

is paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government

A parallel update step of a sampling-free ENMF-type filter

SAND2021-6946C

Philippe Bisaillon¹, Ajit Desai^{1,5}, Mohammad Khalil², Chris Pettit³, Dominique Poirel⁴
and Abhijit Sarkar¹

¹Department of Civil and Environmental Engineering
Carleton University, Canada

²Quantitative Modeling & Analysis
Sandia National Laboratories, Livermore, California 94551, USA

³Aerospace Engineering Department
United States Naval Academy, Annapolis, Maryland, USA

⁴Department of Mechanical and Aerospace Engineering
Royal Military College of Canada

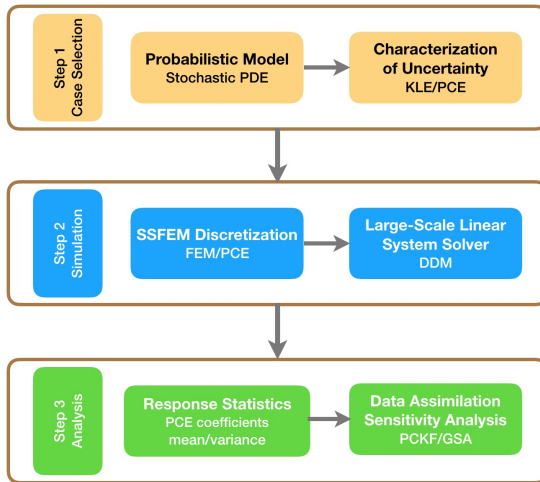
⁵Currently at Bank of Canada
Ottawa, Canada

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

Introduction

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

Uncertainty Quantification Framework



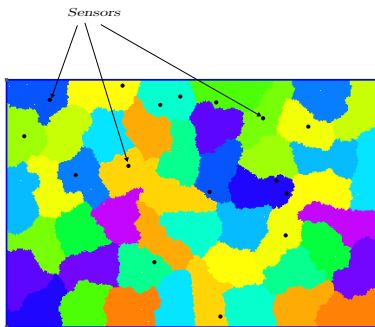
Bayesian Estimation using Nonlinear Filtering

- Model Equation

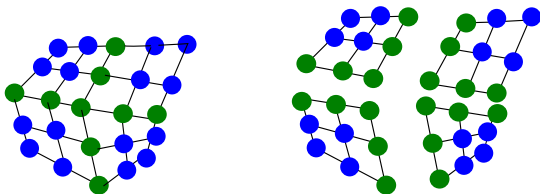
$$\mathbf{u}_{k+1} = \psi_k(\mathbf{u}_k, \mathbf{f}_k, \mathbf{q}_k) \quad -- \quad \text{Forecast Step}$$

- Measurement Equation

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



Domain Decomposition Method for Stochastic PDEs



- Spatial decomposition

$$\begin{bmatrix} \mathbf{A}_{ll}^s(\theta) & \mathbf{A}_{l\Gamma}^s(\theta) \\ \mathbf{A}_{\Gamma l}^s(\theta) & \mathbf{A}_{\Gamma\Gamma}^s(\theta) \end{bmatrix} \begin{Bmatrix} \mathbf{u}_l^s(\theta) \\ \mathbf{u}_{\Gamma}^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_l^s \\ \mathbf{f}_{\Gamma}^s \end{Bmatrix} .$$

- Polynomial Chaos expansion

$$\sum_{i=0}^L \psi_i \begin{bmatrix} \mathbf{A}_{ll,i}^s & \mathbf{A}_{l\Gamma,i}^s \\ \mathbf{A}_{\Gamma l,i}^s & \mathbf{A}_{\Gamma\Gamma,i}^s \end{bmatrix} \begin{Bmatrix} \mathbf{u}_l^s(\theta) \\ \mathbf{u}_{\Gamma}^s(\theta) \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_l^s \\ \mathbf{f}_{\Gamma}^s \end{Bmatrix} .$$

Domain Decomposition Method for Stochastic PDEs

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

Domain Decomposition Method for Stochastic PDEs

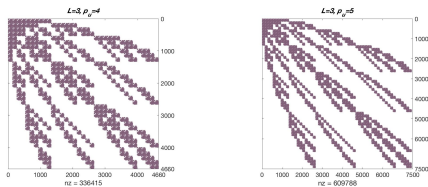
$$\begin{bmatrix} \mathcal{A}_{II}^1 & \dots & 0 & \mathcal{A}_{II}^1 \mathcal{R}_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & \mathcal{A}_{II}^{n_s} & \mathcal{A}_{II}^{n_s} \mathcal{R}_{n_s} \\ \mathcal{R}_1^T \mathcal{A}_{II}^1 & \dots & \mathcal{R}_{n_s}^T \mathcal{A}_{II}^{n_s} & \sum_{s=1}^{n_s}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

