Sparse Operator Compression of Elliptic Operators with Multiscale Coefficients

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Big Data Meets Computation, IPAM
Motivations

Dimension reduction appears nearly everywhere in science and engineering.

- Solving elliptic equations with multiscale coefficients: multiscale finite element basis for the elliptic operator.
- Principal component analysis (PCA): principle modes of the covariance operator.
- Quantum chemistry: eigen states of the Hamiltonian.

For computational efficiency and/or good interpretability, localized basis functions are preferred.

- Sparse principle modes obtained by Sparse PCA or sparse dictionary learning: Zou-Hastie-Tibshirani-04, Witten-Tibshirani-Hastie-09, etc.
- Compressed Wannier modes: Ozoliņš-Lai-Caflisch-Osher-13, E-Li-Lu-10, Lai-Lu-Osher-15, etc.
Consider an elliptic operator in the divergence form

\[ L u = \sum_{0 \leq |\sigma|, |\gamma| \leq k} (-1)^{|\sigma|} D^\sigma (a_{\sigma\gamma}(x) D^\gamma u), \tag{1} \]

where the coefficients \( a_{\sigma\gamma} \in L^\infty(D) \), \( D \) is a bounded domain in \( \mathbb{R}^d \), \( \sigma = (\sigma_1, \ldots, \sigma_d) \) is a \( d \)-dimensional multi-index.

- \( L \) is self-adjoint and positive definite in a Hilbert space \( H^k_B(D) \).
- \( H^k_B(D) \subset H^k(D) \) incorporates the boundary condition for the elliptic operator.

- For any \( f \in L^2(D) \), \( Lu = f \) has a unique weak solution in \( H^k_B(D) \), denoted as \( u := L^{-1} f \).

- Given \( n \) basis functions \( \Psi = [\psi_1, \ldots, \psi_n] \subset H^k_B(D) \), we define the operator compression error:

\[ E_{oc}(\Psi; L^{-1}) := \min_{K_n \in \mathbb{R}^{n \times n}, K_n \succeq 0} \| L^{-1} - \Psi K_n \Psi^T \|_2, \tag{2} \]

which is the optimal approximation error of \( L^{-1} \) among all positive semidefinite operators with range space spanned by \( \Psi \).
Main results of sparse operator compression

Definition

Given $n$ basis functions $Ψ = [ψ_1, \ldots, ψ_n] \subset H_B^k(D)$, we define the operator compression error:

$$E_{oc}(Ψ; L^{-1}) := \min_{K_n ∈ \mathbb{R}^{n×n}, K_n ≥ 0} ∥L^{-1} − Ψ K_n Ψ^T∥_2,$$

which is the optimal approximation error of $L^{-1}$ among all positive semidefinite operators with range space spanned by $Ψ$.

For any $n ∈ \mathbb{N}$, we construct $n$ localized basis functions $\{ψ_{i}^{loc}\}_{i=1}^n$ such that

1. $|\text{supp}(ψ_{i}^{loc})| ≤ \frac{C_l \log(n)}{n}$, $∀1 ≤ i ≤ n.$ \hspace{1cm} (3)

2. $E_{oc}(Ψ_{loc}; L^{-1}) ≤ C_e λ_n(L^{-1})$, \hspace{1cm} (4)

The constants $C_l$ and $C_e$ are independent of $n$ and multiscale features in $a_{σγ}$. 
Potential Applications I. Solving elliptic equations.

\( \mathcal{L} \) is an elliptic operator of order \( 2k \) \((k \geq 1)\) with rough multiscale coefficients in \( L^\infty(D) \), and the load \( f \in L^2(D) \).

\[
\mathcal{L} u = f, \quad u \in H^k_0(D).
\] (5)

- \( k = 1 \): heat equation, subsurface flow; \( k = 2 \): beam equation, plate equation, etc...
- We construct nearly optimally localized basis functions \( \{\psi_{i}^{loc}\}_{i=1}^{n} \subset H^k_0(D) \). For a given mesh \( h \), we have
  \[
  \left| \text{supp}(\psi_{i}^{loc}) \right| \leq C_l h \log(1/h) \quad 1 \leq i \leq n.
  \]
- The multiscale finite element solution \( u_{ms} := \Psi^{loc} L^{-1}_n (\Psi^{loc})^T f \) satisfies
  \[
  \|u - u_{ms}\|_H \leq C_e h^k \|f\|_2 \quad \forall f \in L^2(D),
  \]
  where \( \| \cdot \|_H \) is the energy norm, \( C_e \) is indep. of small scale of \( a_{\sigma\gamma} \).
- Sparsity/locality: computational efficiency.
The Matérn class covariance in spatial statistics

\[
K_\nu(x, y) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \sqrt{2\nu} \frac{|x - y|}{\rho} \right)^\nu K_\nu \left( \sqrt{2\nu} \frac{|x - y|}{\rho} \right)
\] (6)

