Quantification of Epistemic Uncertainties in the $k - \varepsilon$ Model Coefficients

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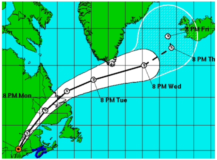
Introduction

Uncertainty

"Uncertainty is the only certainty there is, and knowing how to live with insecurity is the only security."

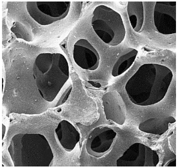
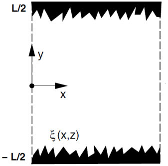
— John Allen Paulos

- **Uncertainties** are present in most engineering and practical applications.





- **Sources of Uncertainty**:
  - ✓ physical properties
  - ✓ initial conditions
  - ✓ boundary conditions
  - ✓ geometry
  - ✓ model parameters
  - ✓ etc.

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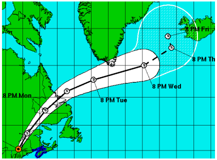



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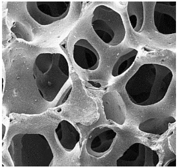
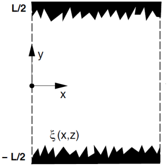



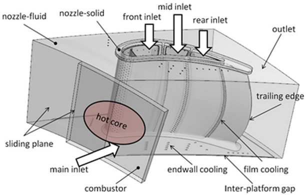
Despite these uncertainties can predictions be trusted?

Uncertainty in Turbomachines

- Turbomachines can be intensely sensitive to the uncertainties.
- Aleatory uncertainties:
  - ✓ Operating conditions
  - ✓ Geometry
- Operational: Volumetric flow rate, turbulence properties, rotational speed.
- Geometrical:
  - ✓ Manufacturing tolerances.
  - ✓ Turbomachines are designed to run for years: in-service erosion and corrosion.







Uncertainty Quantification Using Polynomial Chaos Expansion

Uncertainty Quantification

- How do input uncertainties affect objective functions are affected?
- Non-deterministic CFD is a growing field. (e.g. NUMECA)
- First step: identification of the sources of uncertainties and their PDFs.

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Quantitative characterization and reduction of uncertainties in applications.

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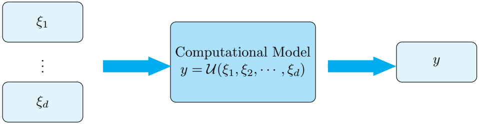
Determinstic system



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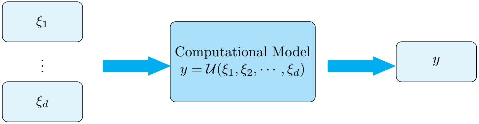
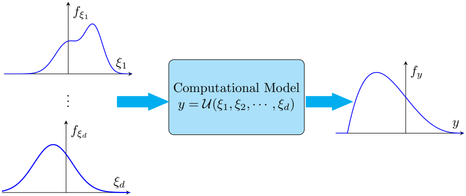


Stochastic system



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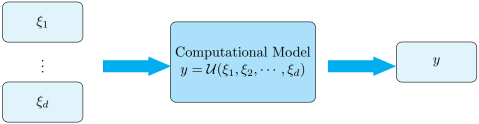

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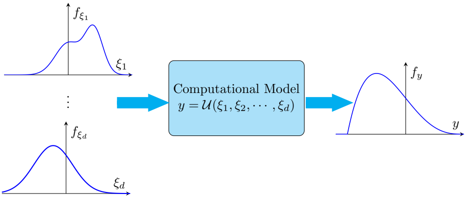

Statistics:

$$\langle y \rangle = \int_{-\infty}^{+\infty} z f_y(z)\, \mathrm{d}z$$

$$\sigma^2 = \int_{-\infty}^{+\infty} (z - \mathbb{E}[y])^2 f_y(z)\, \mathrm{d}z$$

$$\mu_3 = \int_{-\infty}^{+\infty} (z - \mathbb{E}[y])^3 f_y(z)\, \mathrm{d}z$$

$$\mu_4 = \int_{-\infty}^{+\infty} (z - \mathbb{E}[y])^4 f_y(z)\, \mathrm{d}z$$

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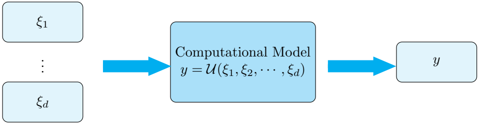

