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Domain Decomposition of Stochastic PDEs using FEniCS

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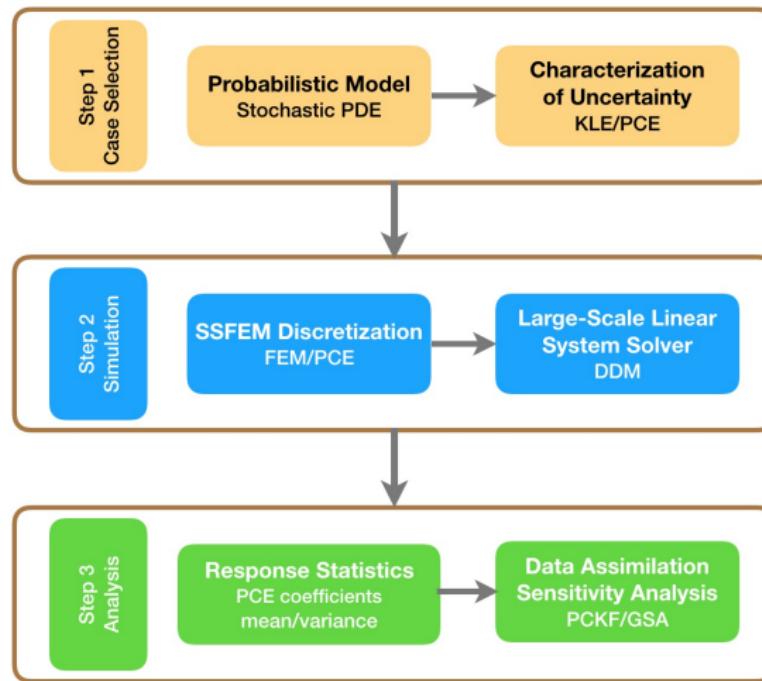
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Ottawa, Canada

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Introduction

- Motivation
 - Uncertainty quantification for high resolution numerical models.
 - *fine mesh resolution*
 - *many random parameters/variables*
- Objective
 - Develop scalable (numerical and parallel) algorithms to quantify uncertainty in large-scale computational models.
- Methodology
 - Exploit non-overlapping domain decomposition methods in conjunction with an intrusive polynomial chaos approach.

Uncertainty Quantification Framework



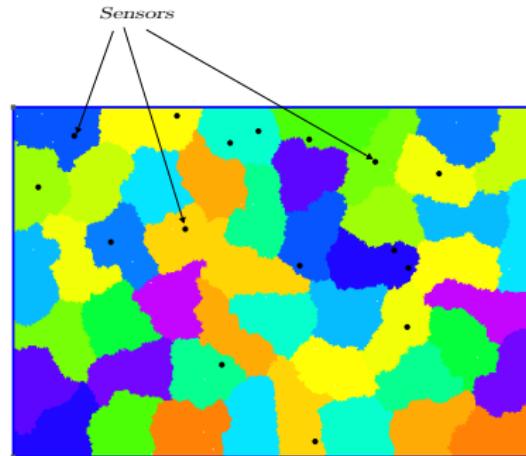
Bayesian Estimation using Nonlinear Filtering

- Model Equation

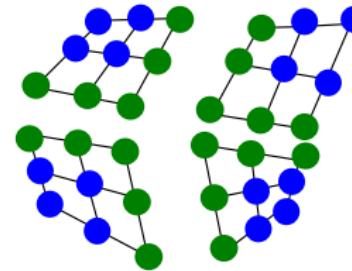
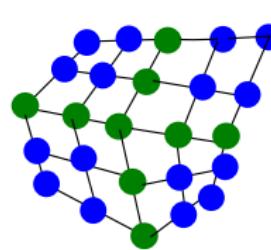
$$\mathbf{u}_{k+1} = \psi_k (\mathbf{u}_k, \mathbf{f}_k, \mathbf{q}_k) \quad -- \text{ Forecast Step}$$

- Measurement Equation

$$\mathbf{d}_k = \mathbf{h}_k (\mathbf{u}_k, \epsilon_k) \quad -- \text{ Assimilation Step}$$



Domain Decomposition Method for Stochastic PDEs



- Spatial decomposition

$$\begin{bmatrix} \mathbf{A}_{II}^s(\theta) & \mathbf{A}_{IG}^s(\theta) \\ \mathbf{A}_{GI}^s(\theta) & \mathbf{A}_{GG}^s(\theta) \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s(\theta) \\ \mathbf{u}_G^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_G^s \end{Bmatrix} .$$

- Polynomial Chaos expansion

$$\sum_{i=0}^L \Psi_i \begin{bmatrix} \mathbf{A}_{II,i}^s & \mathbf{A}_{IG,i}^s \\ \mathbf{A}_{GI,i}^s & \mathbf{A}_{GG,i}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_I^s(\theta) \\ \mathbf{u}_G^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_I^s \\ \mathbf{f}_G^s \end{Bmatrix} .$$

Domain Decomposition Method for Stochastic PDEs

$$\begin{aligned}
 & \left\langle \sum_{i=0}^L \Psi_i(\theta) \begin{bmatrix} \mathbf{A}_{II,i}^1 & \dots & 0 & \mathbf{A}_{I\Gamma,i}^1 \mathbf{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathbf{A}_{II,i}^{n_s} & \mathbf{A}_{I\Gamma,i}^{n_s} \mathbf{R}_{n_s} \\ \mathbf{R}_1^T \mathbf{A}_{I\Gamma,i}^1 & \dots & \mathbf{R}_{n_s}^T \mathbf{A}_{I\Gamma,i}^{n_s} & \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{A}_{I\Gamma,i}^s \mathbf{R}_s \end{bmatrix} \right. \\
 & \quad \left. \sum_{j=0}^N \Psi_j(\theta) \begin{Bmatrix} \mathbf{u}_{I,j}^1 \\ \vdots \\ \mathbf{u}_{I,j}^{n_s} \\ \mathbf{u}_{\Gamma,j} \end{Bmatrix} \right\rangle \Psi_k(\theta) \rangle \\
 & = \left\langle \begin{Bmatrix} \mathbf{f}_I^1 \\ \vdots \\ \mathbf{f}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathbf{R}_s^T \mathbf{f}_{\Gamma}^s \end{Bmatrix} \right\rangle \Psi_k(\theta) \rangle, \quad k = 0, \dots, N.
 \end{aligned}$$