- \( \nu = 1/2: \ K_{1/2}(x, y) = \sigma^2 \exp(-|x - y|/\rho) \)
- \( \nu \to \infty: \ \lim_{\nu \to \infty} K_\nu(x, y) = \sigma^2 \exp \left( -\frac{|x-y|^2}{2\rho^2} \right) \).

\[\text{Figure: Left: samples of human faces. Right: sparse principal modes.} \]

\[\text{\[Wang-Jia-Hu-Turk, IJPRAI, 2005}\]
The Matérn class covariance

\[ K_\nu(x, y) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \sqrt{2\nu} \frac{|x - y|}{\rho} \right)^\nu K_\nu \left( \sqrt{2\nu} \frac{|x - y|}{\rho} \right), \]

- It is the solution operator of high-order elliptic operators

\[ \mathcal{L} = C_{\nu, \lambda} \sigma^2 \left( \frac{2\nu}{\lambda^2} - \Delta \right)^{\nu + d/2}. \]

- We construct nearly optimally localized basis functions \( \{\psi_{i}^{loc}\}_{i=1}^{n} \):

\[ |\text{supp}(\psi_{i}^{loc})| \leq \frac{C_{l} \log(n)}{n} \quad 1 \leq i \leq n. \]

- We can approximate \( K_\nu \) by rank-\( n \) operator with optimal accuracy:

\[ \left\| K_\nu - \Psi^{loc} K_n \left( \Psi^{loc} \right)^T \right\|_2 \leq C_e \lambda_n(K_\nu). \]

- Sparsity/locality: better interpretability and computational efficiency.
Maximally-localized generalized Wannier functions for composite energy bands

Nicola Marzari and David Vanderbilt

Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08855-0849, USA
(July 10, 1997)

We discuss a method for determining the optimally-localized set of generalized Wannier functions associated with a set of Bloch bands in a crystalline solid. By “generalized Wannier functions” we mean a set of localized orthonormal orbitals spanning the same space as the specified set of Bloch bands. Although we minimize a functional that represents the total spread \( \sum_n \langle r^2 \rangle^2_n \) of the Wannier functions in real space, our method proceeds directly from the Bloch functions as represented on a mesh of k-points, and carries out the minimization in a space of unitary matrices \( U_{\text{MN}} \) describing the rotation among the Bloch bands at each k-point. The method is thus suitable for use in connection with conventional electronic-structure codes. The procedure also returns the total electric polarization as well as the location of each Wannier center. Sample results for Si, GaAs, molecular C\(_2\)H\(_4\) and LiCl will be presented.

\[
i\hbar \partial_t u(t, x) = \left( -\frac{\hbar^2}{2} \Delta_x + V(x) \right) u \quad \Rightarrow \quad \begin{cases} \mathcal{L} e_m = \lambda_m e_m \\ u(x, t) = \sum \alpha_m(t) e_m(x) \end{cases}
\]

Hamiltonian: \( \mathcal{L} \)

Sparsity/locality: better interpretability and computational efficiency.

\(^2\)Marzari-Vanderbilt, PRB (56), 97
We construct nearly optimally localized basis functions \( \{ \psi_i^{loc} \}_{i=1}^n \) that optimally approximates the eigenspace in the sense of

\[
E_{oc}(\Psi^{loc}; L^{-1}) := \min_{K_n \in \mathbb{R}^{n \times n}, K_n \succeq 0} \| L^{-1} - \psi^{loc} K_n (\psi^{loc})^T \|_2 \leq C e \lambda_n(L^{-1}),
\]

Another natural choice to define the compression error:

\[
\tilde{E}_{oc}(\Psi) = \| P_{V_n} - P_{\Psi} \|_2 = \left\| \sum_{i=1}^n e_i e_i^T - P_{\Psi} \right\|_2,
\]

where \( V_n \) is the first \( n \)-dimensional eigenspace span\( \{ e_1, \ldots, e_n \} \) and \( P_V \) is the orthogonal projection from \( L^2(D) \) to its subspace \( V \).

