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INEXACT METHODS FOR SYMMETRIC STOCHASTIC EIGENVALUE PROBLEMS

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Overview

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2. Problem definition: symmetric stochastic eigenvalue problem
3. Sampling-based methods
4. Stochastic Galerkin method
    - Two inexact iterative solvers
    - Preconditioners
5. Numerical experiments
6. Conclusion

1. Motivation

- Stochastic eigenvalue problem
  - **Eigenvalue analysis**: modeling of vibration of mechanical structures, neutron transport criticality computations, or stability of dynamical systems
  - **Stochastic Eigenvalue analysis**: eigenvalue problems parameterized by random variables
    - The behavior of the mathematical models depends on **proper choice of parameters** (e.g., coefficients, boundary conditions or forces)
    - In practice, the exact values of these parameters are not known and are modeled as **random processes**
- Existing solvers for stochastic eigenvalue problem
  - Monte Carlo methods [Nightingale and Umrigar 2007] => robust but slow
  - Perturbation methods [Shinozuka and C. J. Astill 1972] => limited to low variability
  - Spectral stochastic finite element methods (SSFEMs) [Verhoosel, Guti´errez, and Hulshoff 2006] [Hakula, Kaarnioja, and Laaksonen 2015] [Ghanem and Ghosh 2007] [Benner, Onwunta, and Stoll 2018] => effective but require solutions of large systems of nonlinear equations

2. Problem definition

- Symmetric stochastic eigenvalue problem:

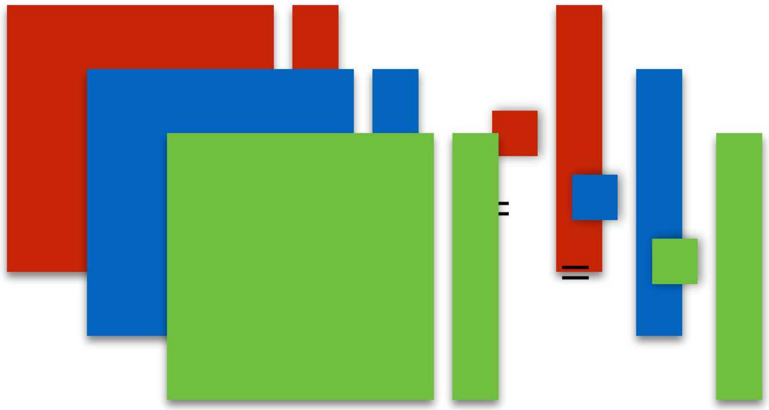
$$A(\xi)u^s(\xi) = \lambda^s(\xi)u^s(\xi)$$

- $A(\xi) \in \mathbb{R}^{n\times n}$: linear operator, a matrix-valued function
- $u^s(\xi) \in \mathbb{R}^n$: eigenvector, a vector-valued function
- $\lambda^s(\xi) \in \mathbb{R}$: eigenvalue, a scalar function
- $\xi = [\xi_1, \dots, \xi_{m_\xi}]^\mathrm{T}$: a set of i.i.d. random variables, $\xi \sim P(\xi)$

$$A(\xi^{(1)})u^s(\xi^{(1)}) = \lambda^s(\xi^{(1)})u^s(\xi^{(1)})$$

$$A(\xi^{(2)})u^s(\xi^{(2)}) = \lambda^s(\xi^{(2)})u^s(\xi^{(2)})$$

$$A(\xi^{(3)})u^s(\xi^{(3)}) = \lambda^s(\xi^{(3)})u^s(\xi^{(3)})$$



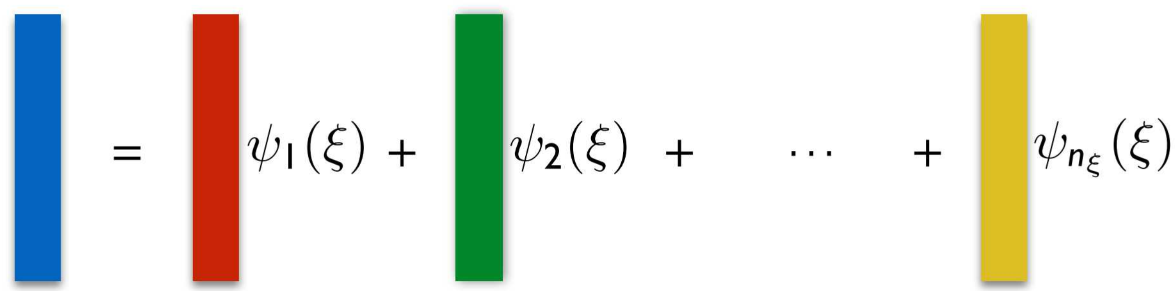
- $A(\xi) = A(\xi)^\mathrm{T}$: symmetric operator
- $u^s(\xi)^\mathrm{T}u^s(\xi) = \mathrm{I}$: orthonormal eigenvectors

Problem definition

- Spectral approximation of random functions via gPC expansion [Xiu and Karniadakis 2002]
  - gPC expansion: with generalized polynomial chaos basis $\psi_i(\xi) \in \mathbb{R}$

$$f(\xi) = \sum_{i=1}^{n_\xi} f_i \psi_i(\xi) = \underbrace{f_1\psi_1(\xi)}_{\text{mean}} + f_2\psi_2(\xi) + \cdots + f_{n_\xi}\psi_{n_\xi}(\xi), \qquad f(\xi),\, f_i \in \mathbb{R}^{n_f}$$

Degrees of polynomials increase



$$= \begin{bmatrix} \psi_1(\xi) & & & \psi_2(\xi) & & & & \psi_{n_\xi}(\xi) & & \\ & \ddots & & & \ddots & & \cdots & & \ddots & \\ & & \psi_1(\xi) & & & \psi_2(\xi) & & & & \psi_{n_\xi}(\xi) \end{bmatrix}$$

$$= (\Psi(\xi)^{\mathsf{T}} \otimes I)\bar{f}$$

$$\Psi(\xi)^{\mathsf{T}} = \begin{bmatrix} \psi_1(\xi) & \cdots & \psi_{n_\xi}(\xi) \end{bmatrix}$$

