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Domain Decomposition of Stochastic PDEs: High Resolution Computational Mesh with Large Stochastic Dimension

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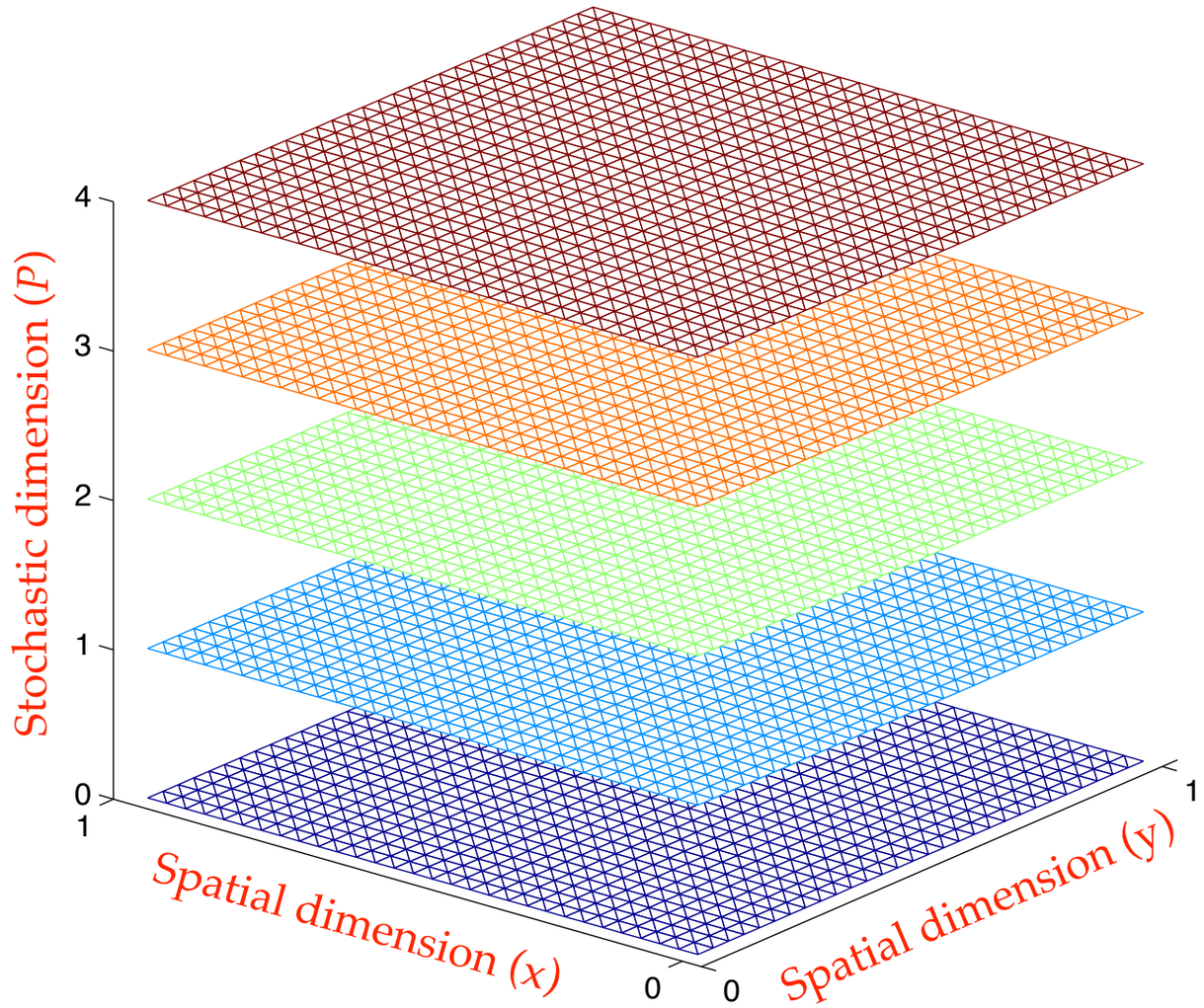
Uncertainty Quantification at Extreme Scale

- Deterministic finite element method with spatial mesh resolution ***N = 100,000***.



- Stochastic finite element method with stochastic discretization using ***P = 100*** PCE terms will leads to the total problem of size,

$$N \times P = 10 \text{ million} \longrightarrow \textbf{HPC}$$

Introduction

- **Motivation**
  - Efficient uncertainty quantification algorithms for extreme-scale stochastic systems, leveraging modern high-performance computing.

- **Objective**
  - Develop parallel scalable algorithms for uncertainty quantification of systems with high resolution in both stochastic and physical domain.

- **Methodology**
  - Employ intrusive polynomial chaos expansion based Stochastic FEM.
  - Develop non-overlapping domain decomposition based solvers.
  - Efficient use of memory and floating-point-operations using PETSc.

Stochastic Partial Differential Equation (SPDE)

- Stationary stochastic diffusion equation.

$$-\nabla \cdot \left(\; c_d(\boldsymbol{x}, \theta) \;\; \nabla u(\boldsymbol{x}, \theta) \; \right) = f(\boldsymbol{x}), \qquad D \times \Omega$$

- Diffusion coefficient (c_d) is modelled as a lognormal stochastic process.

$$c_d(\boldsymbol{x}, \theta) = \exp \left(g(\boldsymbol{x}, \theta) \right)$$

- Obtained from underlying Gaussian process (g) with 2D exponential covariance.

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

Stochastic Spectral Finite Element Method (SSFEM)

- **Stochastic Input** : Truncated Karhunen-Loève Expansion (KLE)

$$g(\boldsymbol{x},\theta) = g_0(\boldsymbol{x}) + \sum_{i=1}^{L} \sqrt{\lambda_i}\; g_i(\boldsymbol{x})\; \xi_i(\theta)$$

- **Model parameters/Solution process** : Polynomial Chaos Expansion (PCE)

$$\alpha\left(\boldsymbol{x},\xi(\theta)\right) = \sum_{j=0}^{P} \alpha_j(\boldsymbol{x})\; \Psi_j(\xi(\theta))$$

$$P = \frac{(L+p)!}{L!\; p!} - 1$$

where $\boldsymbol{P}$ is a number of PCE terms, $\boldsymbol{p}$ is order of chaos and $\boldsymbol{L}$ is dimensionality of stochastic space.

