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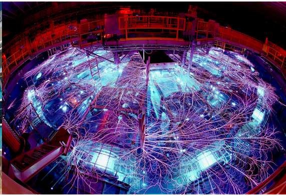

Scalable methods for nonlocal models

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Theoretical and Applied Aspects for Nonlocal Models
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U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

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Elliptic nonlocal operators

Let $\delta \in (0, \infty]$ be the *horizon*, $\Omega \subset \mathbb{R}^d$ a bounded open domain, define the *interaction domain*

$$\Omega_I := \{\mathbf{y} \in \mathbb{R}^d \setminus \Omega : |\mathbf{x} - \mathbf{y}| \leq \delta, \quad \text{for } \mathbf{x} \in \Omega\}.$$

We want to numerically solve equations involving the nonlocal operator

$$\mathcal{L}u(\mathbf{x}) = \text{p.v.} \int_{\Omega \cup \Omega_I} (u(\mathbf{y}) - u(\mathbf{x}))\gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y}, \qquad \mathbf{x} \in \Omega,$$

with

$$\begin{aligned} &\gamma(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x}, \mathbf{y}) \, |\mathbf{x} - \mathbf{y}|^{-\beta(\mathbf{x}, \mathbf{y})} \, \mathcal{X}_{|\mathbf{x}-\mathbf{y}| \leq \delta}, \qquad && \mathbf{x}, \mathbf{y} \in \Omega \cup \Omega_I, \\ &\phi(\mathbf{x}, \mathbf{y}) > 0. \end{aligned}$$

- Examples:
  - Integral fractional Laplacian: $\phi \sim$ const, $\beta = d + 2s$, $s \in (0, 1)$, $\delta = \infty$
  - Tempered fractional Laplacian: $\phi(\mathbf{x}, \mathbf{y}) \sim \exp(-\lambda |\mathbf{x} - \mathbf{y}|)$
  - Truncated fractional Laplacian: δ finite
  - Variable order fractional Laplacians with varying coefficient: $\beta(\mathbf{x}, \mathbf{y}) = d + 2s(\mathbf{x}, \mathbf{y})$, $\phi(\mathbf{x}, \mathbf{y}) > 0$
  - Integrable kernels: constant kernel ($\beta = 0$), "peridynamic" kernel ($\beta = 1$)
- Assumptions (for now):
  - γ is symmetric.
  - Interaction domain is defined wrt ℓ_2-norm.

- Nonlocal Poisson's equation:

$$\begin{aligned} -\mathcal{L}u &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{in } \Omega_I. \end{aligned}$$

- Nonlocal heat equation:

$$\begin{aligned} u_t - \mathcal{L}u &= f \quad \text{in } (0,T) \times \Omega, \\ u &= 0 \quad \text{in } (0,T) \times \Omega_I, \\ u &= u_0 \quad \text{on } \{0\} \times \Omega. \end{aligned}$$

- Source control
- Parameter learning:

$$\min_{u,s,\delta,\dots} \frac{1}{2} \|u - u_d\|_{L^2}^2 + \mathcal{R}(s, \delta, \dots)$$

  subject to nonlocal equation.
- Remark: Homogeneous Dirichlet "boundary" condition for simplicity.

Goal

Assemble and solve nonlocal equations in similar complexity & memory as their local counterparts, i.e. $\mathcal{O}(n \log n)$.

Bilinear form

- We consider

$$a(u,v) = \frac{1}{2}\int_{\Omega} d\mathbf{x} \int_{\Omega} d\mathbf{y}\; \left[\left(u\left(\mathbf{x}\right) - u\left(\mathbf{y}\right)\right)\left(v\left(\mathbf{x}\right) - v\left(\mathbf{y}\right)\right)\right]\gamma(\mathbf{x},\mathbf{y})$$
$$+ \int_{\Omega} d\mathbf{x} \int_{\Omega_I} d\mathbf{y}\, u\left(\mathbf{x}\right) v\left(\mathbf{x}\right) \gamma(\mathbf{x},\mathbf{y}).$$

posed on $\widetilde{H}^s\left(\Omega\right)$ or $L^2\left(\Omega\right)$ respectively, where

$$H^s\left(\Omega\right) := \left\{u \in L^2\left(\Omega\right) \mid \|u\|_{H^s(\Omega)} < \infty\right\}, \quad \widetilde{H}^s\left(\Omega\right) := \left\{u \in H^s\left(\mathbb{R}^d\right) \mid u = 0 \text{ in } \Omega^c\right\},$$

and

$$\|u\|^2_{H^s(\Omega)} = \|u\|^2_{L^2(\Omega)} + \int_{\Omega} d\mathbf{x} \int_{\Omega} d\mathbf{y}\, \frac{(u(\mathbf{x}) - u(\mathbf{y}))^2}{|\mathbf{x}-\mathbf{y}|^{d+2s}},$$
$$\|u\|^2_{\widetilde{H}^s(\Omega)} = \int_{\mathbb{R}^d} d\mathbf{x} \int_{\mathbb{R}^d} d\mathbf{y}\, \frac{(u(\mathbf{x}) - u(\mathbf{y}))^2}{|\mathbf{x}-\mathbf{y}|^{d+2s}}.$$