\[
E_{oc}(\Psi; L^{-1}) = \min_{K_n \in \mathbb{R}^{n \times n}, K_n \succeq 0} \left\| \sum_{i=1}^\infty \frac{1}{\lambda_i} e_i e_i^T - \psi K_n \psi^T \right\|_2.
\]

We believe that \( E_{oc}(\Psi; L^{-1}) \) is a better criterion for operator compression because it takes into consideration the decay of the eigenvalues of the solution operator \( L^{-1} \).
Our construction and theoretical results

**Figure:** Left: 8 localized basis functions for $-\Delta$ with periodic BC. Middle and right: 2 localized basis functions for $\Delta^2$ with homogeneous Dirichlet BC.
Our construction of \( \{ \psi_{i,loc}^{n} \}_{i=1}^{n} \)

1. Choose \( h > 0 \). Partition the physical domain \( D \) using a regular partition \( \{ \tau_i \}_{i=1}^{m} \) with mesh size \( h \).

2. Choose \( r > 0 \), say \( r = 2h \log(1/h) \). For each patch \( \tau_i \), \( S_r \) is the union of the subdomains \( \tau_{i'} \) intersecting \( B(x_i, r) \) (for some \( x_i \in \tau_i \)).

3. \( P_{k-1}(\tau_i) \) is the space of all \( d \)-variate polynomials of degree at most \( k - 1 \) on the patch \( \tau_i \). \( Q = \binom{k+d-1}{d} \) is its dimension.

\( \{ \varphi_{i,q} \}_{q=1}^{Q} \) is a set of orthogonal basis functions for \( P_{k-1}(\tau_i) \).

\[
\psi_{i,q}^{loc} = \arg \min_{\psi \in H^{k}_B} \| \psi \|^{2}_{H} \\
\text{s.t. } \int_{S_r} \psi \varphi_{j,q'} = \delta_{i,q,j,q'}, \quad \forall 1 \leq j \leq m, 1 \leq q' \leq Q, \\
\psi(x) \equiv 0, \quad x \in D \setminus S_r,
\]

where \( H^{k}_B \) is the solution space (with some prescribed BC), \( \| \cdot \|_{H} \) is the energy norm associated with \( \mathcal{L} \) and the BC.

**Figure:** A regular partition, local patch \( \tau_i \) and its associated \( S_r \).
Our construction \( \Psi^{\text{loc}} := \{\psi^{\text{loc}}_{i,q}\}_{i=1,q=1}^{m,Q} \)

**Theorem (Hou-Zhang-2016)**

Suppose \( H^k_B = H^k_0(D) \) and \( \mathcal{L}u = (-1)^k \sum_{|\sigma|=|\gamma|=k} D^\sigma (a_{\sigma \gamma} D^\gamma u) \). Assume that \( \mathcal{L} \) is self-adjoint, positive definite and strongly elliptic, and that there exists \( \theta_{\text{min}}, \theta_{\text{max}} > 0 \) such that

\[
\theta_{\text{min}} \| \xi \|^2_k \leq \sum_{|\sigma|=|\gamma|=k} a_{\sigma \gamma} \xi^\sigma \xi^\gamma \leq \theta_{\text{max}} \| \xi \|^2_k, \quad \forall \xi \in \mathbb{R}^d.
\]

Then for \( r \geq C_r h \log(1/h) \), we have

1. \[
\| \mathcal{L}^{-1} f - \Psi^{\text{loc}} L_n^{-1} (\Psi^{\text{loc}})^T f \|_H \leq \frac{C_e h^k}{\sqrt{\theta_{\text{min}}}} \| f \|_2 \quad \forall f \in L^2(D), \quad (7)
\]

   where \( L_n \) is the stiffness matrix under basis functions \( \Psi^{\text{loc}} \).

2. \[
E_{\text{oc}}(\Psi^{\text{loc}}; \mathcal{L}^{-1}) \leq \frac{C_e^2 h^{2k}}{\theta_{\text{min}}}. \quad (8)
\]

Here, the constant \( C_r \) only depends on the contrast \( \frac{\theta_{\text{max}}}{\theta_{\text{min}}} \), and \( C_e \) is independent of the coefficients.
Several remarks

- Theorem (Hou-Zhang-2016) also applies to $\mathcal{L}$ with low order terms, i.e. $\mathcal{L}u = (-1)^k \sum_{|\sigma|,|\gamma| \leq k} D^{\sigma} (a_{\sigma\gamma} D^{\gamma} u)$.