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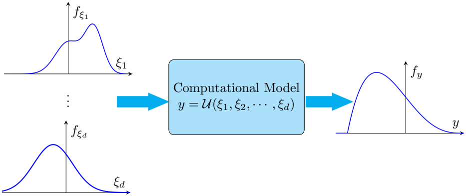

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UQ Methods

Introduce mathematical approaches to solve above integrals.

Polynomial Chaos Expansion

- *Uncertainty Quantification* approaches
  - ✓ Sampling methods (non-intrusive)
  - ✓ Quadrature methods (non-intrusive)
  - ✓ Spectral methods (intrusive): Polynomial Chaos Expansion
- The stochastic field $\mathcal{U}(\boldsymbol{x};\boldsymbol{\xi})$ is decomposed

PC Expansion

$$\mathcal{U}(\boldsymbol{x};\boldsymbol{\xi}) = \sum_{0\leqslant|\boldsymbol{\alpha}|\leqslant p} u_{\boldsymbol{\alpha}}(\boldsymbol{x})\boldsymbol{\psi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

- The number of unknown coefficients (u_i's) is: $P+1 = \binom{p+n_s}{p}$
- Curse of dimensionality
- Functions $\psi_i(\xi)$'s are the orthogonal polynomials with respect to input PDFs.
- Regression approach is employed to calculate the PCE coefficients.
- Sobol' sampling scheme
- Variance based sensitivity analysis using Sobol' indices.

Sparse Reconstruction of Polynomial Chaos Expansion Using Compressed Sensing

Introduction

- Industrial problems: large number of random variables.
- *Curse of dimensionality*: Computational cost of PCE grows exponentially with the number variables.
- Remedy: *efficient* methods

Efficient methods

✓ Adaptive methods
✓ Reduced basis methods
✓ Multifidelity methods
✓ Sparse methods

- Sparse reconstruction approaches:
  - ✓ Hyperbolic sparse
  - ✓ Compressed sensing

$$\mathcal{U}(\boldsymbol{x};\boldsymbol{\xi}) = \sum_{0\leqslant|\boldsymbol{\alpha}|\leqslant p} u_{\boldsymbol{\alpha}}(\boldsymbol{x})\psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

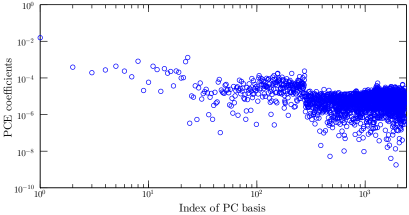


FIGURE: PCE coefficient of drag coefficient of the RAE2822 airfoil with stochastic geometry and operating condition

Compressed Sensing

Definition

Recover a sparse signal from a set of incomplete observations

- Optimization problem (ℓ_0-minimization):

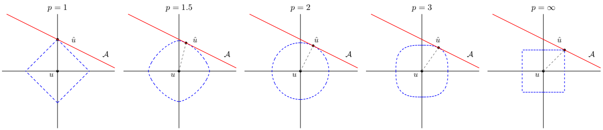
$$\hat{\boldsymbol{u}} = \operatorname{argmin}_{\boldsymbol{u}} \|\boldsymbol{u}\|_0 \quad \text{subject to} \quad \boldsymbol{\Psi}\boldsymbol{u} = \mathcal{Y}$$

- ℓ_0-minimization is NP-hard! Hence, ℓ_1-minimization

$$\hat{\boldsymbol{u}} = \operatorname{argmin}_{\boldsymbol{u}} \|\boldsymbol{u}\|_1 \quad \text{subject to} \quad \boldsymbol{\Psi}\boldsymbol{u} = \mathcal{Y}$$