- Eigenvector: $u^s(\xi) = \sum_{k=1}^{n_\xi} u_k^s \psi_k(\xi) = (\Psi(\xi)^{\mathsf{T}} \otimes I)\bar{u}^s, \quad u_k^s \in \mathbb{R}^n,\ \bar{u}^s \in \mathbb{R}^{n n_\xi}$
- Eigenvalue: $\lambda^s(\xi) = \sum_{k=1}^{n_\xi} \lambda_k^s \psi_k(\xi) = \bar{\lambda}^{s\mathsf{T}} \Psi(\xi), \quad \lambda_k^s \in \mathbb{R},\ \bar{\lambda}^s \in \mathbb{R}^{n_\xi}$

3. Sampling-based methods

- Computing the unknown coefficients via discrete projections:
  - Orthonormality of the gPC basis: $\langle \psi_i(\xi), \psi_j(\xi) \rangle = \mathbb{E}[\psi_i(\xi)\psi_j(\xi)] = \int_\Gamma \psi_i(\xi)\psi_j(\xi) dP(\xi)$

$$\langle \psi_i(\xi), \psi_j(\xi) \rangle = \mathbb{E}[\psi_i(\xi)\psi_j(\xi)] = 0, \qquad i \neq j$$

  - Discrete projection:

$$\mathbb{E}[f(\xi)\psi_i(\xi)] = \mathbb{E}[f_1\psi_1(\xi)\psi_i(\xi) + \cdots + f_{n_\xi}\psi_{n_\xi}(\xi)\psi_i(\xi)] = f_i\,\mathbb{E}[\psi_i(\xi)\psi_i(\xi)] = f_i$$

  - Need to evaluate

$$\mathbb{E}[f(\xi)\psi_i(\xi)] = \int_\Gamma f(\xi)\psi_i(\xi) dP(\xi)$$

- Two methods for discrete projections
  - Monte Carlo method:

$$f_k = \frac{1}{n_{MC}} \sum_{q=1}^{n_{MC}} f(\xi^{(q)})\psi_k(\xi^{(q)})$$

  - Stochastic collocation method: [Xiu 2007]

$$f_k = \sum_{q=1}^{n_q} f(\xi^{(q)})\psi_k(\xi^{(q)})w^{(q)}$$

4. Stochastic Galerkin method

- Galerkin (orthogonal) projection:

$$(\Psi(\xi)^{\mathsf{T}} \otimes A(\xi))\bar{u}^s = (\bar{\lambda}^{s\mathsf{T}}\Psi(\xi)\Psi(\xi)^{\mathsf{T}} \otimes I)\bar{u}^s$$
$$\bar{u}^{s\mathsf{T}}(\Psi(\xi)\Psi(\xi)^{\mathsf{T}} \otimes I)\bar{u}^s = 1$$

gPC approximation:

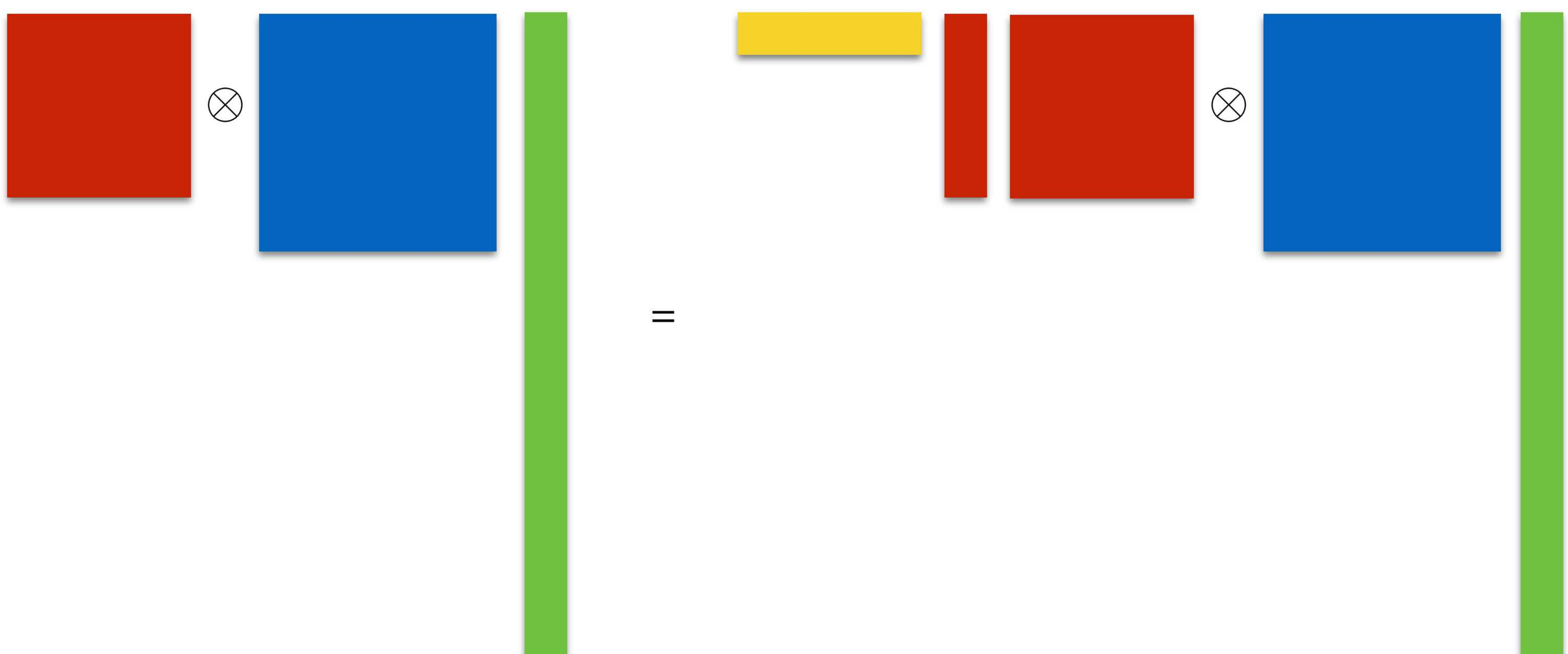
$$\lambda^s(\xi) = \bar{\lambda}^{s\mathsf{T}}\Psi(\xi)$$
$$u^s(\xi) = (\Psi(\xi)^{\mathsf{T}} \otimes I)\bar{u}^s$$