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

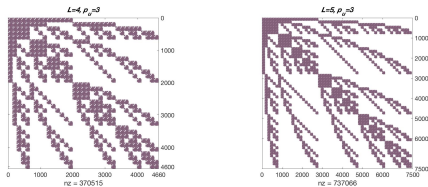
$$\mathcal{U}_I^m = (\mathbf{u}_{I,0}^m, \dots, \mathbf{u}_{I,N}^m)^T \quad ; \quad \mathcal{U}_\Gamma = (\mathbf{u}_{\Gamma,0}, \dots, \mathbf{u}_{\Gamma,N})^T.$$

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

Block Sparsity Structure



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



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

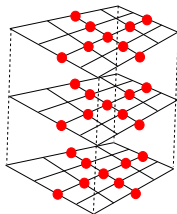
Extended Interface Problem

- 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

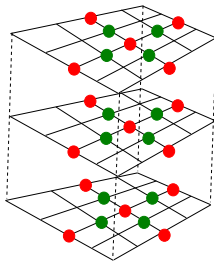
$$\kappa(M^{-1}S) \leq C \frac{1}{H^2} (1 + \log \frac{H}{h})^2$$

- Two-level preconditioner

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

Two-Level Domain Decomposition Methods for SPDEs

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



$$\mathcal{U}_I^s = \left\{ \begin{array}{c} \mathcal{U}_r^s \\ \mathcal{U}_c^s \end{array} \right\}$$

Probabilistic Balancing Domain Decomposition with Constraints

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

$$\mathcal{M}_{NNC}^{-1} = \sum_{s=1}^{n_s} \mathcal{R}_s^T \mathcal{D}_s \mathcal{R}_s^r [\mathcal{S}_{rr}^s]^{-1} \mathcal{R}_s^r \mathcal{D}_s \mathcal{R}_s + \mathcal{R}_0^T [\mathcal{F}_{cc}]^{-1} \mathcal{R}_0,$$

$$\mathcal{R}_0 = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{R}_s^c - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{R}_s^r) \mathcal{D}_s \mathcal{R}_s.$$

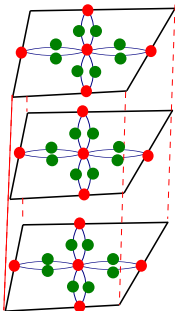
$$\mathcal{F}_{cc} = \sum_{s=1}^{n_s} \mathcal{B}_c^{sT} (\mathcal{S}_{cc}^s - \mathcal{S}_{cr}^s [\mathcal{S}_{rr}^s]^{-1} \mathcal{S}_{rc}^s) \mathcal{B}_c^s,$$

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

Probabilistic Dual Primal Domain Decomposition

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

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



Two-Level Domain Decomposition Methods for SPDEs

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

	$\mathcal{H}'_i$	$[\mathcal{S}'_i]^{-1}$	$\mathcal{H}_0$	$[\mathcal{S}_c]^{-1}$
a	$\mathcal{R}'_i \mathcal{D}_i \mathcal{R}_i$	$[\mathcal{S}'_i]^{-1}$	$\sum_{\alpha=1}^n \mathcal{B}'_c{}^T (\mathcal{R}'_i - \mathcal{S}'_\alpha [\mathcal{S}'_i]^{-1} \mathcal{R}'_\alpha) \mathcal{D}_i \mathcal{R}_i$	$\sum_{\alpha=1}^n \mathcal{B}'_c{}^T (\mathcal{S}'_\alpha - \mathcal{S}'_\alpha [\mathcal{S}'_i]^{-1} \mathcal{S}'_\alpha) \mathcal{B}'_c$
b	$\mathcal{D}'_i \mathcal{B}'_i$	$[\mathcal{S}'_i]^{-1}$	$\sum_{\alpha=1}^n \mathcal{B}'_c{}^T \mathcal{S}'_\alpha [\mathcal{S}'_i]^{-1} \mathcal{D}'_i \mathcal{B}'_i$	$\sum_{\alpha=1}^n \mathcal{B}'_c{}^T (\mathcal{S}'_\alpha - \mathcal{S}'_\alpha [\mathcal{S}'_i]^{-1} \mathcal{S}'_\alpha) \mathcal{B}'_c$
c	$\mathcal{B}'_i{}^T$	$[\mathcal{S}'_i]^{-1}$	$\sum_{\alpha=1}^n \mathcal{B}'_c{}^T \mathcal{S}'_\alpha [\mathcal{S}'_i]^{-1} \mathcal{B}'_i{}^T$	$\sum_{\alpha=1}^n \mathcal{B}'_c{}^T (\mathcal{S}'_\alpha - \mathcal{S}'_\alpha [\mathcal{S}'_i]^{-1} \mathcal{S}'_\alpha) \mathcal{B}'_c$