Domain Decomposition Method for Stochastic PDEs

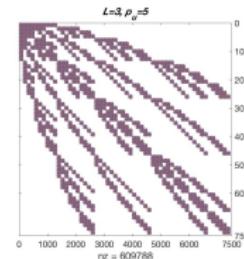
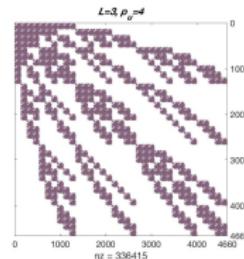
$$\begin{bmatrix} \mathcal{A}_{II}^1 & \dots & 0 & \mathcal{A}_{I\Gamma}^1 \mathcal{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathcal{A}_{II}^{n_s} & \mathcal{A}_{I\Gamma}^{n_s} \mathcal{R}_{n_s} \\ \mathcal{R}_1^T \mathcal{A}_{\Gamma I}^1 & \dots & \mathcal{R}_{n_s}^T \mathcal{A}_{\Gamma I}^{n_s} & \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{A}_{\Gamma\Gamma}^s \mathcal{R}_s \end{bmatrix} \begin{Bmatrix} \mathcal{U}_I^1 \\ \vdots \\ \mathcal{U}_I^{n_s} \\ \mathcal{U}_{\Gamma} \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_I^1 \\ \vdots \\ \mathcal{F}_I^{n_s} \\ \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{F}_{\Gamma}^s \end{Bmatrix}, \quad (1)$$

$$[\mathcal{A}_{\alpha\beta}^s]_{jk} = \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_{\alpha\beta,i}^s \quad ; \quad \mathcal{F}_{\alpha,k}^s = \langle \Psi_k \mathbf{f}_{\alpha}^s \rangle, \quad (2)$$

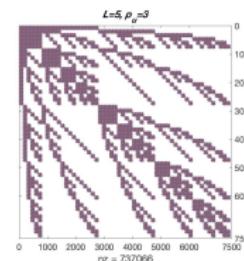
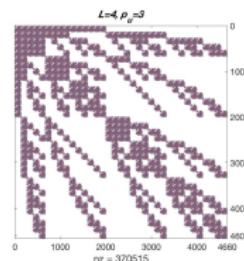
$$\mathcal{U}_I^m = (\mathbf{u}_{I,0}^m, \dots, \mathbf{u}_{I,N}^m)^T \quad ; \quad \mathcal{U}_{\Gamma} = (\mathbf{u}_{\Gamma,0}, \dots, \mathbf{u}_{\Gamma,N})^T.$$

Sarkar, A. Benabbou, N. and Ghanem, R., IJNME, 2009.

Block Sparsity Structure



$L = 3$ and $p_u = 4, 5.$



$p_u = 3$ and $L = 4, 5.$

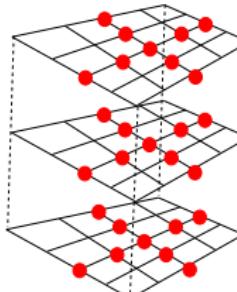
Extended Interface Problem

- The Extended Schur Complement System

$$\mathcal{S}\mathcal{U}_\Gamma = \mathcal{G}_\Gamma.$$

$$\mathcal{S} = \sum_{s=1}^{n_s} \mathcal{R}_s^T [\mathcal{A}_{\Gamma\Gamma}^s - \mathcal{A}_{\Gamma I}^s (\mathcal{A}_{II}^s)^{-1} \mathcal{A}_{I\Gamma}^s] \mathcal{R}_s.$$

- Develop parallel iterative algorithms.
- Formulate scalable preconditioners.
- Application to 2D and 3D Stochastic PDEs with non-Gaussian coefficients.



Two-Level Domain Decomposition Methods for SPDEs

$$\mathcal{M}^{-1} = \sum_{s=1}^{n_s} \mathcal{H}_f^s{}^T [\mathcal{S}_f^s]^{-1} \mathcal{H}_f^s + \mathcal{H}_0^T [\mathcal{S}_c]^{-1} \mathcal{H}_0,$$

- Condition Number Bound of Deterministic System
 - One-level preconditioner

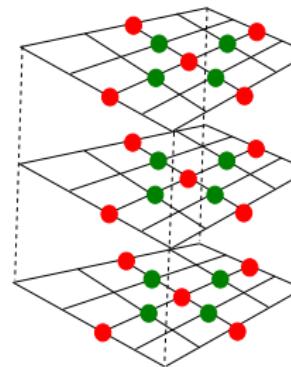
$$\kappa(M^{-1}S) \leq C \frac{1}{H^2} \left(1 + \log \frac{H}{h}\right)^2$$

- Two-level preconditioner

$$\kappa(M^{-1}S) \leq C \left(1 + \log \frac{H}{h}\right)^2$$

Two-Level Domain Decomposition Methods for SPDEs

- Partitioning the interface nodes into remaining (■) and corner(●) nodes



$$\mathcal{U}_\Gamma^s = \left\{ \begin{array}{l} \mathcal{U}_r^s \\ \mathcal{U}_c^s \end{array} \right\}$$

Probabilistic Balancing Domain Decomposition with Constraints

$$\left[\begin{array}{ccc} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \mathcal{B}_c^s \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \mathcal{B}_c^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^s \mathcal{T} \mathcal{A}_{ci}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^s \mathcal{T} \mathcal{A}_{cr}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^s \mathcal{T} \mathcal{A}_{cc}^s \mathcal{B}_c^s \end{array} \right] \left\{ \begin{array}{c} \mathcal{X}^s \\ \mathcal{U}_r^s \\ \mathcal{U}_c \end{array} \right\} = \left\{ \begin{array}{c} \mathbf{0} \\ \mathcal{F}_r^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^s \mathcal{T} \mathcal{F}_c^s \end{array} \right\}$$

$$\mathcal{M}_{NNC}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{R}_s^T [\mathcal{S}_{rr}^s]^{-1} \mathcal{R}_s^r \mathcal{D}_s \mathcal{R}_s + R_0^T [F_{cc}]^{-1} R_0,$$

$$R_0 = \sum_{s=1}^{n_s} \mathcal{B}_c^s \mathcal{T} (\mathcal{R}_s^c - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{R}_s^r) \mathcal{D}_s \mathcal{R}_s.$$