Domain Decomposition Method (DDM)

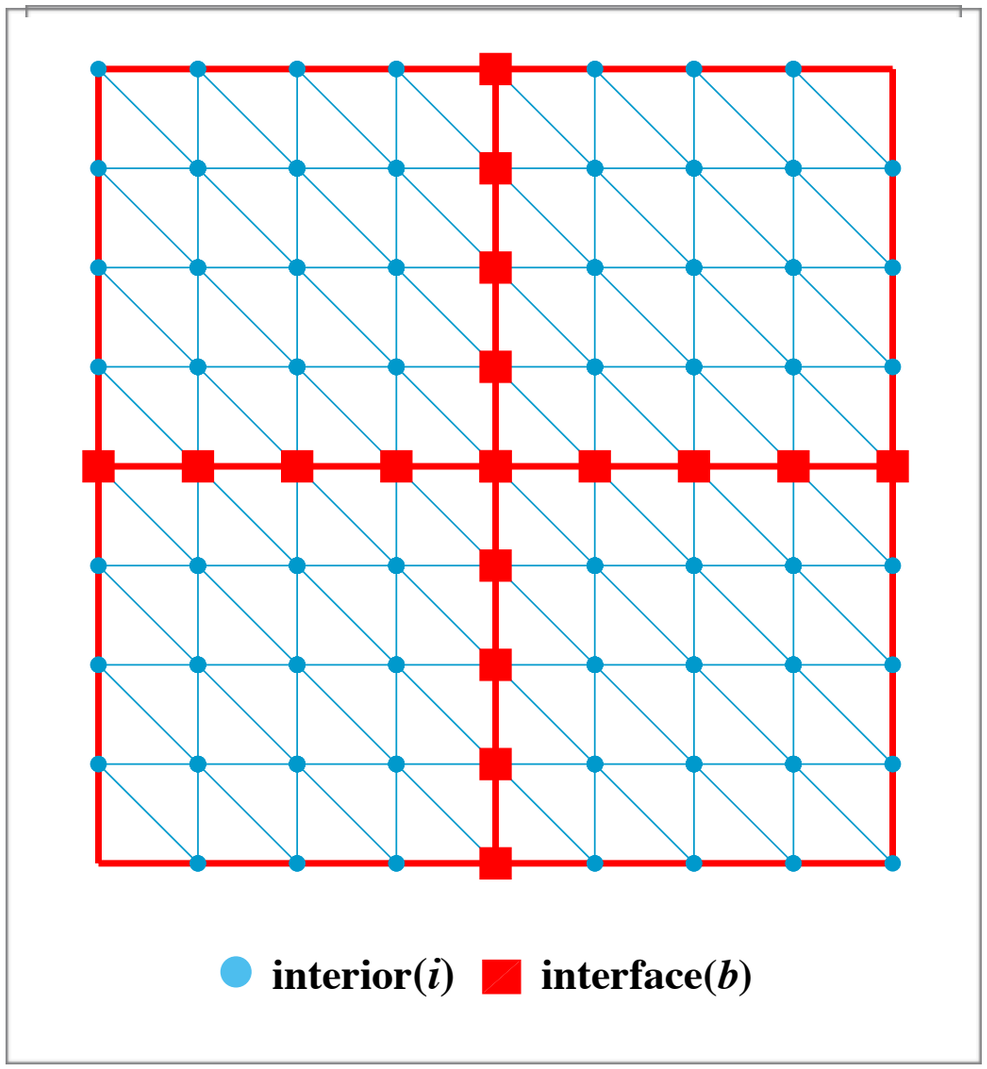
- Finite element approximation of the SPDE

$$\mathbf{A}(\theta)\ \mathbf{u}(\theta) = \mathbf{f}$$

- Spatial domain D is divided into n_s non-overlapping subdomains

$$\begin{bmatrix} \mathbf{A}_{ii}^{s} & \mathbf{A}_{ib}^{s} \\ \mathbf{A}_{bi}^{s} & \mathbf{A}_{bb}^{s} \end{bmatrix} \begin{Bmatrix} \mathbf{u}_{i}^{s} \\ \mathbf{u}_{b}^{s} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_{i}^{s} \\ \mathbf{f}_{b}^{s} \end{Bmatrix}$$

$$s = 1,\ 2,\ \ldots,\ n_s$$



DDM for Stochastic PDEs : Intrusive Approach

- PCE substitution, Galerkin projection, enforce global assembly

$$\begin{bmatrix} A^1_{ii} & \dots & 0 & A^1_{ib}R_1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & A^{n_s}_{ii} & A^{n_s}_{ib}R_{n_s} \\ R^T_1 A^1_{bi} & \dots & R^T_{n_s} A^{n_s}_{bi} & \sum_{s=1}^{n_s} R^T_s A^s_{bb} R_s \end{bmatrix} \begin{Bmatrix} u^1_i \\ \vdots \\ u^{n_s}_1 \\ u_b \end{Bmatrix} = \begin{Bmatrix} f^1_i \\ \vdots \\ f^{n_s}_i \\ \sum_{s=1}^{n_s} R^T_s f^s_b \end{Bmatrix}$$

where

$$\left[A^s_{\alpha\beta}\right]_{jk} = \sum_{i=0}^{L} \langle \Psi_i \Psi_j \Psi_k \rangle \left[\mathbf{A^s_{\alpha\beta}}\right]_i$$

Extended Schur Complement System : Primal Approach

- Eliminating interior degree of freedom,

$$Su_b = g_b$$

$$S = \sum_{s=0}^{n_s} R_s^T \left[A_{bb}^s - A_{bi}^s [A_{ii}^s]^{-1} A_{ib}^s \right] R_s$$

$$g_b = \sum_{s=1}^{n_s} R_s^T [f_b^s - A_{bi}^s [A_{ii}^s]^{-1} f_i^s]$$

- Preconditioned Schur complement system to solve :

$$M^{-1} S u_b = M^{-1} g_b$$

Preconditioned Conjugate Gradient Method (PCGM)

- One-Level preconditioner :

$$M_1^{-1} = \sum_{s=1}^{n_s} R_s^T [M_s]^{-1} R_s$$

$$k(M_1^{-1}S) \leq C \frac{1}{H^2} \left(1 + log \frac{H}{h}\right)^2$$

- Two-Level preconditioner :

