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

Isuru Fernando, Andreas Klöckner

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Outline

- Introduction to Multipole and Local expansions
- Compressed Taylor Series based Multipole and Local expansions
- Results - Accuracy and Time complexity

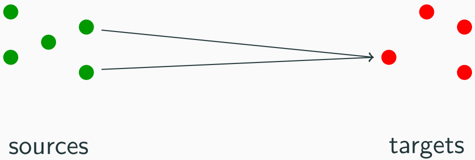
N-body problem

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,

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



If the number of sources are S and number of targets are T then, calculating the potential of all targets takes $\mathcal{O}(ST)$ time.

Local Expansion

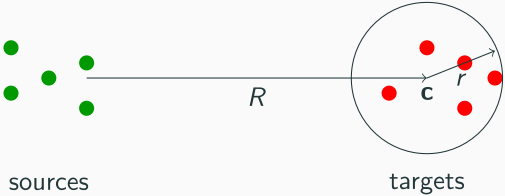
Potential function $\psi(t, s)$ can be written as a Taylor expansion.

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

Error term in Taylor expansion for Laplace 3D is,

$$\approx \sum_{|m|=p+1} K_m \left(\frac{\mathbf{t} - \mathbf{c}}{\mathbf{s} - \mathbf{c}} \right)^m$$

It's convergent if all sources are outside the circle around targets.



Local Expansion

Coefficients can be computed in $\mathcal{O}(Sp^d)$ time where p is the order of the Taylor series and d is the number of dimensions.

Sum can be calculated in $\mathcal{O}(Tp^d)$ time.

Cost of the algorithm is $\mathcal{O}(Sp^d) + \mathcal{O}(Tp^d)$ instead of $\mathcal{O}(ST)$ for calculating the interaction directly.

Useful for solving partial differential equations with Integral equation methods where integrals of the form,

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

needs to be evaluated.

Multipole Expansion

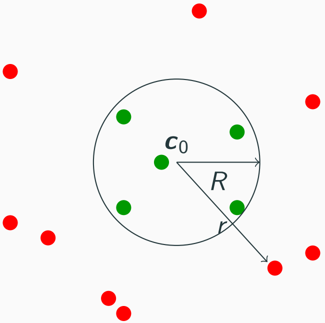
Taylor expansion is,

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

Changing the variable of differentiation, we get multipole expansion,

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

Multipole Expansion



Error for the multipole expansion is

$$\sum_{|m|=p+1} K_m \left(\frac{\mathbf{s}-\mathbf{c}}{\mathbf{t}-\mathbf{c}}\right)^m$$

and the expansion is convergent if all targets are outside the circle.

Multipole Expansion

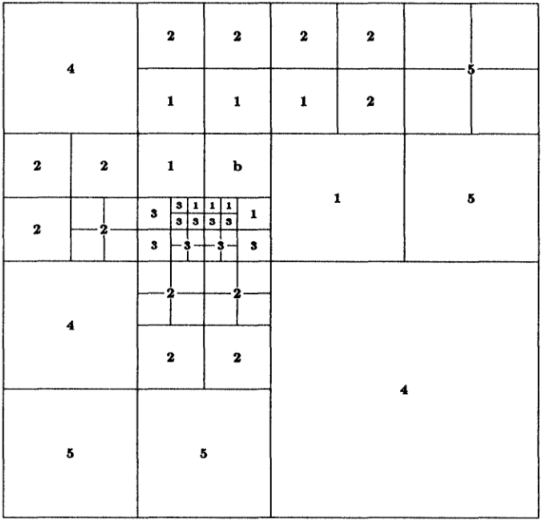


Figure 1: Carrier et al, 1988

Time complexities

	P2L	P2M	M2M	M2L	L2L	L2P	M2P
Taylor Series	p^3	p^3	p^6	p^6	p^6	p^3	p^3
Spherical Harmonic Series	p^2	p^2	$p^2 \log(p)$	$p^2 \log(p)$	$p^2 \log(p)$	p^2	p^2

