SAND2019-2005C

Large-Scale Uncertainty Propagation via Overlapping Domain Decomposition

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SIAM Conference on Computational Science and Engineering
Spokane, Washington, USA
February 25 - March 1, 2019

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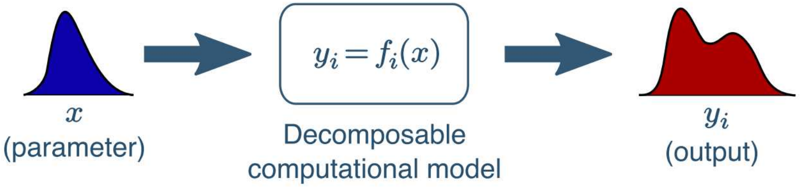
Overview

UQ in Decomposable Systems

- Objective: UQ Solvers for decomposable systems at extreme scale



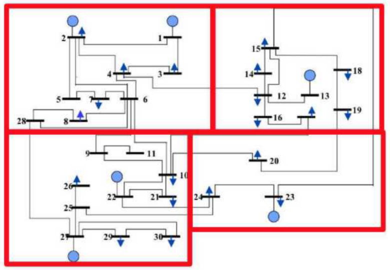
$y_i = f_i(x)$

x
(parameter)

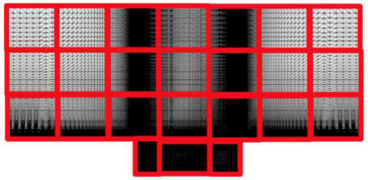
Decomposable
computational model

y_i
(output)

- Decomposable systems characterize many complex scientific/engineering applications
  - Multiple subsystems
  - Subsystems:
    - Characterized by different physics or scales
    - Different discretization schemes and deterministic solution techniques
    - Tailored uncertainty analysis schemes



Source: Lesieutre, Pinar, and Roy. "Power system extreme event detection:The vulnerability frontier." Hawaii International Conference on System Sciences, Proceedings of the 41st Annual. IEEE, 2008.



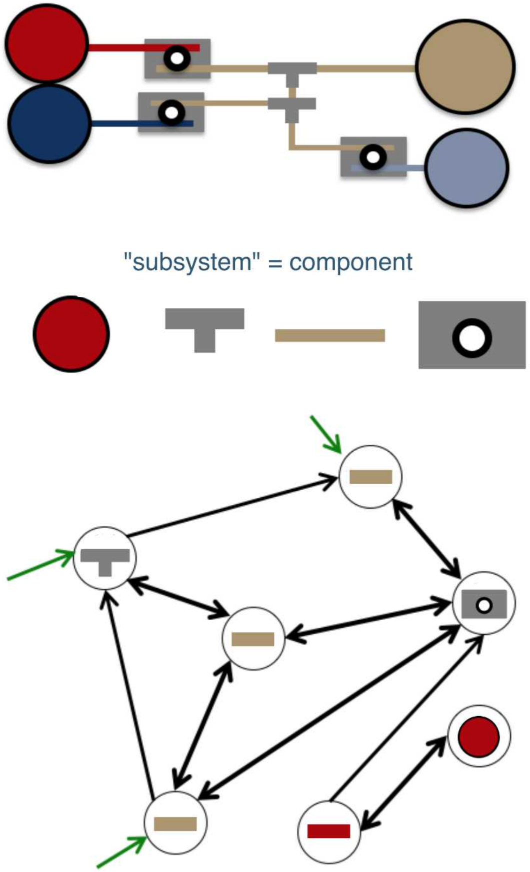
Source: nnsa.energy.gov

Challenges for UQ in Decomposable Systems

- For extreme-scale decomposable systems, high-fidelity simulation and UQ are typically achievable at the subsystem level, but intractable for the full system:
    - Long full-system simulation times
    - Limits on the problem size that can be reliability simulated
    - Integrating subsystem models possessing different physics or scales
- Full-system surrogate models, which are typically employed to make UQ tractable, may not be possible to construct, as they rely on a training set of these (possibly infeasible) simulations
- Proposed approach performs extensive UQ at the (tractable) subsystem level while propagating coupling information using new techniques inspired by domain decomposition

UQ Solvers for Decomposable Systems

- Idea: Model as subsystem network
  - ✦ UQ at subsystem level
  - ✦ System-level coordination for compatibility
  - \+ Promotes subsystem independence
  - \+ Focuses computational effort locally
  - \+ Tailored uncertainty analysis, discretizations, and solvers can be applied to each subsystem separately
- Method: DDUQ
  - ✦ Assigns each subsystem to a node in a directed graph, and coupling random variables to edges
  - ✦ New domain decomposition methods for UQ to enforce statistical compatibility
  - \+ Full-system UQ from subsystem analyses