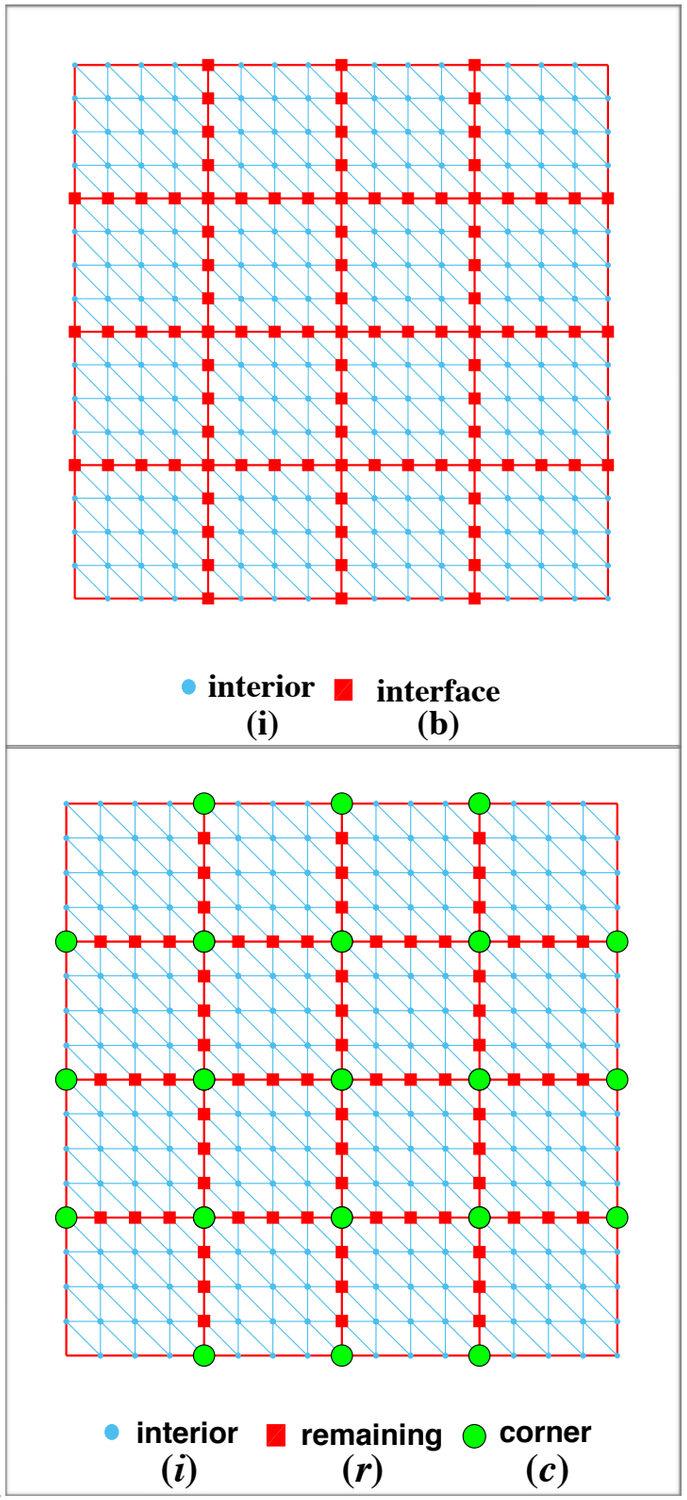
$$M_2^{-1} = \sum_{s=1}^{n_s} R_s^T [M_s]^{-1} R_s + R_0^T [M_0]^{-1} R_0$$

Fine **Coarse**

$$k(M_2^{-1}S) \leq C \left(1 + log \frac{H}{h}\right)^2$$

*Condition number bound of **deterministic** systems.

where ***h*** is the finite element mesh size and ***H*** is the subdomain size.



FETI-DP: Dual-Primal Approach

- Preconditioned Lagrange multiplier system of PCE coefficients

$$M_D^{-1}\left[F_{rr} + F_{rc}[F_{cc}]^{-1}F_{cr}\right]\Lambda = M_D{}^{-1}(d_r - F_{rc}[Fcc]^{-1}d_c)$$

- One-level Dirichlet preconditioner

$$M_D^{-1} = \sum_{s=1}^{n_s} B_r^s D_r^s [S_{rr}^s] D_r^s B_r^{s\tau},$$

where

$$F_{cc} = \sum_{s=1}^{n_s} B_c^{s\tau}(S_{cc}^s - S_{cr}^s[S_{rr}^s]^{-1}S_{rc}^s)B_c^s$$

$$S_{\alpha\beta}^s = A_{\alpha\beta}^s - A_{\alpha i}^s[A_{ii}^s]^{-1}A_{i\beta}^s$$

PCGM Algorithm : Parallel Implementation

$$M^{-1}Su_b = M^{-1}g_b$$

1: **Compute :** $r_{b_0} = g_b - Su_{b_0}$
2: **Precondition :** $z_0 = M^{-1}r_{b_0}$
3: **Compute :** $p_0 = z_0$
4: **Compute :** $\delta_0 = (r_{b_0}, z_0)$
5: **for** $i = 0, 1, 2, \ldots$, **do**
6: **Compute :** $q_i = Sp_i$
7: **Compute :** $\gamma_i = (q_i \ , \ p_i)$
8: **Compute :** $\alpha_i = \delta_i / \gamma_i$
9: **Update :** $u_{i+1} = u_i + \alpha_i p_i$
10: **Update :** $r_{b_{i+1}} = r_{b_i} - \alpha_i q_i$
11: **If** *iterate has converged,* **Exit**
12: **Precondition :** $z_{i+1} = M^{-1}r_{b_{i+1}}$
13: **Compute :** $\delta_{i+1} = (r_{b_{i+1}}, z_{i+1})$
14: **Compute :** $\beta_i = \delta_{i+1} / \delta_i$
15: **Update :** $p_{i+1} = z_{i+1} + \beta_i p_i$
16: **end for**

(a): Mat-Vec Product: $q_i = \sum_{s=0}^{n_s} R_s^T \left[S_s\right] R_s p_i$

13: **for** $s = 1, 2, \ldots$, **do**
14: Scatter : $p_i^s = R_s \ p_i$
15: Solve : $out2 = A_{ii}^{s\,-1}(A_{ib}^s \ p_i^s)$
16: Compute : $q_i^s = A_{bb}^s \ p_i^s - A_{bi}^s * out2$
17: Gather : $q_i = \sum_{s=0}^{n_s} R_s^T q_i^s$
18: **end for**

(b): Preconditioning: $z_{i+1} = \sum_{s=0}^{n_s} R_s^T \left[M_s^{-1}\right] R_s r_{bi+1}$

24: **for** $s = 1, 2, \ldots$, **do**
25: Scatter : $r_{b_{i+1}}^s = R_s r_{b_{i+1}}$
26: Solve : $z_i^s = M_s^{-1} r_{b_{i+1}}^s$
27: Gather : $z_{i+1} = \sum_{s=0}^{n_s} R_s^T z_i^s$
28: **end for**

