Automatic Synthesis of Low Complexity Translation Operators for the Fast Multipole Method

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February 28, 2021

Outline

- Introduction to Taylor series based Fast Multipole Method
- Compressed Taylor Series based Multipole and Local expansions
- Results - accuracy and time complexity

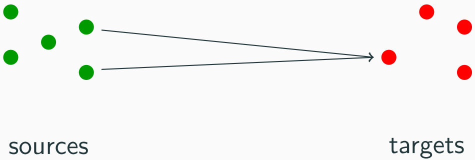
N-body problem

Let $\mathbf{s}$ be sources and $\mathbf{t}$ be targets. Potential at target $\mathbf{t}_i$ is the sum of all potentials from the sources $\mathbf{s}$ given by,

$$\psi(\mathbf{t}, \mathbf{s})_i = \sum_j G(t_i, s_j).$$

For example,

$$G(t_i, s_j) = \frac{1}{\text{dist}(t_i, s_j)}.$$



If the number of sources and and targets are both n then, calculating the potential of all targets takes $\mathcal{O}(n^2)$ time.

Fast Multipole Method

Algorithm by Greengard and Rokhlin (1987) to compute the potentials in $\mathcal{O}(n)$ time.

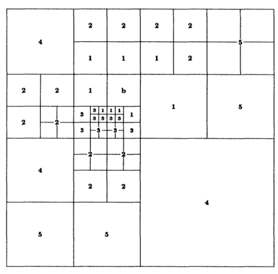


Figure 1: Carrier et al, 1988

Useful for solving partial differential equations with Integral equation methods where integrals of the following form are evaluated.

$$\int G(x,y)\sigma_y dy.$$

Taylor Series based FMM

Local expansion:

$$\psi(\mathbf{t},\mathbf{s}) = \sum_{|m|\le k} \underbrace{\frac{D^m_{\mathbf{t}}\psi(\mathbf{t},\mathbf{s})\Big|_{\mathbf{t}=\mathbf{c}}}{m!}}_{\text{depends on src/ctr}} \underbrace{(\mathbf{t}-\mathbf{c})^m}_{\text{depends on tgt/ctr}}$$

Multipole expansion:

$$\psi(\mathbf{t},\mathbf{s}) = \sum_{|m|\le k} \underbrace{\frac{D^m_{\mathbf{s}}\psi(\mathbf{t},\mathbf{s})\Big|_{\mathbf{s}=\mathbf{c}}}{m!}}_{\text{depends on tgt/ctr}} \underbrace{(\mathbf{s}-\mathbf{c})^m}_{\text{depends on src/ctr}}$$

Taylor Series based FMM

Expansion Types:

- Special purpose expansions (Spherical harmonics, Fourier-bessel based)
- Linear Algebra (Eg: Kernel-independent FMM)
- Taylor series based expansions

Pros	Cons
- Works for all Green's functions	- Expansions $\mathrm{O}(p^3)$ compared to $\mathrm{O}(p^2)$
	- Translations $\mathrm{O}(p^6)$ compared to $\mathrm{O}(p^2 \log(p))$
	- Stability issues

Table 1: Pros and cons of Taylor series based expansions

Compressed Multipole Expansion

When the potential ψ satisfies the 2D Helmholtz equation we have,

$$\psi_{xx} + \psi_{yy} + \kappa^2 \psi = 0$$

Recall,

$$\psi(\mathbf{t}, \mathbf{s}) = \sum_{|m| \le p} \underbrace{\frac{D_{\mathbf{s}}^m \psi(\mathbf{t}, \mathbf{s})\Big|_{\mathbf{s}=\mathbf{c}}}{m!}}_{\text{depends on tgt/ctr}} \underbrace{(\mathbf{s} - \mathbf{c})^m}_{\text{depends on src/ctr}}$$