- For $\delta = \infty$, if $\gamma(\mathbf{x},\mathbf{y}) = \nabla_{\mathbf{y}} \cdot \mathbf{\Gamma}(\mathbf{x},\mathbf{y})$, can reduce integral from $\Omega \times \Omega^c$ to $\Omega \times \partial\Omega$. (E.g. $\Gamma(\mathbf{x},\mathbf{y}) \sim \frac{\mathbf{x}-\mathbf{y}}{|\mathbf{x}-\mathbf{y}|^{d+2s}}$ for the constant-order fractional kernel.)

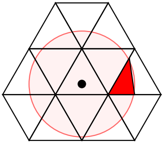
Finite element approximation

- Partition domain into shape-regular mesh $\mathcal{P}_h = \{K\}$ with edges e on the boundary $\partial\Omega$.
- Set $V_h \subset \widetilde{H}^s(\Omega)$ the space of continuous, piecewise linear functions.

$$
\begin{aligned}
a(u,v) =& \frac{1}{2} \sum_K \sum_{\tilde{K}} \int_K d\mathbf{x} \int_{\tilde{K}} d\mathbf{y}\, (u(\mathbf{x}) - u(\mathbf{y}))\, (v(\mathbf{x}) - v(\mathbf{y}))\, \gamma(\mathbf{x},\mathbf{y}) \\
&+ \sum_K \sum_e \int_K d\mathbf{x}\, u(\mathbf{x})\, v(\mathbf{x}) \int_e d\mathbf{y}\, \mathbf{n}_e \cdot \Gamma(\mathbf{x},\mathbf{y}).
\end{aligned}
$$

$\dim V_h =: n$

- Approximate cut elements with simplices, $\mathcal{O}(h_K^2)$ error[1]



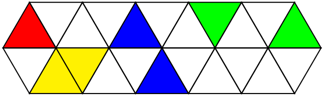
[1] Marta D'Elia, Max Gunzburger, and Christian Vollmann. "A cookbook for approximating Euclidean balls and for quadrature rules in finite element methods for nonlocal problems". In: *Mathematical Models and Methods in Applied Sciences* 31.08 (2021), pp. 1505–1567.

Quadrature

- In subassembly procedure, use quadrature to evaluate element pair contributions:

$$a^{K\times\tilde{K}}(\phi_i,\phi_j) = \frac{1}{2}\int_K d\mathbf{x}\int_{\tilde{K}} d\mathbf{y}\,(\phi_i(\mathbf{x})-\phi_i(\mathbf{y}))\,(\phi_j(\mathbf{x})-\phi_j(\mathbf{y}))\,\gamma(\mathbf{x},\mathbf{y})$$

- Treatment for element pairs $K\cap\tilde{K}\neq\emptyset$:



  - split $K\times\tilde{K}$ into sub-simplices,
  - Duffy transform onto a hypercube, with Jacobian canceling the singularity.
  - Choose quadrature order so that quadrature error $\leq$ discretization error[2]:
    - $|\log h_K|$ if the elements coincide (*red*),
    - $|\log h_K|^2$ if the elements share only an edge (*yellow*),
    - $|\log h_K|^3$ if the elements share only a vertex (*blue*),
    - $|\log h_K|^4$ if the elements are "near neighbours" (*green*), and
    - C if the elements are well separated.

[2] Mark Ainsworth and Christian Glusa. "Aspects of an adaptive finite element method for the fractional Laplacian: A priori and a posteriori error estimates, efficient implementation and multigrid solver". In: *Computer Methods in Applied Mechanics and Engineering* (2017).

$\mathcal{O}(n \log n)$ approximations to the stiffness matrix

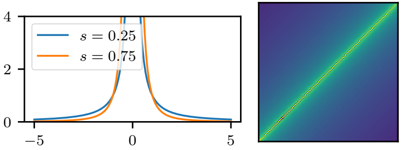


Figure: *Left:* Fractional kernels in $d = 1$ dimensions. *Right:* Magnitude of matrix entries.

Depending on δ and h:

- Straightforward discretization can lead to a fully dense matrix.
- Assembly and solve would have at least $\mathcal{O}(n^2)$ complexity and memory requirement.

Better approach

Panel clustering / Fast Multipole Method / hierarchical matrix approximation

- Find low-rank representations of off-diagonal matrix blocks.
- Lots of methods for computing a structurally sparse approximation, varying level of intrusiveness. I will show what I use: *panel clustering*.
- Important: we don't want to assemble a dense matrix and then compress it.
- Approximation incurs error. The game is to control it so that it is dominated by discretization error.

Cluster method: admissible clusters

First question: Which sub-blocks of the matrix do we want to compress?