Challenges

- Memory required to assemble and store the blocks of subdomain level (local) stochastic FE matrices.

$$[A^s_{ii}],\ [A^s_{bb}],\ [A^s_{cc}],\ \text{etc}\ldots$$

PETSc-*Mat* for Stochastic Sparse Matrix Assembly

- Time required to solve the local problems.

$$[A^s_{ii}]^{-1},\ [A^s_{bb}]^{-1}\ \text{and}\ \ [A^s_{cc}]^{-1}$$

PETSc-*Ksp* Sparse Iterative Solver

- Time, memory and FLOPS for local matrix-vector products.

$$A^s_{ii}v^s, A^s_{ib}v^s, A^s_{bb}v^s, etc\ldots$$

PETSc-*MatMult* for Sparse Mat-Vec Products

One Level PCGM : PETSc-PCGM for Local Problems

Original Problem

$$Au = f$$

Schur Complement
One Level PCGM

$$M_1^{-1} S u_b = M_1^{-1} g_b$$

Mat-Vec Product
~~**Dense-Cholesky**~~
PETSc-PCGM : (1)

$$v_i^s = [A_{ii}^s]^{-1} p_i^s$$

Preconditioning
~~**Dense-Cholesky**~~
PETSc-PCGM : (2)

$$v_b^s = [A_{bb}^s]^{-1} r_b^s$$

NNC/FETI-DP PCGM : PETSc-PCGM for Local Problems

Original Problem

$$Au = f$$

NNC-PCGM

Schur Complement System
Two-Level PCGM

$$M_2^{-1} S u_b = M_2^{-1} g_b$$

FETIDP-PCGM

Lagrange Multiplier System:
One-Level PCGM

$$M_D^{-1}\left[F_{rr} + F_{rc}[F_{cc}]^{-1}F_{cr}\right]\Lambda = M_D^{-1}\left(d_r - F_{rc}[Fcc]^{-1}\, d_c\right)$$

NNC-MVP

NNC-PP

FETIDP-PP

FETIDP-MVP

Local
PETSc-PCGM : (1)

$$v_i^s = [A_{ii}^s]^{-1} p_i^s$$

Global Coarse
One-Level PCGM

$$M_1^{-1} F_{cc} z_c = M_1^{-1} d_c$$

Local Fine
PETSc-PCGM : (2)

$$z_r^s = [S_{rr}^s]^{-1} v_r^s$$

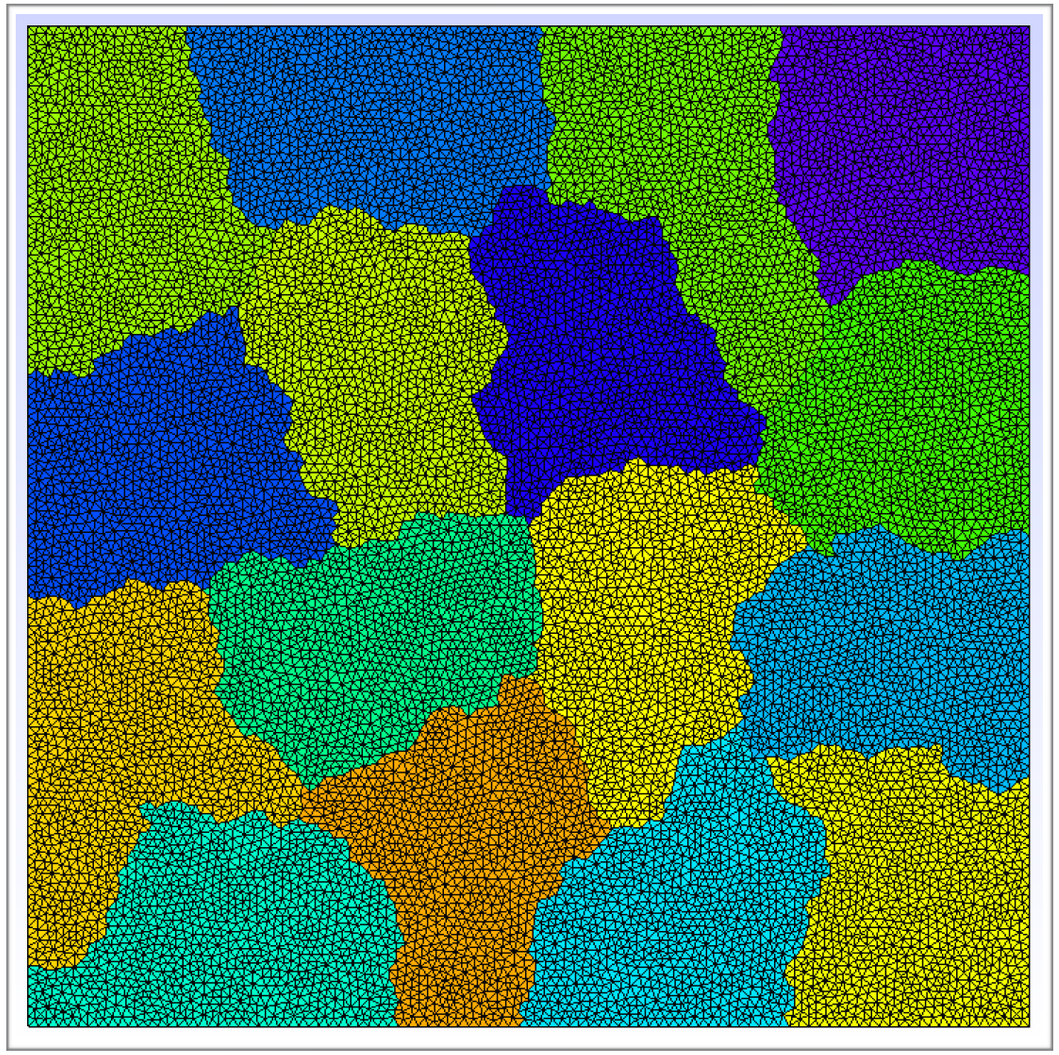
Mat-Vec Product
PETSc-PCGM : (3)