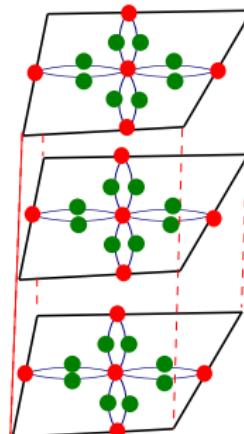
$$F_{cc} = \sum_{s=1}^{n_s} \mathcal{B}_c^s \mathcal{T} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s,$$

$$\mathcal{S}_{\alpha\beta}^s = \mathcal{A}_{\alpha\beta}^s - \mathcal{A}_{\alpha i}^s [\mathcal{A}_{ii}^s]^{-1} \mathcal{A}_{i\beta}^s, \quad [\mathcal{A}_{\alpha\beta}^s]_{jk} = \sum_{i=0}^L \langle \Psi_i \Psi_j \Psi_k \rangle \mathbf{A}_{\alpha\beta,i}^s$$

Probabilistic Dual Primal Domain Decomposition

$$\begin{bmatrix} \mathcal{A}_{ii}^s & \mathcal{A}_{ir}^s & \mathcal{A}_{ic}^s \mathcal{B}_c^s & 0 \\ \mathcal{A}_{ri}^s & \mathcal{A}_{rr}^s & \mathcal{A}_{rc}^s \mathcal{B}_c^s & \mathcal{B}_r^s T \\ \sum_{s=1}^{n_s} \mathcal{B}_c^s T \mathcal{A}_{ci}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^s T \mathcal{A}_{cr}^s & \sum_{s=1}^{n_s} \mathcal{B}_c^s T \mathcal{A}_{cc}^s \mathcal{B}_c^s & 0 \\ 0 & \sum_{s=1}^{n_s} \mathcal{B}_r^s & 0 & 0 \end{bmatrix} \begin{Bmatrix} \mathcal{U}_i^s \\ \mathcal{U}_s^s \\ \mathcal{U}_c \\ \Lambda \end{Bmatrix} = \begin{Bmatrix} \mathcal{F}_i^s \\ \mathcal{F}_r^s \\ \sum_{s=1}^{n_s} \mathcal{B}_c^s T \mathcal{F}_c^s \\ 0 \end{Bmatrix},$$

$$(\bar{F}_{rr} + \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{F}_{cr})\Lambda = \bar{d}_r - \bar{F}_{rc}[\bar{F}_{cc}]^{-1}\bar{d}_c,$$



Two-Level Domain Decomposition Methods for SPDEs

$$\mathcal{M}^{-1} = \sum_{s=1}^{n_s} \mathcal{H}_f^s{}^T [\mathcal{S}_f^s]^{-1} \mathcal{H}_f^s + \mathcal{H}_0^T [\mathcal{S}_c]^{-1} \mathcal{H}_0,$$

	\mathcal{H}_r	$[\mathcal{S}_n^r]^{-1}$	\mathcal{H}_0	$[\mathcal{S}_n]^{-1}$
a	$\mathcal{R}_r^T \mathcal{D}_r \mathcal{R}_r$	$[\mathcal{S}_n^r]^{-1}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{R}_r^T - \mathcal{S}_r^s [\mathcal{S}_n^r]^{-1} \mathcal{R}_r^s) \mathcal{D}_r \mathcal{R}_r$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_n^r - \mathcal{S}_n^s [\mathcal{S}_n^s]^{-1} \mathcal{S}_n^r) \mathcal{B}_c^s$
b	$\mathcal{D}_r^T \mathcal{B}_r^s$	$[\mathcal{S}_n^r]^{-1}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_n^s [\mathcal{S}_n^s]^{-1} \mathcal{D}_r^T \mathcal{B}_r^s$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_n^r - \mathcal{S}_n^s [\mathcal{S}_n^s]^{-1} \mathcal{S}_n^r) \mathcal{B}_c^s$
c	\mathcal{B}_r^{sT}	$[\mathcal{S}_n^r]^{-1}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} \mathcal{S}_n^s [\mathcal{S}_n^s]^{-1} \mathcal{B}_r^{sT}$	$\sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_n^r - \mathcal{S}_n^s [\mathcal{S}_n^s]^{-1} \mathcal{S}_n^r) \mathcal{B}_c^s$

a) Neumann-Neumann with Coarse grid, **b)** Primal-Primal, **c)** Dual-Primal Operator.

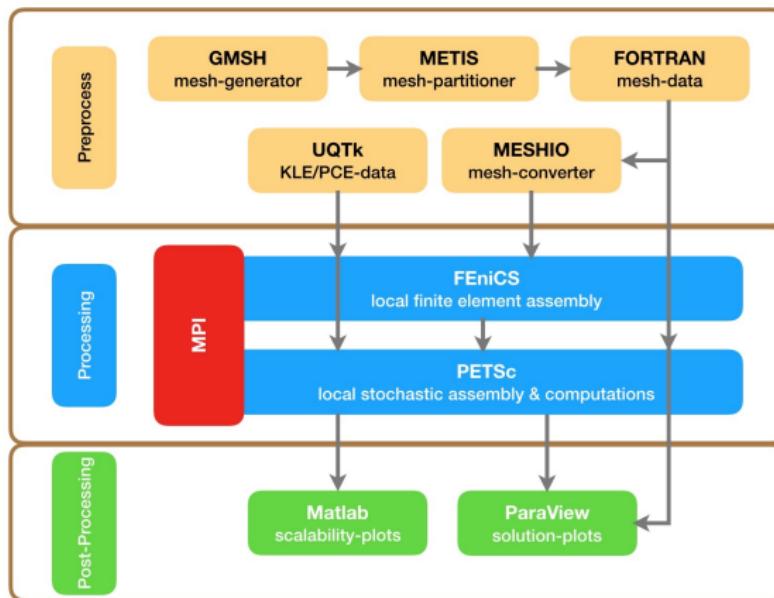
Investigated numerical and parallel scalabilities:

Subber, W. and Sarkar, A., JCP, 2014

Subber, W. and Sarkar, A., CMAME, 2013

Desai, A., Khalil, M., Pettit, C., Poirel, D. and Sarkar, A., CMAME 2017

Implementational Framework



Problem Setup for Numerical Experiments

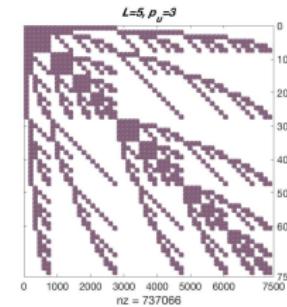
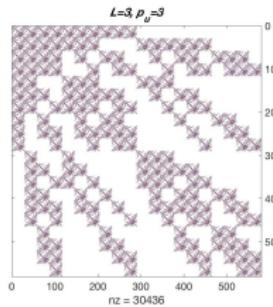
- Model Problem:

$$\begin{aligned} -\nabla \cdot (c_d(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) &= F(\mathbf{x}), & \Omega \times \mathcal{W}, \\ u(\mathbf{x}, \theta) &= 0, & \delta\Omega \times \mathcal{W}, \end{aligned}$$

- Diffusion coefficient c_d modelled as a lognormal process with the underlying a Gaussian process having mean μ , variance σ^2 and exponential covariance function C (on a 2D domain).