Build tree of clusters of DoFs.

- root contains all unknowns
- subdivision based on coordinates
- distributed computations: first level given by partition of unknowns

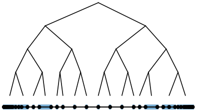


Figure: A cluster tree in $d = 1$ dimensions.

- Find cluster pairs (P, Q) that are *admissible* for approximation: sufficient separation compared to sizes.
- Matrix entries that are not part of any admissible cluster pair are assembled directly into the sparse near-field matrix A_{near}.

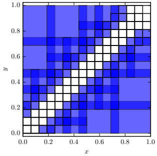


Figure: Elements of admissible cluster pairs in blue. Overlaps in dark blue.

Cluster method – $\mathcal{H}$-matrices

Let $P, Q \subset \Omega$, P and Q admissible.
Let ϕ, ψ be FE basis functions with $\operatorname{supp}\phi \subset P$, $\operatorname{supp}\psi \subset Q$.

$$a(\phi, \psi) = -\int_\Omega \int_\Omega \gamma(\mathbf{x}, \mathbf{y})\, \phi(\mathbf{x})\, \psi(\mathbf{y})\,.$$

Let $\boldsymbol{\xi}_\alpha^P$ be Chebyshev nodes in P and L_α^P the associated Lagrange polynomials. Then

$$\gamma(\mathbf{x}, \mathbf{y}) \approx \sum_{\alpha,\beta=1}^{m^d} \gamma\left(\boldsymbol{\xi}_\alpha^P, \boldsymbol{\xi}_\beta^Q\right) L_\alpha^P(\mathbf{x})\, L_\beta^Q(\mathbf{y})\,, \quad \mathbf{x} \in P,\ \mathbf{y} \in Q.$$

and

$$a(\phi, \psi) \approx -\sum_{\alpha,\beta=1}^{m^d} \gamma\left(\boldsymbol{\xi}_\alpha^P, \boldsymbol{\xi}_\beta^Q\right) \int_P \phi(\mathbf{x})\, L_\alpha^P(\mathbf{x})\ d\mathbf{x} \int_Q \psi(\mathbf{y})\, L_\beta^Q(\mathbf{y})\ d\mathbf{y}.$$

- Decouples ϕ and ψ, "sparsifies" off-diagonal matrix blocks.
- Replaces subblock of $a(\cdot,\cdot)$ with a low rank approximation $U_P \Sigma_{(P,Q)} U_Q^T$ with tall and skinny U_P, U_Q.
- If we stop now, we have constructed a so-called $\mathcal{H}$-matrix approximation:

$$A \approx A_{\text{near}} + A_{\text{far}} = A_{\text{near}} + \sum_{(P,Q)\text{ admissible}} U_P \Sigma_{(P,Q)} U_Q^T.$$

Cluster method – $\mathcal{H}^2$-matrices

For $\boldsymbol{x}$ in a sub-cluster P of Q, i.e. $P \subset Q$,

$$L_\alpha^Q(\boldsymbol{x}) = \sum_{\beta=1}^{m^d} L_\alpha^Q\left(\boldsymbol{\xi}_\beta^P\right) L_\beta^P(\boldsymbol{x}).$$

Need to compute

- Far-field coefficients $\int_P \phi(\boldsymbol{x}) L_\alpha^P(\boldsymbol{x}) \, d\boldsymbol{x}$ only for leaves of the cluster tree,
- shift coefficients $L_\alpha^Q\left(\boldsymbol{\xi}_\beta^P\right)$,
- kernel approximations $\gamma\left(\boldsymbol{\xi}_\alpha^P, \boldsymbol{\xi}_\beta^Q\right)$,
- near-field entries.

$\mathcal{H}^2$-matrix approximation[3][4]

FE assembly and matrix-vector product in $\mathcal{O}\left(n \log^{2d} n\right)$ operations.

- Finite δ: need to be able to form clusters that fit within the horizon.
- Less intrusive but more costly way of computing far-field interactions via entry sampling: Adaptive Cross Approximation (ACA)

[3] Mark Ainsworth and Christian Glusa. "Towards an efficient finite element method for the integral fractional Laplacian on polygonal domains". In: *Contemporary Computational Mathematics-A Celebration of the 80th Birthday of Ian Sloan*. Springer, 2018, pp. 17–57.

[4] Mark Ainsworth and Christian Glusa. "Aspects of an adaptive finite element method for the fractional Laplacian: A priori and a posteriori error estimates, efficient implementation and multigrid solver". In: *Computer Methods in Applied Mechanics and Engineering* (2017).

Operator interpolation[5,6]

Parameter learning problem requires operators for different values of s and δ.