- Noisy signal:

$$\hat{\boldsymbol{u}} = \operatorname{argmin}_{\boldsymbol{u}} \|\boldsymbol{u}\|_1 \quad \text{subject to} \quad \|\boldsymbol{\Psi}\boldsymbol{u} - \mathcal{Y}\|_2 \leqslant \epsilon$$



Original

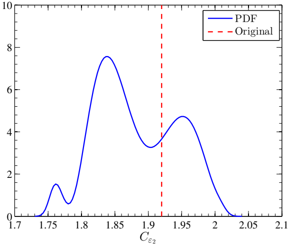
Reduced to 10% of the wavelet coefficients

LIMITATION OF CLASSIC PCE

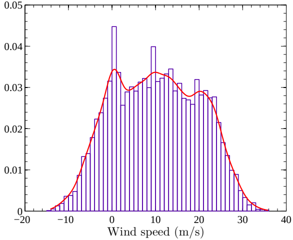
- PCE basis should be orthogonal with respect to the PDF of the uncertain input parameters.
- The Wiener-Askey polynomial: exponential convergence for a limited number of PDFs.
- What about arbitrary PDFs?
- Gram-Schmidt orthogonalization method.
- Exponential convergence for arbitrary distributions.
- The GSPCE is revisited and for the first time used with the regression method.

Distribution	Polynomials	Support
Gaussian	Hermite	$(-\infty, \infty)$
Uniform	Legendre	$[-1, 1]$
Gamma	Laguerre	$[0, \infty)$
Beta	Jacobi	$[-1, 1]$

$$\mathcal{U}(\boldsymbol{x};\boldsymbol{\xi}) = \sum_{0\leqslant|\boldsymbol{\alpha}|\leqslant p} u_{\boldsymbol{\alpha}}(\boldsymbol{x})\boldsymbol{\psi}_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$



PDF of $C_{\varepsilon 2}$ in $k-\varepsilon$ model.



PDF of wind speed from measured meteorological data (www.umass.edu)

Gram-Schmidt Orthogonalization Method

- One-dimensional monic orthogonal polynomials:

$$\psi_j(\xi) = e_j(\xi) - \sum_{k=0}^{j-1} c_{jk}\psi_j(\xi), \quad j = 1, 2, \cdots, p,$$

with

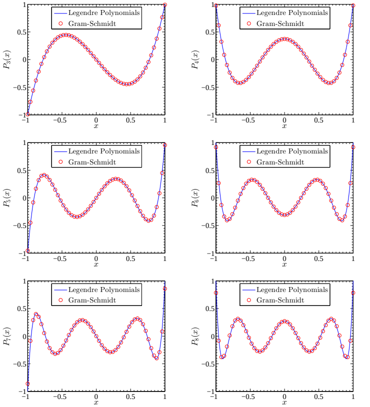
$$\psi_0 = 1 \quad c_{jk} = \frac{\langle e_j(\xi), \psi_k(\xi)\rangle}{\langle \psi_k(\xi), \psi_k(\xi)\rangle},$$

where the polynomials $e_j(\xi)$ are polynomials of exact degree j.

- The polynomials are normalized as:

$$\psi_j(\xi) = \frac{\psi_j(\xi)}{\langle \psi_j(\xi), \psi_j(\xi)\rangle}$$

Legendre (Uniform)



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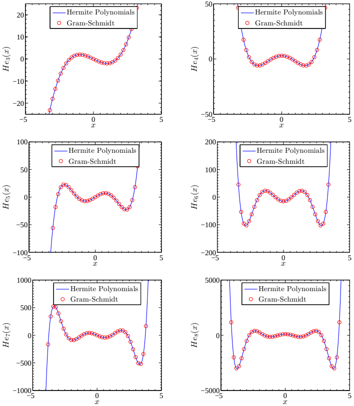
Hermite (Gaussian)



Numerical Example: Quantification of epistemic uncertainties in the $k - \varepsilon$ model coefficients in OpenFOAM channel flow