- Theorem (Hou-Zhang-2016) also applies to other homogeneous boundary conditions, like periodic BC, Robin BC and mixed BC.

- For $H_B^k = H^1_0(D)$, i.e. second order elliptic operators with zero Dirichlet BC, Theorem (Hou-Zhang-2016) have been proved in Owhadi-2015. A similar result for $H_B^k = H^1_0(D)$ was also provided in Målqvist-Peterseim-2014. In this case, Our proof improves the estimates of the constants $C_r$ and $C_e$.

- For other BCs, operators with lower order terms, and high-order elliptic operators, new techniques and concepts have been developed. Among them, the most important three new techniques are
  - a projection-type polynomial approximation property in $H^k(D)$,
  - the notion of the strong ellipticity $^3$,
  - an inverse energy estimate for functions in $\Psi := \text{span}\{\psi_{i,q} : 1 \leq i \leq m, 1 \leq q \leq Q\}$.

$^3$Equivalent to uniform ellipticity when $d = 1, 2$ or $k = 1$. Slightly stronger than uniform ellipticity in other cases; counter examples exist but difficult to construct.
Theorem (An error estimate based on projection-type approximation)

Suppose there is a $n$-dimensional subspace $\Phi \subset L^2(D)$ with basis $\{\varphi_i\}_{i=1}^n$ such that

$$\|u - P_{\Phi}^{(L^2)} u\|_{L^2} \leq k_n \|u\|_H \quad \forall u \in H^k(D).$$

(9)

Let $\Psi$ be the $n$-dimensional subspace in $H^k(D)$ (also in $H^k_{\mathcal{B}}(D)$) spanned by $\{\mathcal{L}^{-1} \varphi_i\}_{i=1}^n$. Then

1. For any $f \in L^2(D)$ and $u = \mathcal{L}^{-1} f$, we have

$$\|u - P_{\Psi}^{(H^k_{\mathcal{B}})} u\|_H \leq k_n \|f\|_{L^2}.$$  

(10)

2. We have

$$E_{oc}(\Psi; \mathcal{L}^{-1}) \leq k_n^2.$$  

(11)

- $k = 1$: $\Phi$ piecewise constant functions. By the Poincare inequality, it is easy to obtain $\|u - P_{\Phi}^{(L^2)} u\|_{L^2} \leq \frac{C_p h}{\sqrt{\theta_{min}}} \|u\|_H$.

- $k \geq 2$: $\Phi$ piecewise polynomials with degree no more than $k - 1$. By a projection-type polynomial approximation property in $H^k(D)$, see Thm 3.1 in Hou-Zhang-PartII, we have $\|u - P_{\Phi}^{(L^2)} u\|_{L^2} \leq \frac{C_p h^k}{\sqrt{\theta_{min}}} \|u\|_H$. 

Roadmap of the proof: Error estimate, discussions

Take $H^k_B = H^1_0(D)$ as an example, where $\Phi$ is the space of piecewise constant functions.

- Based on a projection-type approximation property, we obtain the error estimates of the GFEM in the energy norm, i.e.

$$\|u - P^{(L^2)}_{\Phi} u\|_{L^2} \leq C_{proj} h \|u\|_H \Rightarrow \|u - P^{(H^1_0)}_{\Psi} u\|_H \leq C_{proj} h \|f\|_{L^2}.$$  

$C_{proj}$ does not depend on the small scales in the coefficients.

- Traditional interpolation-type estimation requires higher regularity of the solution $u$: assume $u \in H^2(D)$

$$|u - I_h u|_{1,2,D} \leq C h |u|_{2,2,D} \Rightarrow \|u - I_h u\|_H \leq C_{interp} h \|f\|_{L^2}.$$  

$C_{interp}$ depends on the small scales in the coefficients.