Propagating Uncertainties in Networks

- Goal: propagate uncertainties from subsystems to the full system
- Current state of the art:
  - Simplified probability representations [Gu, Renaud, Penninger ,2006; Du and Chen, 2005; Chiralaksanakul and Mahadevan, 2005]
  - Simplifying assumptions on network topology: Feed-forward systems [Amaral, Allaire, Willcox, 2014]
  - Two-component systems [Arnst, Ghanem, Phipps, Red-Horse, 2014; Parks, Bochev, Lehoucq, 2008; Olson, D., Bochev, P., Luskin, M., Shapeev, 2014; Constantine, Phipps, Wildey, 2014]
  - Enforce compatibility for deterministic solves/samples [Liao and Willcox, 2015]
  - Enforce compatibility (weakly) in distributions [Liao and Willcox, 2015; Ghoreishi, Allaire, 2017]
  - Domain Decomposition for SPDEs [Sarkar, Benabbou, Ghanem, 2009; Desai, Khalil, Pettit, Poirel, Sarkar, 2018; Zhang, Babaee, Karniadakis, 2018]
- Proposed framework:
  - Rigorous: Enforces strong compatibility (matching random variables)
  - Scalable: Handles multiple components
  - General: Components as black-boxes (beyond stochastic PDEs)
  - Flexible: Tackles arbitrary networks with general inter-connectivity
  - Parallelizable: exhibits excellent weak parallel scalability

Representing Uncertainties

- We represent uncertainties probabilistically using random variables (RVs)
- Use functional representations to preserve coupling of RVs across the network
- Strategy: Use well-established Polynomial Chaos Expansion
  - ✦ Represent model inputs/outputs as RVs
  - ✦ Construct PCEs for uncertain parameters
  - ✦ Obtain PCEs for model outputs using *Non-intrusive Spectral Projection*:
    - ■ *Sampling*-based
    - \+ Relies on black-box utilization of the subcomponent computational model
    - ■ Evaluate projection integrals *numerically* using
      - – Quadrature/Sparse-Quadrature methods
        - \+ Fast convergence
  - ✦ Given a *germ* $\boldsymbol{\xi}(\omega) = \{\xi_1, \cdots, \xi_n\}$ – a set of *i.i.d.* RVs
  - ✦ Any RV in $L^2(\Omega, \mathfrak{S}(\boldsymbol{\xi}), P)$ can be written as a PCE:

$$u(\omega) \simeq \sum_{k=0}^{P} u_k \Psi_k(\boldsymbol{\xi}(\omega))$$

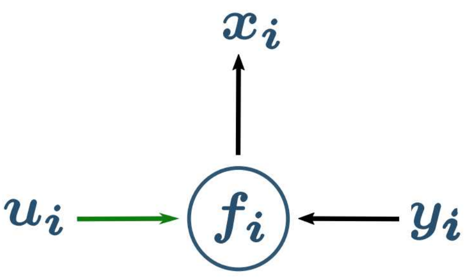
- – u_k are coefficients (deterministic)
- – $\Psi_k(\cdot)$ are functions orthogonal w.r.t. $p(\boldsymbol{\xi})$

DDUQ Formulation

- Subsystem uncertainty propagation of PCE coefficients

$$\boldsymbol{x_i} = \boldsymbol{f_i}\left(\boldsymbol{y_i}, \boldsymbol{u_i}\right)$$

  - Exogenous inputs: $\boldsymbol{u_i}$ (Vector of PCE coefficients)
  - Endogenous inputs: $\boldsymbol{y_i}$ (Vector of PCE coefficients)
  - Outputs: $\boldsymbol{x_i}$ (Vector of PCE coefficients)
  - Uncertainty propagation operator: $\boldsymbol{f_i}$



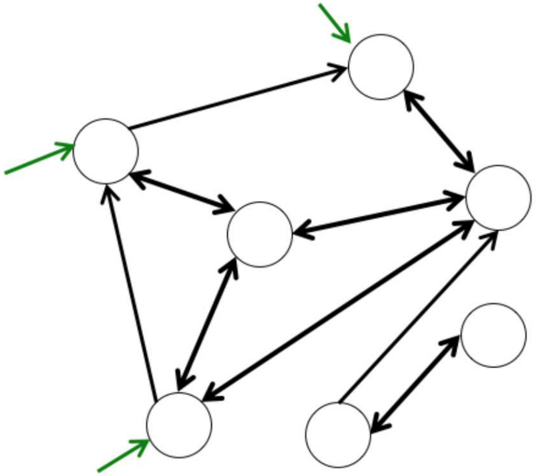
- Full-system uncertainty propagation

$$\boldsymbol{x} = \boldsymbol{f}\left(\boldsymbol{y}, \boldsymbol{u}\right)$$

  - Adjacency matrix satisfies $\boldsymbol{y} = \boldsymbol{I_x^y}\,\boldsymbol{x}$