Table 1: Time complexities for expansions, translations and evaluations

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

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,

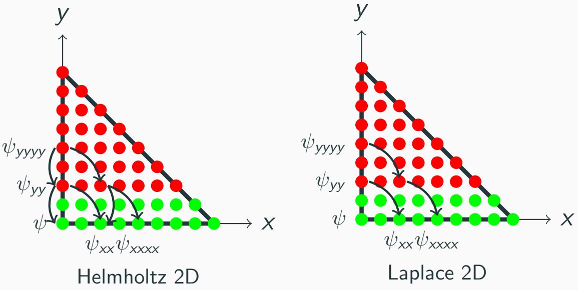
$$\begin{aligned} c_1 \psi_{xx} + c_2 \psi_{yy} + c_3 \psi &= c_1 \psi_{xx} + c_2(-\psi_{xx} - \kappa^2 \psi) + c_3 \psi \\ &= (c_1 - c_2)\psi_{xx} + 0\psi_{yy} + \psi(c_3 - \kappa^2 c_2). \end{aligned}$$

Compressed Multipole Expansion

For 2D Helmholtz equation we also have,

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

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



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,

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

Note that the coefficients are derivative terms and using the PDE, we can find linear combinations for the coefficients.

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 $\mathcal{O}(p^{d-1})$.

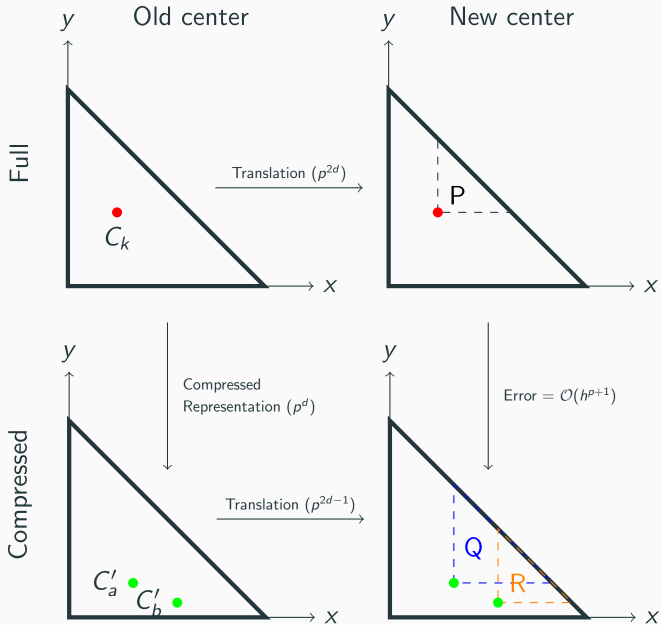
Compressed Multipole Translation

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

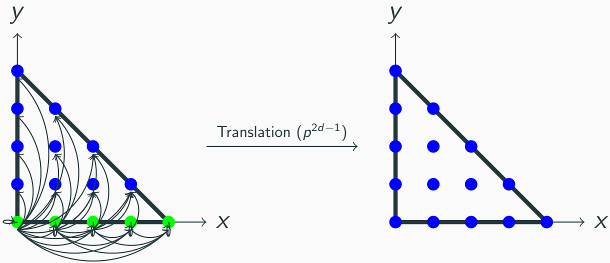
$$\begin{aligned}(\mathbf{s} - \mathbf{c})^k &= \left((\mathbf{s} - \mathbf{c}_1) + (\mathbf{c}_1 - \mathbf{c})\right)^k \\ &= \sum_{l \le k} \binom{k}{l} (\mathbf{s} - \mathbf{c}_1)^l (\mathbf{c}_1 - \mathbf{c})^{k-l} \\ &= \sum_{l \le k} \beta_{k,l} (\mathbf{s} - \mathbf{c}_1)^l\end{aligned}$$

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

Compressed Multipole Translation

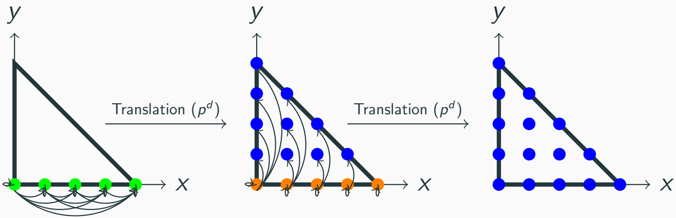


Compressed Multipole Translation



Source coefficients

Target coefficients



Source coefficients

Intermediate coefficients

Target coefficients

Compressed Multipole to Local Translation

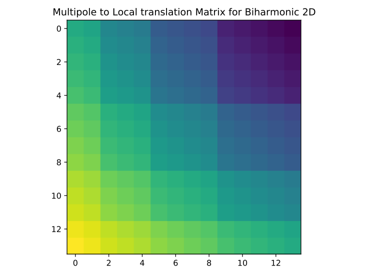
From multipole expansion, we get,

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

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.