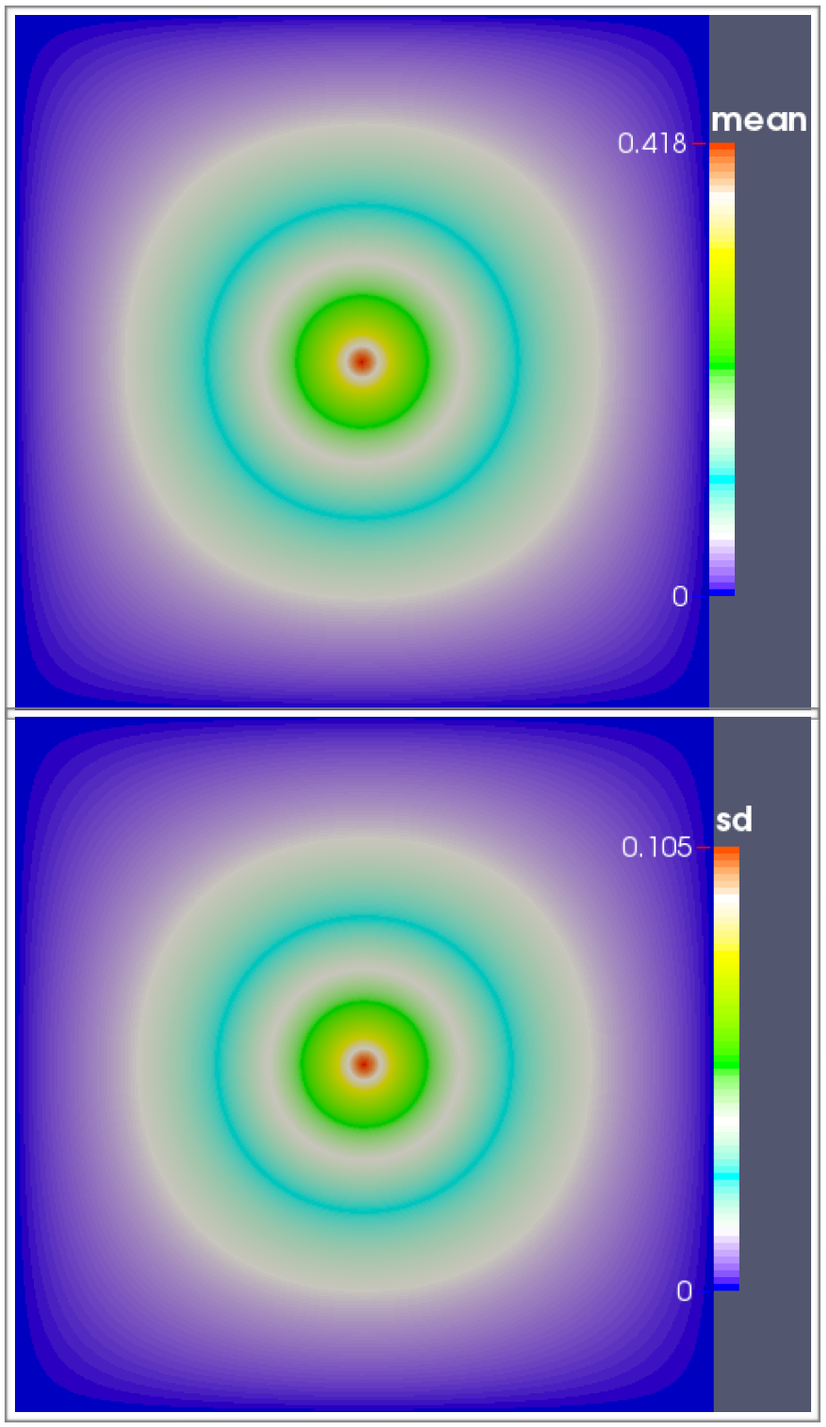
$$v_i^s = [A_{ii}^s]^{-1} p_i^s$$

Preconditioning
PETSc-PCGM : (4)

$$v_c^s = [A_{cc}^s]^{-1} r_c^s$$

Numerical Results : 2D Stochastic Diffusion Equation



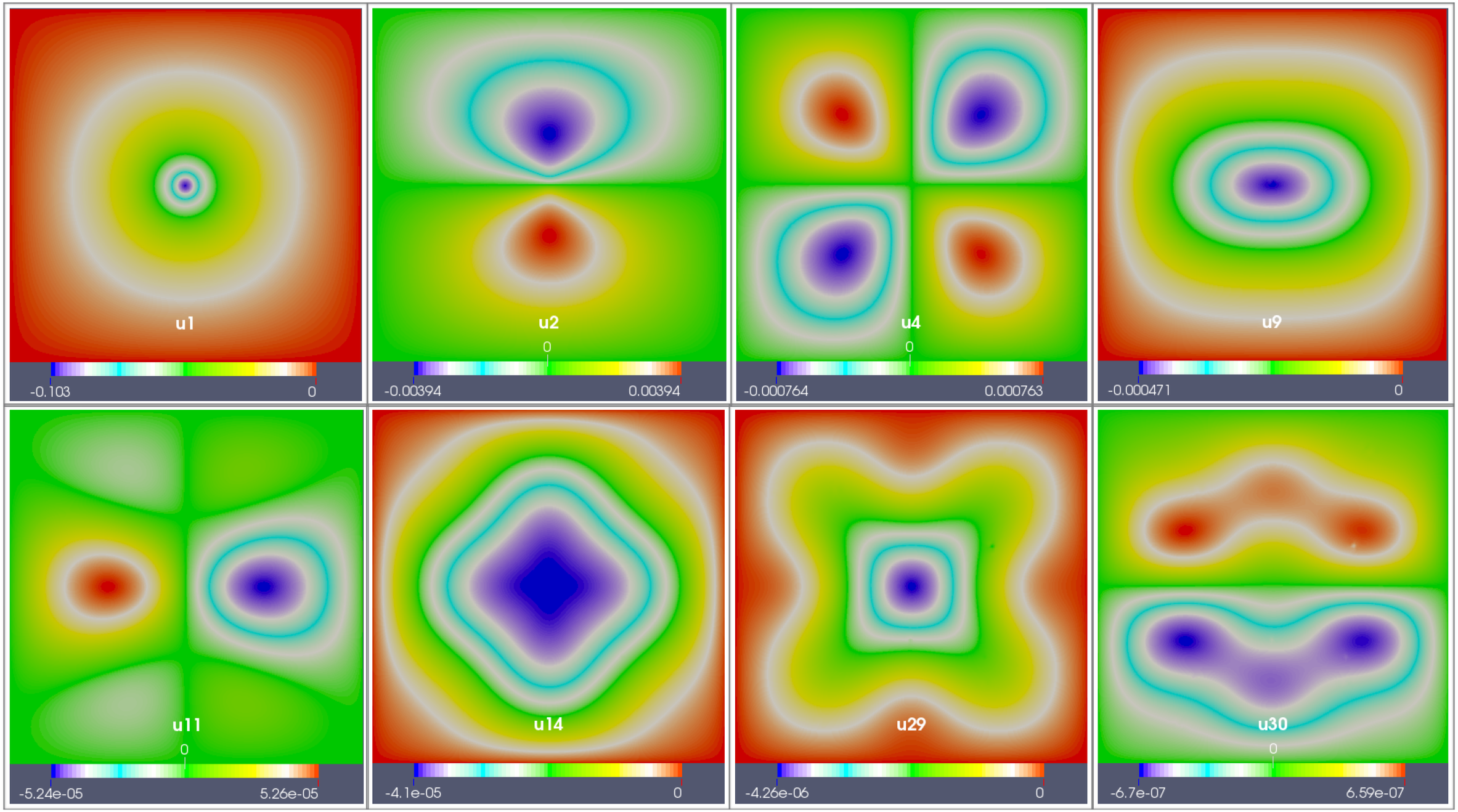


Exponential covariance function with numerical parameters :

