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.

- Localized multiscale finite element basis: Babuska-Caloz-Osbron-94, Hou-Wu-1997, Hughes-Feijóo-Mazzei-98, E-Engquist-03, Owhadi-Zhang-07, Målqvist-Peterseim-14, Owhadi-15, etc.
- 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.

Operator compression

Consider an elliptic operator in the divergence form

$$\mathcal{L}u = \sum_{0\le|\sigma|,|\gamma|\le k} (-1)^{|\sigma|} D^\sigma (a_{\sigma\gamma}(x) D^\gamma u), \tag{1}$$

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.

- $\mathcal{L}$ is self-adjoint and positive definite in a Hilbert space $H^k_{\mathcal{B}}(D)$. $H^k_{\mathcal{B}}(D) \subset H^k(D)$ incorporates the boundary condition for the elliptic operator.
- For any $f \in L^2(D)$, $\mathcal{L}u = f$ has a unique weak solution in $H^k_{\mathcal{B}}(D)$, denoted as $u := \mathcal{L}^{-1} f$.
- Given n basis functions $\Psi = [\psi_1, \ldots, \psi_n] \subset H^k_{\mathcal{B}}(D)$, we define the operator compression error:

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

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

Main results of sparse operator compression

Definition

Given n basis functions $\Psi = [\psi_1, \ldots, \psi_n] \subset H^k_{\mathcal{B}}(D)$, we define the operator compression error:

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

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

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

- $$\left|\mathrm{supp}(\psi_i^{loc})\right| \leq \frac{C_l \log(n)}{n}, \quad \forall 1 \leq i \leq n. \tag{3}$$
- $$E_{oc}(\Psi^{loc}; \mathcal{L}^{-1}) \leq C_e \lambda_n(\mathcal{L}^{-1}), \tag{4}$$
- The constants C_l and C_e are independent of n and multiscale features in $a_{\sigma\gamma}$.

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 $f \in L^2(D)$.

$$\mathcal{L}u = f, \qquad u \in H_0^k(D). \tag{5}$$

- $k = 1$: heat equation, subsurface flow; $k = 2$: beam equation, plate equation, etc...
- We construct nearly optimally localized basis functions $\{\psi_i^{loc}\}_{i=1}^n \subset H_0^k(D)$. 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 $u_{ms} := \Psi^{loc} L_n^{-1} \left(\Psi^{loc}\right)^T f$ 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.

Potential Applications II. Sparse PCA.

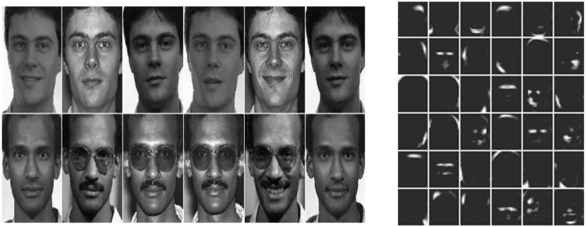


Figure: Left: samples of human faces. Right: sparse principal modes. [1]

The Matérn class covariance in spatial statistics

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

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

[1] Wang-Jia-Hu-Turk, IJPRAI, 2005

Potential Applications II. Sparse PCA continued.

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 $\{\psi_i^{loc}\}_{i=1}^n$:

$$\left|\mathsf{supp}(\psi_i^{loc})\right| \leq \frac{C_l \log(n)}{n} \quad 1 \leq i \leq n.$$

- We can approximate K_ν 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.

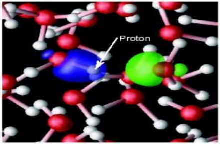
Potential Applications III. Quantum chemistry.