From the PDE we have

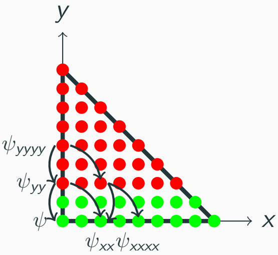
$$\begin{aligned} c_1 \psi_{xx} + c_2 \psi_{yy} + c_3 \psi &= c_1 \psi_{xx} + c_2(-\psi_{xx} - \kappa^2 \psi) + c_3 \psi \\ &= (c_1 - c_2)\psi_{xx} + 0\psi_{yy} + \psi(c_3 - \kappa^2 c_2). \end{aligned}$$

Compressed Multipole Expansion

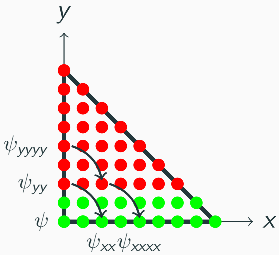
For 2D Helmholtz equation we also have,

$$\psi_{xxyy} + \psi_{yyyy} + \kappa^2 \psi_{yy} = 0$$

$$\psi_{xxxx} + \psi_{xxyy} + \kappa^2 \psi_{xx} = 0$$



Helmholtz 2D



Laplace 2D

All the coefficients represented by red dots get zeroed.

Multipole expansion coefficients go from $\mathcal{O}(p^d)$ to $\mathcal{O}(p^{d-1})$.

Compressed Local Expansion

Recall,

$$\psi(\mathbf{t}, \mathbf{s}) = \sum_{|m| \le p} \underbrace{\frac{D_{\mathbf{t}}^{m} \psi(\mathbf{t}, \mathbf{s})\Big|_{\mathbf{t}=\mathbf{c}}}{m!}}_{\text{depends on src/ctr}} \underbrace{(\mathbf{t} - \mathbf{c})^{m}}_{\text{depends on tgt/ctr}}$$

Out of $\mathcal{O}(p^d)$ coefficients, only $\mathcal{O}(p^{d-1})$ are independent.

This makes the number of terms of a local expansion to be $\mathcal{O}(p^{d-1})$.

Calculating derivatives for Local Expansion

Tausch (2003) proposes an algorithm which has an amortized $\mathcal{O}(p)$ time.

We found several formulae to calculate these in amortized $\mathcal{O}(1)$ time.

For Laplace 3D

$$
\begin{aligned}
r^2 \frac{\partial^{n+m+l}}{\partial x^n y^m z^l}\left(\frac{1}{r}\right) = &-(2n-1)x \frac{\partial^{n+m-1}}{\partial x^{n-1} y^m z^l}\left(\frac{1}{r}\right) - (n-1)^2 \frac{\partial^{n+m-2}}{\partial x^{n-2} y^m z^l}\left(\frac{1}{r}\right) - 2my \frac{\partial^{n+m-1}}{\partial x^n y^{m-1} z^l}\left(\frac{1}{r}\right) \\
&- m(m-1) \frac{\partial^{n+m-2}}{\partial x^n y^{m-2} z^l}\left(\frac{1}{r}\right) - 2lz \frac{\partial^{n+m-1}}{\partial x^n y^m z^{l-1}}\left(\frac{1}{r}\right) - l(l-1) \frac{\partial^{n+m-2}}{\partial x^n y^m z^{l-2}}\left(\frac{1}{r}\right)
\end{aligned}
$$

.

For Biharmonic 2D,

$$
\begin{aligned}
r^2 \frac{\partial^{n+m}}{\partial x^n y^m}\left(r^2 \log(r)\right) = &-2(n-2)x \frac{\partial^{n+m-1}}{\partial x^{n-1} y^m}\left(r^2 \log(r)\right) - (n-1)(n-4) \frac{\partial^{n+m-2}}{\partial x^{n-2} y^m}\left(r^2 \log(r)\right) \\
&- 2my \frac{\partial^{n+m-1}}{\partial x^n y^{m-1}}\left(r^2 \log(r)\right) - m(m-1) \frac{\partial^{n+m-2}}{\partial x^n y^{m-2}}\left(r^2 \log(r)\right).
\end{aligned}
$$