$\sigma = 0.3,\ b_1 = b_2 = 1.0$ and

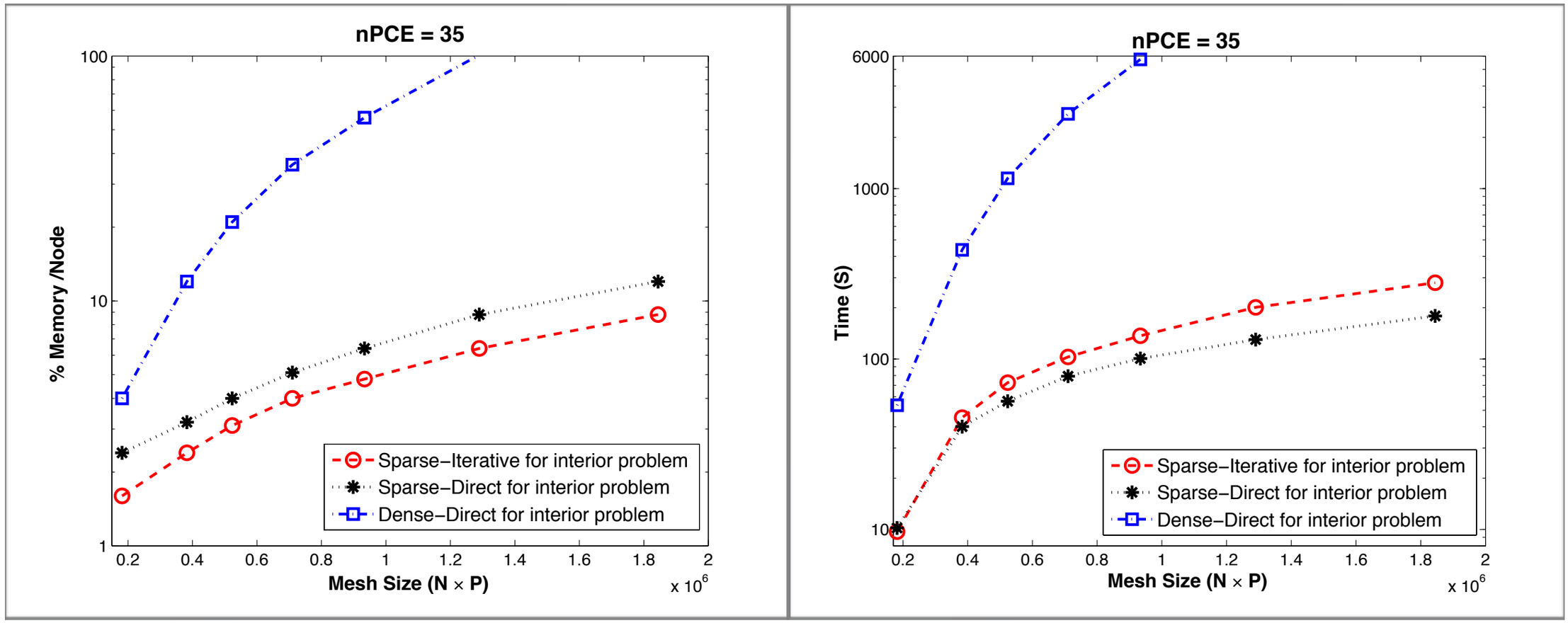
$L = 4,\ p = 3,\ \mathbf{P} = 35$

Few Higher Order PCE Coefficients



One Level PCGM: Dense vs PETSc-Sparse

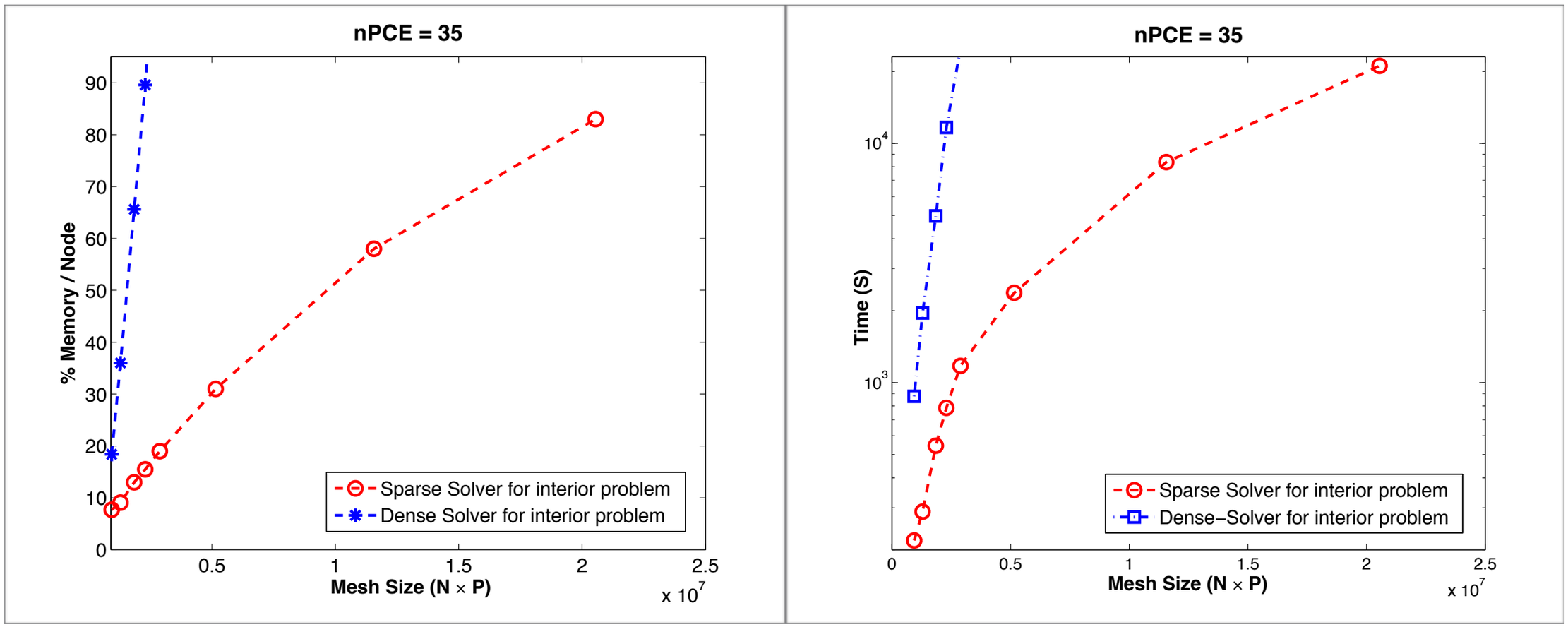
- **Total execution time (including assembly) and memory occupied / node :**
  For fixed number of processors (nProc = 60), with increasing problem size.