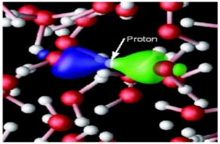
Maximally-localized generalized Wannier functions for composite energy bands

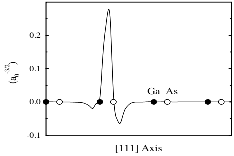
Nicola Marzari and David Vanderbilt
Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08855-0849, USA
(July 10, 1997)

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 $\sum_n \langle r^2\rangle_n - \langle \mathbf{r}\rangle_n^2$ 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 $U_{mn}^{(\mathbf{k})}$ 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_2H_4 and LiCl will be presented. [2]

$$\mathrm{i}\hbar\partial_t u(t,x) = \underbrace{\left(-\frac{\hbar^2}{2}\Delta_x + V(x)\right)}_{\text{Hamiltonian : } \mathcal{L}} u \quad \Rightarrow \quad \begin{cases} \mathcal{L}e_m = \lambda_m e_m \\ u(x,t) = \sum \alpha_m(t) e_m(x) \end{cases}$$







Sparsity/locality: better interpretability and computational efficiency.

[2] Marzari-Vanderbilt, PRB (56), 97

Potential Applications III. Quantum chemistry continued.

- We construct nearly optimally localized basis functions $\{\psi_i^{loc}\}_{i=1}^n$ that optimally approximates the eigenspace in the sense of

$$E_{oc}(\Psi^{loc};\mathcal{L}^{-1}) := \min_{\substack{K_n\in\mathbb{R}^{n\times n}\\ K_n\succeq 0}} \|\mathcal{L}^{-1} - \Psi^{loc}K_n\left(\Psi^{loc}\right)^T\|_2 \le C_e\lambda_n(\mathcal{L}^{-1}),$$

- Another natural choice to define the compression error:

$$\widetilde{E}_{oc}(\Psi) = \|\mathcal{P}_{V_n} - \mathcal{P}_\Psi\|_2 = \left\|\sum_{i=1}^n e_i e_i^T - \mathcal{P}_\Psi\right\|_2,$$

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

-

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

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

Our construction and theoretical results

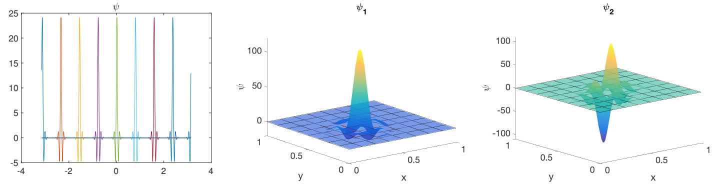


Figure: Left: 8 localized basis functions for $-\Delta$ with periodic BC. Middle and right: 2 localized basis functions for Δ^2 with homogeneous Dirichlet BC.

Our construction of $\{\psi_i^{loc}\}_{i=1}^n$

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 τ_i, S_r is the union of the subdomains $\tau_{i'}$ intersecting $B(x_i, r)$ (for some $x_i \in \tau_i$).
3. $\mathcal{P}_{k-1}(\tau_i)$ is the space of all d-variate polynomials of degree at most $k-1$ on the patch τ_i. $Q = \binom{k+d-1}{d}$ is its dimension. $\{\varphi_{i,q}\}_{q=1}^Q$ is a set of orthogonal basis functions for $\mathcal{P}_{k-1}(\tau_i)$.

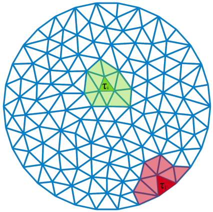


Figure: A regular partition, local patch τ_i and its associated S_r.

$$
\begin{aligned}
\psi_{i,q}^{loc} = \arg\min_{\psi \in H_{\mathcal{B}}^k} \quad & \|\psi\|_H^2 \\
\text{s.t.} \quad & \int_{S_r} \psi \varphi_{j,q'} = \delta_{iq,jq'}, \quad \forall 1 \le j \le m,\ 1 \le q' \le Q, \\
& \psi(x) \equiv 0, \quad x \in D \backslash S_r,
\end{aligned}
$$

where $H_{\mathcal{B}}^k$ is the solution space (with some prescribed BC), $\|\cdot\|_H$ is the energy norm associated with $\mathcal{L}$ and the BC.

Our construction $\Psi^{loc} := \{\psi_{i,q}^{loc}\}_{i=1,q=1}^{m,Q}$

Theorem (Hou-Zhang-2016)

Suppose $H_{\mathcal{B}}^k = H_0^k(D)$ *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* $\theta_{min}, \theta_{max} > 0$ *such that*

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

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

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

   where L_n *is the stiffness matrix under basis functions* Ψ^{loc}.