Galerkin projection $\Downarrow$ orthogonal projection onto trial basis,

$$\Psi(\xi)^{\mathsf{T}} = \begin{bmatrix}\psi_1(\xi) & \cdots & \psi_{n_\xi}(\xi)\end{bmatrix}$$

$$\mathbb{E}[\Psi\Psi^{\mathsf{T}} \otimes A]\bar{u}^s = \mathbb{E}[(\bar{\lambda}^{s\mathsf{T}}\Psi)\Psi\Psi^{\mathsf{T}} \otimes I)]\bar{u}^s$$

$$\mathbb{E}[\Psi \otimes (\bar{u}^{s\mathsf{T}}(\Psi\Psi^{\mathsf{T}} \otimes I)\bar{u}^s)] = \mathbb{E}[\Psi \otimes 1]$$



Two inexact solvers for SG formulation

- Inexact stochastic inverse subspace iteration
  - Stochastic inverse subspace iteration (SISI): a stochastic extension of inverse subspace iteration [Meidani and Ghanem 2012, 2014, Sousedik and Elman 2016]
  - **Inexact variant of SISI**
  - **Efficient preconditioners for inexact SISI**
- Inexact Newton method for stochastic eigenvalue problems
  - Newton iteration (NI) for SG formulation [Ghanem and Ghosh 2007]
  - Inexact variant of NI [Benner, et al 2018]
  - **Efficient preconditioners for inexact NI**

Inexact SISI

- Inverse subspace iteration: $Au^s = \lambda^s u^s$
  - Approximate eigenvectors via an iterative procedure:
    1. solve $Av^{s,(i)} = u^{s,(i)}$
    2. orthonormalize $[u^{1,(i)}, u^{2,(i)}, \cdots] := \textbf{Gram-Schmidt}([v^{1,(i)}, v^{2,(i)}, \cdots])$
  - Compute eigenvalue via Rayleigh quotient: $\lambda^s = u^{s,(i)\mathsf{T}} A u^{s,(i)}$
- Stochastic inverse subspace iteration:
  - Extension of ISI to solve $A(\xi)u^s(\xi) = \lambda^s(\xi)u^s(\xi)$ in SG formulation
  - Modifications: approximate stochastic eigenvector via an iterative procedure:
    1. solve $\boxed{\mathbb{E}[\Psi\Psi^\mathsf{T} \otimes A]\bar{v}^{s,i} = \bar{u}^{s,i}}$
    2. Gram-Schmidt and Rayleigh quotient are tailored to stochastic expansions
- Inexact SISI:
  - Solve the linear systems at each nonlinear step only approximately using preconditioned conjugate gradient method (stopping criteria: relative residual)
  - Adaptive stopping tolerance: based on the previous nonlinear residual

Inexact Newton iteration

- Need to solve a nonlinear system of equations:

$$R(\bar{u}^s, \bar{\lambda}^s) = \begin{bmatrix} F(\bar{u}^s, \bar{\lambda}^s) \\ G(\bar{u}^s) \end{bmatrix} = \begin{bmatrix} \mathbb{E}[\Psi\Psi^{\mathsf{T}} \otimes A]\bar{u}^s - \mathbb{E}[(\bar{\lambda}^{s\,\mathsf{T}}\Psi)\Psi\Psi^{\mathsf{T}} \otimes I]\bar{u}^s \\ \mathbb{E}[\Psi \otimes \big((\bar{u}^{s\,\mathsf{T}}(\Psi\Psi^T \otimes I)\bar{u}^s) - 1\big)] \end{bmatrix} = 0$$

- Newton iteration:

$$\boxed{\mathcal{J}(\bar{u}^{s,(n)}, \bar{\lambda}^{s,(n)}) \begin{bmatrix} \delta\bar{u}^{s,(n)} \\ \delta\bar{\lambda}^{s,(n)} \end{bmatrix} = -R(\bar{u}^{s,(n)}, \bar{\lambda}^{s,(n)})}$$

$$\begin{bmatrix} \bar{u}^{s,(n+1)} \\ \bar{\lambda}^{s,(n+1)} \end{bmatrix} = \begin{bmatrix} \bar{u}^{s,(n)} \\ \bar{\lambda}^{s,(n)} \end{bmatrix} + \begin{bmatrix} \delta\bar{u}^{s,(n)} \\ \delta\bar{\lambda}^{s,(n)} \end{bmatrix}$$

  - Jacobian:

$$\mathcal{J}(\bar{u}^s, \bar{\lambda}^s) = \begin{bmatrix} \frac{\partial F}{\partial \bar{u}^s}(\bar{u}^s, \bar{\lambda}^s) & \frac{\partial F}{\partial \bar{\lambda}^s}(\bar{u}^s, \bar{\lambda}^s) \\ \frac{\partial G}{\partial \bar{u}^s}(\bar{u}^s, \bar{\lambda}^s) & 0 \end{bmatrix}$$

- Inexact computation: solves the systems only approximately using Krylov-subspace methods (GMRES)
  - Stopping criteria for GMRES: relative residual
  - Adaptive tolerance: based on nonlinear residual at the previous nonlinear iteration step

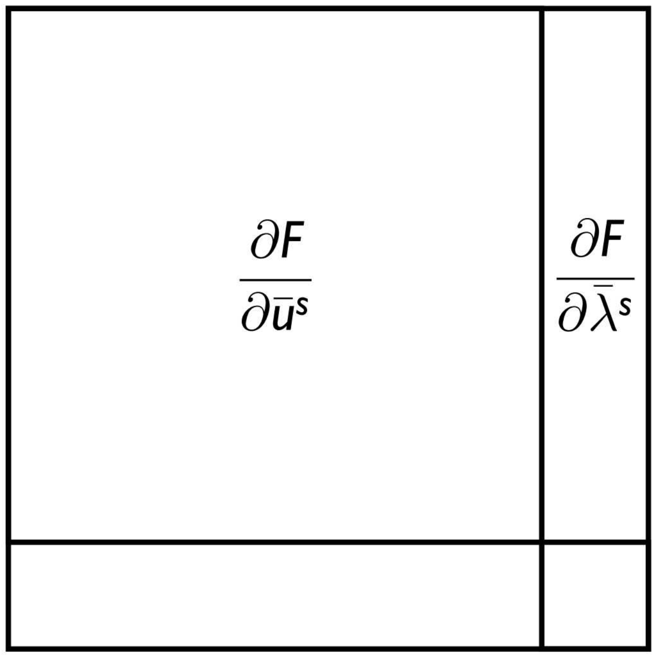
$$\frac{\|R_n + \mathcal{J}_n x\|_2}{\|R_n\|_2} < \tau \, \|R_{n-1}\|_2$$