- Execution time and memory required using **dense solver** (**LAPACK-Cholesky**) increase exponentially as compared to **sparse-iterative-solver** (**PETSc-PCGM**) **sparse-direct-solver** (**PETSc-MUMPS**) for subdomain-level-interior-problems.

Two Level PCGM: Dense vs PETSc-Sparse

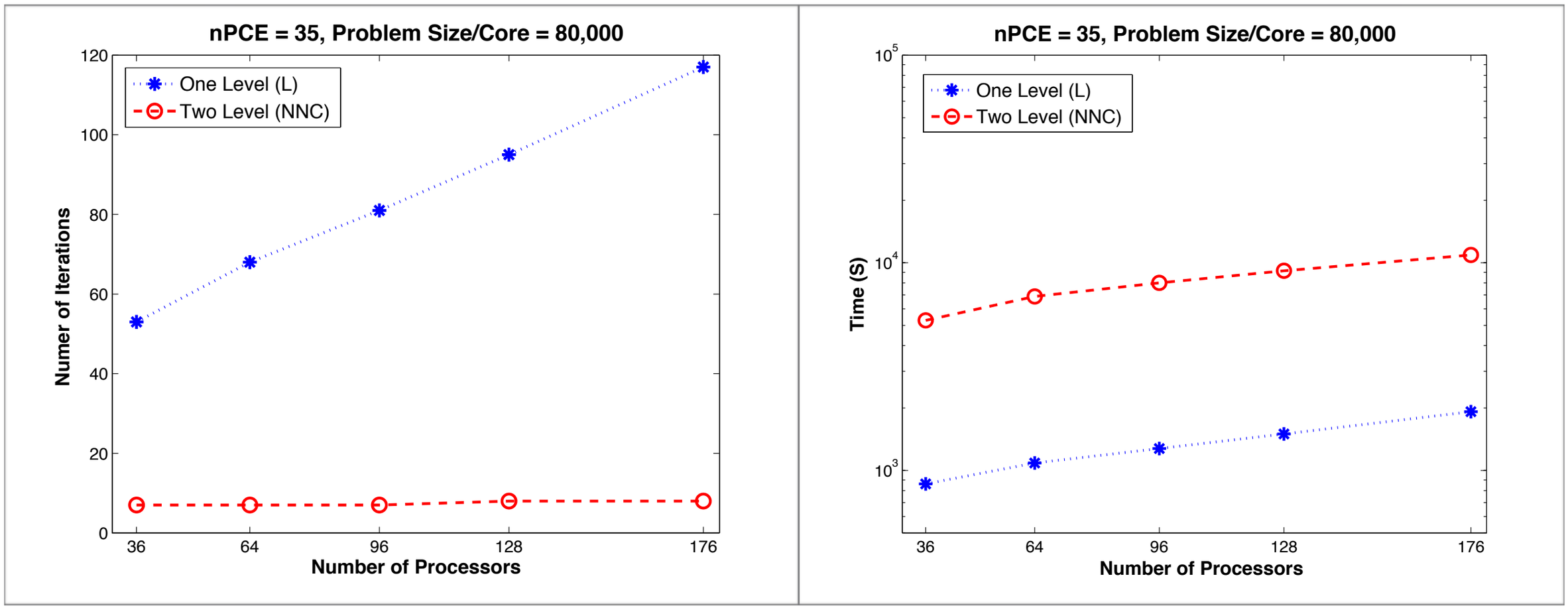
- **Total execution time (including assembly) and memory occupied / node :**
  For fixed number of processors (nProc = 176), with increasing problem size.



- Execution time and memory required using **dense-solver** (**LAPACK-Cholesky**) increase exponentially as compared to **sparse-solve** (**PETSc-PCGM**).