- Basis functions for $I_h u$: optimally localized linear nodal basis

- Basis functions for $P^{(H^1_0)}_{\Psi} u$: global basis functions $\{\mathcal{L}^{-1} \varphi_i\}_{i=1}^n$
Roadmap of the proof: Basis with exponential decay

Global energy minimizing basis functions

\[
\psi_{i,q} = \arg \min_{\psi \in H^k_{\mathcal{B}}} \|\psi\|^2_H \\
\text{s.t.} \int_D \psi_{i,q} \varphi_{j,q'} = \delta_{ij,qq'}, \forall 1 \leq q' \leq Q, 1 \leq j \leq m.
\]

(12)

Theorem (Energy minimizing basis functions with exponential decay)

- \{\psi_{i,q} : 1 \leq i \leq m, 1 \leq q \leq Q\} and \{\mathcal{L}^{-1}\varphi_{i,q} : 1 \leq i \leq m, 1 \leq q \leq Q\} span the same space \(\Psi\).
- \(\psi_{i,q}\) decays exponentially fast away from its associated patch \(\tau_i\).
Roadmap of the proof: Basis with exponential decay

Global energy minimizing basis functions

\[
\psi_{i,q} = \arg\min_{\psi \in H^k_B} \|\psi\|^2_H \\
\text{s.t. } \int_D \psi_{i,q} \varphi_{j,q'} = \delta_{i_q,j_q'}, \forall 1 \leq q' \leq Q, 1 \leq j \leq m.
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(12)

Theorem (Energy minimizing basis functions with exponential decay)

- \{\psi_{i,q} : 1 \leq i \leq m, 1 \leq q \leq Q\} and \{\mathcal{L}^{-1}\varphi_{i,q} : 1 \leq i \leq m, 1 \leq q \leq Q\} span the same space \(\Psi\).
- \psi_{i,q} decays exponentially fast away from its associated patch \(\tau_i\).

Intuition: We apply a linear transform to \{\mathcal{L}^{-1}\varphi_{i,q} : 1 \leq i \leq m, 1 \leq q \leq Q\} such that the new basis function \(\psi_{i,q}\) has zero moments up to the \((k - 1)\)-th order on any patch other than \(\tau_i\).
Roadmap of the proof: Basis with exponential decay

\[ \psi_{i,q} = \arg \min_{\psi \in H^k_B} \| \psi \|_H^2 \]

s.t. \[ \int_D \psi_{i,q} \varphi_{j,q'} = \delta_{i q, j q'}, \forall 1 \leq q' \leq Q, 1 \leq j \leq m. \]

1D second order elliptic operator with Robin BC:

\[ \mathcal{L}u = -\frac{1}{2}u'' + \frac{1}{2}u, \]

\[ u(0) - u'(0) = 0, \quad u(1) + u'(1) = 0, \]

1D Matérn covariance with \( \nu = 1/2 \):

\[ K_{1/2}(x, y) = \exp(-|x - y|), \]

\[ \mathcal{L}^{-1} f = \int_0^1 K_{1/2}(x, y) f(y) dy. \]
Roadmap of the proof: Basis with exponential decay

\[ \psi_{i,q} = \arg \min_{\psi \in H^k_B} \| \psi \|_H^2 \]

\[ \text{s.t. } \int_D \psi_{i,q} \varphi_{j,q'} = \delta_{i,q,j,q'}, \forall 1 \leq q' \leq Q, 1 \leq j \leq m. \]

1D second order elliptic operator with Robin BC:

\[ L u = -\frac{1}{2} u'' + \frac{1}{2} u, \]
\[ u(0) - u'(0) = 0, \ u(1) + u'(1) = 0, \]

\[ H^k_B = H^1([0, 1]), \quad \| u \|_H^2 = \frac{1}{2} \left( u(0)^2 + u(1)^2 + \int_0^1 (u')^2 + \int_0^1 u^2 \right). \]

1D Matérn covariance with \( \nu = 1/2 \):

\[ K_{1/2}(x, y) = \exp(-|x - y|), \]
\[ L^{-1} f = \int_0^1 K_{1/2}(x, y) f(y) dy. \]

Figure: The basis function associated with patch \([1/2 - h, 1/2], \ h = 1/64.\)
Localized energy minimizing basis functions

\[ \psi_{i,q}^{loc} = \arg \min_{\psi \in H^k_{\mathcal{B}}} \| \psi \|_H^2 \]

s.t. \[ \int_{S_r} \psi \varphi_{j,q'} = \delta_{iq,jq'}, \quad \forall 1 \leq j \leq m, 1 \leq q' \leq Q, \]
Roadmap of the proof: Localized basis