Preconditioners for Newton iteration

- Preconditioners: (inexpensive) approximations to Jacobian matrices
  - Mean-based (MB) preconditioner [Powell and Elman 2009]
  - Constraint mean-based (MB) preconditioner [Keller, et al 2000]
  - Constraint hierarchical Gauss—Seidel (chGS) preconditioner [Sousedik and Ghanem 2014]

Preconditioners for Newton iteration

- Structure of Jacobian matrices

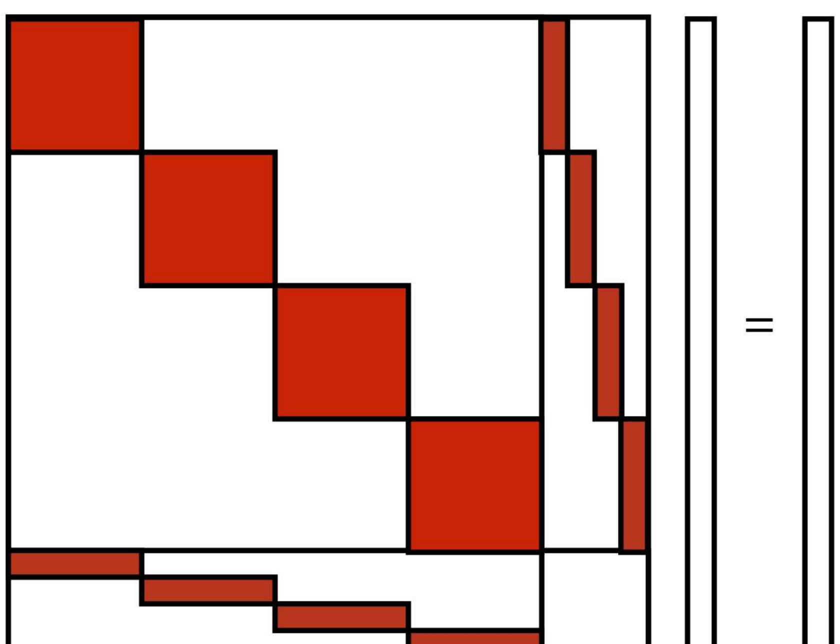


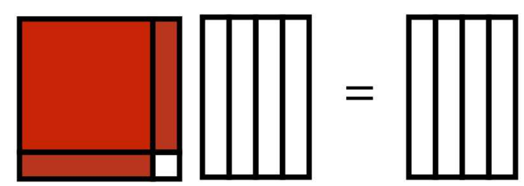
$$\frac{\partial F}{\partial \bar{u}^s} = \mathbb{E}[\Psi\Psi^T \otimes A] - \mathbb{E}[(\bar{\lambda}^{sT}\Psi)\Psi\Psi^T \otimes I]$$

$$A(\xi) = \sum_{k=1}^{n_a} A_k \psi_k(\xi), \quad A_k \in \mathbb{R}^{n\times n}$$

$$\mathbb{E}[\Psi\Psi^T \otimes A] = \sum_{k=1}^{n_a} H_k \otimes A_k, \qquad H_k = \mathbb{E}[\psi_k \Psi\Psi^T]$$

- Consider the mean-component only: $H_1 \otimes A_1, \qquad H_1 = \mathbb{E}[\psi_1 \Psi\Psi^T] = I$





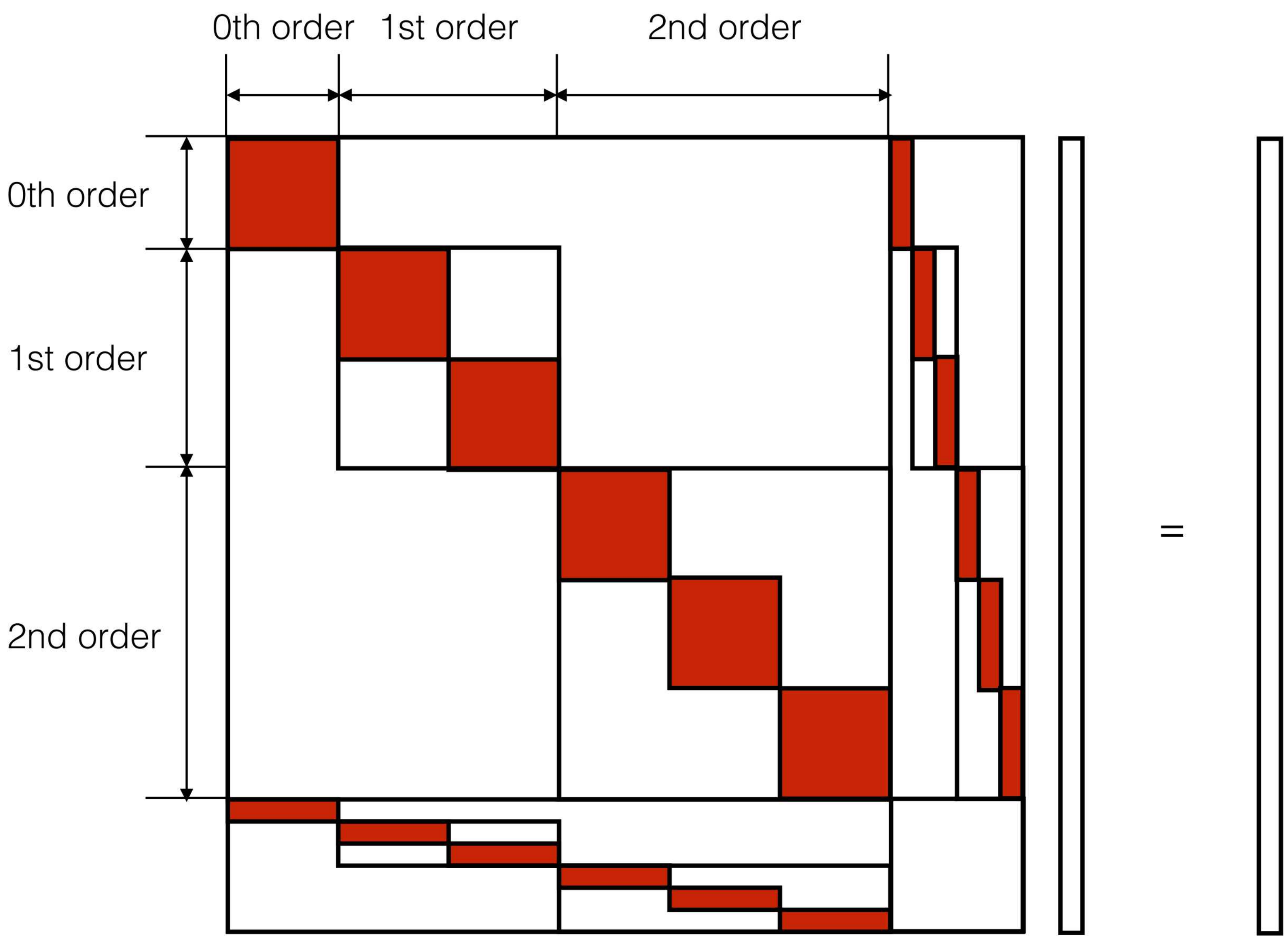
$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix}$$