$$\boldsymbol{x} = \boldsymbol{f}\left(\boldsymbol{I_x^y}\,\boldsymbol{x}, \boldsymbol{u}\right)$$

fixed-point problem



DDUQ Solvers

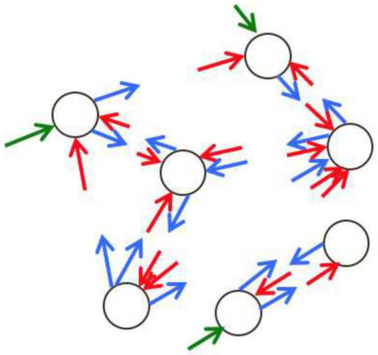
$$\boxed{\boldsymbol{x} = \boldsymbol{f}\left(\boldsymbol{I}^{\boldsymbol{y}}_{\boldsymbol{x}}\,\boldsymbol{x}, \boldsymbol{u}\right)}$$

- Jacobi iterations with relaxation

$$\bar{\boldsymbol{x}} = \boldsymbol{f}\left(\boldsymbol{I}^{\boldsymbol{y}}_{\boldsymbol{x}}\,\boldsymbol{x}^{(k)}, \boldsymbol{u}\right)$$

$$\boldsymbol{x}^{(k+1)} = \omega\bar{\boldsymbol{x}} + (1-\omega)\,\boldsymbol{x}^{(k)}$$

  - ✦ Independent subsystems at each iteration

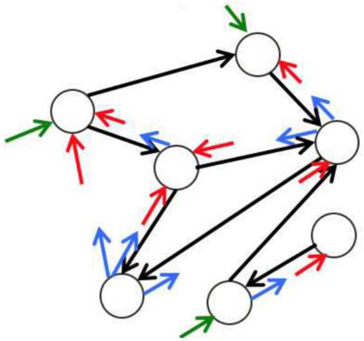


- Gauss–Seidel iterations with relaxation

$$\bar{\boldsymbol{x}} = \boldsymbol{f}\left(\omega\left[\boldsymbol{P}^{(y_i)}_{(p_i)}\right]^T\boldsymbol{L}\left[\boldsymbol{P}^{(x_i)}_{(p_i)}\right]\bar{\boldsymbol{x}} + \left[\boldsymbol{P}^{(y_i)}_{(p_i)}\right]^T\left((1-\omega)\,\boldsymbol{L} + \boldsymbol{D} + \boldsymbol{U}\right)\left[\boldsymbol{P}^{(x_i)}_{(p_i)}\right]\boldsymbol{x}^{(k)}, \boldsymbol{u}\right)$$

$$\boldsymbol{x}^{(k+1)} = \omega\bar{\boldsymbol{x}} + (1-\omega)\,\boldsymbol{x}^{(k)}$$

  - ✦ Feed-forward network (directed acyclic graph) at each iteration
  - ✦ Permutation matrix $\left[\boldsymbol{P}^{(y_i)}_{(p_i)}\right]$ determines DAG



A priori error bound

- PCE truncation within the network may lead to errors in the computed solution
- Let's define $\boldsymbol{g} : (\boldsymbol{\chi}, \boldsymbol{v}) \mapsto \boldsymbol{f}(\boldsymbol{I}_{\boldsymbol{x}}^{\boldsymbol{y}} \boldsymbol{\chi}, \boldsymbol{v})$ such that overall problem becomes

$$\boldsymbol{x} = \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{u})$$

- The 'truth' model associated with a high-fidelity representation of the network (e.g. high-order PCE) leads to the following fixed-point problem

$$\boldsymbol{x}_\star = \boldsymbol{g}_\star(\boldsymbol{x}_\star, \boldsymbol{u}).$$

  - $\boldsymbol{x} \in \mathbb{R}^{\mathsf{x}}$, $\boldsymbol{x}_\star \in \mathbb{R}^{\mathsf{x}_\star}$, with $\mathsf{x}_\star > \mathsf{x}$
  - Prolongation operator $\boldsymbol{I}_H^h : \mathbb{R}^{\mathsf{x}} \to \mathbb{R}^{\mathsf{x}_\star}$
  - Restriction operator $\boldsymbol{I}_h^H : \mathbb{R}^{\mathsf{x}_\star} \to \mathbb{R}^{\mathsf{x}}$ such that $\boldsymbol{I}_h^H \boldsymbol{I}_H^h = \boldsymbol{I}$
- Under mild assumptions, the error can be bounded as

$$\|\boldsymbol{I}_h^H \boldsymbol{x}_\star - \boldsymbol{x}\| \leq \frac{1}{1 - L_{\boldsymbol{g}_\star}^H} \|\boldsymbol{I}_h^H \boldsymbol{g}_\star(\boldsymbol{I}_H^h \boldsymbol{x}, \boldsymbol{u}) - \boldsymbol{x}\|$$