Epistemic Uncertainties in the $k-\varepsilon$ Model Coefficients

- Sources of uncertainties in RANS models:
  - Model formulation
  - Coefficients
- The Launder-Shrama $k-\varepsilon$ model:
  - ✓ Boussinesq (eddy-viscosity) hypothesis:

$$\overline{u_i u_j} = -\nu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \frac{2}{3} k \delta_{ij}$$

  - ✓ Turbulent viscosity:

$$\nu_t = C_\mu f_\mu \frac{k^2}{\varepsilon}$$

  - ✓ To obtain ν_t, transport equations are solved:

$$\frac{\partial}{\partial x_j}(U_j k) = \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + P_k - \tilde{\varepsilon} - 2\nu\left(\frac{\partial \sqrt{k}}{\partial x_j}\right)^2$$

$$\frac{\partial}{\partial x_j}(U_j \tilde{\varepsilon}) = \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\varepsilon}\right)\frac{\partial \tilde{\varepsilon}}{\partial x_j}\right] + C_{\varepsilon 1}\frac{\tilde{\varepsilon}}{\sigma_\varepsilon} P_k - C_{\varepsilon 2} f_2 \frac{\tilde{\varepsilon}^2}{k} + E \quad (1)$$

Launder-Sharma $k - \varepsilon$ model coefficients

- The empirical coefficients of low-Re Launder-Sharma $k - \varepsilon$ model

C_μ	σ_k	σ_ϵ	C_{ε_1}	C_{ε_2}
0.09	1.0	1.3	1.44	1.92

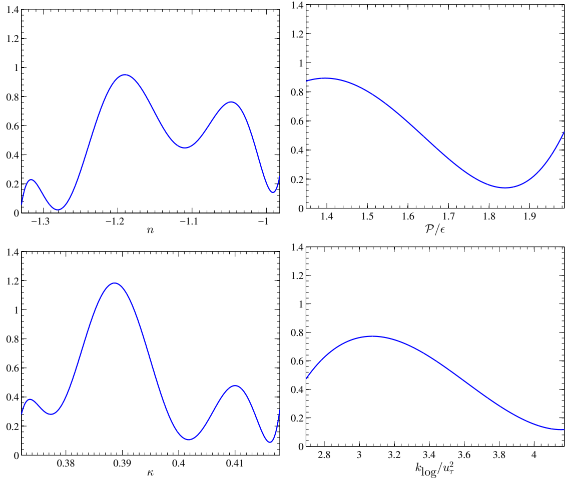
- The coefficients are related to some basic physical quantities (Durbin and Reif, 2011):
  - ✓ The decay exponent in decaying homogeneous, isotropic turbulence, n
  - ✓ The production to dissipation in homogeneous shear flow, $\mathcal{P}/\varepsilon$
  - ✓ The Von-Karman constant, κ
  - ✓ The dimensionless turbulent kinetic energy in the logarithmic layer, $k_{\log}/u_\tau^2$

$$C_\mu = \left(\frac{k_{\log}}{u_\tau^2}\right)^{-2}, \qquad C_{\varepsilon 1} = \frac{C_{\varepsilon 2} - 1}{\mathcal{P}/\varepsilon} + 1,$$

$$C_{\varepsilon 2} = \frac{1-n}{n}, \qquad \sigma_\varepsilon = \frac{\kappa^2}{\sqrt{C_\mu}(C_{\varepsilon 2} - C_{\varepsilon 1})}.$$

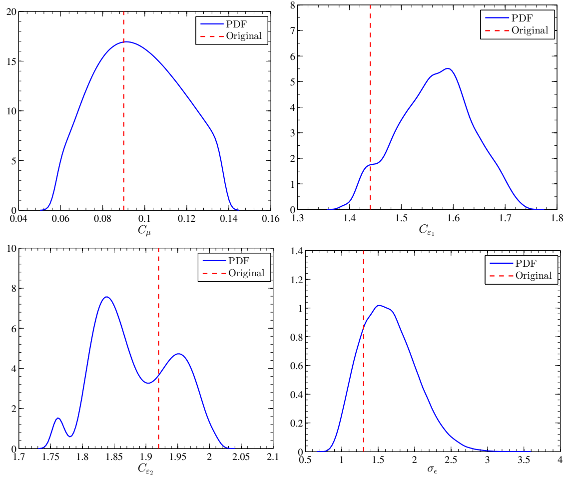
- The reported data for these quantities in the literature are collected and presented as PDFs (Margheri et al., 2014)

