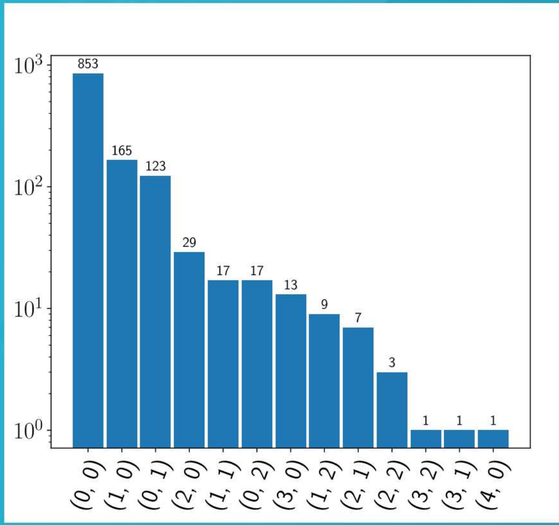


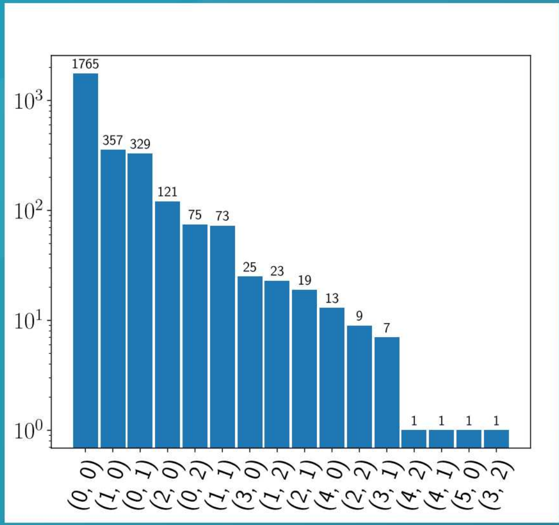


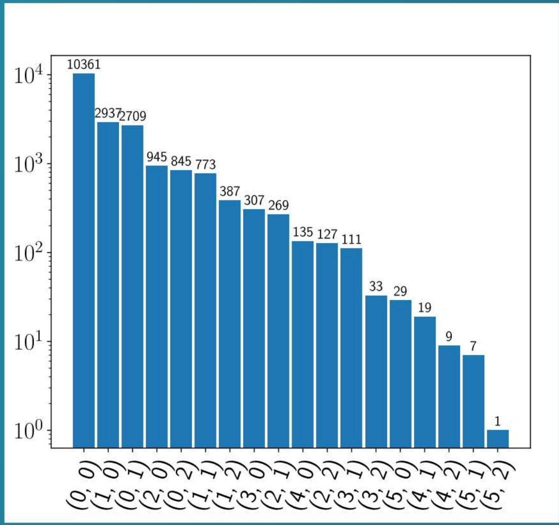
Transient advection-diffusion









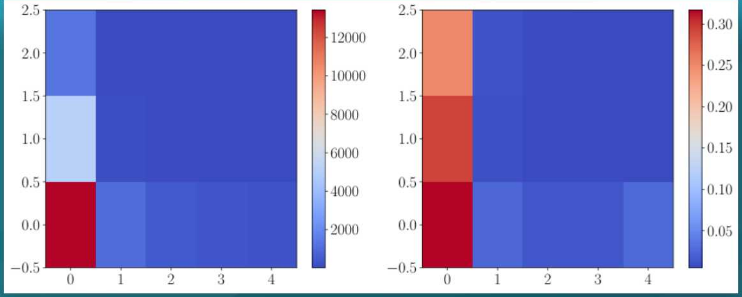


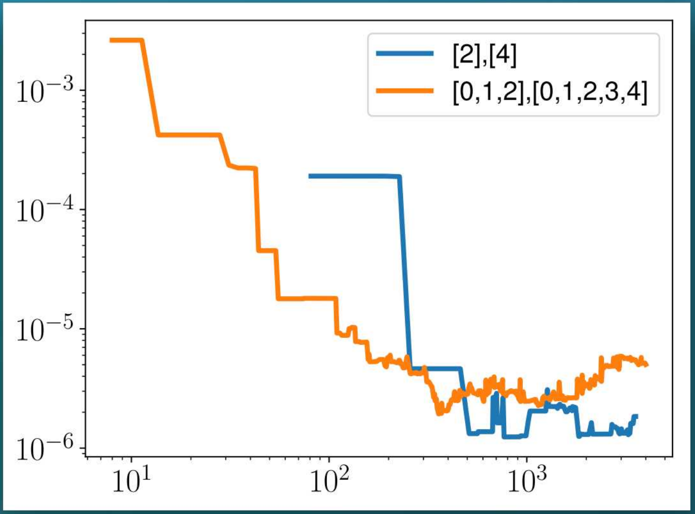
Nozzle Model

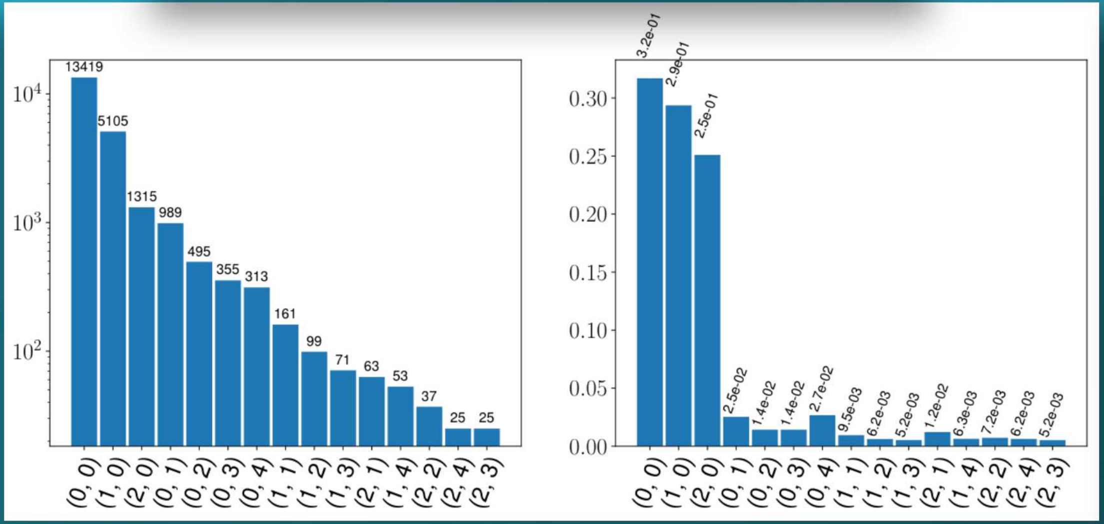