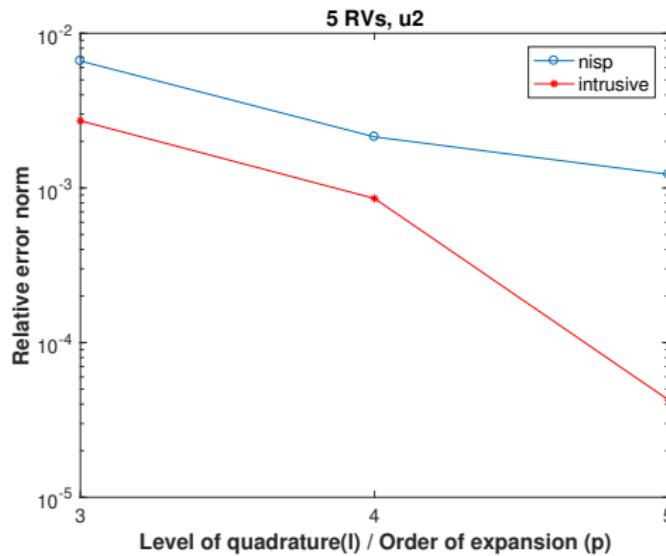
$$C(x_1, y_1; x_2, y_2) = \sigma^2 e^{-|x_2 - x_1|/b_1 - |y_2 - y_1|/b_2},$$

Block-Sparsity Structures



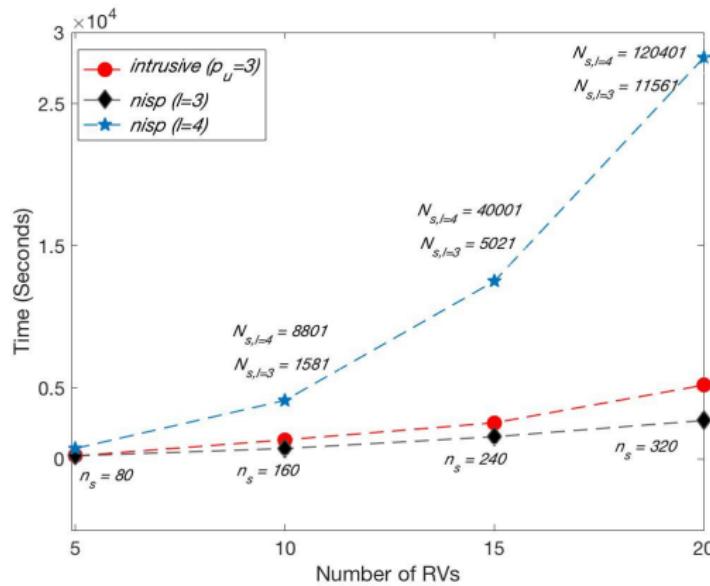
Fixed mesh resolution $N \approx 150$, $P_u = 3$ with $L = 3$ and $L = 5$.

Errors Analysis of PCE Coefficients of Solution Process:
Intrusive Vs Non-Intrusive



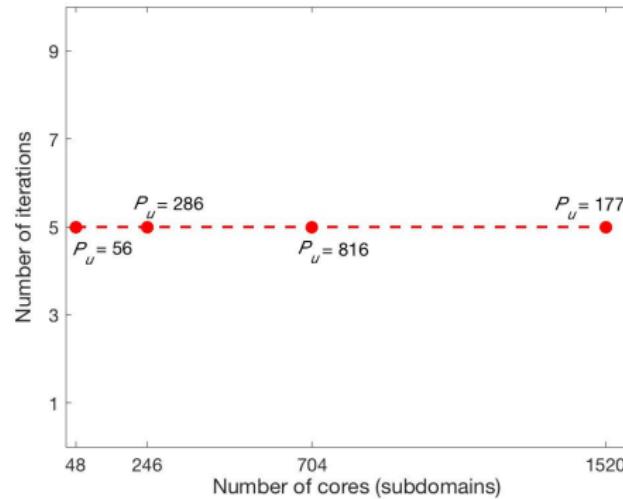
Relative error norm = $\frac{\|u_{iH} - u_{ih}\|}{\|u_{iH}\|}$, 5 random variables, error in $(\hat{\mathbf{u}}_2)$, coarse mesh ($N \approx 150$)

Scalability against Stochastic Dimensions: Intrusive vs Non-Intrusive (Sparse Grid)

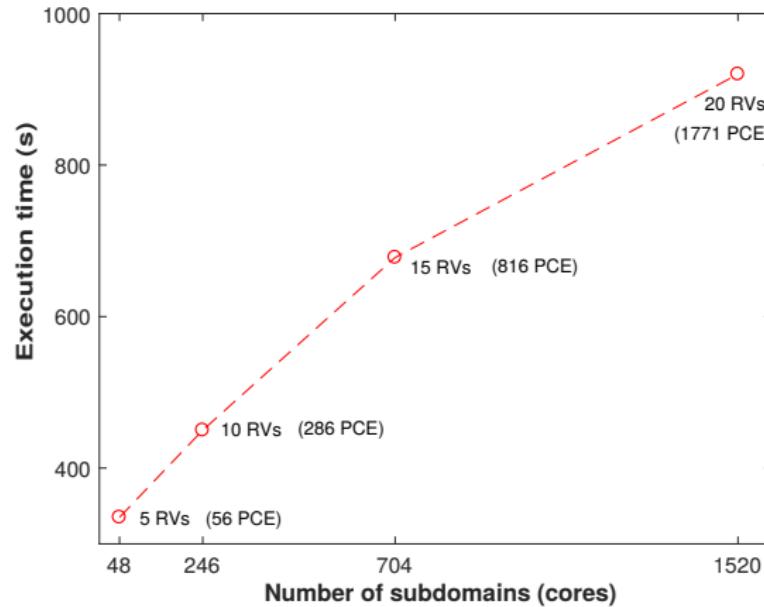


Fixed mesh resolution (52704 nodes and 105410 elements) and third order PCE for intrusive. Smolyak sparse grid with $l = 3$ and $l = 4$ for non-intrusive.