- **Localized** energy minimizing basis functions

\[
\psi_{i,q}^{\text{loc}} = \arg \min_{\psi \in H^k_B} \|\psi\|_H^2
\]

\[
\text{s.t. } \int_{S_r} \psi \varphi_{j,q'} = \delta_{iq,jq'}, \quad \forall 1 \leq j \leq m, 1 \leq q' \leq Q,
\]

\[
\psi(x) \equiv 0, \quad x \in D \setminus S_r.
\]
Roadmap of the proof: Localized basis

- **Localized** energy minimizing basis functions

\[
\psi_{i,q}^{loc} = \arg \min_{\psi \in H^k_B} \|\psi\|_H^2
\]

s.t. \[
\int_{S_r} \psi \varphi_{j,q'} \, d\nu = \delta_{iq,jq'}, \quad \forall 1 \leq j \leq m, 1 \leq q' \leq Q,
\]

\[
\psi(x) \equiv 0, \quad x \in D \setminus S_r.
\]

- Because \(\psi_{i,q}\) decays exponentially fast away from patch \(\tau_i\),

\[
r = O(h \log(1/h))
\]

is sufficient to preserve the good error estimate of \(\Psi\):

\[
\|u - P_{\Psi}^{(H^k_B)} u\|_H \leq \frac{C_p h^k}{\sqrt{\theta_{\min}}} \|f\|_{L_2} \Rightarrow \|u - P_{\Psi_{loc}}^{(H^k_B)} u\|_H \leq \frac{2C_p h^k}{\sqrt{\theta_{\min}}} \|f\|_{L_2}.
\]
Roadmap of the proof: Localized basis

- **Localized** energy minimizing basis functions

\[
\psi_{i,q}^{\text{loc}} = \arg \min_{\psi \in H^k_B} \|\psi\|_H^2
\]

s.t. \[\int_{S_r} \psi \varphi_{j,q'} = \delta_{iq,jq'}, \quad \forall 1 \leq j \leq m, 1 \leq q' \leq Q, \]

\[\psi(x) \equiv 0, \quad x \in D \setminus S_r.\]

- Because \(\psi_{i,q}\) decays exponentially fast away from patch \(\tau_i, r = \mathcal{O}(h \log(1/h))\) is sufficient to preserve the good error estimate of \(\Psi\):

\[
\|u - P^{(H^k_B)}_\Psi u\|_H \leq \frac{C_p h^k}{\sqrt{\theta_{\text{min}}}} \|f\|_{L^2} \Rightarrow \|u - P^{(H^k_B)}_{\Psi^{\text{loc}}} u\|_H \leq \frac{2C_p h^k}{\sqrt{\theta_{\text{min}}}} \|f\|_{L^2}.
\]

- With the Aubin-Nitsche duality argument, we have proved

\[
E_{oc}(\Psi^{\text{loc}}; \mathcal{L}^{-1}) \leq \frac{4C_p^2 h^{2k}}{\theta_{\text{min}}}. \]
Roadmap of the proof: Localized basis

\[ \mathcal{L}u = -\frac{1}{2}u''(x) + \frac{1}{2}u, \quad u(0) - u'(0) = 0, \quad u(1) + u'(1) = 0. \]

**Figure:** A few basis functions for the case \( m = 2^7 \) and \( r = 2.4h \log_2(1/h) \).

**Figure:** \( E(\Psi^{loc}; \mathcal{L}^{-1}) \) with localized basis functions \( \Psi^{loc} \).
Compare with the $l^1$-minimization approach

**Sparse Operator Compression**

\[
\min_{\psi \in H^k_B} \|\psi\|_H^2 \\
\text{s.t.} \quad \int_{S_r} \psi \varphi_{j,q'} = \delta_{i_q,j_q'}, \forall j,q' \\
\psi(x) \equiv 0, \quad x \in D \setminus S_r,
\]

Sparsity/locality from moment condition and exponential decay

**$l^1$ minimization**

\[
\min_{\psi \subset H^k_B} \sum_{i=1}^n \|\psi_i\|_H^2 + \mu \sum_{i=1}^n \|\psi_i\|_1, \\
\text{s.t.} \quad \int_D \psi_i \psi_j = \delta_{i,j} \forall 1 \leq i,j \leq n.
\]