- Mean-based (MB) preconditioner: $\begin{bmatrix} A & 0 \\ 0 & BA^{-1}B^T \end{bmatrix}$

- Constraint MB (cMB) preconditioner: $\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix}$

Preconditioners for Newton iteration

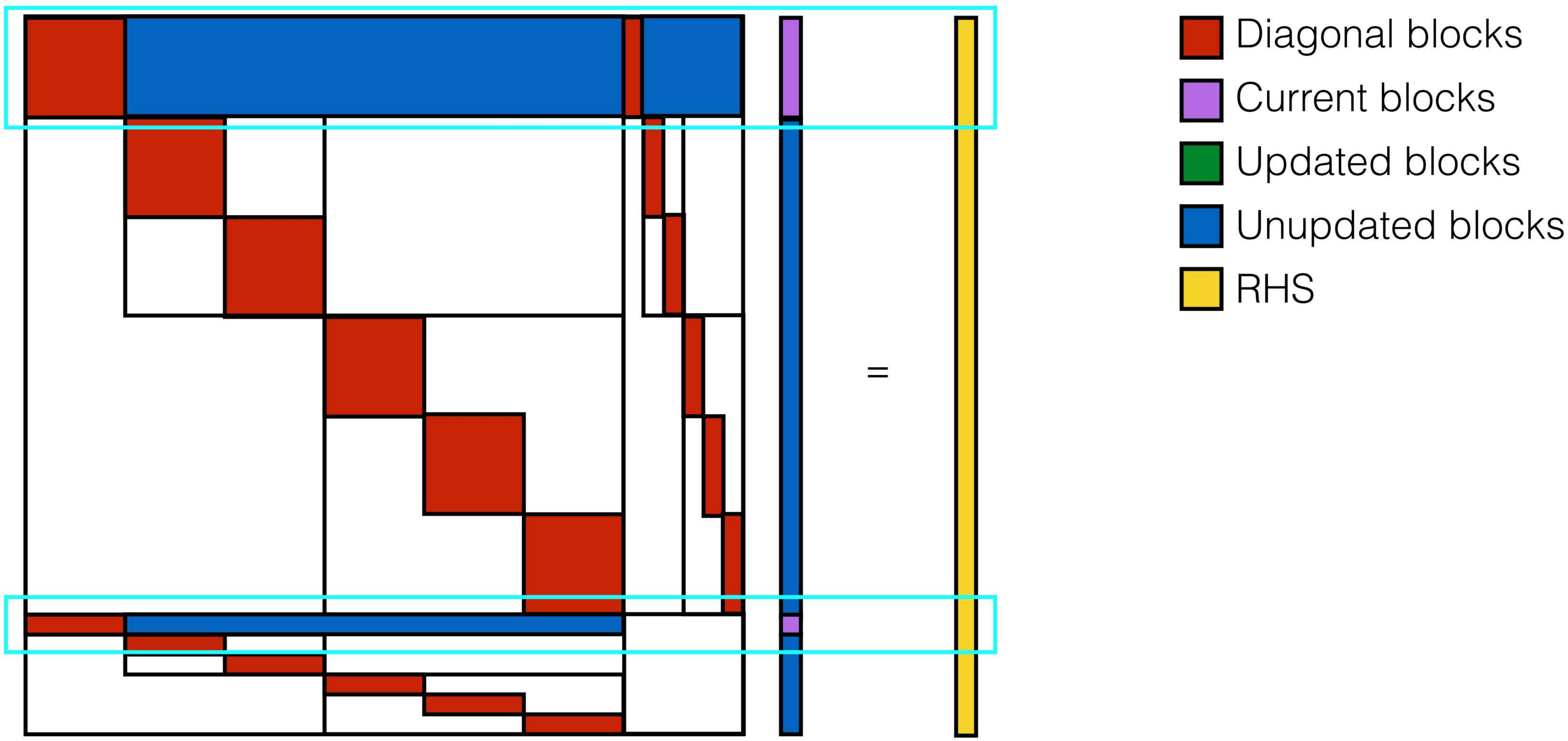
- Consider a hierarchical structure: Gauss—Seidel update