- Piecewise Chebyshev interpolation in s:

Lemma

Let $s \in [s_{\min}, s_{\max}] \subset (0,1)$, $\delta \in (0,\infty)$, and let $\eta > 0$. Assume that $u(s) \in H_{\Omega}^{s+1/2-}(\mathbb{R}^n)$, $v \in H_{\Omega}^{s}(\mathbb{R}^n)$. There exists a partition of $[s_{\min}, s_{\max}]$ into sub-intervals $\mathcal{S}_k$ and interpolation orders M_k such that the piecewise Chebyshev interpolant $\tilde{a}(\cdot,\cdot;s,\delta)$ satisfies:

$$\left|a(u(s),v;s,\delta) - \tilde{a}(u(s),v;s,\delta)\right| \leq \eta \left\|u(s)\right\|_{H_{\Omega}^{\bar{s}_2(s)}(\mathbb{R}^n)} \left\|v\right\|_{H_{\Omega}^{s}(\mathbb{R}^n)},$$

and the total number of interpolation nodes satisfies

$$\sum_{k=1}^{K} (M_k + 1) \leq C \left|\log \eta\right|.$$

The constant C depends on δ and $s_{\max}$.

- Combined with hierarchical matrix approach: $\mathcal{O}(n \log^{2d+1} n)$ complexity & memory.
- Also allows to evaluate derivatives wrt s.
- Assembly for different values of δ is achieved by splitting the kernel into infinite horizon, singular part, and δ-dependent regular part.

[5] Olena Burkovska and Max Gunzburger. "Affine approximation of parametrized kernels and model order reduction for nonlocal and fractional Laplace models". In: *SIAM Journal on Numerical Analysis* 58.3 (2020), pp. 1469–1494.

[6] Olena Burkovska, Christian Glusa, and Marta D'Elia. "An optimization-based approach to parameter learning for fractional type nonlocal models". In: *Computers & Mathematics with Applications* (2021).

Conditioning and scalable solvers

- $\mathcal{O}(n \log n)$ matrix-vector product in all cases $\rightarrow$ can explore iterative solvers
- Steady-state:
  - Fractional kernel, $\delta = \infty$[7]: $\kappa(\mathbf{A}) \sim h^{-2s} \sim n^{2s/d}$
  - Fractional kernel, $\delta \leq \delta_0$[8]: $\kappa(\mathbf{A}) \sim \delta^{2s-2} h^{-2s} \sim \delta^{2s-2} n^{2s/d}$
  - Constant kernel, δ finite[8]: $\kappa(\mathbf{A}) \sim \delta^{-2}$
- Time-dependent:
  - $\kappa(\mathbf{M} + \Delta t \mathbf{A}) \sim 1 + \Delta t\, \kappa(\mathbf{A})$
  - Depending on time-stepper and CFL condition, this is well-conditioned for small s, large δ.

- Scalable solver options:
  - Multigrid
    - Geometric (GMG)
    - Algebraic (AMG)
  - Domain decomposition
    - Substructuring
    - Schwarz methods
  - Krylov methods
    The matrix is well-conditioned in the certain parameter regimes, e.g.
    - constant kernel, δ large, or
    - or fractional kernel, s small, δ large.

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[7] Mark Ainsworth, William McLean, and Thanh Tran. "The conditioning of boundary element equations on locally refined meshes and preconditioning by diagonal scaling". In: *SIAM Journal on Numerical Analysis* 36.6 (1999), pp. 1901–1932.

[8] Burak Aksoylu and Zuhal Unlu. "Conditioning analysis of nonlocal integral operators in fractional Sobolev spaces". In: *SIAM Journal on Numerical Analysis* 52.2 (2014), pp. 653–677.

Geometric multigrid (GMG)

- Hierarchy of meshes from uniform or adaptive refinement
- Restriction / prolongation given by nesting of FE spaces
- Assembly into hierarchical or CSR matrix format on every level
- Smoothers:
  - Jacobi,
  - Chebyshev,
  - Gauss-Seidel when CSR matrix format is used.
- Coarse solve: convert to dense or CSR matrix

Numerical Examples in 2D – Timings

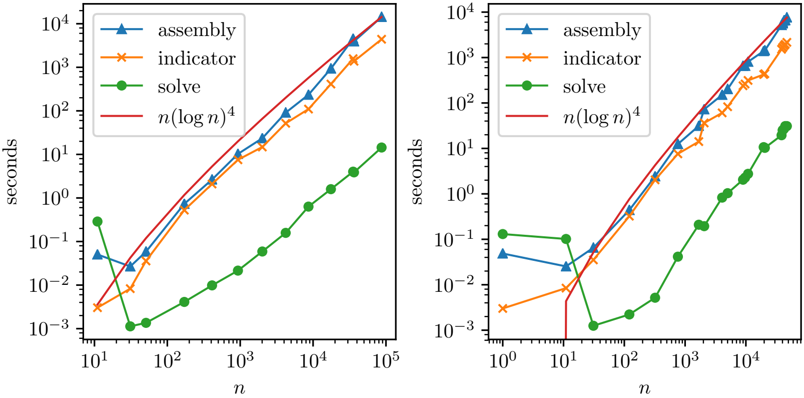
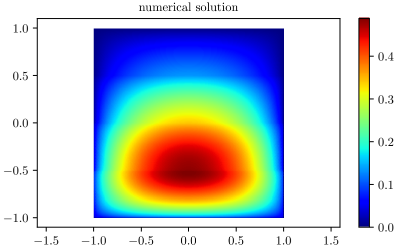
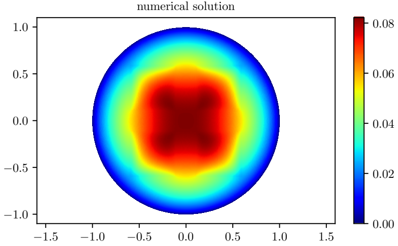