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

Here, the constant C_r *only depends on the contrast* $\frac{\theta_{max}}{\theta_{min}}$, *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. $\mathcal{L}u = (-1)^k \sum_{|\sigma|,|\gamma| \le k} D^\sigma(a_{\sigma\gamma} D^\gamma u)$.
- Theorem (Hou-Zhang-2016) also applies to other homogeneous boundary conditions, like periodic BC, Robin BC and mixed BC.
- For $H^k_{\mathcal{B}} = H^1_0(D)$, i.e. second order elliptic operators with zero Dirichlet BC, Theorem (Hou-Zhang-2016) have been proved in Owhadi-2015. A similar result for $H^k_{\mathcal{B}} = H^1_0(D)$ 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 $\Psi := \mathrm{span}\{\psi_{i,q} : 1 \le i \le m, 1 \le q \le Q\}$.

[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.

Roadmap of the proof: Error estimate

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

$$\|u - \mathcal{P}_{\Phi}^{(L^2)} u\|_{L^2} \leq k_n \|u\|_H \qquad \forall u \in H^k(D). \tag{9}$$

Let Ψ 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*

$$\|u - \mathcal{P}_{\Psi}^{(H^k_{\mathcal{B}})} u\|_H \leq k_n \|f\|_{L_2}\,. \tag{10}$$

2. *We have*

$$E_{oc}(\Psi; \mathcal{L}^{-1}) \leq k_n^2\,. \tag{11}$$

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

Roadmap of the proof: Error estimate, discussions

Take $H^k_{\mathcal{B}} = H^1_0(D)$ as an example, where Φ 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.

  $$\|u - \mathcal{P}_{\Phi}^{(L^2)} u\|_{L^2} \leq C_{proj} h \|u\|_H \Rightarrow \|u - \mathcal{P}_{\Psi}^{(H_0^1)} u\|_H \leq C_{proj} h \|f\|_{L_2}.$$

  C_{proj} does not depends on the small scales in the coefficients.
- Tranditional interpolation-type estimation requires higher regularity of the solution u: assume $u \in H^2(D)$

  $$|u - \mathcal{I}_h u|_{1,2,D} \leq C h |u|_{2,2,D} \Rightarrow \|u - \mathcal{I}_h u\|_H \leq C_{interp} h \|f\|_{L_2}.$$

  C_{interp} depends on the small scales in the coefficients.
- Basis functions for $\mathcal{I}_h u$: optimally localized linear nodal basis
  Basis functions for $\mathcal{P}_{\Psi}^{(H_0^1)} u$: global basis functions $\{\mathcal{L}^{-1}\varphi_i\}_{i=1}^n$

Roadmap of the proof: Basis with exponential decay

Global energy minimizing basis functions

$$\boxed{\begin{aligned} \psi_{i,q} = & \operatorname*{arg\,min}_{\psi \in H^k_{\mathcal{B}}} \quad \|\psi\|_H^2 \\ & \text{s.t.} \quad \int_D \psi_{i,q} \varphi_{j,q'} = \delta_{iq,jq'}, \forall 1 \le q' \le Q, 1 \le j \le m. \end{aligned}} \tag{12}$$

Theorem (Energy minimizing basis functions with exponential decay)

- $\{\psi_{i,q} : 1 \le i \le m, 1 \le q \le Q\}$ *and* $\{\mathcal{L}^{-1}\varphi_{i,q} : 1 \le i \le m, 1 \le q \le Q\}$ *span the same space* Ψ*.*
- $\psi_{i,q}$ *decays exponentially fast away from its associated patch* τ_i*.*

Roadmap of the proof: Basis with exponential decay

Global energy minimizing basis functions

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Intuition: We apply a linear transform to $\{\mathcal{L}^{-1}\varphi_{i,q} : 1 \le i \le m, 1 \le q \le Q\}$ such that the new basis function $\psi_{i,q}$ has zero moments up to the $(k-1)$-th order on any patch other than τ_i.