PDFs of Basic Physical Quantities



$$C_\mu = \left(\frac{k_{\log}}{u_\tau^2}\right)^{-2}, \quad C_{\varepsilon 1} = \frac{C_{\varepsilon 2} - 1}{\mathcal{P}/\varepsilon} + 1, C_{\varepsilon 2} = \frac{1-n}{n}, \quad \sigma_\varepsilon = \frac{\kappa^2}{\sqrt{C_\mu}(C_{\varepsilon 2} - C_{\varepsilon 1})}.$$

PDFs of $k - \varepsilon$ Coefficients



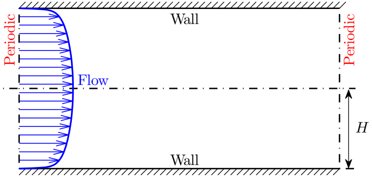
- The PDFs of Launder-Sharma Coefficients are computed using a Monte-Carlo simulation
- Reported standard values lie within its PDF range

TEST CASE: CHANNEL FLOW

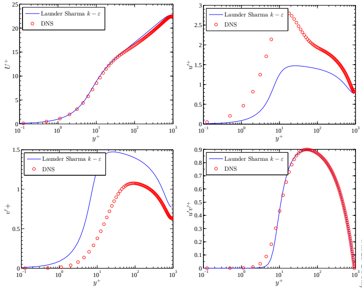
- Fully-developed turbulent channel flow
- Friction Reynolds number

$$\mathrm{Re}_\tau = \frac{u_\tau H}{\nu} = 950$$

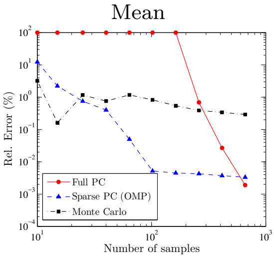
- OpenFOAM Solver: `boundaryFoam`
- Steady-state solver for incompressible, 1D turbulent flow
- grad $\bar{p} = \mathrm{div}\bar{\tau}$
- Number of stochastic parameters $n_s = 4$
- UQ analyses preformed with $p = 7$
- Reference solution: 8th order full PC

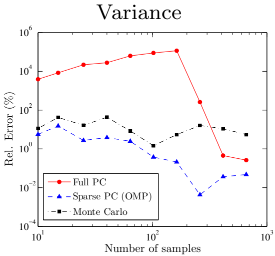


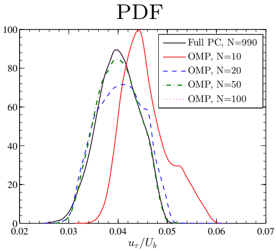
- Turbulence model: `LaunderSharmaKE`
- Discretization:
  - ✓ `gradSchemes: linear`
  - ✓ `divSchemes: linear`
  - ✓ `divSchemes: linear`
- Linear solvers:
  - ✓ `U: PCG, DIC`
  - ✓ `k: smoothSolver, symGaussSeidel`
  - ✓ `epsilon: smoothSolver, symGaussSeidel`

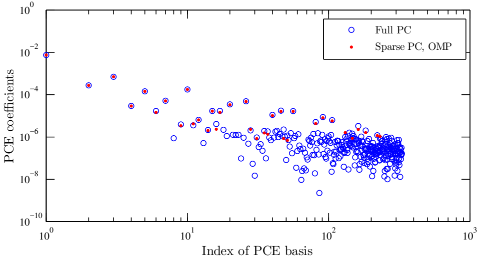


CONVERGENCE OF FRICTION VELOCITY (u_τ) STATISTICS



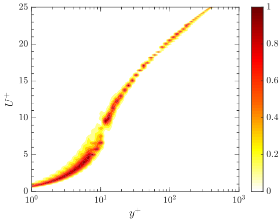




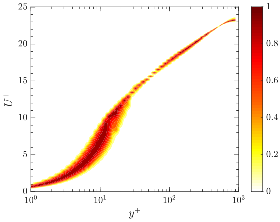


- Sparse method converged much faster.
- OMP with $N = 100$ sample method has successfully explored the important basis in the PCE.