  - $L_{\boldsymbol{g}_\star}^H < 1$ is the restricted Lipschitz constant of the fixed-point mapping $\boldsymbol{g}_\star$
- *Self-consistent* UQ methods: The right-hand side of above inequality will be zero
  - Non-intrusive Spectral Projection with fixed quadrature rule

2D stationary stochastic nonlinear heat equation

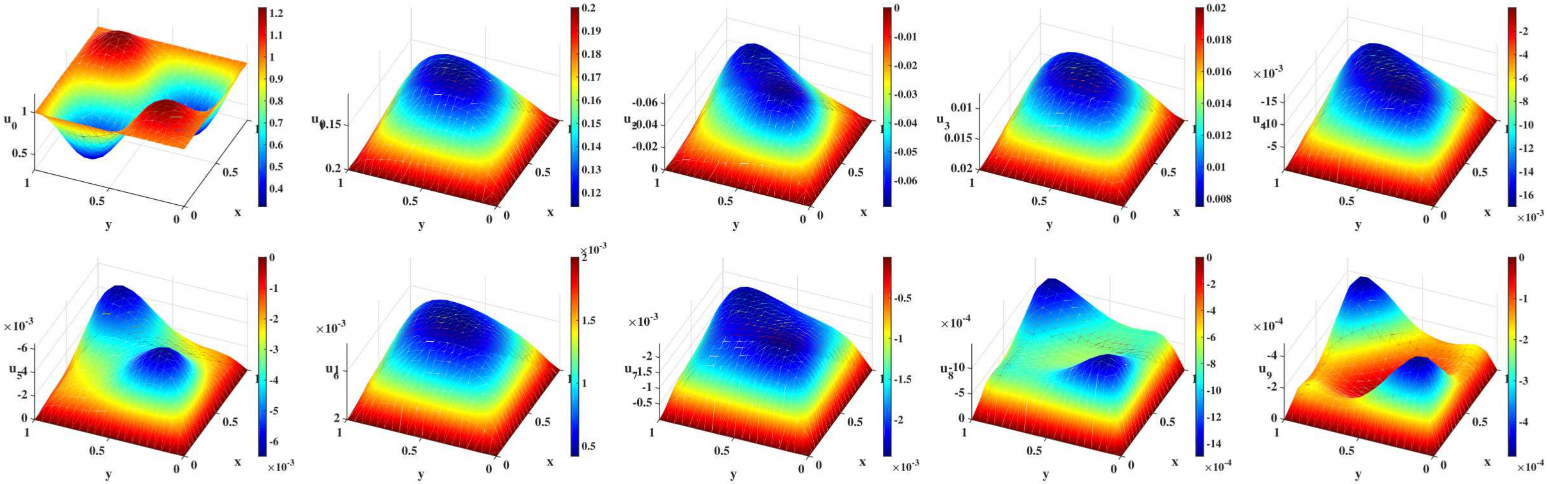
- Two-dimensional stationary nonlinear heat equation with uncertain diffusion and boundary condition

$$-\nabla u + \left(e^{\mu u} - 1\right) = 10\sin\left(2\pi x_1\right)\sin\left(2\pi x_2\right)\ , \qquad x \in \Omega := (0,1)^2$$

$$u_\Gamma = T_1(\xi) = 1.0 + 0.2\xi_1 + 0.02\left(\xi_1^2 - 1\right) + 0.002\left(\xi_1^3 - 3\xi_1\right)$$
$$\mu = T_2(\xi) = 1.0 + 0.2\xi_2 + 0.02\left(\xi_2^2 - 1\right) + 0.002\left(\xi_2^3 - 3\xi_2\right)$$