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

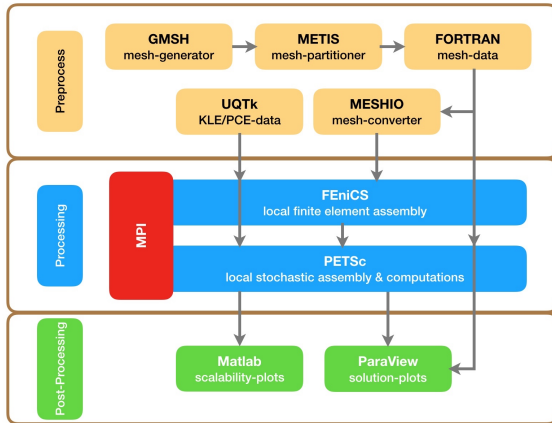
Investigated numerical and parallel scalabilities:

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

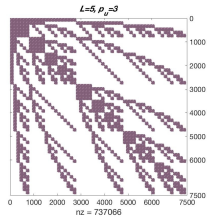
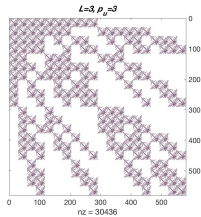
- Model Problem:

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

- 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).

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

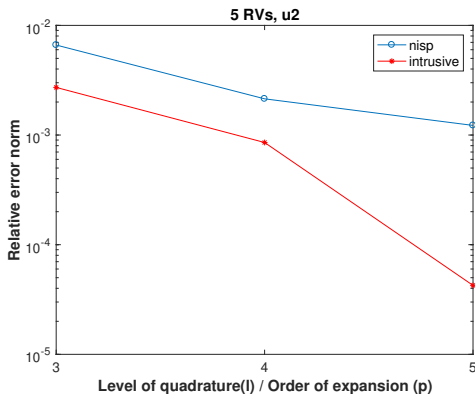
Block-Sparsity Structures



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

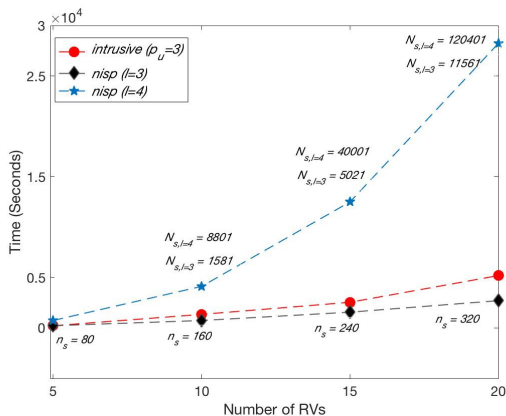
Errors Analysis of PCE Coefficients of Solution Process:

Intrusive Vs Non-Intrusive



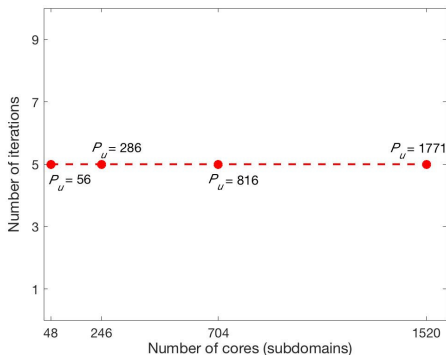
Relative error norm = $\frac{\|u_{iH} - u_{ih}\|}{\|u_{iH}\|}$, 5 random variables, error in ($\hat{u}_2$),
coarse mesh ($N \approx 150$)

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



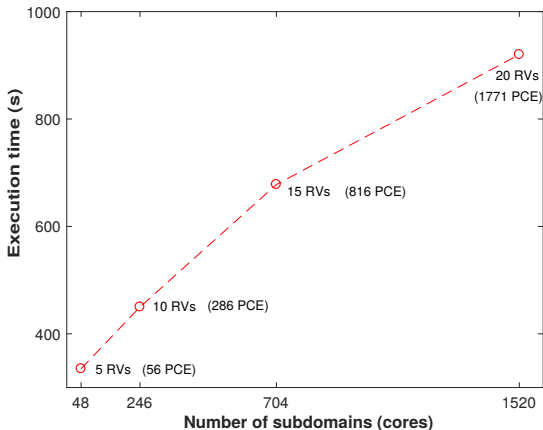
Fixed mesh resolution (52704 nodes and 105410 elements) and third order PCE for intrusive. Smolyak sparse grid with $l = 3$ and $l = 4$ for non-intrusive.