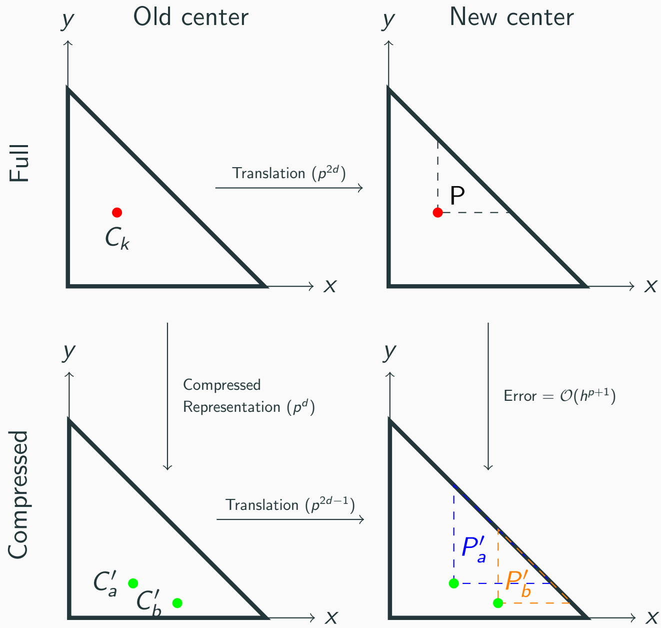
Compressed Multipole Translation

Let $\alpha_k = (\mathbf{s} - \mathbf{c}_1)^k$ be already computed multipole coefficients around center $\mathbf{c}_1$. Then,

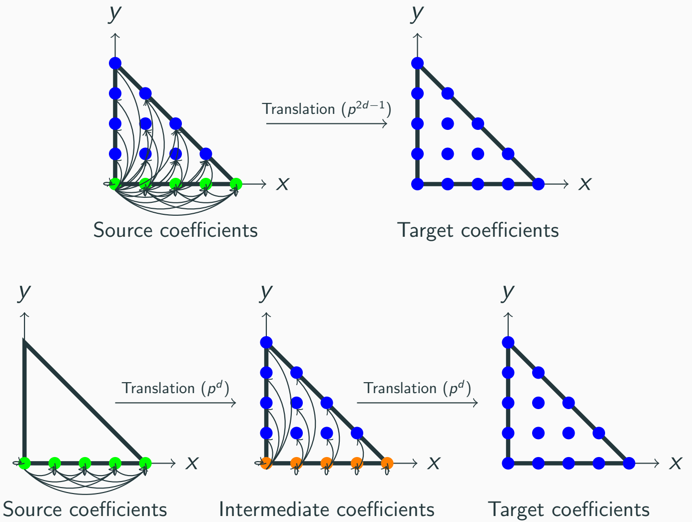
$$\begin{aligned}(\mathbf{s} - \mathbf{c})^k &= \left((\mathbf{s} - \mathbf{c}_1) + (\mathbf{c}_1 - \mathbf{c})\right)^k \\ &= \sum_{l \le k} \binom{k}{l} (\mathbf{s} - \mathbf{c}_1)^l (\mathbf{c}_1 - \mathbf{c})^{k-l} \\ &= \sum_{l \le k} \beta_{k,l} (\mathbf{s} - \mathbf{c}_1)^l\end{aligned}$$

Cost: $\mathcal{O}(p^{2d})$.