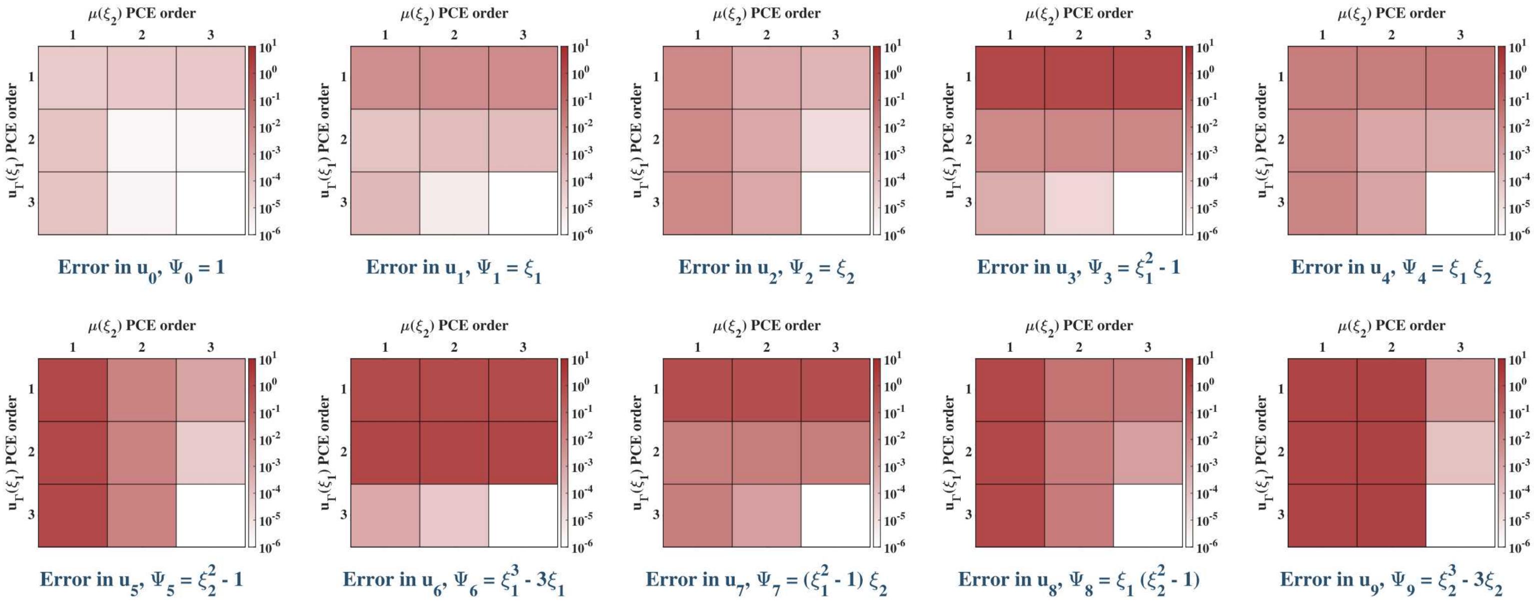
  - ✦ $\xi = (\xi_1, \xi_2)$ iid standard normal random variables
  - ✦ The basis functions $\{\Psi_k\}$ are 2D Hermite polynomials of order at most $p = 3$

- Output PCE coefficients (10 coefficients for a 2nd-order 2D PCE)):



Error analysis

- Examine the effect of using a lower fidelity input on the system response
- Utilize lower-order (truncated) input parameter PCEs
- Normalized L_2 error norms for the 3rd-order output PCE coefficients:



Error in u_0, $\Psi_0 = 1$

Error in u_1, $\Psi_1 = \xi_1$

Error in u_2, $\Psi_2 = \xi_2$

Error in u_3, $\Psi_3 = \xi_1^2 - 1$

Error in u_4, $\Psi_4 = \xi_1 \xi_2$

Error in u_5, $\Psi_5 = \xi_2^2 - 1$

Error in u_6, $\Psi_6 = \xi_1^3 - 3\xi_1$

Error in u_7, $\Psi_7 = (\xi_1^2 - 1)\, \xi_2$

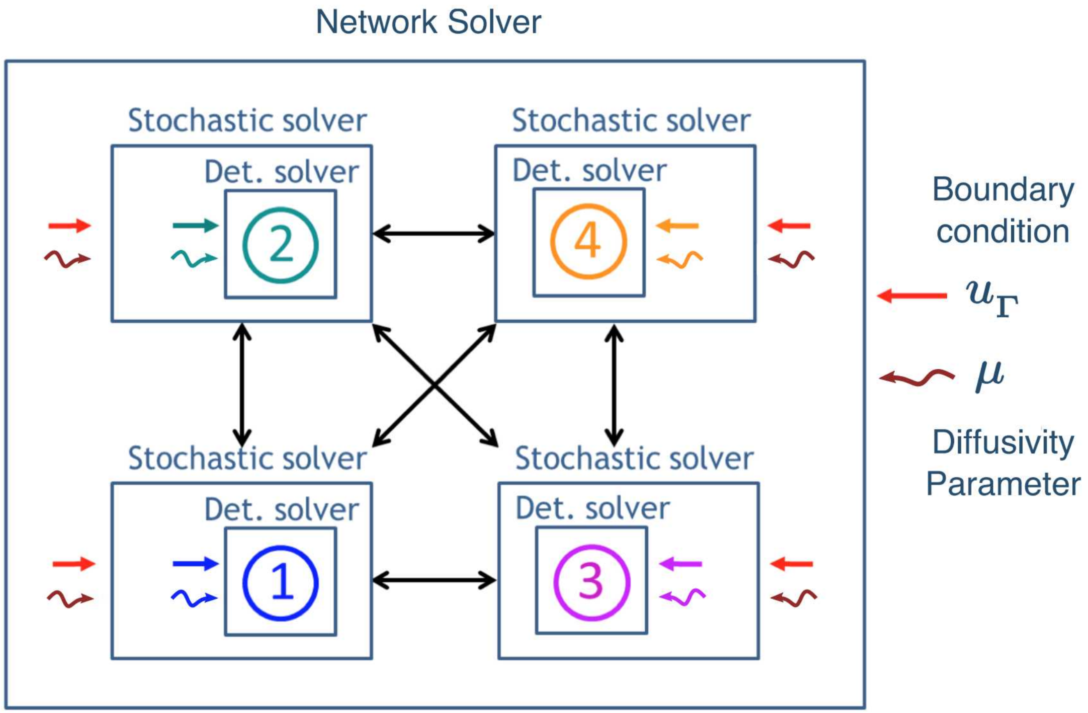
Error in u_8, $\Psi_8 = \xi_1\, (\xi_2^2 - 1)$