DAKOTA

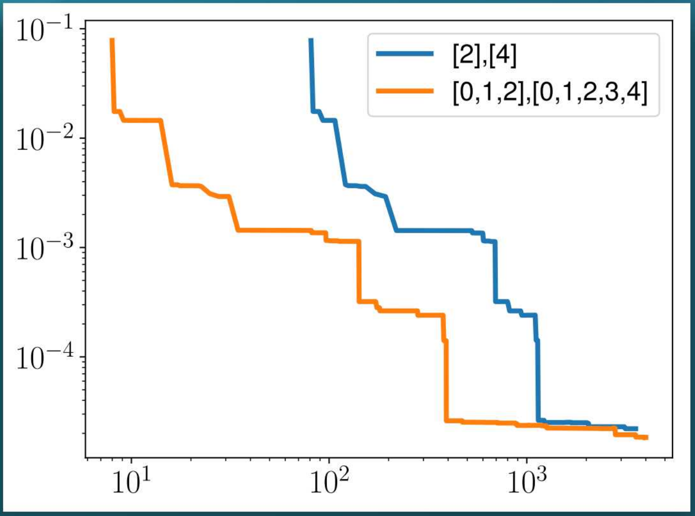
2D Euler nozzle model costs in seconds

α_1 \ α_2	1	2	3	4	5	5
0	36.3	39.3	44.2	61.5	131.2	347.9
1	88.5	90.5	95.7	113.1	184.2	386.8
2	293.6	297.4	300.0	317.5	384.5	609.2









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