Implementing Fast Multipole Methods with High Level Interpreted Languages

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Motivation - the N Body Problem

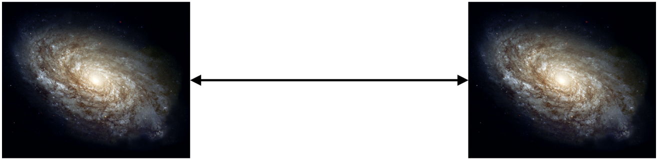
- e.g. Electrostatics, Gravitation
- $\{x_i\}_{i=1,..,N}$ Source Particles
- $\{y_j\}_{j=1,..,M}$ Target Particles

$$\Phi(y_j) = \sum_{i=1}^{N} K(x_i, y_j) q_i, \tag{1}$$

$$\text{where, } K(x, y) = \frac{1}{\|x - y\|} \tag{2}$$

- FMM reduces complexity from $O(N^2)$ to $O(N)$

Motivation - Intuition

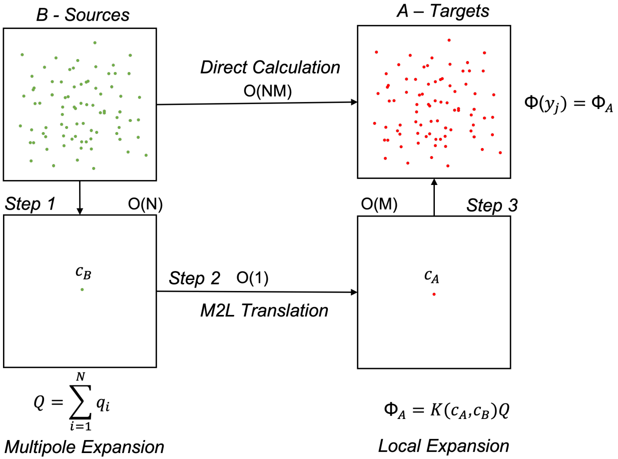


Galaxy A

Galaxy B

Motivation - Intuition

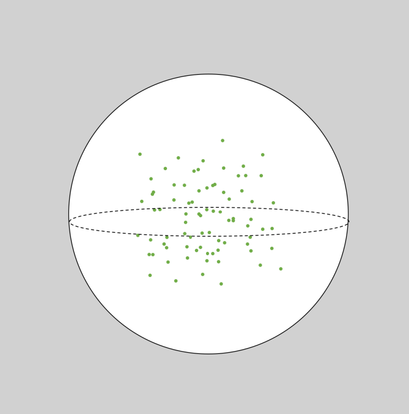
Motivation - Three Step Procedure



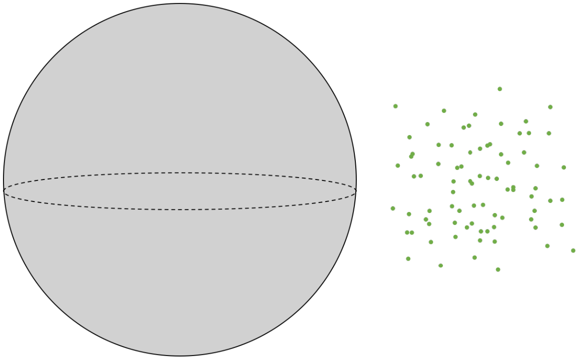
Analytic FMM - Concept

Idea: Use compressed representations of far field potentials to reduce complexity, in a recursive fashion

Analytic FMM - Multipole Expansion



Analytic FMM - Local Expansion

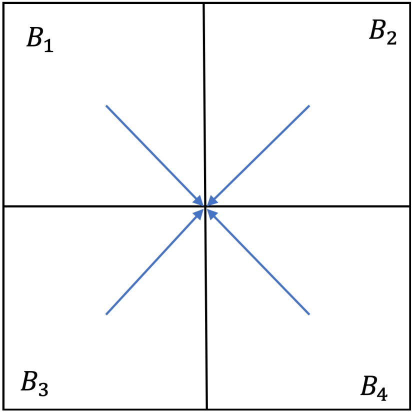


- For 3D Laplace kernel, can write multipole and local expansions using sph. harmonics, these can be truncated to required accuracy
- Exact operators exist for this kernel to shift between multipole and local expansion coefficients
- Exact bounds on error also exist, with respect to direct computation [2]