Roadmap of the proof: Basis with exponential decay

$$\boxed{\begin{aligned}\psi_{i,q} = &\mathop{\arg\min}_{\psi \in H^k_{\mathcal{B}}} \quad \|\psi\|_H^2 \\ &\text{s.t.} \quad \int_D \psi_{i,q}\varphi_{j,q'} = \delta_{iq,jq'}, \forall 1 \le q' \le Q, 1 \le j \le m.\end{aligned}}$$

1D second order elliptic operator with Robin BC:

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

1D Matérn covariance with $\nu = 1/2$:

$$K_{1/2}(x,y) = \exp(-|x-y|),$$
$$\mathcal{L}^{-1}f = \int_0^1 K_{1/2}(x,y)f(y)\mathrm{d}y.$$

Roadmap of the proof: Basis with exponential decay

$$\boxed{\begin{aligned} \psi_{i,q} &= \arg\min_{\psi \in H^k_{\mathcal{B}}} \quad \|\psi\|_H^2 \\ &\text{s.t.} \quad \int_D \psi_{i,q}\varphi_{j,q'} = \delta_{iq,jq'}, \forall 1 \le q' \le Q, 1 \le j \le m. \end{aligned}}$$

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

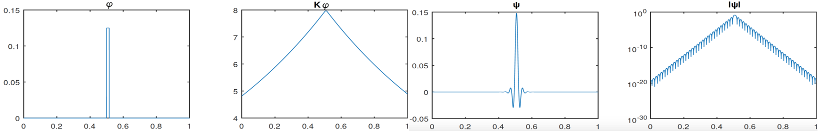

Figure: The basis function associated with patch $[1/2-h, 1/2]$, $h = 1/64$.

Roadmap of the proof: Localized basis

- Localized energy minimizing basis functions

$$\psi_{i,q}^{loc} = \underset{\psi \in H_{\mathcal{B}}^k}{\arg\min} \quad \|\psi\|_H^2$$

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

Roadmap of the proof: Localized basis

- Localized energy minimizing basis functions

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Roadmap of the proof: Localized basis

- Localized energy minimizing basis functions

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

$$\|u - \mathcal{P}_{\Psi}^{(H_{\mathcal{B}}^k)} u\|_H \le \frac{C_p h^k}{\sqrt{\theta_{min}}} \|f\|_{L_2} \Rightarrow \|u - \mathcal{P}_{\Psi^{loc}}^{(H_{\mathcal{B}}^k)} u\|_H \le \frac{2 C_p h^k}{\sqrt{\theta_{min}}} \|f\|_{L_2}.$$

Roadmap of the proof: Localized basis

- Localized energy minimizing basis functions

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

$$E_{oc}(\Psi^{loc}; \mathcal{L}^{-1}) \le \frac{4C_p^2 h^{2k}}{\theta_{min}}.$$

Roadmap of the proof: Localized basis

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

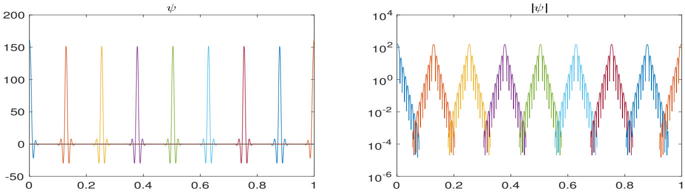


Figure: A few basis functions for the case $m = 2^7$ and $r = 2.4h\log_2(1/h)$.

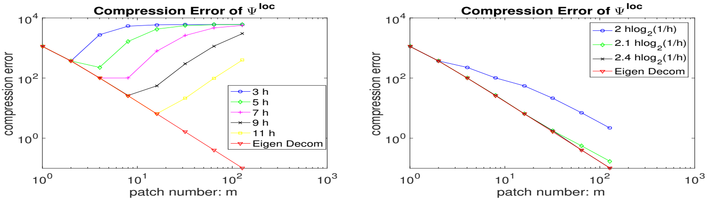


Figure: $E(\Psi^{loc}; \mathcal{L}^{-1})$ with localized basis functions Ψ^{loc}.