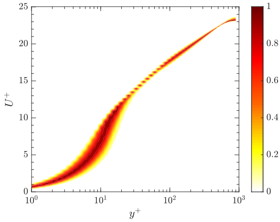
2D PDFs of Velocity Field



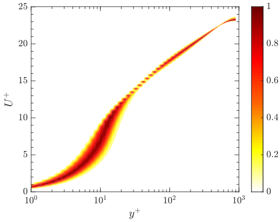
(a) OMP, $N = 10$



(b) OMP, $N = 50$



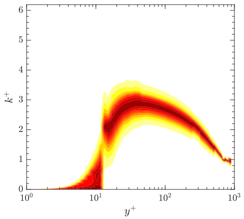
(c) OMP, $N = 100$



(d) Full PC, $N = 990$

- Normalized 2D PDFs (PDF/max(PDF)).
- Increasing number of samples improves reconstructed 2D PDFs.
- Using $N = 100$ samples the constructed 2D PDF is very similar to the full PC.
- **The sparse method is 9 times faster!**

2D PDFs of Turbulence Field



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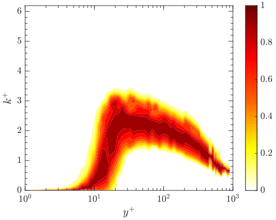

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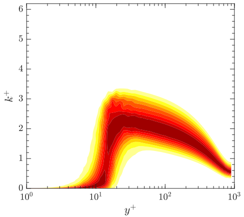

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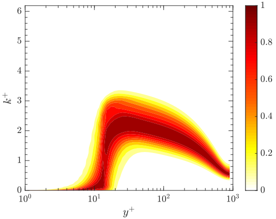

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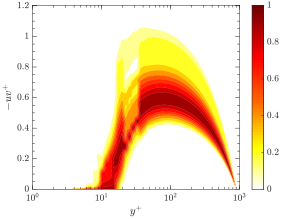

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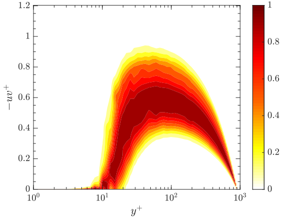

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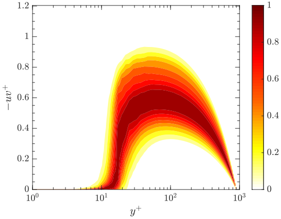
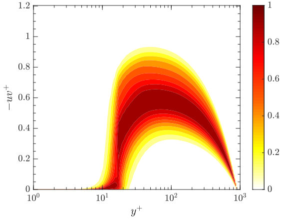


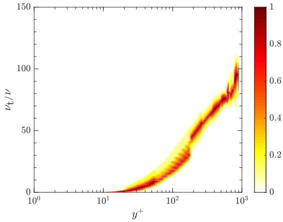
(c) OMP, $N = 100$



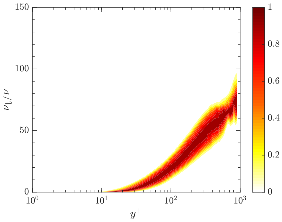
(d) Full PC, $N = 990$

- Normalized 2D PDFs (PDF/max(PDF)).
- Increasing number of samples improves reconstructed 2D PDFs.
- Using $N = 100$ samples the constructed 2D PDF is very similar to the full PC.
- **The sparse method is 9 times faster!**