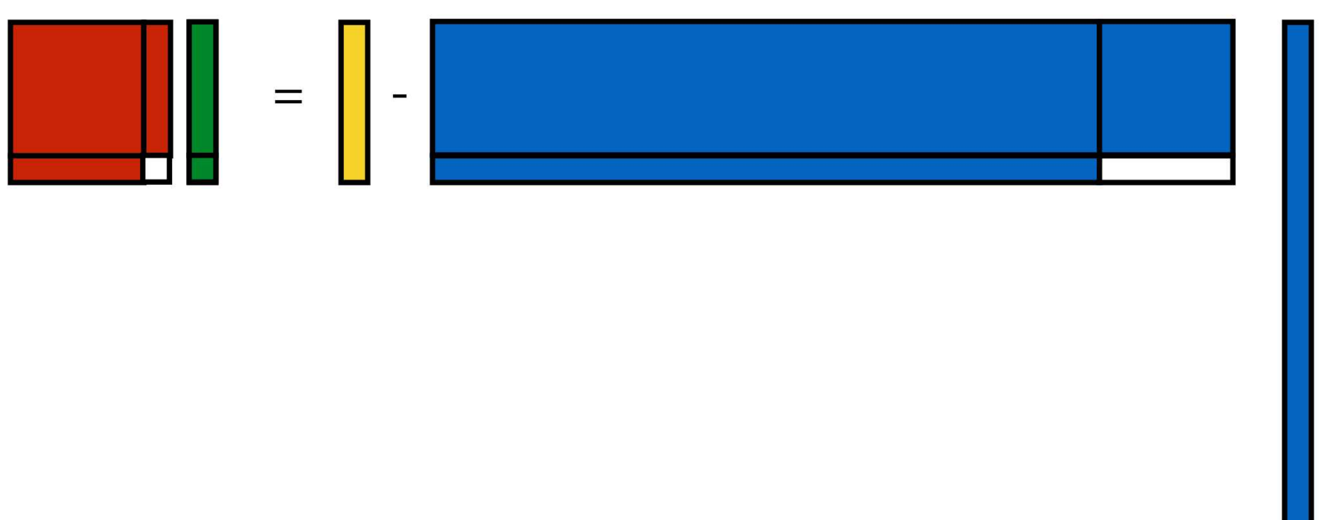


$$[H_k]_{ij} = \mathbb{E}[\psi_k \psi_i \psi_j]$$

Preconditioners for Newton iteration

- Consider a hierarchical structure: Gauss—Seidel update



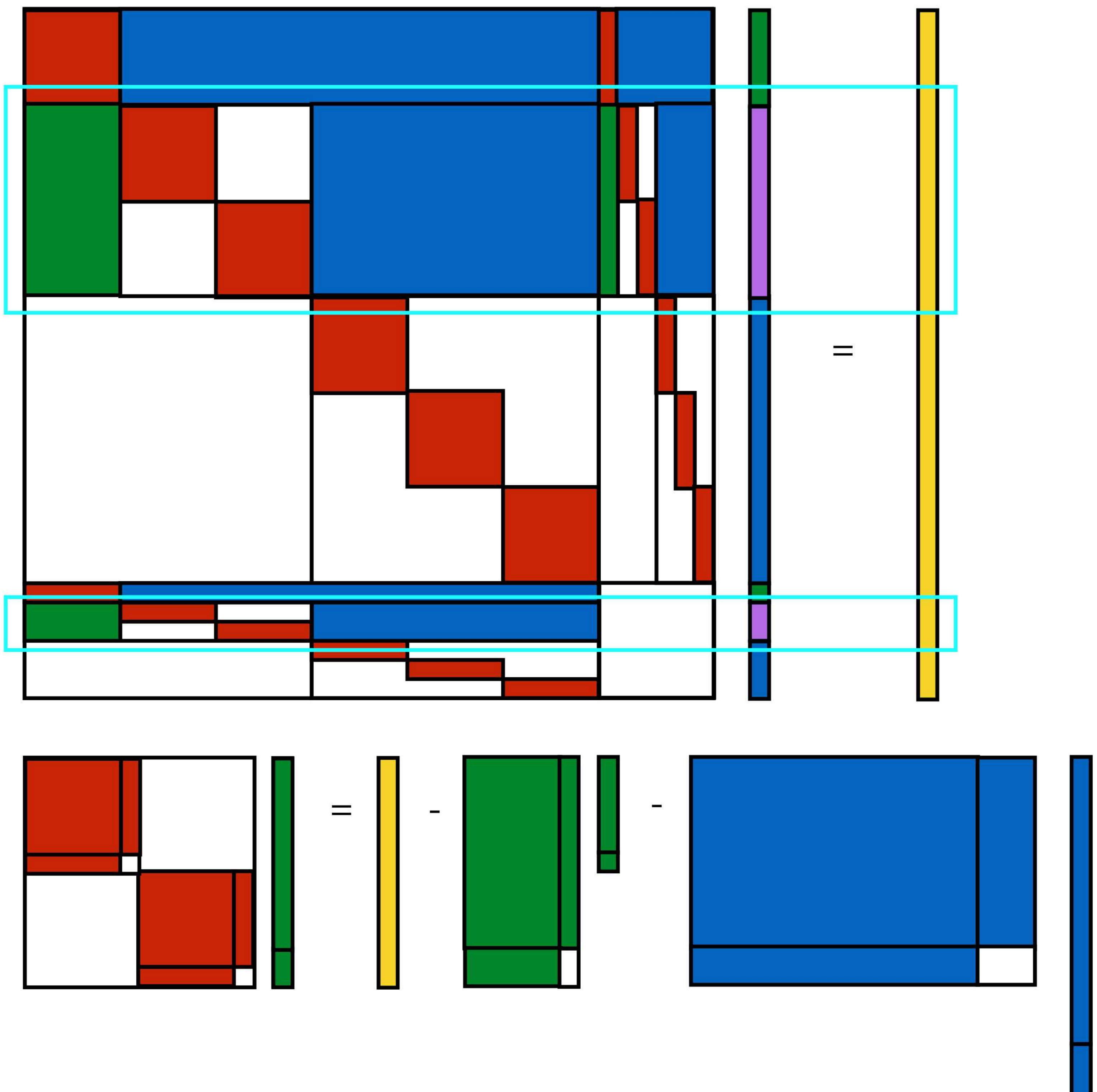


Solve diagonal blocks with cMB

Constraint hierarchical GS: chGS

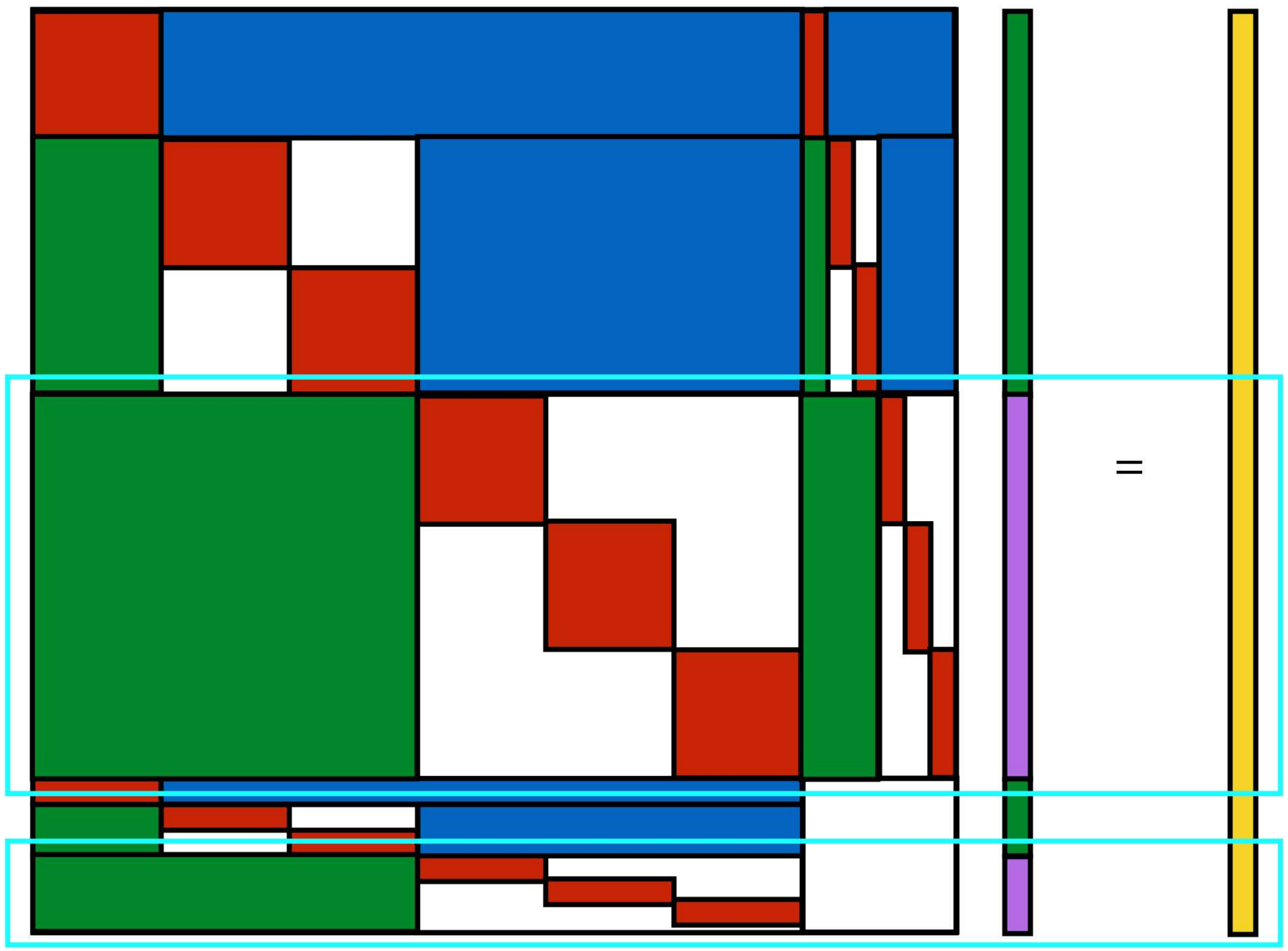
Preconditioners for Newton iteration

- Consider a hierarchical structure: Gauss—Seidel update



Preconditioners for Newton iteration

- Consider a hierarchical structure: Gauss—Seidel update



5. Numerical experiments

- Model problem: stochastic diffusion problem with lognormal coefficient

$$