Compare with the l^1-minimization approach

Sparse Operator Compression

$$\boxed{\begin{aligned} \min_{\psi\in H^k_{\mathcal{B}}} \quad & \|\psi\|_H^2 \\ \text{s.t.} \quad & \int_{S_r} \psi\varphi_{j,q'} = \delta_{iq,jq'},\ \forall j, q' \\ & \psi(x) \equiv 0, \quad x \in D\backslash S_r, \end{aligned}}$$

Sparsity/locality from moment condition and exponential decay

l^1 minimization

$$\boxed{\begin{aligned} \min_{\Psi\subset H^k_{\mathcal{B}}} \quad & \sum_{i=1}^n \|\psi_i\|_H^2 + \mu \sum_{i=1}^n \|\psi_i\|_1, \\ \text{s.t.} \quad & \int_D \psi_i\psi_j = \delta_{i,j}\ \forall 1 \le i, j \le n. \end{aligned}}$$

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

$$\begin{aligned} \min_{\psi \in H^k_{\mathcal{B}}} \quad & \|\psi\|_H^2 \\ \text{s.t.} \quad & \int_{S_r} \psi \varphi_{j,q'} = \delta_{iq,jq'}, \ \forall j, q' \\ & \psi(x) \equiv 0, \quad x \in D \backslash S_r, \end{aligned}$$

l^1 minimization

$$\begin{aligned} \min_{\Psi \subset H^k_{\mathcal{B}}} \quad & \sum_{i=1}^n \|\psi_i\|_H^2 + \mu \sum_{i=1}^n \|\psi_i\|_1, \\ \text{s.t.} \quad & \int_D \psi_i \psi_j = \delta_{i,j} \ \forall 1 \le i, j \le n. \end{aligned}$$

- 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:

$$\mathcal{L} = -\frac{1}{2}\Delta, \quad D = [0, 50].$$ [5]

- Discretization $\mathcal{L} \in R^{1024\times 1024}$.
- 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.

[5] Lai-Osher, SIAM-JSC, 2014

Sparse OC vs l^1 minimization: 1D free electron

Localized/compressed modes

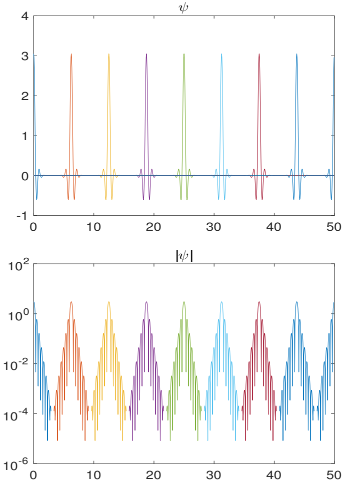


Figure: A few basis functions for the case $m = 2^7$ and $r = h\log_2(1/h)$.

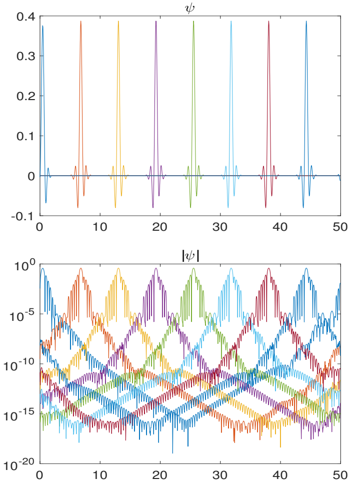


Figure: A few compressed modes, $m = 2^7, \mu = 0.84$

Sparse OC vs l^1 minimization: 1D free electron

Approximate eigenvalues

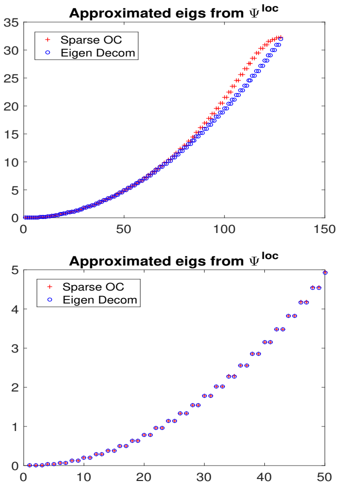


Figure: The eigenvalues of $Q^T H Q$ and H; Q is an orthonormal basis of Ψ^{loc}.