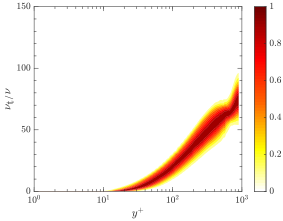
2D PDFs of Turbulence Field



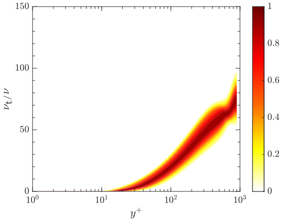
(a) OMP, $N = 10$



(b) OMP, $N = 50$



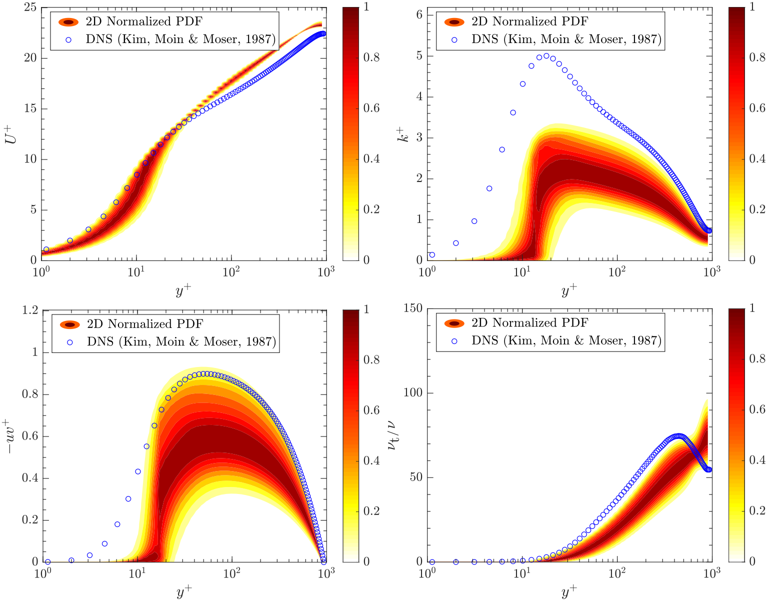
(c) OMP, $N = 100$



(d) Full PC, $N = 990$

- Normalized 2D PDFs (PDF/max(PDF)).
- Increasing number of samples improves reconstructed 2D PDFs.
- Using $N = 100$ samples the constructed 2D PDF is very similar to the full PC.
- **The sparse method is 9 times faster!**

Comparing with DNS Data




Thank
You
Merci
Gracias
TerimaKasih
Spacibo
Danke
KamSahHamnida
Xièxie
Mèsi
Grazie
Chokrane
Dziakuju
GratiasAgimus
GratiasAgo
Motashakkeram
KopKhunKha
Gracie
Hvala
Arigatô
Takk
aDank
BarakAllahuFiik
ThintKo
Buznyg
Blagodaram
Rahmat
Matondo
Mercé
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Dakujem
Gràcies
Faleminderit
Efharisto
NajisTuke
Grandmercé
Nirringrazzjak
Bayarlalaa
Obrigado
Salamat
Saha
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Chnorakaloutioun
TänanVäga
Tak
Sagolun
Dankie
Ačiū
Barkal
Mauruuru
Kiitos
Grazzi
Murakoze
Köszönöm
TapadhLeat
WaadMahadsantahay
Tanemirt
Tenki
Aabhar
Dhanyavaad
Gratzias
KhobChaiDeu


Thank
You
Merci
Gracias
Danke
Spacibo
TerimaKasih
Hvala
Arigatô
KamSahHamnida
Xièxie
Mèsi
Chokrane
Dziakuju
Grazie
Takk
aDank
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GratiasAgimus
GratiasAgo
Motashakkeram
KopKhunKha
Tak
Dankie
TänanVäga
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Tenki
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Mauruuru
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Aćiū
Sagolun
Grazzi
Dhanyavaad
Aabhar
Dakujem
Mamnun
Gratzias
KhobChaiDeu


WHAT?
WHY?
WHEN?
WHERE?
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WHICH?
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WHAT? HOW? WHY?
HOW?