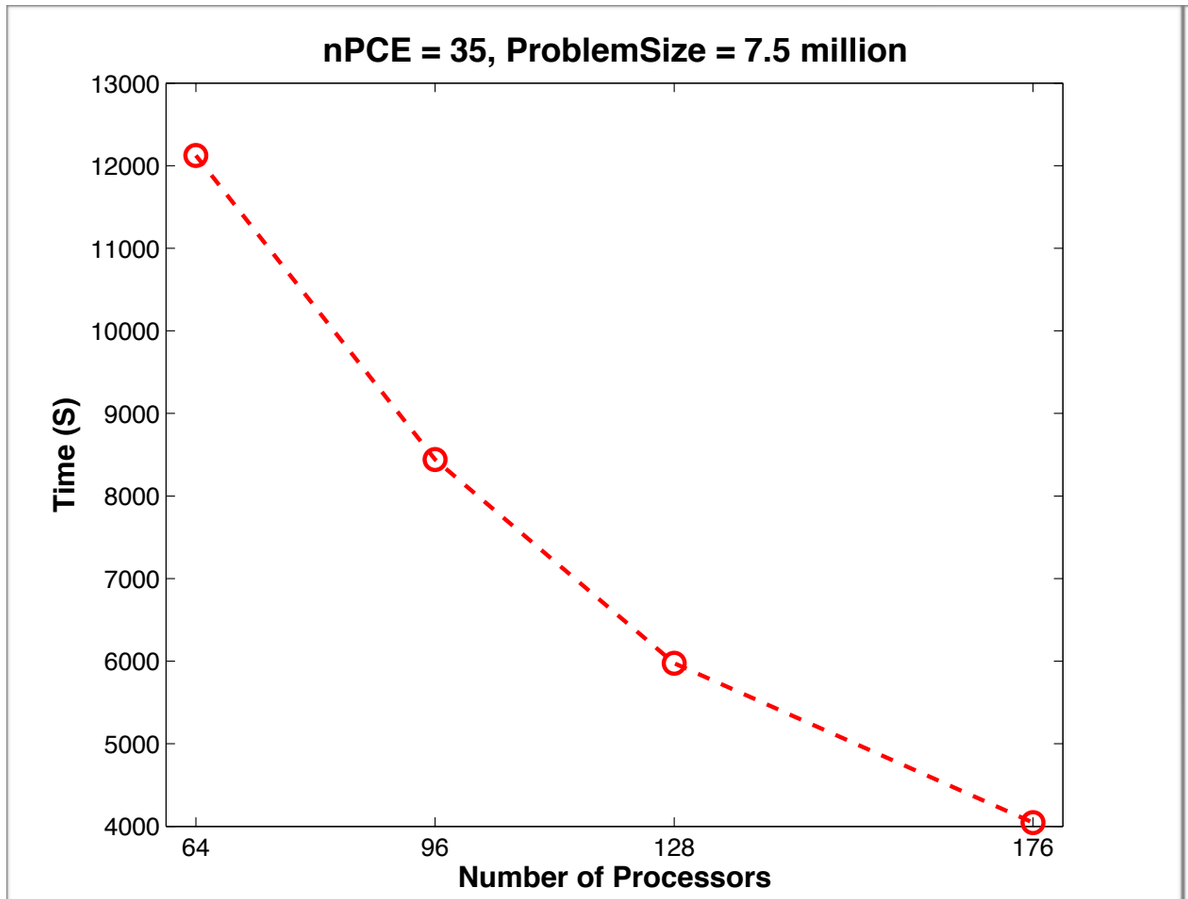
Numerical Scalability : One/Two-Level PCGM

- Scalability studies : performed using Linux-cluster having 22 nodes with 176 processors and 32 GB of memory per node (Quad-Core 3.0 GHz Intel Xeon processors) with InfiniBand interconnect using Message Passing Interface(MPI).

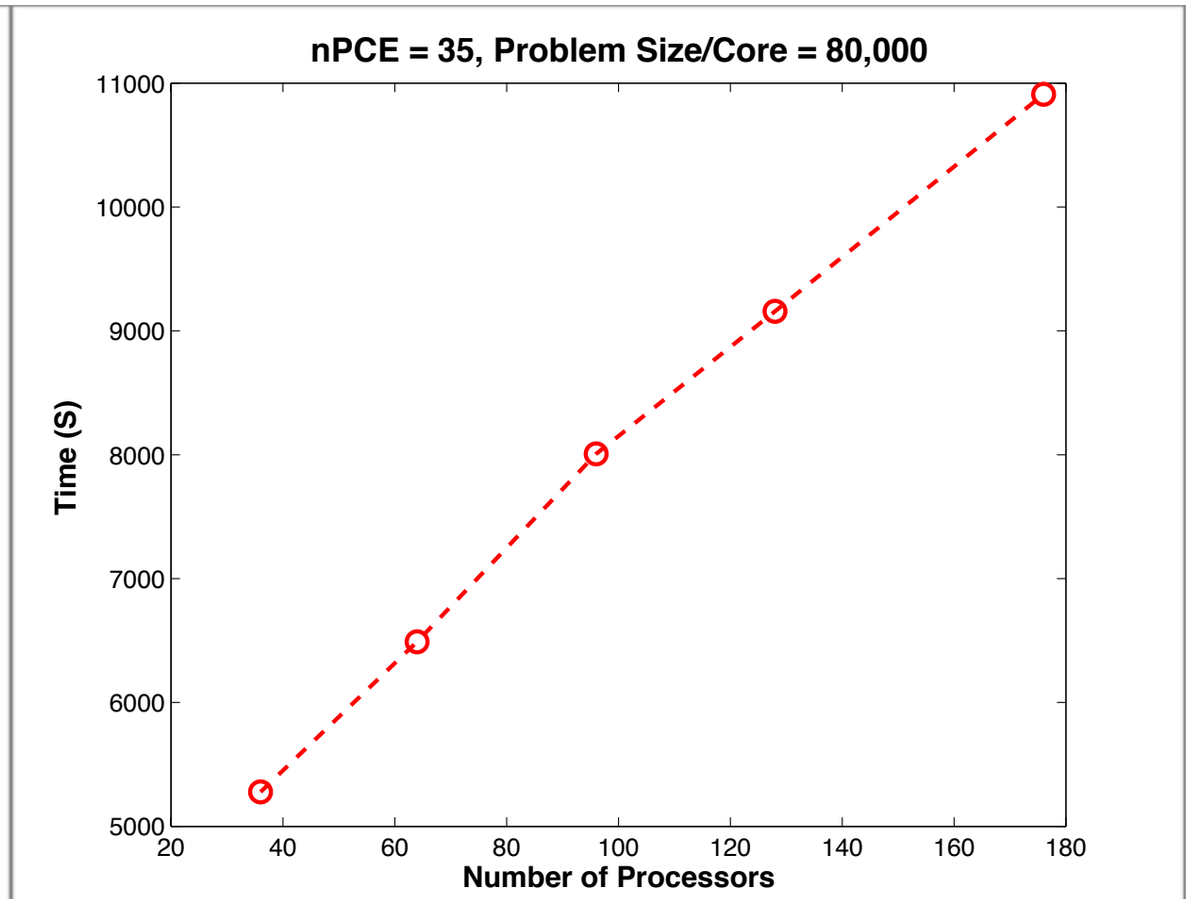


Parallel Scalability : Two-Level PCGM

Strong Scalability



Weak Scalability



- Scalability studies : performed using Linux-cluster with 22 nodes, 2 Quad-Core processors per node, 32 GB of memory per node.

Conclusions

- At extreme scale, the **subdomain-level** i.e. the **local problem** size becomes the bottleneck of the DDM based PCGM algorithms.

  - Optimized sparse memory allocation using **PETSc** objects:
    Mat / Vec / KSP / PC

  - Optimized sparse solvers using **PETSc** routines:
    KSPCG / MUMPS / KSPSolve / PCSetType

  - Optimized FLOPS for algebraic operation using **PETSc** routines:
    MatMult / MatTranspose / VecDot / VecNorm / VecAYPX

- With a given machine, the PETSc-based-DDM-solver could able to solve a much **bigger** problem in **less** time.

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Thank You!

Questions?