Compressed Multipole Translation

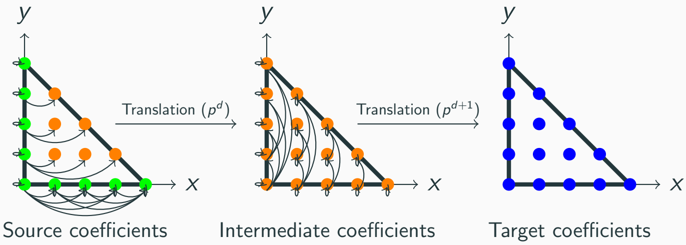


Faster Compressed Multipole Translation

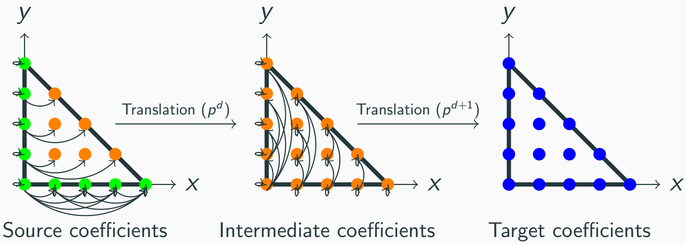


Note: For local to local translation, reverse all arrows.

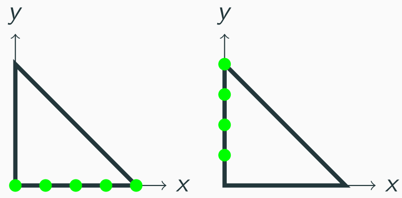
Faster Compressed Multipole Translation



Faster Compressed Multipole Translation



Divide the problem into 2 subproblems



Compressed Multipole to Local Translation

From multipole expansion, we get,

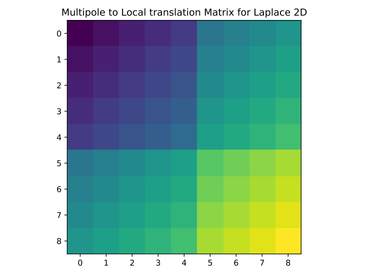
$$\psi(\mathbf{t}, \mathbf{s}) = \sum_{|m| \le k} \underbrace{\frac{D_{\mathbf{s}}^m \psi(\mathbf{t}, \mathbf{s})\Big|_{\mathbf{s}=\mathbf{c}}}{m!}}_{\text{depends on tgt/ctr}} \underbrace{(\mathbf{s} - \mathbf{c})^m}_{\text{depends on src/ctr}}$$

To translate this multipole expansion to a local expansion, we need to get the derivatives of the above expression and evalaute at new center.

Cost: $\mathcal{O}(p^{2d-2})$.

Compressed Multipole to Local Translation

Multipole to local translation matrix is a block Toeplitz matrix of smaller toeplitz matrices.



Compressed Multipole to Local Translation

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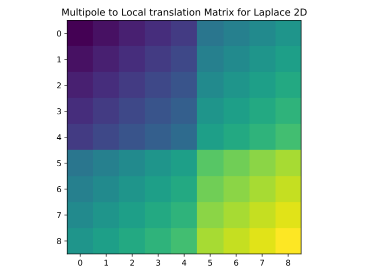
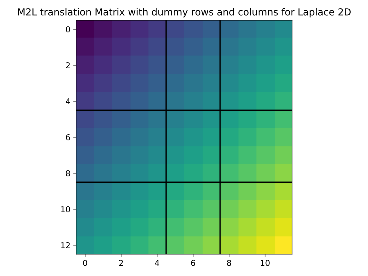




Use a Fast Fourier Transform (FFT) to do the translation.

Cost:

- $\mathcal{O}(p^{d-1}\log(p))$ for elliptic PDEs
- $\mathcal{O}(p^{d}\log(p))$ for other PDEs

Time complexities

	P2L/M2P	P2M/L2P	M2M	M2L	L2L
Taylor Series	p^3	p^3	p^6	p^6	p^6
Compressed Taylor Series without fast derivatives	p^3	p^3	p^3	p^3	p^3
Compressed Taylor Series with fast derivatives	p^2	p^3	p^3	$p^2 \log(p)$	p^3
Spherical Harmonic Series	p^2	p^2	$p^2 \log(p)$	$p^2 \log(p)$	$p^2 \log(p)$

Table 2: Time complexities for expansions, translations and evaluations

All operations are exact except for M2M in Compressed Taylor.