Figure: Timings for assembly of the stiffness matrix for fractional kernels, $\delta = \infty$, solution of linear system using GMG and computation of the error indicators for the two-dimensional problem. $s = 0.25$ on the left, $s = 0.75$ on the right.

Fractional kernel, variable order[9]





$f \equiv 1, \delta = 0.5$

$$s(\mathbf{x}, \mathbf{y}) = \frac{1}{2}(\sigma(\mathbf{x}_1) + \sigma(\mathbf{y}_1))$$

$$\sigma(z) = \begin{cases} 1/5 & \text{if } z < -1/2, \\ 2/5 & \text{if } -1/2 \le z < 0, \\ 3/5 & \text{if } 0 \le z < 1/2, \\ 4/5 & \text{if } 1/2 \le z. \end{cases}$$

$f \equiv 1, \delta = \infty$

$$s(\mathbf{x}, \mathbf{y}) = \begin{cases} 0.25 & \text{if } \mathbf{x}, \mathbf{y} \in \text{islands}, \\ 0.75 & \text{if } \mathbf{x}, \mathbf{y} \notin \text{islands}, \\ 0.75 & \text{else}. \end{cases}$$

[9] Marta D'Elia and Christian A. Glusa. *A fractional model for anomalous diffusion with increased variability. Analysis, algorithms and applications to interface problems*. (Accepted in Numerical Methods for Partial Differential Equations). 2021.

FEM convergence for variable s

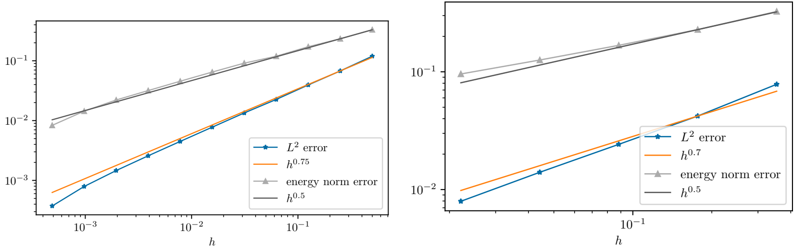


Figure: Convergence in L^2 and energy norm for a 1D example (*left*) and a 2D example with four material layers (*right*).

Rate of convergence, fractional kernels

	$\|\|e\|\|$	$\|\|e\|\|_{L^2}$
constant kernels (literature)	$h^{1/2-\varepsilon}$	$h^{\min\{1,1/2+s\}-\varepsilon}$
variable kernels (observed)	$h^{1/2-\varepsilon}$	$h^{\min\{1,1/2+\underline{s}\}-\varepsilon}$

$\underline{s} = \min s(\boldsymbol{x}, \boldsymbol{y})$

$\Rightarrow$ Possibly straightforward extension of regularity theory?

Solvers for Time-Dependent Problems: CG and GMG

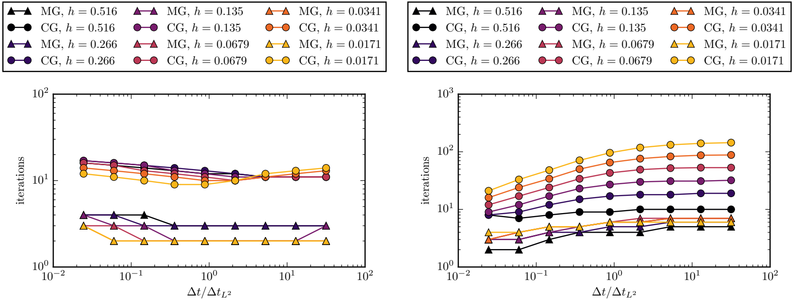


Figure: Fractional kernel. Number of iterations for CG and GMG depending on Δt for $s = 0.25$ (*left*) and $s = 0.75$ (*right*). Δt_{L^2} is the time-step that balances discretisation errors in time and space with respect to the L^2-norm.

Conjugate gradient is a competitive solver when the fractional order s is small and the time step Δt is not too large.