Error in u_9, $\Psi_9 = \xi_2^3 - 3\xi_2$

- Observations:
  - ✦ The mean response (u_0 coefficient) converges rapidly: mean response of a system normally depends on lower order moments of the uncertain inputs.
  - ✦ Higher-order output PCE coefficients: strong correlation between input order and error in the output PCE coefficient multiplying polynomials of corresponding seed

Workflow in Network Solver

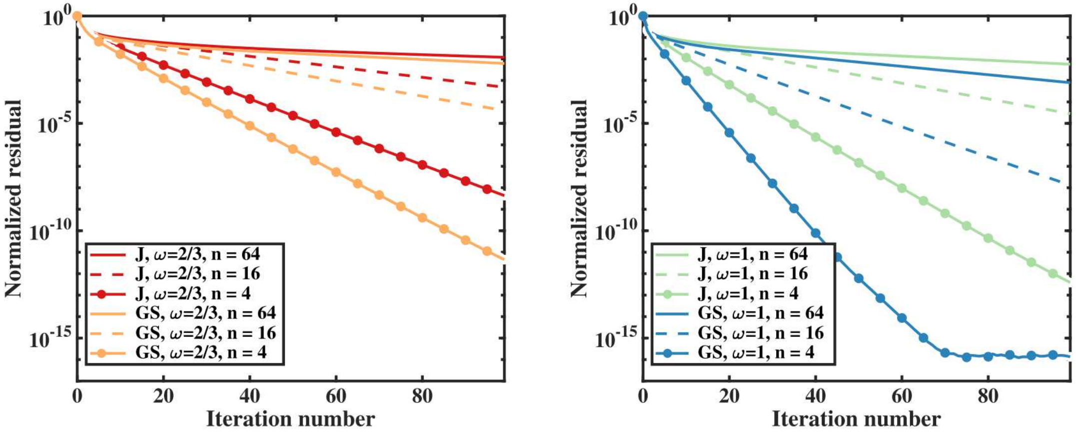
- Schematic of workflow for network solver in tackling the 2D heat equation: 4 subdomains (subcomponents)



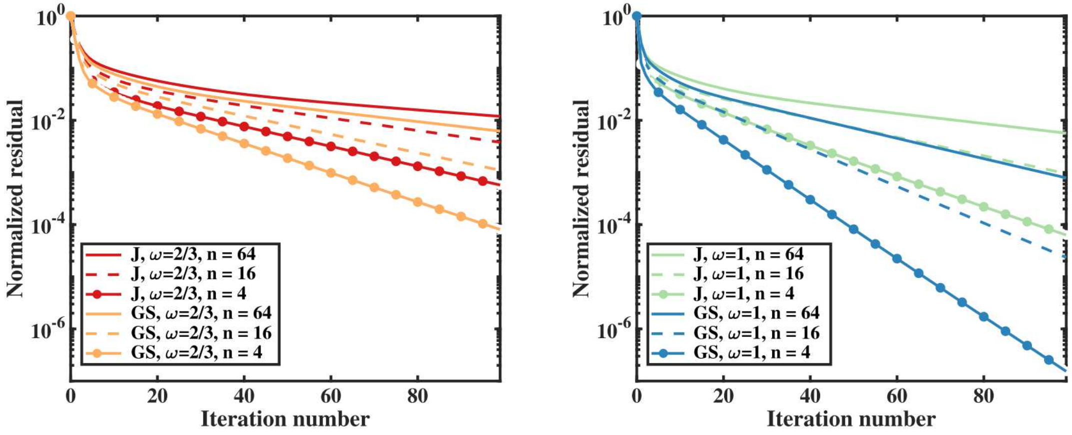
- Modularity: network, stochastic, deterministic solvers independent
- Flexibility: Tailored deterministic solvers for each subsystem
- Extensiblity: new application requires new deterministic solver only