\begin{aligned}
-\nabla \cdot (a(x,\xi)\nabla u(x,\xi)) &= \lambda(\xi) u(x,\xi) \quad &&\text{in } D \times \Gamma,\\
u(x,\xi) &= 0 &&\text{on } \partial D \times \Gamma,
\end{aligned}
$$

where the diffusion coefficient is a truncated lognormal process:

$$
a(x,\xi) = \sum_{\ell=1}^{n_a} a_\ell(x)\psi_\ell(\xi)
$$

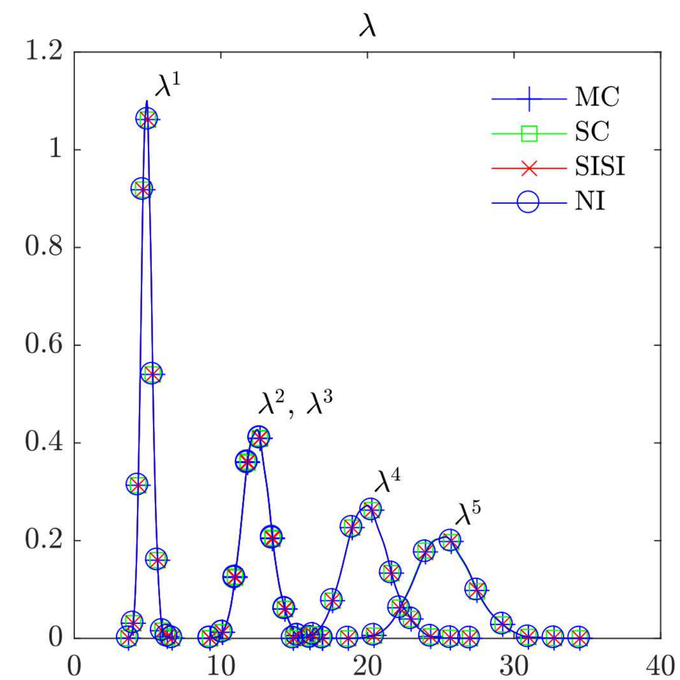
- Finite element discretization:

$$
A(\xi)u^s(\xi) = \lambda^s(\xi)u^s(\xi)
$$

where $A(\xi) = \sum_{\ell=1}^{n_a} A_\ell \psi_\ell(\xi) = \sum_{\ell=1}^{n_a} \left[L^{-1}K_\ell L^{-T}\right]\psi_\ell(\xi)$ with K_ℓ a stiffness matrix weighted by $a_\ell(x)$ and $M = LL^T$ is a mass matrix.