Algebraic multigrid (WIP)

Motivation:

- Adaptively refined / graded meshes can make geometric multigrid painful.
- Use of established algebraic multigrid framework: Trilinos/MueLu
  - Lots of features (more smoothers, coarse solvers, multigrid cycles, etc)
  - Able to handle coefficient and mesh variations
  - Runs on lots of different computing architectures (CPU, threads, GPUs, etc)

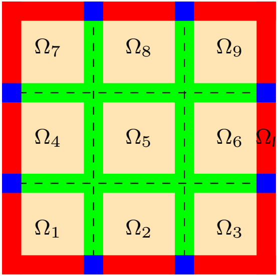
Approach:

- Algebraic multigrid constructs coarse problems using sparsity patterns and matrix entries
  $\rightarrow$ Cannot directly use matrix $\boldsymbol{A}$ when $\delta \gg h$ and hierarchical matrix format is used.
- Construct hierarchy for an auxiliary operator:
  - PDE operators, e.g. $(\nabla u, \nabla v)$,
  - (distance) Graph Laplacian wrt mesh,
  - near field part of hierarchical matrix after some filtering.
- Triple matrix products $\boldsymbol{A}_c = \boldsymbol{RAP}$ where $\boldsymbol{R}$ and $\boldsymbol{P}$ are sparse and $\boldsymbol{A}$ an $\mathcal{H}$- or $\mathcal{H}^2$-matrix
- Recompression of coarse matrix $\boldsymbol{A}_c$

		memory (finest level)		iterations (time)
unknowns	# MPI ranks	dense	$\mathcal{H}^2$	CG+AMG
11,193	4	0.93 GB	0.18 GB	7 (0.22s)
45,169	18	15.2 GB	0.89 GB	9 (0.82s)
181,473	72	245 GB	5.1 GB	15 (2.1s)
727,489	288	3,943 GB	17.8 GB	9 (3.75s)
n	$\sim n$	$\sim n^2$	$\sim n \log^4 n$	constant # iterations?

Table: 2d fractional Poisson problem, $s = 0.75$, $\delta = \infty$, smoothed aggregation

Substructuring[10,11,12]



- Assume $\delta = \mathcal{O}(h)$.
- Cover with overlapping subdomains $\Omega \cup \Omega_I = \bigcup \Omega_i$, diam $(\Omega_i \cap \Omega_j) \sim \delta$ for adjacent subdomains.
- Duplicate unknowns in overlaps:

$$\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f} \Leftrightarrow \begin{pmatrix} \boldsymbol{A}_{\epsilon\epsilon} & \boldsymbol{M}^T \\ \boldsymbol{M} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_\epsilon \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_\epsilon \\ 0 \end{pmatrix}$$

  - $\boldsymbol{A}_{\epsilon\epsilon}$ is block diagonal by subdomain, partition-of-unity type scaling included.
  - For floating subdomains, local matrix $\boldsymbol{A}_p$ is singular.
  - $\boldsymbol{M}$ has entries $\{\pm 1, 0\}$, encodes the identity constraints on the overlaps (non-redundant).

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[10] Giacomo Capodaglio, Marta D'Elia, Pavel Bochev, and Max Gunzburger. "An energy-based coupling approach to nonlocal interface problems". In: *Computers & Fluids* 207 (2020), p. 104593.

[11] Xiao Xu, Christian Glusa, Marta D'Elia, and John T. Foster. "A FETI approach to domain decomposition for meshfree discretizations of nonlocal problems". In: *Computer Methods in Applied Mechanics and Engineering* 387 (2021), p. 114148.

[12] WIP with Bochev, Capodaglio, D'Elia, Gunzburger, Klar, Vollmann

Reduced system and Dirichlet preconditioner

- Let nullspace of $\boldsymbol{A}_{\epsilon\epsilon}$ be given by $\boldsymbol{Z}$.
- Eliminate primal variables from

$$\begin{pmatrix} \boldsymbol{A}_{\epsilon\epsilon} & \boldsymbol{M}^T \\ \boldsymbol{M} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_\epsilon \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_\epsilon \\ 0 \end{pmatrix}$$

  and obtain

$$\begin{aligned} \boldsymbol{P}_0 K \lambda &= \boldsymbol{P}_0 (\boldsymbol{M}\boldsymbol{A}_{\epsilon\epsilon}^\dagger \boldsymbol{f}_\epsilon) \\ \boldsymbol{G}^T \boldsymbol{\lambda} &= \boldsymbol{Z}^T \boldsymbol{f}_\epsilon, \end{aligned}$$