Convergence results

- Examine convergence of PCE coefficients (unknowns)
- Weak scalability: The subdomain problem size (i.e. number of subdomain-level finite-element nodes) fixed while increasing the number of subdomains

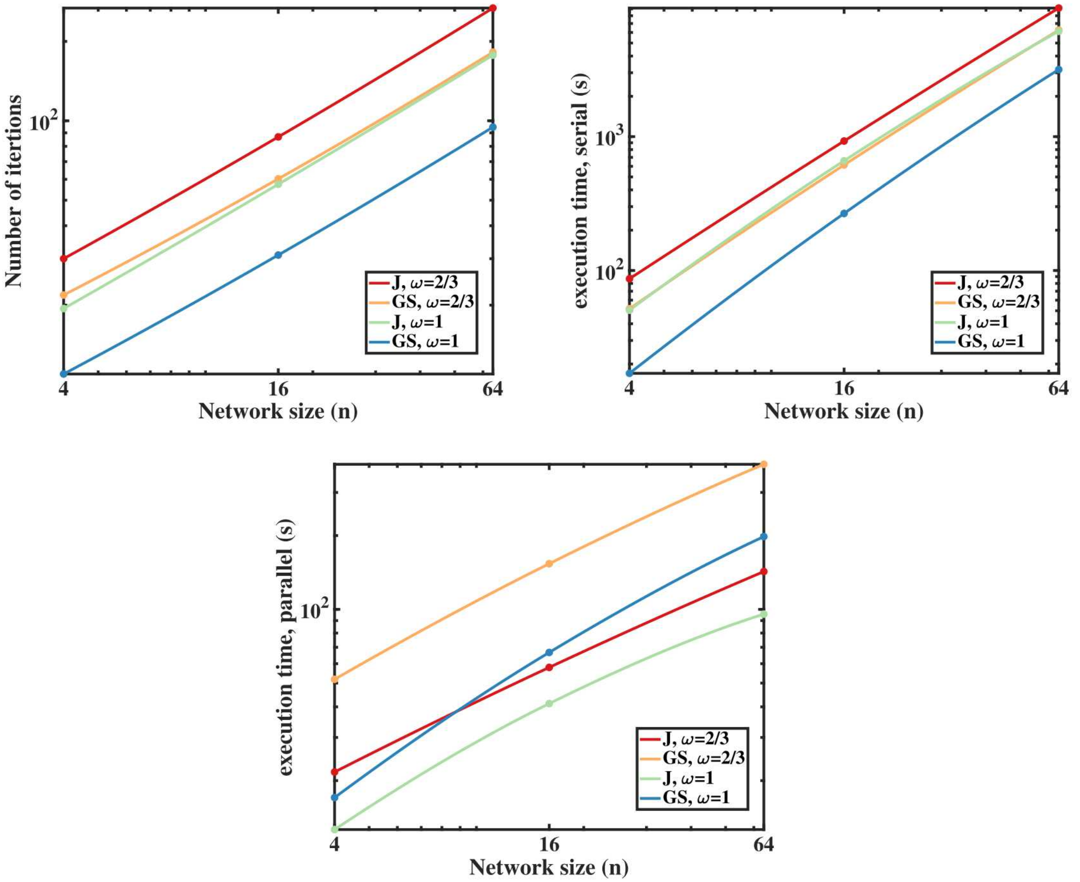


- Strong scalability: The global problem size (i.e. number of global finite-element nodes) fixed while increasing the number of subdomains