Scalability against Number of Random Variables: NNC/BDDC



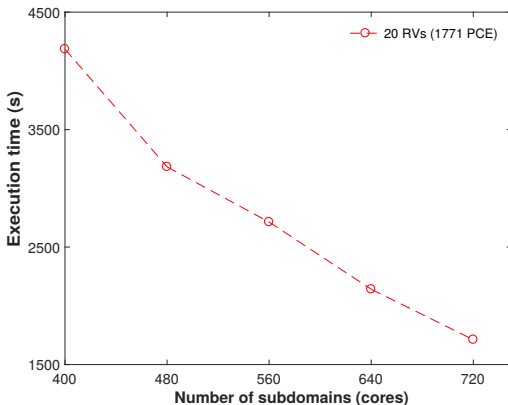
Fixed mesh resolution (52704 nodes and 105410 elements), fixed problem size per subdomain ($\approx 60,000$) and third order PCE (linear system of order max. ≈ 93 million)

Scalability against Number of Random Variables: NNC/BDDC



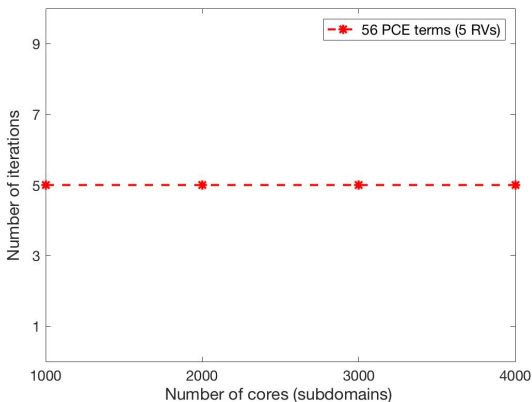
Fixed mesh (52704 nodes and 105410 elements), fixed problem size per subdomain ($\approx 60,000$) and third order PCE

Parallel Scalability (Strong): NNC/BDDC



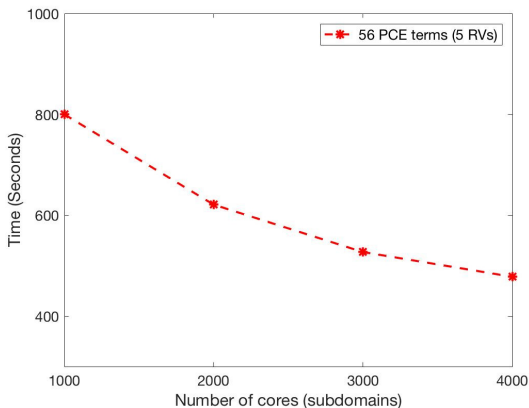
Fixed global problem, mesh with (52704 nodes and 105410 elements) and number of PCE terms $P_u = 1771$.

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 ($P_u = 56$).

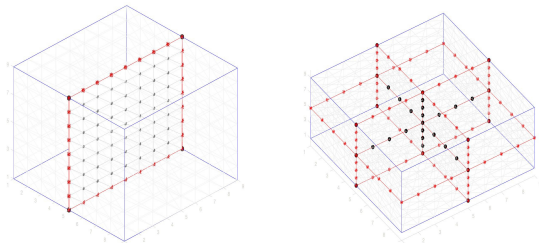
Scalability using Large-Scale HPC Cluster



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, Bjorstad 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

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

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

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

Modified BDDC/NNC Preconditioner:

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

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

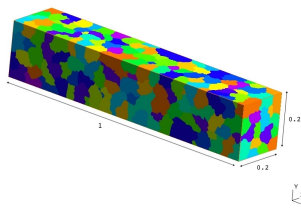
Numerical Experiments: Wirebasket based BDDC/NNC solver

- Diffusion equation

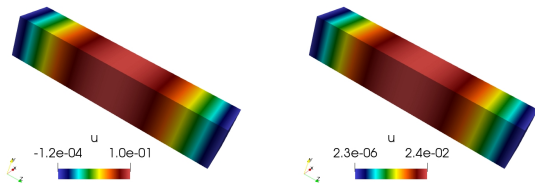
$$\begin{aligned} -\nabla \cdot (c_d(\mathbf{x}, \theta) \nabla u(\mathbf{x}, \theta)) &= F(\mathbf{x}), & \Omega \times \mathcal{W}, \\ u(\mathbf{x}, \theta) &= 0, & \delta\Omega \times \mathcal{W}, \end{aligned}$$

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

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

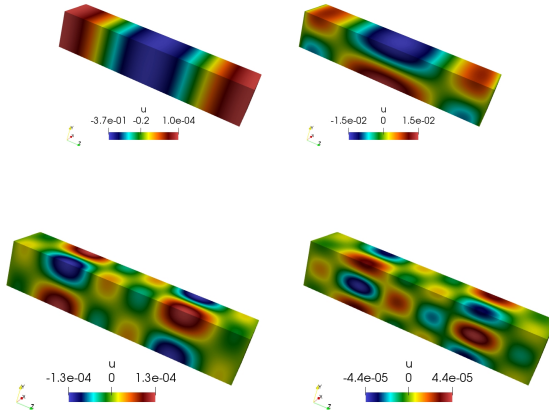


Characteristics of the Solution Process:
Diffusion Equation



Mean and standard deviation.