  where $\boldsymbol{K} = \boldsymbol{M}\boldsymbol{A}_{\epsilon\epsilon}^\dagger \boldsymbol{M}^T$, $\boldsymbol{G} = \boldsymbol{M}\boldsymbol{Z}$, $\boldsymbol{P}_0 = \boldsymbol{I} - \boldsymbol{G}(\boldsymbol{G}^T\boldsymbol{G})^\dagger \boldsymbol{G}^T$.
- Use projected CG to solve system.
- $\boldsymbol{P}_0$ acts as a "coarse grid".
- Preconditioner for $\boldsymbol{K}$:
  - Let $\boldsymbol{A}_p$, $\boldsymbol{M}_p$ be local parts of $\boldsymbol{A}_{\epsilon\epsilon}$ and $\boldsymbol{M}$.
  - Write $\boldsymbol{K} = \sum_{p=1}^{P} \boldsymbol{M}_p \boldsymbol{A}_p^\dagger \boldsymbol{M}_p^T = \sum_{p=1}^{P} \widetilde{\boldsymbol{M}}_p \boldsymbol{S}_p^\dagger \widetilde{\boldsymbol{M}}_p^T$.
  - Dirichlet preconditioner: $\boldsymbol{Q} = \sum_{p=1}^{P} \widetilde{\boldsymbol{M}}_p \boldsymbol{S}_p \widetilde{\boldsymbol{M}}_p^T$.
- Results shown use Manuel Klar's (U of Trier) assembly code
  `https://gitlab.uni-trier.de/klar/nonlocal-assembly`

Weak scaling – 2D, constant kernel

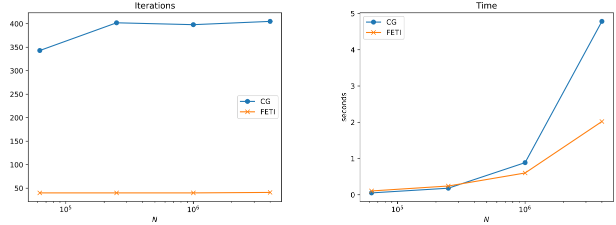

Figure: $\delta = 8e - 3 \rightarrow \kappa \sim$ const

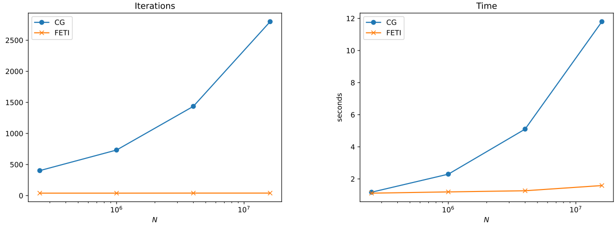

Figure: $\delta = 4h \rightarrow \kappa \sim N$

Weak scaling – 2D, fractional kernel, $s = 0.4$

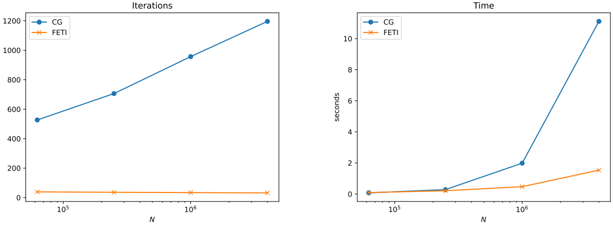

Figure: $\delta = 8e - 3 \rightarrow \kappa \sim N^s$

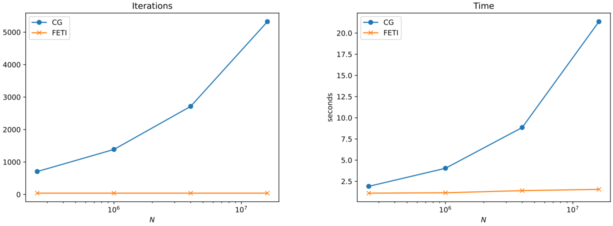

Figure: $\delta = 4h \rightarrow \kappa \sim N$

Strong scaling, 2D

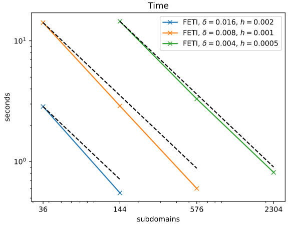

Figure: constant kernel, $\delta = 8h$.

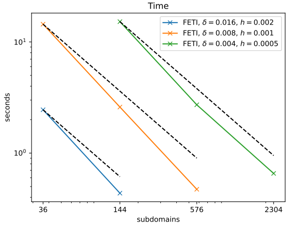

Figure: fractional kernel, $s = 0.4$, $\delta = 8h$.

Schwarz methods (WIP, with Pierre Marchand (INRIA))