Here P is Point, L is Local expansion and M is Multipole expansion.

Code generation

With Compressed Taylor generating code for Stokes

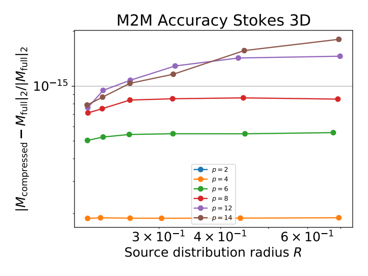
$$\mu\nabla^2\mathbf{u} - \boldsymbol{\nabla} p + \mathbf{f} = \mathbf{0}$$
$$\boldsymbol{\nabla}\cdot\mathbf{u} = 0$$

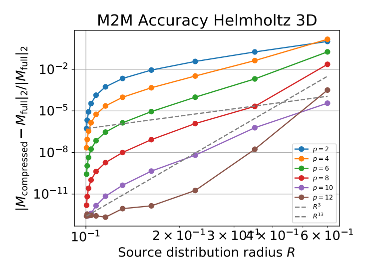
is done simply by giving the PDE as,

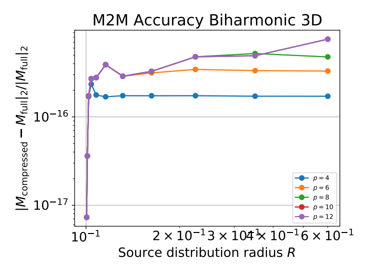
```
w = make_pde_syms(dim, dim+1)
mu = sym.Symbol("mu")
u = w[:dim]
p = w[-1]
pdes = PDE(mu * laplacian(u) - grad(p), div(u))
```

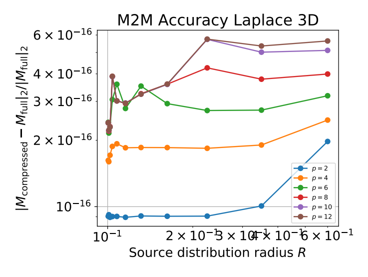
which generates code for the expansion, translations and evaluations.

Results - Error M2M

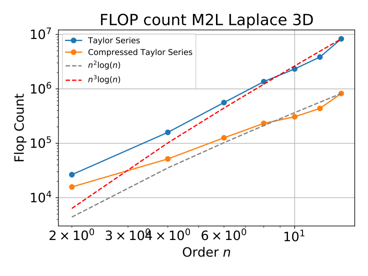


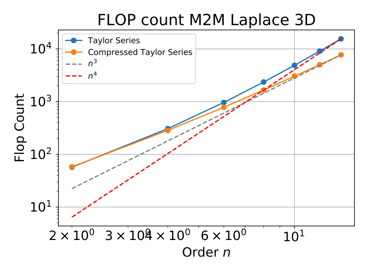


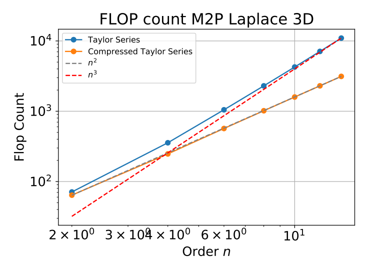


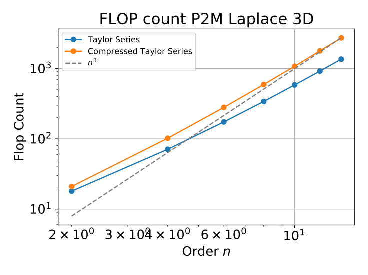


Results - FLOP count









Summary

- Kernel generic method for elliptic constant coefficient linear PDEs.
- Only needs the PDE and the Green's function for the PDE.
- Asymptotically better than full Taylor Series in,
    - Number of FLOPs
    - Storage
- Next goal: A fast Stokes solver on a GPU.

Ackowledgements:

- NSF grants 19-11019 and 16-54756
- Siam travel grant