Scalability against Number of Random Variables: NNC/BDDC

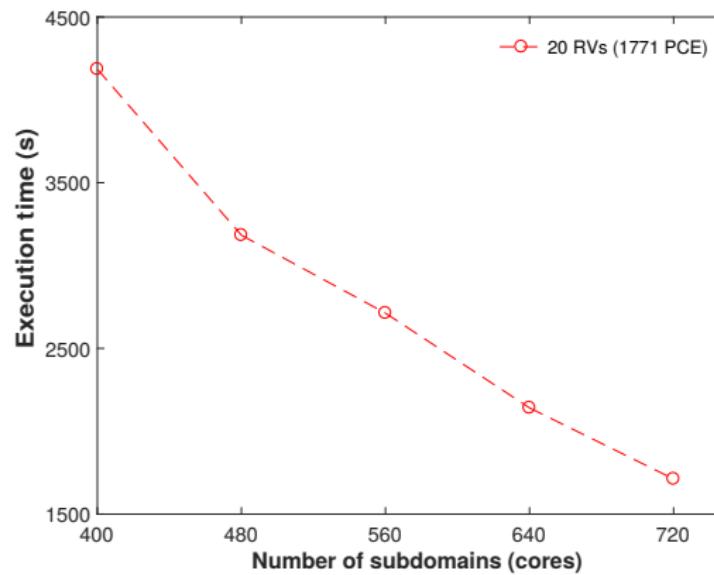


Fixed mesh resolution (52704 nodes and 105410 elements), fixed problem size per subdomain ($\approx 60,000$) and third order PCE (linear system of order max. ≈ 93 million)

Scalability against Number of Random Variables: NNC/BDDC

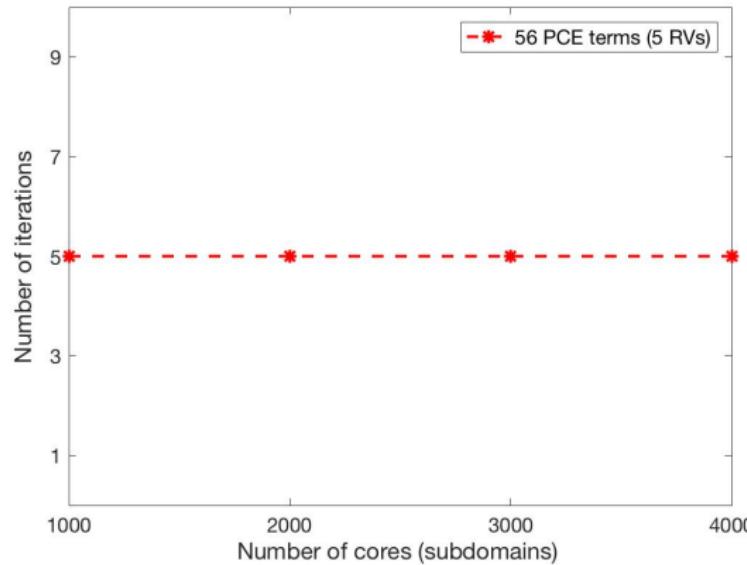
Fixed mesh (52704 nodes and 105410 elements), fixed problem size per subdomain ($\approx 60,000$) and third order PCE

Parallel Scalability (Strong): NNC/BDDC



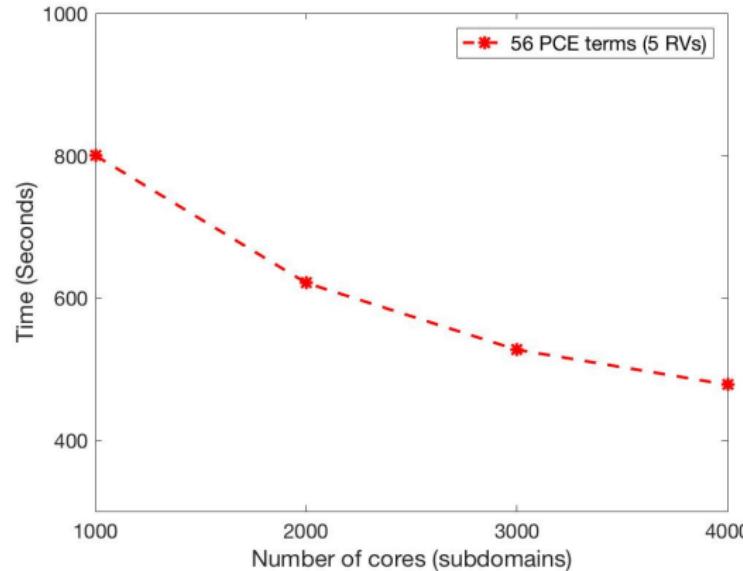
Fixed global problem, mesh with (52704 nodes and 105410 elements) and number of PCE terms $P_u = 1771$.

Scalability using Large-Scale HPC Cluster



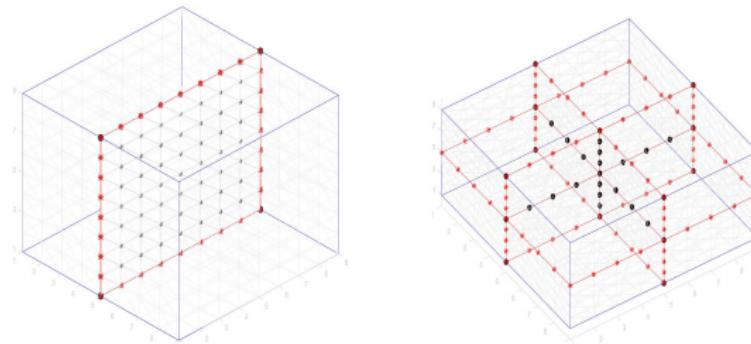
For the fixed mesh resolution (0.332 million nodes and 0.664 million elements.) and fixed number of PCE terms ($P_u = 56$).

Scalability using Large-Scale HPC Cluster



For the fixed mesh resolution (0.332 million nodes and 0.664 million elements.) and fixed number of PCE terms ($P_u = 56$).

*Probabilistic Coarse Grid in Three Dimensions:
Extended Wirebasket Grid*



(-) - the global interface edge, (●) - vertices (★) - interface-edges
and (●) - interface-faces.