- Drawback of substructuring: cannot handle $\delta \gg h$.
- Schwarz method
  - overlapping subdomain restrictions $\{\boldsymbol{R}_p\}$, local matrices $\boldsymbol{A}_p = \boldsymbol{R}_p \boldsymbol{A} \boldsymbol{R}_p^T$
  - partition of unity $\sum_{p=1}^{P} \boldsymbol{R}_p^T \boldsymbol{D}_p \boldsymbol{R}_p = \boldsymbol{I}$, with $\{\boldsymbol{D}_p\}$ diagonal
  - additive Schwarz preconditioner: $\boldsymbol{Q}_1 := \sum_{p=1}^{P} \boldsymbol{R}_p^T \boldsymbol{A}_p^{-1} \boldsymbol{R}_p$, or restricted additive Schwarz
- No global information exchange $\rightarrow$ need a coarse grid
- GenEO approach:
  Span coarse space using solutions of subdomain eigenvalue problems
  $\boldsymbol{D}_p \boldsymbol{A}_p \boldsymbol{D}_p \boldsymbol{v}_{p,k} = \lambda_{p,k} \boldsymbol{B}_p \boldsymbol{v}_{p,k}$, where $\boldsymbol{B}_p$ is similar to $\boldsymbol{A}_p$, but assembled over a modified local mesh.
- Distributed $\mathcal{H}$-matrix is built using Pierre Marchand's Htool library
  `https://github.com/htool-ddm/htool`
- HPDDM library for DD and GenEO `https://github.com/hpddm/hpddm`
- 2D fractional Poisson problem, $s = 0.75$, $\delta = \infty$

		memory (finest level)		iterations (time)
unknowns	# MPI ranks	dense	$\mathcal{H}$	GMRES+DD
65,025	72	31.5 GB	5.4 GB	21 (1.34s)
261,121	288	508 GB	12.6 GB	23 (0.96s)
1,046,529	1152	8,160 GB	86 GB	24 (2.4s)

- Caveats:
  - solver setup needs improvement, working on alternative low-rank approximations
  - direct solves (subdomain, coarse) and eigenvalue problems in dense format

Advertisement: PyNucleus, a FEM code for nonlocal problems

- Written in Python, lots of optimized kernels compiled to C via Cython.
- Compatible with NumPy/SciPy
- Simplical meshes in 1D, 2D, (3D); uniform refinement with boundary snapping options
- Mesh (re)partitioning using (PAR)METIS
- Finite Element discretizations: discontinuous P_0, continuous P_1, P_2, P_3
- Assembly of local differential operators
- Lots of solvers (direct, Krylov, simple preconditioners),
  and in particular geometric multigrid
  WIP: AMG (Trilinos/MueLu), DD (Htool&HPDDM)
- MPI distributed computations via mpi4py
- Assembly of the nonlocal operators in weak form:

$$a(u,v) = \frac{1}{2} \iint_{(\Omega\cup\Omega_I)^2} (u(\mathbf{x}) - u(\mathbf{y}))(v(\mathbf{x}) - v(\mathbf{y}))\gamma(\mathbf{x},\mathbf{y})d\mathbf{y}d\mathbf{x}$$

  into
  - CSR sparse matrix ($\delta \sim h$),
  - dense matrix ($\delta \gg h$),
  - $\mathcal{H}^2$ hierarchical matrix ($\delta \gg h$; only tested for fractional kernels)
- For fractional kernels: quadrature orders are tuned for optimal convergence.
- Code: `https://github.com/sandialabs/PyNucleus`
- Documentation and examples: `https://sandialabs.github.io/PyNucleus`

Code example


```python
from PyNucleus import (kernelFactory, nonlocalMeshFactory, dofmapFactory,
                       functionFactory, HOMOGENEOUS_DIRICHLET, solverFactory)

# Infinite horizon fractional kernel
kernel = kernelFactory('fractional', dim=2, s=0.75, horizon=inf)

# Mesh for unit disc, no interaction domain for homogeneous Dirichlet
mesh, _ = nonlocalMeshFactory('disc', kernel=kernel,
                              boundaryCondition=HOMOGENEOUS_DIRICHLET,
                              hTarget=0.15)

dm = dofmapFactory('P1', mesh)                                # P1 finite elements
f = functionFactory('constant', 1.)                           # constant forcing
b = dm.assembleRHS(f)                                         # $\int_\Omega f\phi_i$
A = dm.assembleNonlocal(kernel, matrixFormat='h2')            # $a(\phi_i, \phi_j)$, hierarchical
u = dm.zeros()                                                # solution vector

# solve with diagonally preconditioned CG
solver = solverFactory('cg-jacobi', A=A, setup=True)
solver(b, u)
u.plot()
```

- The documentation contains two examples of how to setup and solve local and nonlocal problems with a lot more explanations.
- The repository contains several drivers that demonstrate some of the code capabilities.

Conclusion

- Discretized fractional equations are dense, but not structurally dense.
  $\rightarrow$ approximation of off-diagonal matrix blocks
- Multigrid and domain decomposition solvers are optimal for nonlocal problems.
- Resulting approaches have essentially the same complexity as PDE case, allow for complex domains.

Thanks for listening!

MATNIP

Funding:
The MATNIP LDRD project (PI: Marta D'Elia) develops for the first time a rigorous nonlocal interface theory based on physical principles that is consistent with the classical theory of partial differential equations when the nonlocality vanishes and is mathematically well-posed. This will improve the predictive capability of nonlocal models and increase their usability at Sandia and, more in general, in the computational-science and engineering community. Furthermore, this theory will provide the groundwork for the development of nonlocal solvers, reducing the burden of prohibitively expensive computations.

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