Weak scalability results

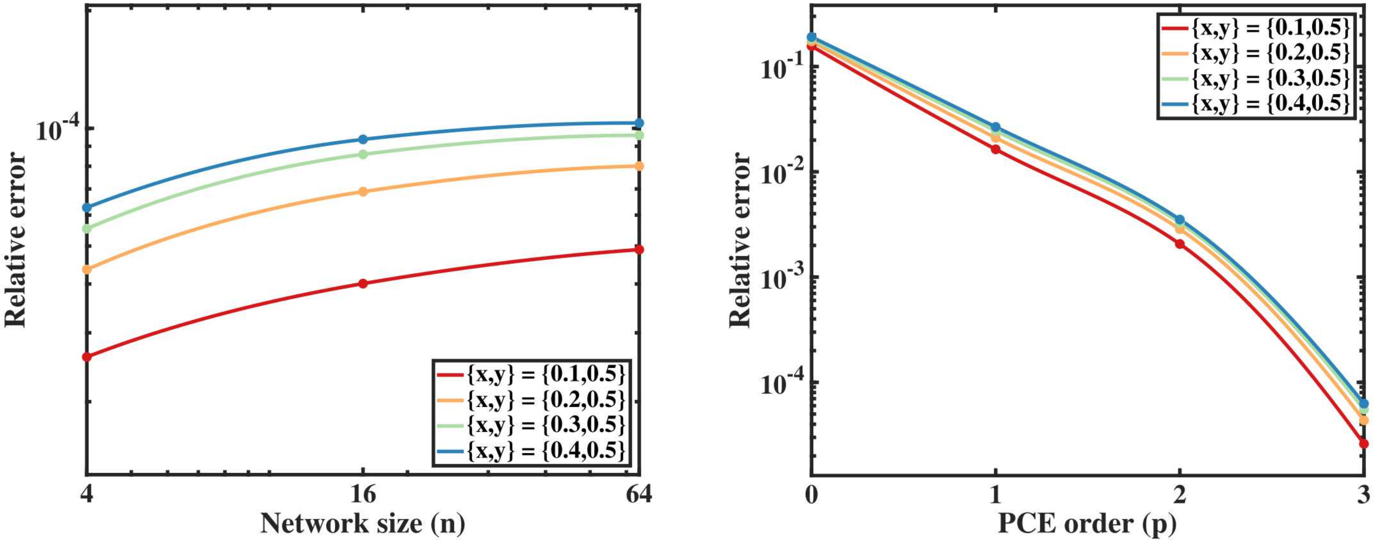
- All timings are obtained by performing calculations on an Intel(R) Xeon(R) Core(TM) i7-5557U CPU @ 3.10GHz with 16 GB RAM



- Observations:
  - \+ Iteration count *weakly* dependent on network size
  - \+ Jacobi faster (for parallel implementations) than Gauss–Seidel

Error Analysis

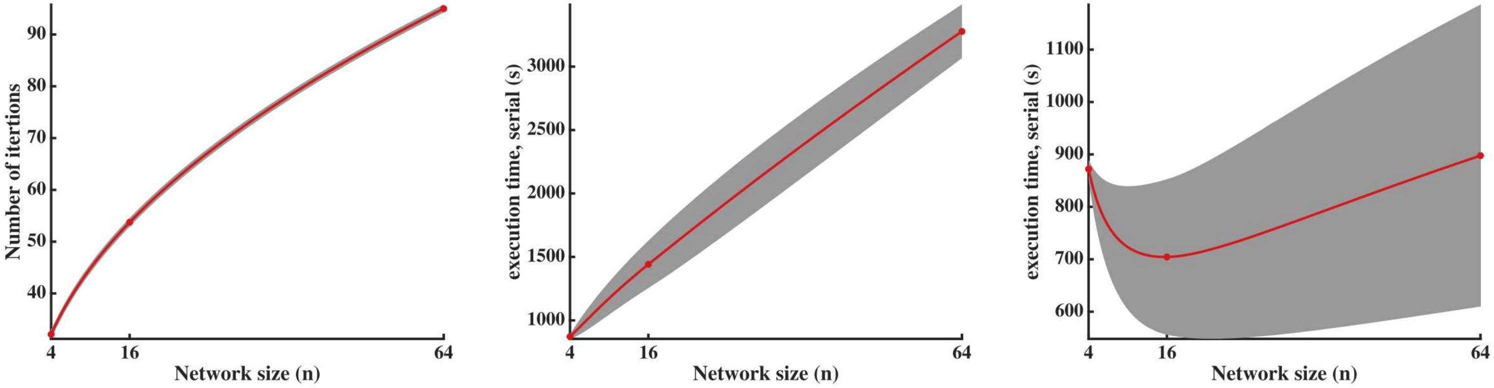
- Normalized error for solution (PC coefficients) at isolated physical locations for
  - ✦ varying network size (fixed PCE-order of unknowns)
  - ✦ varying PCE-order representation of unknowns (fixed network size of 4)



- Observations:
  - + Errors relatively small
  - ✦ Errors increase with (1) distance from boundary, (2) network size, (3) lower-fidelity PCE representation

Gauss-Seidel Iterations: Effect of Permutation Matrix

- Strong scalability results for Gauss-Seidel iterations with random permutation matrix (10 Monte Carlo samples)



- Observations:
  - \+ Minimal impact on the total number of iterations
  - \+ Weak impact on the serial execution time
  - \- Strong impact on the parallel execution time
    - \+ Extreme gains to be had in using optimal permutation matrix

Summary

- Presented a framework for propagation of uncertainties through decomposable systems
- Network-based UQ with coupling information propagated using new techniques inspired by domain decomposition
- Proposed methodology extends existing suite of techniques:
    - Rigorous: Enforces strong compatibility (matching random variables)
    - Scalable: Handles multiple components
    - General: Components as black-boxes (beyond stochastic PDEs)
    - Flexible: Tackles arbitrary networks with general inter-connectivity
    - Parallelizable: exhibits excellent weak parallel scalability
- Application: 2D nonlinear stochastic static heat equation with uncertain parameters and boundary conditions