Deterministic Setting: Condition Number Bound Vertex vs Wirebasket-based Methods

Ref. Book by Smith, Bjørstad and Gropp, 2004

For the vertex-based method in two dimensions

$$\kappa \leq C(1 + \log(H/h))^2,$$

For the vertex-based method in three dimensions

$$\kappa \leq C(H/h)(1 + \log(H/h)).$$

For the wirebasket-based methods in three dimensions

$$\kappa \leq C(1 + \log(H/h))^2.$$

Probabilistic BDDC/NNC using Extended Wirebasket-based Coarse Grid

$$\mathcal{F}_{WW} \mathcal{U}_W = d_W,$$

$$\mathcal{F}_{WW} = \sum_{s=1}^{n_s} \mathcal{B}_W^s {}^T \left(\mathcal{S}_{WW}^s - \mathcal{S}_{WF}^s [\mathcal{S}_{FF}^s]^{-1} \mathcal{S}_{FW}^s \right) \mathcal{B}_W^s,$$
$$d_W = \sum_{s=1}^{n_s} \mathcal{B}_W^s {}^T \left(f_W^s - \mathcal{S}_{WF}^s [\mathcal{S}_{FF}^s]^{-1} f_F^s \right).$$

Modified BDDC/NNC Preconditioner:

$$\mathcal{M}_{NNW}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s {}^T \mathcal{D}_s (\mathcal{R}_s^F {}^T [\mathcal{S}_{FF}^s]^{-1} \mathcal{R}_s^F) \mathcal{D}_s \mathcal{R}_s + \mathcal{R}_0 {}^T [\mathcal{F}_{WW}]^{-1} \mathcal{R}_0.$$

$$\mathcal{R}_0 = \sum_{s=1}^{n_s} \mathcal{B}_W^s {}^T (\mathcal{R}_s^W - \mathcal{S}_{WF}^s [\mathcal{S}_{FF}^s]^{-1} \mathcal{R}_s^F) \mathcal{D}_s \mathcal{R}_s,$$

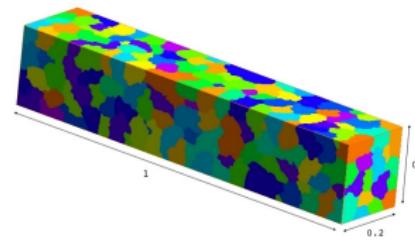
Numerical Experiments: Wirebasket based BDDC/NNC solver

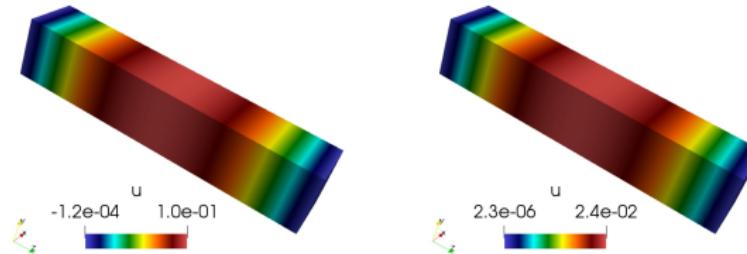
- Diffusion equation

$$\begin{aligned} -\nabla \cdot (c_d(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) &= F(\mathbf{x}), & \Omega \times \mathcal{W}, \\ u(\mathbf{x}, \theta) &= 0, & \delta\Omega \times \mathcal{W}, \end{aligned}$$

- Diffusion coefficient c_d - lognormal process having underlying a Gaussian process with exponential covariance C

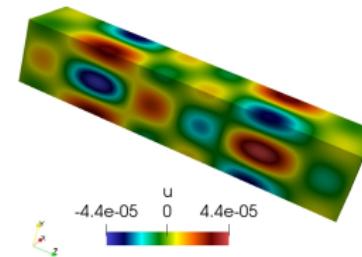
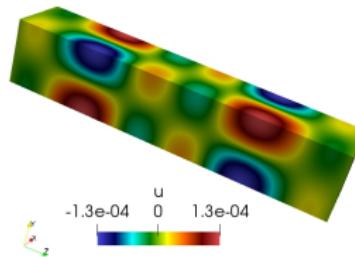
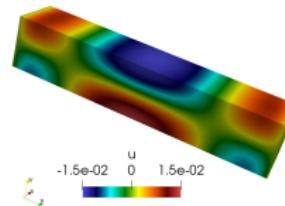
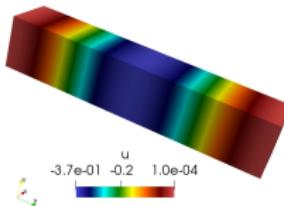
$$C(x_1, y_1, z_1; x_2, y_2, z_2) = \sigma^2 e^{-|x_2-x_1|/b_x - |y_2-y_1|/b_y - |z_2-z_1|/b_z}.$$



*Characteristics of the Solution Process:**Diffusion Equation*

Mean and standard deviation.

Characteristics of the Solution Process



Selected PCE coefficients.

Numerical Experiments: Wirebasket based BDDC/NNC solver for PDE System

- Linear Elasticity

$$\begin{aligned} -\nabla \cdot \sigma(\mathcal{U}(\mathbf{x}, \theta)) &= F(\mathbf{x}) \quad \text{in} \quad \mathcal{D}, \\ \sigma(\mathcal{U}(\mathbf{x}, \theta)) \cdot \hat{\mathbf{n}} &= b_T \quad \text{on} \quad \Gamma_1 = \delta\mathcal{D} \setminus \Gamma_0, \\ \mathcal{U}(\mathbf{x}, \theta) &= 0 \quad \text{on} \quad \Gamma_0. \end{aligned}$$

Stress tensor σ :

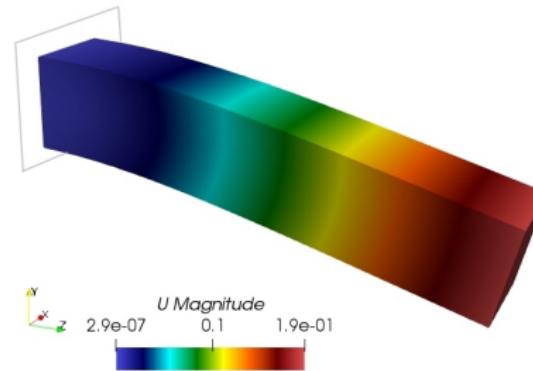
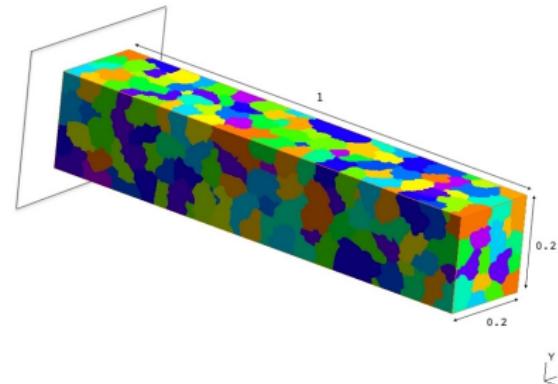
$$\sigma(\mathcal{U}(\mathbf{x}, \theta)) = \lambda(\nabla \cdot \mathcal{U}(\mathbf{x}, \theta))I + 2\mu\epsilon(\mathcal{U}(\mathbf{x}, \theta)),$$