Characteristics of the Solution Process



Selected PCE coefficients.

- Linear Elasticity

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

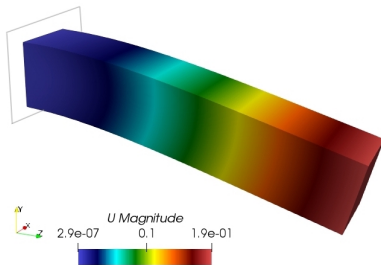
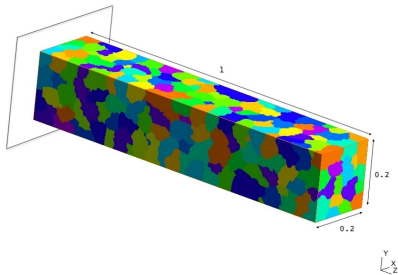
Stress tensor σ :

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

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

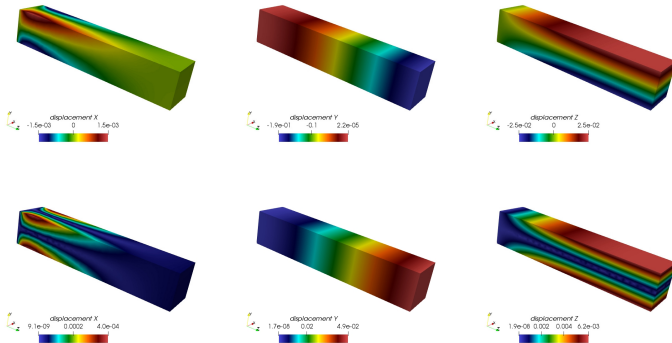
- Young's modulus E - lognormal stochastic process (as before).

Characteristics of the Solution Process:



Characteristics of the Solution Process:

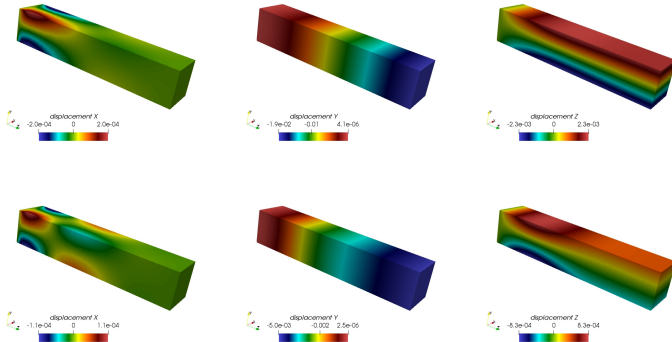
Linear Elasticity



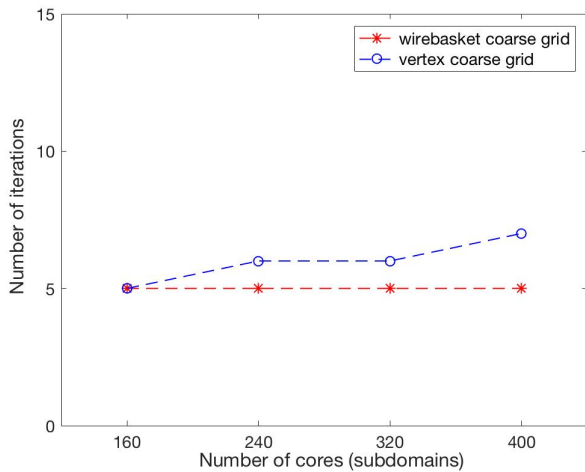
x , y and z components of the mean and standard deviation.