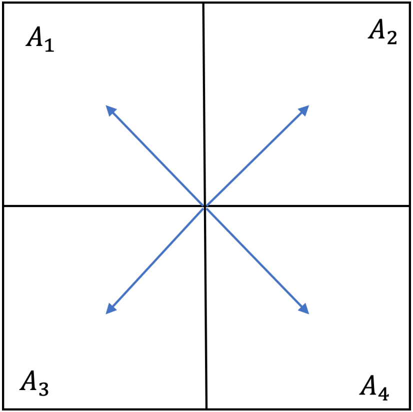
Analytic FMM - Motivating Problem

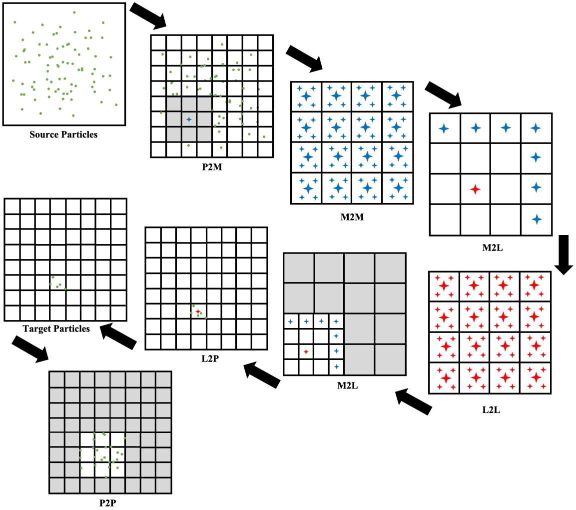
- Consider 2D Problem
- Domain, $\Omega = [0, 1] \times [0, 1]$
- Partition into recursively defined Quadtree
- Each level, l, partitioned into 4^l boxes
- Source and Target particles taken to be the same

Analytic FMM - Shifting Multipole Expansion



Analytic FMM - Shifting Local Expansion





Source Particles
P2M
M2M
M2L
L2L
M2L
L2P
Target Particles
P2P

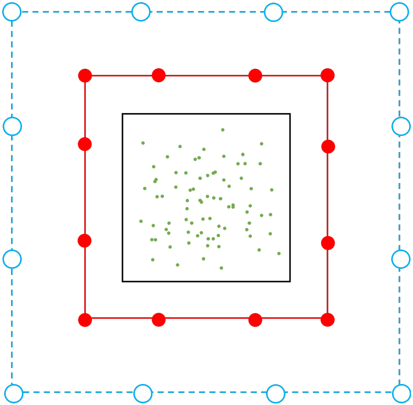
Analytic FMM - Implementation Issues

- Representing problem with efficient data structures: Quad/Octrees
- Computing and storing new expansions for each kernel, may require new software implementations

Kernel Independent FMM

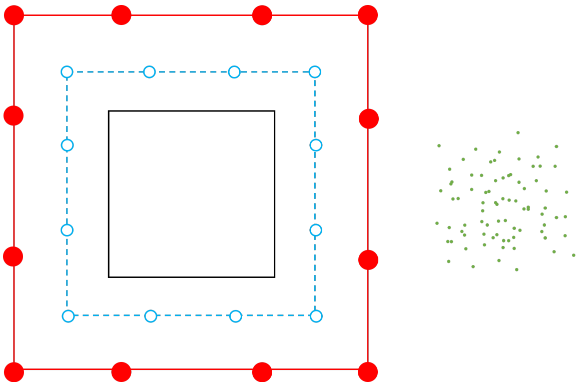
- KIFMM only requires kernel evaluations
- Works by matching potential generated by particles with that generated by an equivalent density in the far field

Kernel Independent FMM - Least Squares Problem



Adapted from [3]

Kernel Independent FMM - Least Squares Problem



Adapted from [3]

Kernel Independent FMM - Least Squares Problem

- Check Surface $x^{B,u}$
- Equivalent Surface $y^{B,u}$
- Equivalent Density $\phi^{B,u}$
- Check Potential $q^{B,u}$
- Indices of source points I_s^B
- Source densities ϕ_i

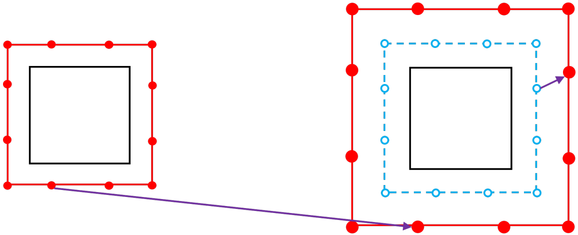
$$\int_{\mathrm{y}^{B,u}} K(\mathrm{x},\mathrm{y})\phi^{B,u} d\mathrm{y} = \sum_{i\in I_s^B} K(\mathrm{x},\mathrm{y})\phi_i = q^{B,u} \text{ for any } \mathrm{x} \in \mathrm{x}^{B,u} \quad (3)$$