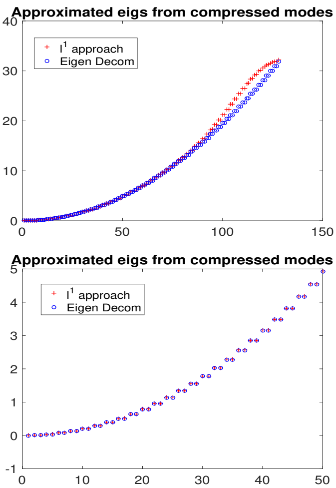


Figure: The eigenvalues of $\Psi^T H \Psi$, $m = 2^7, \mu = 10$

Sparse OC vs l^1 minimization: 1D free electron

Operator compression error

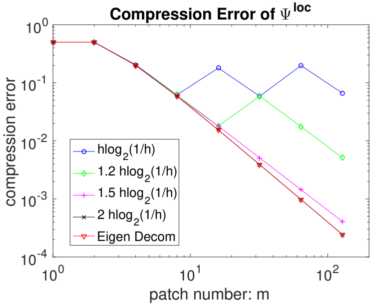


Figure: The operator compression error $E(\Psi;(\mathcal{L}+1)^{-1})$ for the Hamiltonian with localized basis functions Ψ^{loc}.

Sparse OC vs l^1 minimization: 1D free electron

Operator compression error

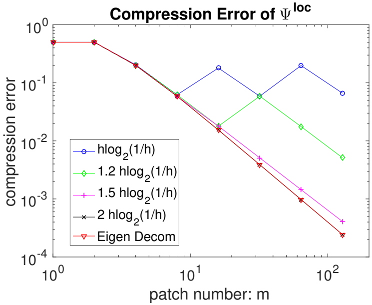


Figure: The operator compression error $E(\Psi; (\mathcal{L}+1)^{-1})$ for the Hamiltonian with localized basis functions Ψ^{loc}.

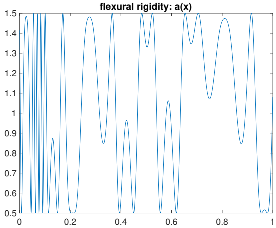
Other related work

- 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

$$\frac{d^2}{dx^2}\left(a(x)\frac{d^2u}{dx^2}\right) = f(x), \quad 0 < x < 1,$$
$$u(0) = u'(0) = 0, \quad u(1) = u'(1) = 0, \tag{13}$$



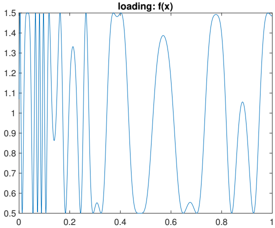
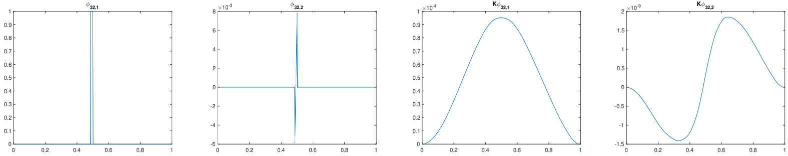
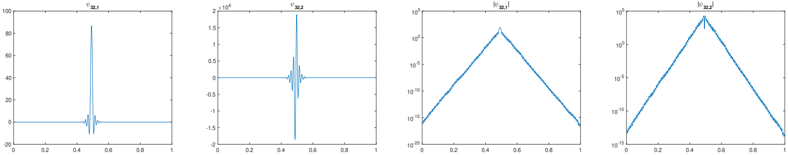


Figure: Highly oscillatory flexural rigidity $a(x)$ and load $f(x)$: no scale separation.

The 1D biharmonic equation: basis functions



(a) Left: $\varphi_{32,1}, \varphi_{32,2}$ for piecewise linear Φ; 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 Φ. 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 $\frac{a_{max}}{a_{min}}$.

The 1D biharmonic equation: finite element solutions

- Φ_0 space of piecewise constant functions $\Rightarrow \Psi_0 \Rightarrow \Psi_0^{loc} \Rightarrow u_{0,h}$
- Φ_0 space of piecewise linear functions $\Rightarrow \Psi_1 \Rightarrow \Psi_1^{loc} \Rightarrow u_{1,h}$

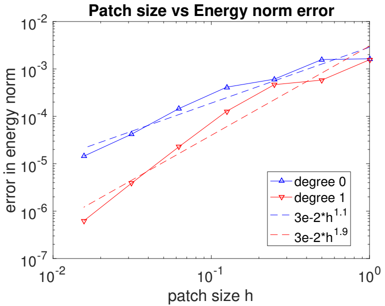


Figure: Error of the finite element solutions: $\|u_{h,0} - u\|_H$ and $\|u_{h,1} - u\|_H$.