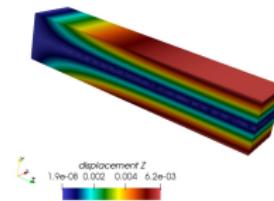
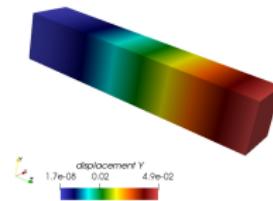
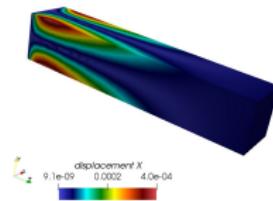
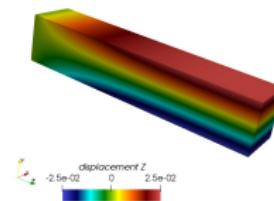
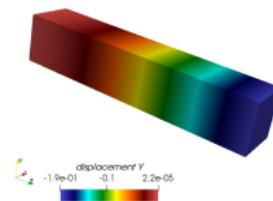
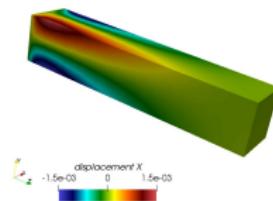
where $\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$ and $\mu = \frac{E}{2(1+\nu)}$ are Lamé constants.

- Young's modulus E - lognormal stochastic process (as before).

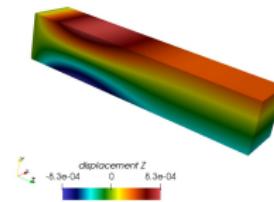
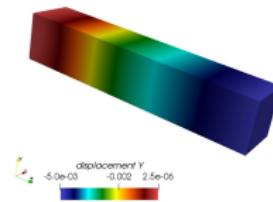
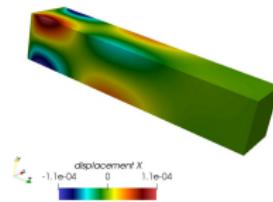
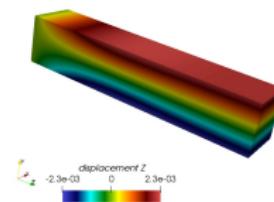
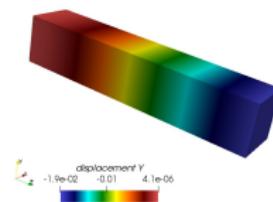
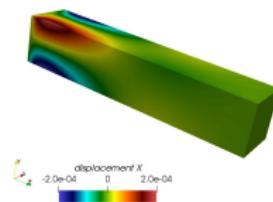
Characteristics of the Solution Process:

Time, space, and solution

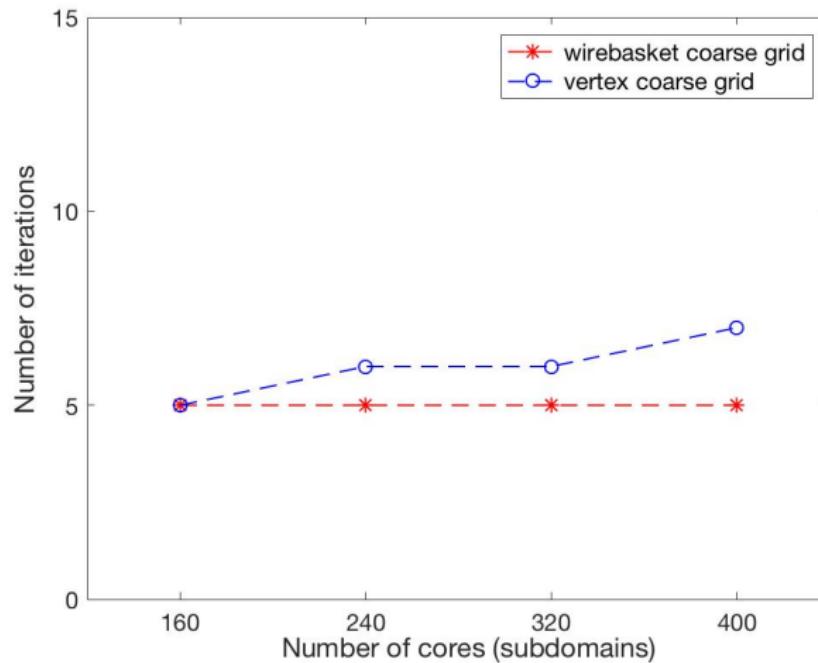


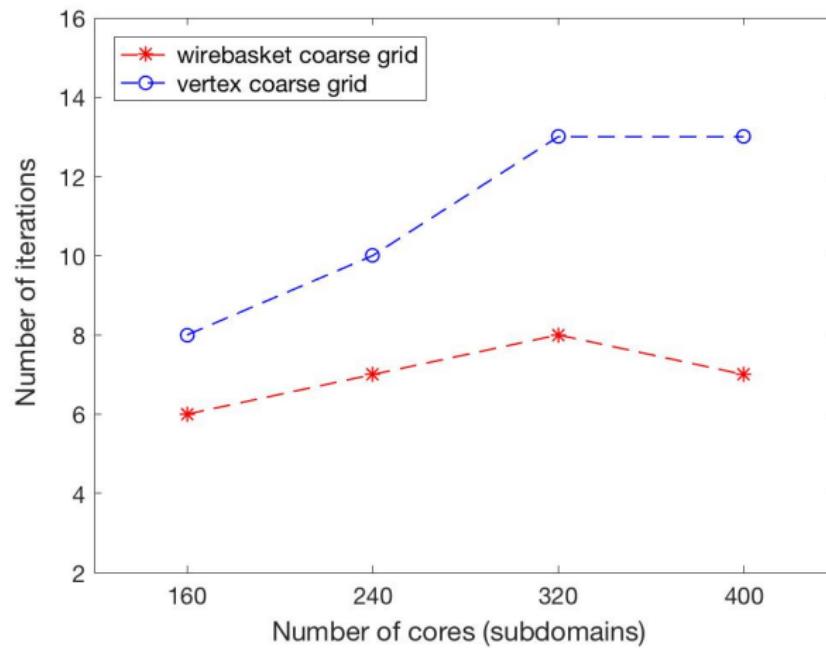
*Characteristics of the Solution Process:**Linear Elasticity*

x, y and z components of the mean and standard deviation.