Numerical experiments

- Results of numerical experiments
  - Eigenvalue: $\lambda^s(\xi) = \sum_{k=1}^{n_\xi} \lambda_k^s \psi_k(\xi) = \bar{\lambda}^{s\mathsf{T}} \Psi(\xi)$
  - gPC coefficients: $\bar{\lambda}^s = [\lambda_1^s, \cdots, \lambda^s]^\mathsf{T}$



Pdf estimates of the five smallest eigenvalues computed via ksdensity

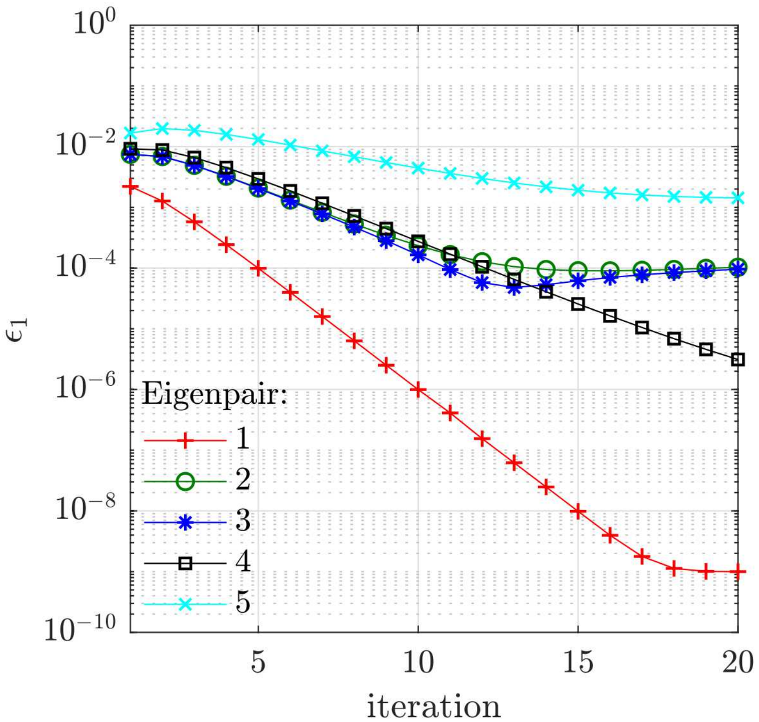
d	k	SC	SISI	NI
0	1	4.9431E+00	4.9431E+00	4.9431E+00
1	2	3.6197E-01	3.6197E-01	3.6197E-01
	3	1.4477E-13	-1.6489E-14	-7.9829E-16
	4	-6.6436E-13	-1.7135E-14	-1.3429E-15
2	5	1.8642E-02	1.8642E-02	1.8642E-02
	6	-5.4534E-13	-9.5178E-17	-7.4261E-17
	7	-3.0909E-13	-1.1628E-15	-9.5249E-17
	8	-1.5442E-03	-1.5442E-03	-1.5442E-03
	9	-9.7700E-15	-1.1200E-15	1.3125E-18
	10	-1.5442E-03	-1.5442E-03	-1.5442E-03

The first 10 coefficients of the gPC expansion of the smallest eigenvalue

MC: Monte Carlo method
SC: Stochastic Collocation method
SISI: Stochastic Inverse Subspace Iteration
NI: Newton iteration

Numerical experiments

- Inexact stochastic inverse subspace iteration (SISI) performance
  - Convergence plot



Convergence history of the inexact stochastic inverse subspace iteration

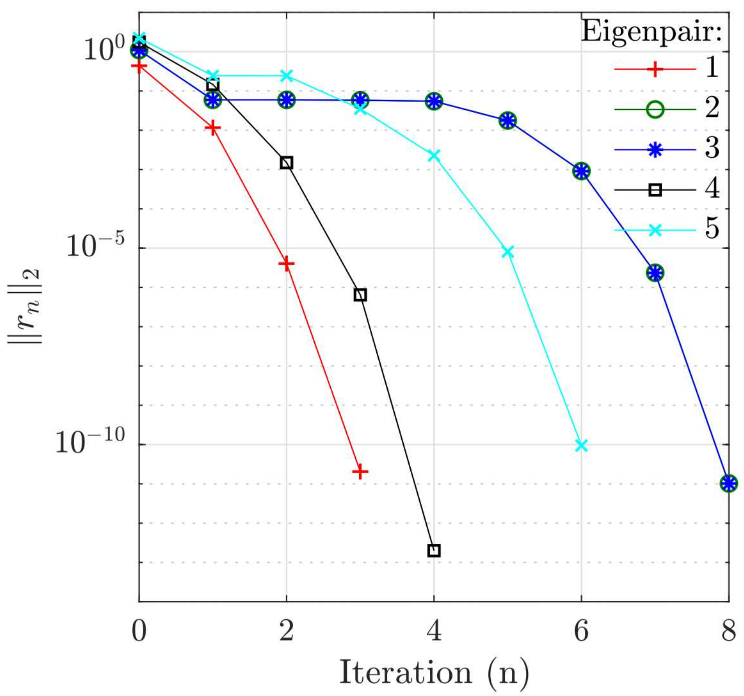
  - Comparison of different preconditioners:

Preconditioner	1st	2nd	3rd	4th	5th
MB	6.45	3.90	3.90	4.60	3.75
hGS (no trunc.)	2.15	1.00	1.00	1.45	1.00

Average number of PCG iterations for computing the five smallest eigenvalues and corresponding eigenvectors

Numerical experiments

- Inexact Newton iteration (NI) performance
  - Convergence plot



Convergence history in terms of the nonlinear residual

- Comparison of different preconditioners:

Preconditioner	1st	2nd	3rd	4th	5th
NMB	13.3	28.9	27.8	16.2	43.0
cMB	4.3	24.7	25.4	5.3	28.0
chGS	2.0	13.8	13.5	2.0	12.3

Average number of MINRES/GMRES iterations for computing the five smallest eigenvalues and corresponding eigenvectors

	1st	4th	1st	4th
Nonlinear step	cMB		chGS	
1	2	2	1	1
2	4	8	2	1
3	7	10	3	2
4		13		4

The number of GMRES iterations for computing the first and the fourth eigenvalues and corresponding eigenvectors

6. Conclusion

- Investigated inexact solvers for symmetric stochastic eigenvalue problems
  - Inexact stochastic inverse subspace iteration (SISI) with PCG
  - Inexact Newton iteration (NI) with GMRES
- Proposed novel preconditioners for efficient computations
  - Hierarchical Gauss-Seidel preconditioner (hGS) for SISI
  - Constraint mean-based (cMB) preconditioner for NI
  - Constraint hierarchical Gauss-Seidel preconditioner for NI
- Demonstrated effectiveness of the preconditions with results of numerical experiments
- Future work:
  - Nonsymmetric stochastic eigenvalue problem
  - Stability analysis of dynamical systems