The 1D biharmonic equation: finite element solutions

- Φ_0 space of piecewise constant functions $\Rightarrow \Psi_0 \Rightarrow \Psi_0^{loc} \Rightarrow u_{0,h}$
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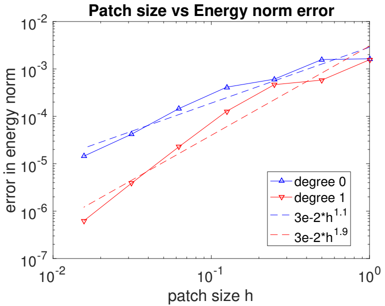

Figure: Error of the finite element solutions: $\|u_{h,0} - u\|_H$ and $\|u_{h,1} - u\|_H$.

To obtain the optimal convergence rate h^k, it is necessary to take Φ as the space of piecewise polynomial space of degree no more than $k-1$.

The 2D biharmonic operator

$$\mathcal{L} = \Delta^2, \quad H^2_{\mathcal{B}} = H^2_0([0,1]^2) \tag{14}$$

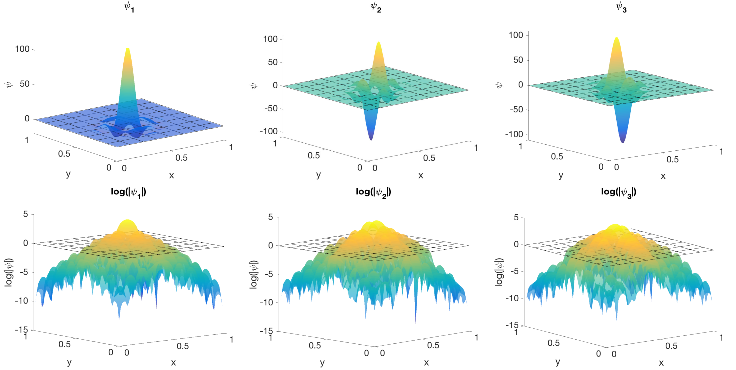

Figure: The three basis functions associated with patch $[1/2 - h_x, 1/2] \times [1/2 - h_y, 1/2]$. They clearly show exponential decay.

Ongoing work and conclusions

Discrete setting: graph Laplacians

$$\mathcal{L}u = -\frac{\mathrm{d}}{\mathrm{d}x}\left(a(x)\frac{\mathrm{d}u}{\mathrm{d}x}\right),$$
$$u(0) = u(1).$$

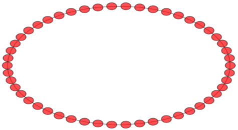

Figure: A 1D circular graph.

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

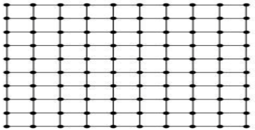

Figure: A 2D lattice graph.

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

$\mathcal{L}$: a graph Laplacian

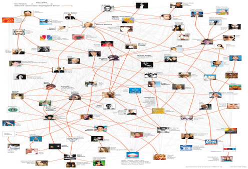

Figure: A social network graph.

- 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.
  - Gödel Prize 2008, 2015.
- Livne-Brandt-2012: Lean Algebraic Multigrid. Practical nearly-linear time algorithm, no theoretical guarantee.
- 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

$$\|u - \mathcal{P}_{\Phi}^{(L^2)} u\|_{L^2} \le C_p \sqrt{\lambda_n(\mathcal{L}^{-1})} \|u\|_H,$$

  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.

References

1. T. Y. Hou and P. Zhang, “Sparse operator compression of elliptic operators Part I: Second order elliptic operators”, preprint, submitted to RMS, 2016.
2. T. Y. Hou and P. Zhang, “Sparse operator compression of elliptic operators Part II: Higher order elliptic operators”, preprint, submitted to RMS, 2016.