Accelerated M2L

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Accelerating the M2L with the SVD

Consider the application of the M2L operator K to a multipole expansion w to get the check potential g.

$$g = Kw \tag{1}$$

This can be approximated with a rank k SVD,

$$\tilde{g} = U_k \Sigma_k V_k^T \tag{2}$$

Stacking the M2L operators for all the source nodes in a given target node's interaction list can be done in two ways, column wise,

$$\begin{aligned} K_{\text{fat}} &= \left[K^1, ..., K^3 16\right] && (3)\\ &= U\Sigma \left[V^{(1)T}, ..., V^{(316)T}\right] && (4) \end{aligned}$$

where we use the fact that there are at most 316 unique orientations for the M2L operator in 3D. Similarly they can be stacked row wise,

$$\begin{aligned} K_{\text{thin}} &= \left[K^1; ...; K^{316}\right] && (5)\\ &= \left[R^{(1)T}; ...; R^{(316)T}\right] \Lambda S^T && (6) \end{aligned}$$

we note that

$$K_{\text{thin}} = K_{\text{fat}}^T \tag{7}$$

for symmetric kernels.

We can do some algebra to reduce the application cost of K when we've done these two SVDs. Consider the application of a single M2L operator corresponding to a single source box in a target box's interaction list,

$$K^{(i)}w = R^{(i)}\Lambda S^T w \tag{8}$$

Using the fact that S is unitary, $S^T S = I$, we can insert into the above equation,

$$\begin{aligned} K^{(i)}w &= R^{(i)}\Lambda S S^T S^T w && (9)\\ &= K^{(i)} S S^T w && (10)\\ &= U\Sigma V^{(i)T} S S^T w && (11)\\ & && (12) \end{aligned}$$

Now using the fact that U is also unitary, such that $U^T U = I$, we find

$$\begin{aligned} K^{(i)}w &= U U^T U \Sigma V^{(i)T} S S^T w && (13)\\ &= U[U^T U \Sigma V^{(i)T} S] S^T w && (14)\\ &= U[U^T K^{(i)} S] S^T w && (15) \end{aligned}$$

The term in the brackets can be calculated using the low rank (k-rank) terms from the SVD,

$$\begin{aligned} [U^T K^{(i)} S] &= \Sigma V^{(i)T} S && (16)\\ &= U^T R^{(i)} \Lambda && (17) \end{aligned}$$

We call this previous equation the compressed M2L operator,

$$C^{i,k} = U^T K^{(i)} S \tag{18}$$

This object can be pre-computed for each unique interaction. The M2L operation can be then broken down into 4 steps

1. Find the 'compressed multipole expansion'

$$w_c = S^T w \tag{19}$$

2. Compute the convolution to find the compressed check potential

$$g_c = \sum_{i \in I} C^{i,k} w_c \tag{20}$$

where the sum is over the interaction list I.

3. A post processing step to recover the check potential

$$g = U g_c \tag{21}$$

4. The calculatation of the local expansion, as usual, in the KIFMM.

Doing this the convolution step is reduced to matrix vector products involving the compressed M2L matrix, which is only of size $k \times k$, rather than $6(p-1)^2 + 2$ where p is the expansion order.