*Characteristics of the Solution Process:**Linear Elasticity*

x, y and z components of the selected PCE coefficients.





Advantages of FEniCS Based Solver

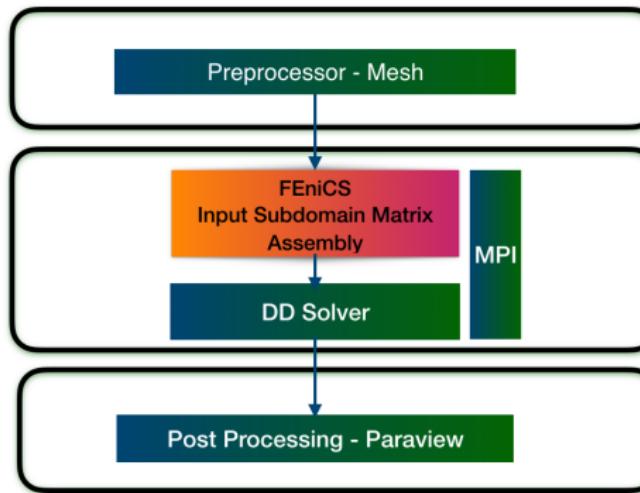
Implementational Efficiency

- Easy to implement stochastic aspects for a wide variety of PDEs (e.g. Poisson, Elasticity etc)
- Enables seamless integration with preprocessing and post-processing modules

Reduced Memory and Time Consumption

Domain Decomposition framework with parallel subdomain level assembly in FEniCS using MPI

SSFEM Solver

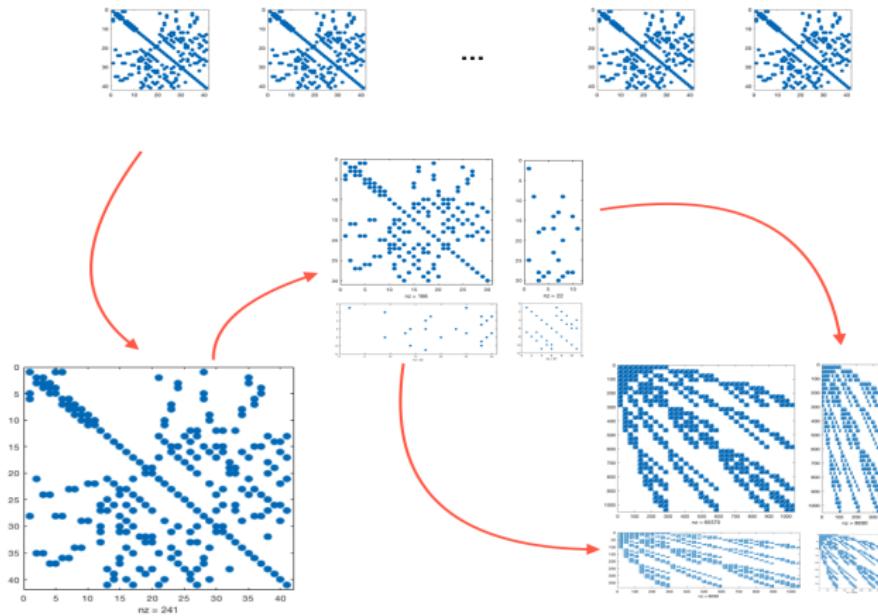


- Polynomial Chaos expansion

$$\sum_{i=0}^L \Psi_i \begin{bmatrix} \mathbf{A}_{H,i}^s & \mathbf{A}_{I,i}^s \\ \mathbf{A}_{II,i}^s & \mathbf{A}_{III,i}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_i^s(\theta) \\ \mathbf{u}_i^c(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_i^s \\ \mathbf{f}_i^c \end{Bmatrix} .$$

Implementational framework of SSFEM solver

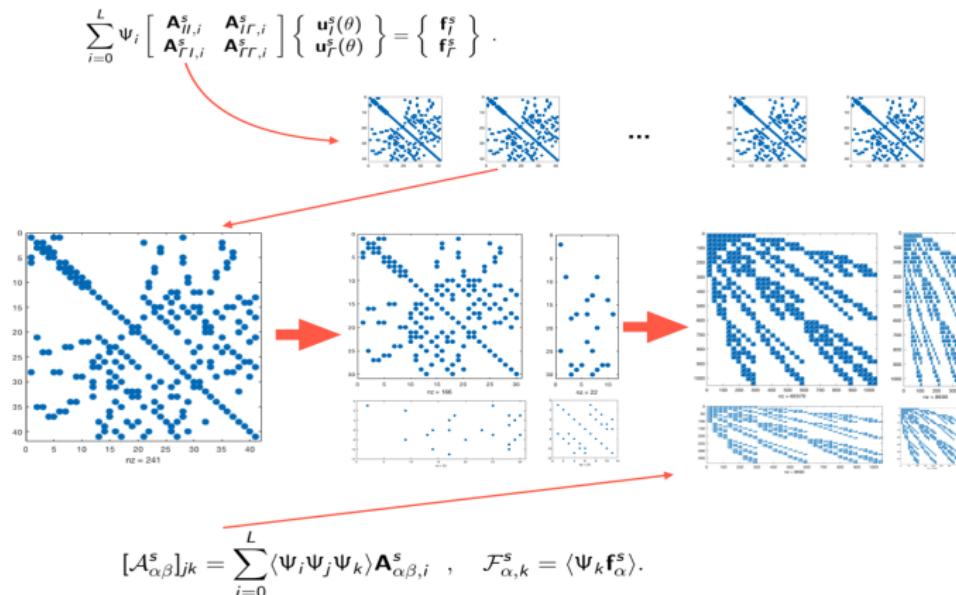
DD Framework using FEniCS



Deterministic and stochastic submatrices

DD Framework using FEniCS

- Polynomial Chaos expansion



Deterministic and stochastic submatrices

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 - **Ontario Innovation Trust**