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	P2M	M2M	M2L	L2L	L2P	M2P
Taylor Series	p^3	p^3	p^6	p^6	p^6	p^3	p^3
Improved Taylor Series	p^3	p^3	p^4	$p^3 \log(p)$	p^4	p^3	p^3
Compressed Taylor Series	p^2	p^3	p^3	$p^2 \log(p)$	p^3	p^3	p^2
Spherical Harmonic Series	p^2	p^2	$p^2 \log(p)$	$p^2 \log(p)$	$p^2 \log(p)$	p^2	p^2

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

Spherical harmonic series requires significant software engineering time for each specific problem.

With Compressed Taylor generating code for Stokes

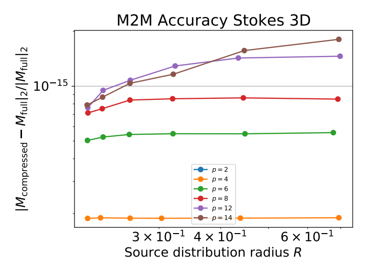
$$\mu\nabla^2\mathbf{u} - \boldsymbol{\nabla} p + \mathbf{f} = \mathbf{0}$$
$$\boldsymbol{\nabla} \cdot \mathbf{u} = 0$$

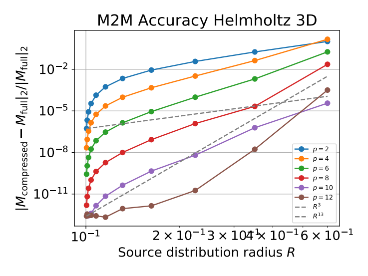
is done simply by giving the PDE as,

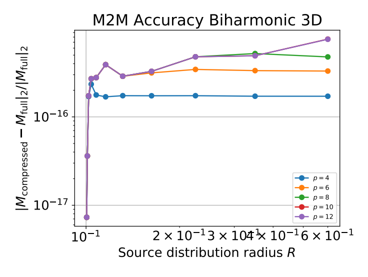
```
w = make_pde_syms(dim, dim+1)
mu = sym.Symbol("mu")
u = w[:dim]
p = w[-1]
pdes = PDE(mu * laplacian(u) - grad(p), div(u))
```

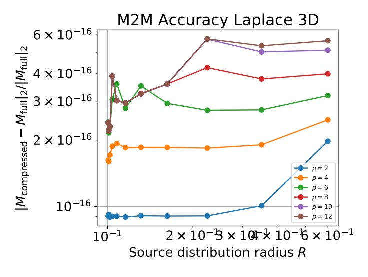
which generates code for the expansion, translations and evaluations.

Results - Error M2M

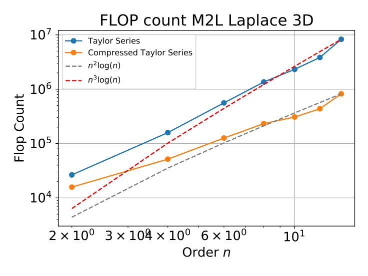


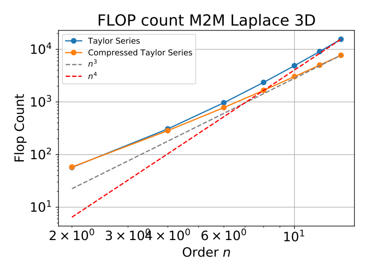


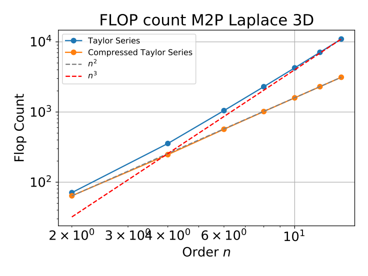


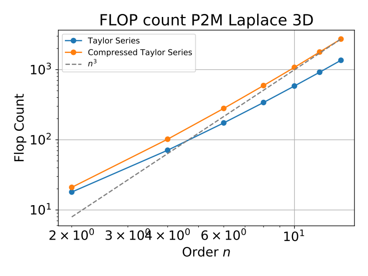


Results - FLOP count









Conclusions

- 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.