Sparsity/locality from the $l^1$ penalty

See e.g. [Ozoliņš-Lai-Caflisch-Osher, PNAS, 2013].
Sparse OC vs $l^1$ minimization: math formulation

Sparse Operator Compression

$$\begin{array}{l}
\min_{\psi \in H^k_B} \quad \|\psi\|_H^2 \\
\text{s.t.} \quad \int_{S_r} \psi \varphi_j, q' = \delta_{iq,jq'}, \forall j, q' \\
\psi(x) \equiv 0, \quad x \in D \setminus S_r,
\end{array}$$

$l^1$ minimization

$$\begin{array}{l}
\min_{\psi \subset H^k_B} \quad \sum_{i=1}^{n} \|\psi_i\|_H^2 + \mu \sum_{i=1}^{n} \|\psi_i\|_1, \\
\text{s.t.} \quad \int_D \psi_i \psi_j = \delta_{i,j} \quad \forall 1 \leq i, j \leq n.
\end{array}$$

- Linear constraints, convex quadratic optimization v.s. orthogonality constraints, non-convex optimization
- Decoupled, parallel implementation v.s. coupled, not easy for parallel computing
- The computational complexity to obtain all $n$ localized basis functions $\{\psi_{i}^{loc}\}_{i=1}^{n}$ is only of order $N \log(N)$, where $N$ is the degree of freedom in the discretization of $\mathcal{L}$.
- The SOC algorithm \(^4\) solves the $l^1$ minimization in an iterative manner, where the computational cost of each iteration is comparable with the total cost of the Sparse OC.

\(^4\) Lai-Osher, SIAM-JSC, 2014
Sparse OC vs $l^1$ minimization: 1D free electron

Free electron with periodic boundary condition:

$$\mathcal{L} = -\frac{1}{2}\Delta, \quad D = [0, 50].$$

- Discretization $\mathcal{L} \in \mathbb{R}^{1024 \times 1024}$.
- Number of compressed/localized modes $n = 128$.
- Sparse OC takes 0.035 sec to obtain all 128 localized modes, without parallel computing.
- After 390 iterations, the $l^1$ approach achieves 1e-7 relative energy decrease, and the iteration is stopped. The total time is 4.426 secs. Each iteration takes 0.013 sec.

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5Lai-Osher, SIAM-JSC, 2014
Sparse OC vs $l^1$ minimization: 1D free electron

Localized/compressed modes

Figure: A few basis functions for the case $m = 2^7$ and $r = h \log_2(1/h)$.

Figure: A few compressed modes, $m = 2^7$, $\mu = 0.84$
Sparse OC vs $l^1$ minimization: 1D free electron

Approximate eigenvalues

Figure: The eigenvalues of $Q^T H Q$ and $H$; $Q$ is an orthonormal basis of $\Psi^{loc}$.

Figure: The eigenvalues of $\Psi^T H \Psi$, $m = 2^7$, $\mu = 10$
Sparse OC vs $l^1$ minimization: 1D free electron

**Figure:** The operator compression error $E(\Psi; (\mathcal{L} + 1)^{-1})$ for the Hamiltonian with localized basis functions $\Psi^{loc}$.
Figure: The operator compression error \( E(\Psi; (\mathcal{L} + 1)^{-1}) \) for the Hamiltonian with localized basis functions \( \Psi^{\text{loc}} \).

Other related work

- E-Li-Lu, PNAS, 2010: localization using weight function (algebraical decay)
- Lai-Lu-Osher, CMS, 2015: convex relaxation of the \( l^1 \) approach
- Hou-Li-Zhang, SIAM-MMS, 2016: ISMD for low rank covariance matrices
Fourth order elliptic operators
The 1D biharmonic equation

\[
\frac{d^2}{dx^2} \left( a(x) \frac{d^2 u}{dx^2} \right) = f(x), \quad 0 < x < 1, \\
\]

\[u(0) = u'(0) = 0, \quad u(1) = u'(1) = 0,\]  \hspace{1cm} (13)

**Figure:** Highly oscillatory flexural rigidity \(a(x)\) and load \(f(x)\): no scale separation.
The 1D biharmonic equation: basis functions

(a) Left: $\varphi_{32,1}, \varphi_{32,2}$ for piecewise linear $\Phi$; Right: $\mathcal{L}^{-1}\varphi_{32,1}, \mathcal{L}^{-1}\varphi_{32,2}$