Characteristics of the Solution Process:

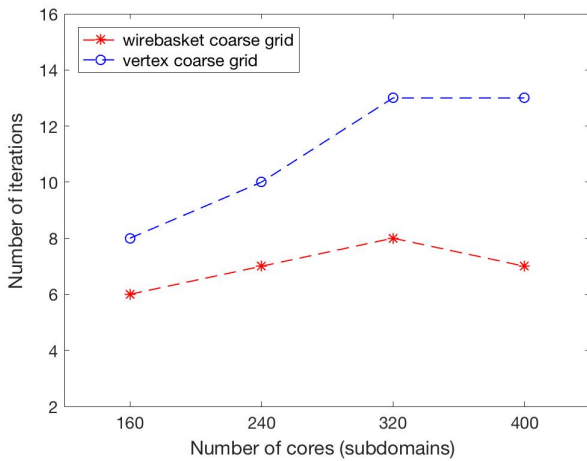
Linear Elasticity



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



Diffusion



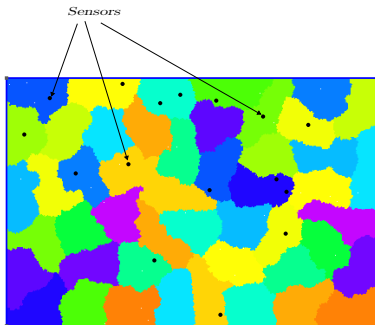
Bayesian Estimation using Nonlinear Filtering

- Model Equation

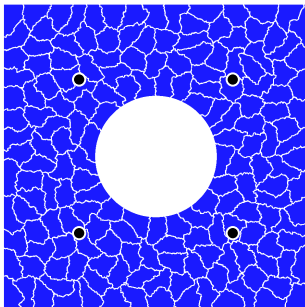
$$\mathbf{u}_{k+1} = \psi_k(\mathbf{u}_k, \mathbf{f}_k, \mathbf{q}_k) \quad \text{-- Forecast Step}$$

- Measurement Equation

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



Diffusion: Experiment with Four Sensors



Parallel Data Assimilation: Polynomial Chaos-Based Kalman Filter (Saad and Ghanem, 2009)

- State Vector Representation

$$\mathbf{u}(\theta) = \sum_{i=0}^N \mathbf{u}_i \Psi_i(\theta) ; \quad \mathbf{P}^f = \sum_{i=1}^N \mathbf{u}_i \mathbf{u}_i' \langle \Psi_i^2 \rangle .$$

$$\mathbb{A}^f = [\mathbf{u}_0, \mathbf{u}_1, \dots, \mathbf{u}_N]$$

- Measurement Vector Representation

$$\mathbf{d} = \sum_{j=0}^N \mathbf{d}_j \Psi_j(\theta) ; \quad \mathbf{\Gamma} = \sum_{i=1}^N \mathbf{d}_i \mathbf{d}_i' \langle \Psi_i^2 \rangle$$

$$\mathbb{D} = [\mathbf{d}_0, \mathbf{d}_1, \dots, \mathbf{d}_N]$$

- Analysis/Update Step (Saad and Ghanem, 2009)

$$\mathbb{A}^a = \mathbb{A}^f + \mathbf{P}^f \mathbf{H}' \left(\mathbf{H} \mathbf{P}^f \mathbf{H}' + \mathbf{\Gamma} \right)^{-1} \left(\mathbb{D} - \mathbf{H} \mathbb{A}^f \right)$$

Parallel Data Assimilation: Analysis Step - Distributed Implementation

- Spatial decomposition of the state vector

$$\mathbf{u}(\theta) = \sum_{i=0}^N \begin{bmatrix} \mathbf{u}_{l,i}^1 \\ \vdots \\ \mathbf{u}_{l,i}^{n_s} \\ \mathbf{u}_{l,i} \\ \mathbf{u}_{r,i} \end{bmatrix} \Psi_i(\theta) .$$

- Decomposition of the state ensemble matrix

$$\mathbb{A}^f = \begin{bmatrix} \mathbf{u}_{l,0}^1 & \mathbf{u}_{l,1}^1 & \cdots & \mathbf{u}_{l,N}^1 \\ \mathbf{u}_{l,0}^2 & \mathbf{u}_{l,1}^2 & \cdots & \mathbf{u}_{l,N}^2 \\ \vdots & \vdots & & \vdots \\ \mathbf{u}_{l,0}^{n_s} & \mathbf{u}_{l,1}^{n_s} & \cdots & \mathbf{u}_{l,N}^{n_s} \\ \mathbf{u}_{r,0} & \mathbf{u}_{r,1} & \cdots & \mathbf{u}_{r,N} \end{bmatrix} = \begin{bmatrix} \left[\mathbb{A}^f \right]_l^1 \\ \left[\mathbb{A}^f \right]_l^2 \\ \vdots \\ \left[\mathbb{A}^f \right]_l^{n_s} \\ \left[\mathbb{A}^f \right]_r \end{bmatrix} ,$$