(b) $\psi_{32,1}, \psi_{32,2}$: normal scale and log-scale

Figure: 1D biharmonic operator: piecewise linear $\Phi$. There are two basis functions associated with each patch. The multiscale effect is visible in the basis functions, but the decay rate only depends on the contrast $\frac{a_{\text{max}}}{a_{\text{min}}}$. 
• \( \Phi_0 \) space of piecewise constant functions \( \Rightarrow \Psi_0 \Rightarrow \Psi_0^{loc} \Rightarrow u_{0,h} \)
• \( \Phi_0 \) space of piecewise linear functions \( \Rightarrow \Psi_1 \Rightarrow \Psi_1^{loc} \Rightarrow u_{1,h} \)

**Figure:** Error of the finite element solutions: \( \|u_{h,0} - u\|_H \) and \( \|u_{h,1} - u\|_H \).
The 1D biharmonic equation: finite element solutions

- \( \Phi_0 \) space of piecewise constant functions \( \Rightarrow \Psi_0 \Rightarrow \Psi_0^{loc} \Rightarrow u_{0,h} \)
- \( \Phi_0 \) space of piecewise linear functions \( \Rightarrow \Psi_1 \Rightarrow \Psi_1^{loc} \Rightarrow u_{1,h} \)

**Figure:** Error of the finite element solutions: \( \|u_{h,0} - u\|_H \) and \( \|u_{h,1} - u\|_H \).

To obtain the optimal convergence rate \( h^k \), it is necessary to take \( \Phi \) as the space of piecewise polynomial space of degree no more than \( k - 1 \).
The 2D biharmonic operator

\[ \mathcal{L} = \Delta^2, \quad H^2_B = H^2_0([0, 1]^2) \]  

(14)

Figure: The three basis functions associated with patch 
\([1/2 - h_x, 1/2] \times [1/2 - h_y, 1/2]\). They clearly show exponential decay.
Ongoing work and conclusions
Discrete setting: graph Laplacians

\[ \mathcal{L}u = -\frac{d}{dx} \left( a(x) \frac{du}{dx} \right), \]
\[ u(0) = u(1). \]

\[ \mathcal{L}u = -\nabla \cdot (a(x) \nabla u), \]
\[ u|_{\partial D} = 0. \]

\[ \mathcal{L}u = f \]
\[ \mathcal{L} : a \text{ graph Laplacian} \]

Figure: A 1D circular graph.
Figure: A 2D lattice graph.
Figure: A social network graph.

- Social networks and transportation networks; genetic data and web pages; spectral clustering of images; electrical resistor circuits; elliptic partial differential equations discretized by finite elements; etc.

- Fundamental problems: fast algorithms for \( \mathcal{L}u = f \) and eigen decomposition of \( \mathcal{L} \).
Discrete setting: graph Laplacians

$$\mathcal{L}u = f$$

- Spielman-Teng (STOC-04, SICOMP-13, SIMAX-14): Nearly-Linear Time Algorithms for Graph Partitioning and Solving Linear Systems
  - Maximal spanning tree, support-graph preconditioners, graph sparsification, etc.
  - Theoretical results, impractical algorithms.


- Sparse operator compression for graph Laplacians? The key is an efficient algorithm to find a partition \( \{\tau_i\}_{i=1}^m \) of the graph vertices such that
  \[
  \|u - P^{(L^2)} \Phi u\|_{L^2} \leq C_p \sqrt{\lambda_n(\mathcal{L}^{-1})}\|u\|_H,
  \]
  which is the Poincare inequality on graphs.

- Implementing the sparse operator compression in a multigrid manner leads to a nearly-linear time algorithm.
Conclusions

- We have developed a general strategy to compress self-adjoint second-order and high-order elliptic operators by localized energy-minimizing basis functions.

- For a self-adjoint, bounded and strongly elliptic operator of order $2k$ ($k \geq 1$), we have proved that with support size $h \log(1/h)$, our localized basis functions can obtain the optimal operator compression rate $O(h^{2k})$.

- We have applied our new operator compression strategy in different applications: solving elliptic equations with multiscale coefficients, Sparse PCA for the Matérn class covariance, and compressing Hamiltonians in quantum chemistry.

- Ongoing work on compressing elliptic operators with high contrast coefficients, new multi-grid algorithms for elliptic operators, and fast algorithms for graph partitioning and solving graph Laplacians.