Parallel Data Assimilation

- Analysis Step - Distributed Implementation

$$\begin{aligned}
 \mathbb{A}^a &= \mathbb{A}^f + \mathbf{P}^f \mathbf{H}' \left(\mathbf{H} \mathbf{P}^f \mathbf{H}' + \mathbf{r} \right)^{-1} \left(\mathbb{D} - \mathbf{H} \mathbb{A}^f \right) \\
 &= \mathbb{A}^f \left[\mathbf{I} + \mathbf{B} \mathbb{D}^{f'} \left(\mathbb{D}^f \mathbf{B} \mathbb{D}^{f'} + \mathbf{D} \mathbf{B} \mathbf{D} \right)^{-1} \left(\mathbb{D} - \mathbb{D}^f \right) \right] \\
 &= \mathbb{A}^f \mathbf{C}
 \end{aligned}$$

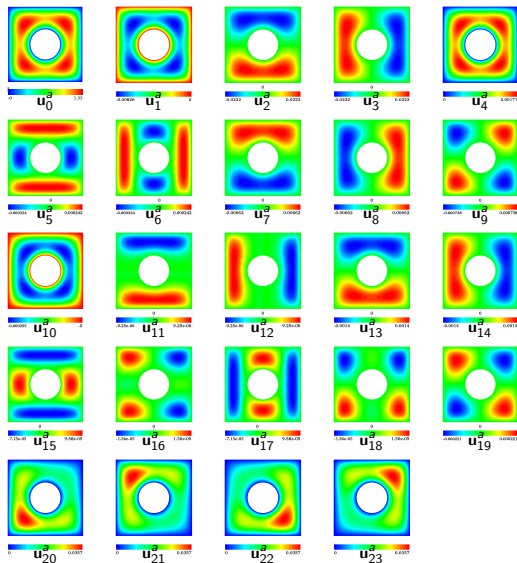
- Compute the forecast observation matrix $\mathbb{D}^f = \mathbf{H} \mathbb{A}^f$ in parallel

$$\begin{aligned}
 \mathbb{D}^f &= \mathbf{H} \mathbb{A}^f \\
 &= \mathbf{H}_I^1 \left[\mathbb{A}^f \right]_I^1 + \mathbf{H}_I^2 \left[\mathbb{A}^f \right]_I^2 + \cdots + \mathbf{H}_I^{n_s} \left[\mathbb{A}^f \right]_I^{n_s} + \mathbf{H}_r \left[\mathbb{A}^f \right]_r \\
 &= \left[\mathbb{D}^f \right]_I^1 + \left[\mathbb{D}^f \right]_I^2 + \cdots + \left[\mathbb{D}^f \right]_I^{n_s} + \left[\mathbb{D}^f \right]_r = \sum_{s=1}^{n_s} \left[\mathbb{D}^f \right]_I^s + \left[\mathbb{D}^f \right]_r .
 \end{aligned}$$

- Perform ensemble update in parallel

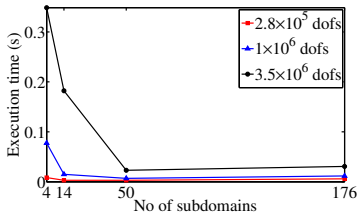
$$\begin{array}{ll}
 \text{Interior nodes, Subdomain 1} & \longrightarrow \\
 \vdots & \\
 \text{Interior nodes, Subdomain } n_s & \longrightarrow \\
 \text{Global boundary nodes} & \longrightarrow
 \end{array}
 \begin{bmatrix} \left[\mathbb{A}^a \right]_I^1 \\ \vdots \\ \left[\mathbb{A}^a \right]_I^{n_s} \\ \left[\mathbb{A}^a \right]_r \end{bmatrix} = \begin{bmatrix} \left[\mathbb{A}^f \right]_I^1 \\ \vdots \\ \left[\mathbb{A}^f \right]_I^{n_s} \\ \left[\mathbb{A}^f \right]_r \end{bmatrix} \mathbf{C} = \begin{bmatrix} \left[\mathbb{A}^f \right]_I^1 \mathbf{C} \\ \vdots \\ \left[\mathbb{A}^f \right]_I^{n_s} \mathbf{C} \\ \left[\mathbb{A}^f \right]_r \mathbf{C} \end{bmatrix}$$

Diffusion: Posterior PCE Coefficients - 4 Sensors

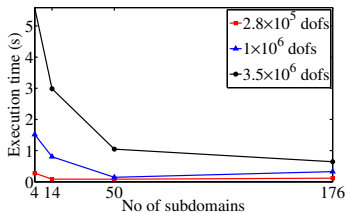


Parallel Scalability

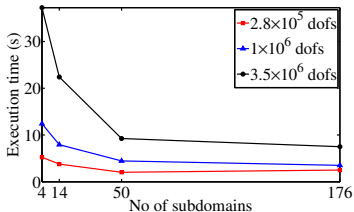
For a fixed problem size and number of measurements:



32 measurements



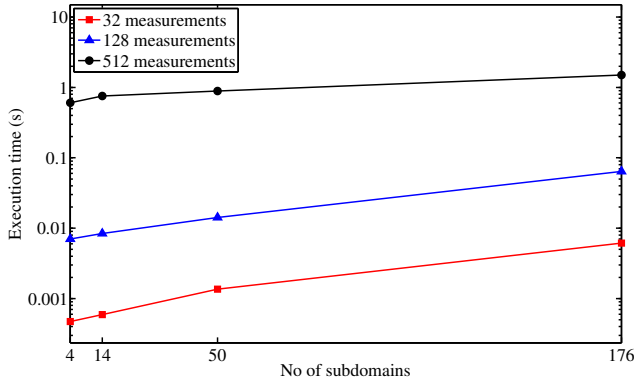
128 measurements



512 measurements

Parallel Scalability

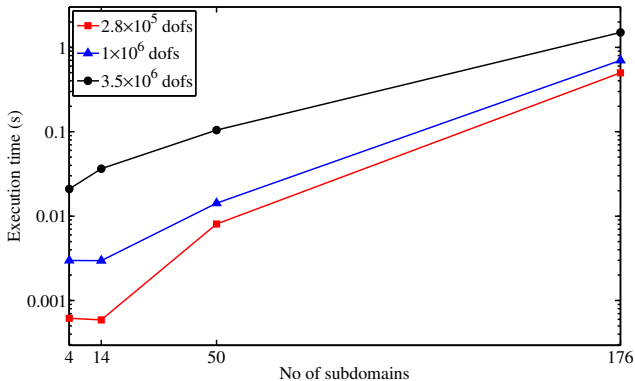
For a fixed problem size per subdomain/core:



20,000 unknowns per subdomain/core

Parallel Scalability

For a fixed number of measurements per subdomain/core:



$$\mathbf{C} = \mathbf{I} + \mathbf{B}\mathbb{D}^{f'} \left(\mathbb{D}^f \mathbf{B}\mathbb{D}^{f'} + \mathbb{D}\mathbf{B}\mathbb{D} \right)^{-1} \left(\mathbb{D} - \mathbb{D}^f \right)$$

Sherman-Morrison Solver

- For independent measurement

$$\mathbf{D}\mathbf{B}_m\mathbf{D}^T = \mathbf{A}_0$$

is a diagonal matrix.

- Rewrite

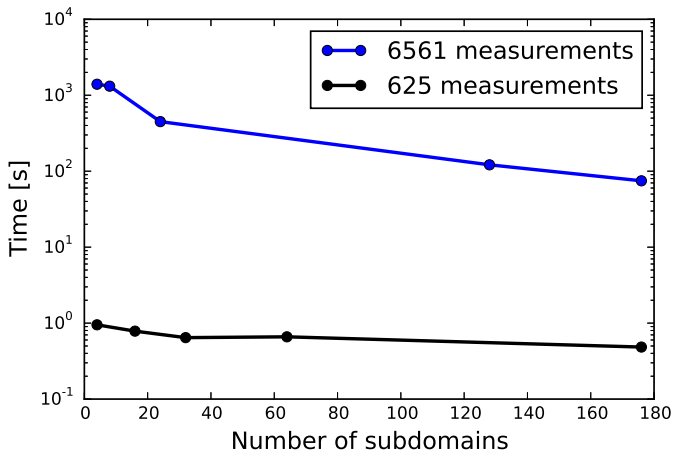
$$\mathbf{A} = \left(\mathbf{D}\mathbf{B}_m\mathbf{D}^T + \mathbf{D}^f\mathbf{B}\mathbf{D}^{fT} \right) = \left(\mathbf{A}_0 + \sum_{i=1}^N \mathbf{u}_i\mathbf{v}_i^T \right)$$

- Use Sherman-Morrison formula recursively

$$(\mathbf{A}_0 + \mathbf{u}\mathbf{v}^T)^{-1} = \mathbf{A}_0^{-1} - \frac{\mathbf{A}_0^{-1}\mathbf{u}\mathbf{v}^T\mathbf{A}_0^{-1}}{1.0 + \mathbf{v}^T\mathbf{A}_0^{-1}\mathbf{u}}$$

Timing

- Problem size: 19602 nodes, 39209 elements



Conclusion

- Development of parallel PCKF that exploits available two-level domain decomposition algorithms for SPDEs.
- Distributed implementation and scalability studies of the parallel PCKF using a stationary stochastic diffusion problem.

Acknowledgment

- **Financial contributions**
 - **Natural Sciences and Engineering Research Council of Canada**
 - **Canada Research Chair Program**
 - **Canada Foundation of Innovation**
 - **Ontario Innovation Trust**