Kernel Independent FMM - Least Squares Problem

$$K_A\phi^A = K_B\phi^B \tag{4}$$

$$\phi^A = (\alpha I + K_A^* K_A)^{-1} K_B \phi^B \tag{5}$$

Kernel Independent FMM - Least Squares Problem, M2L



Kernel Independent FMM - Least Squares Problem, M2L

- Check Surface $x^{B,u}$
- Downward Equivalent Surface $y^{B,d}$
- Upward Equivalent Surface $y^{A,u}$
- Downward Equivalent Density $\phi^{B,d}$
- Upward Equivalent Density $\phi^{A,u}$

$$\int_{\mathrm{y}^{A,u}} K(\mathrm{x},\mathrm{y})\phi^{A,u} d\mathrm{y} = \int_{\mathrm{y}^{B,d}} K(\mathrm{x},\mathrm{y})\phi^{B,d} d\mathrm{y}, \text{ for any } \mathrm{x} \in \mathrm{x}^{B,d} \quad (6)$$

Kernel Independent FMM - Implementation Issues

- No need for new software implementation for large class of compatible Kernels
- Can built singly, extensible, and optimisable software implementation

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Motivation

- Python has emerged as a standard in scientific and data intensive computing
- Desire a high quality software implementation which is also highly performant and easily portable
- Tradeoff performance of compiled languages for engineering ease, and portability

Goals

- Create a performant 3D Python implementation of the KIFMM
- Write software in an extensible and well tested way
- Take advantage of distributed and parallel computing concepts as much as possible

Outcomes - Vectorised Data Structures

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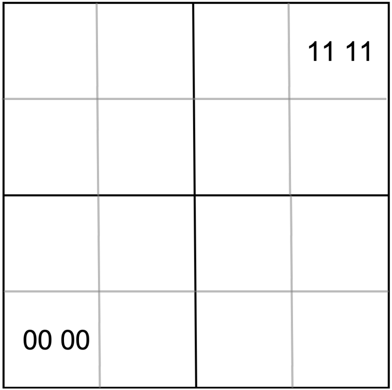
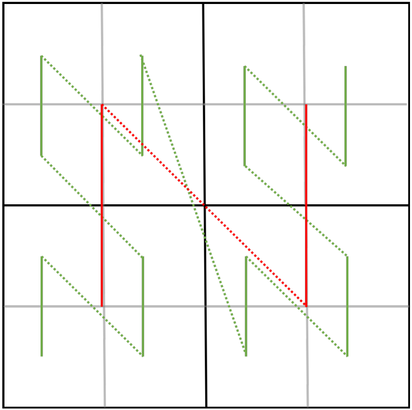
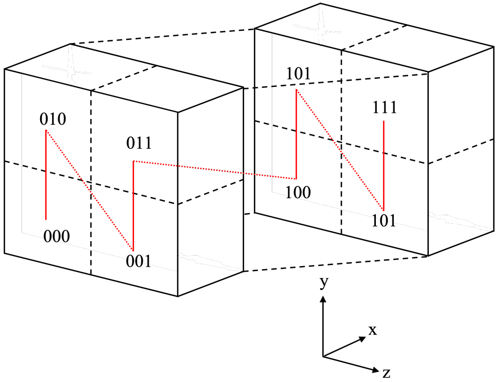
Outcomes - Vectorised Data Structures



Outcomes - Vectorised Data Structures



Outcomes - Vectorised Data Structures



Outcomes - JIT Compilation

- Pre-analyse interpreted bytecode for reused calculations, compile into assembly and cache
- Use Numba on top of Numpy Containers

Outcomes - Multiprocessing & Operator caching

- Pre-compute and cache all operators, used in rhs of least squares problem, $(\phi^A = (\alpha I + K_A^* K_A)^{-1} K_B \phi^B)$
- Use process level parallelism to distribute the computation
- Use HDF5 for rapid loading to memory in comparison to simple serialisation

Outcomes - Low-Rank SVD Compression

- I - number of source boxes in interaction list of a given target box

$$K_{\text{source}} = (\alpha I + K^{*}_{\text{source}} K_{\text{source}})^{-1} K_{\text{target}} \tag{7}$$

$$K_{\text{concatenated}} = [K_1 | K_2 | ... | K_I] \quad \text{, where, } \{K_i | i \in [1, 2, ..., I]\} \tag{8}$$

Outcomes - Low-Rank SVD Compression

- The rank of the full concatenated matrix is r
- Can truncate sum to target rank, k, and tune to retain most of the action of the matrix

$$K_{\text{concatenated}} = U\Sigma V^* \tag{9}$$

$$K_{\text{concatenated}} = \sum_{j=1}^{r} \sigma_j u_j v_j^* \tag{10}$$

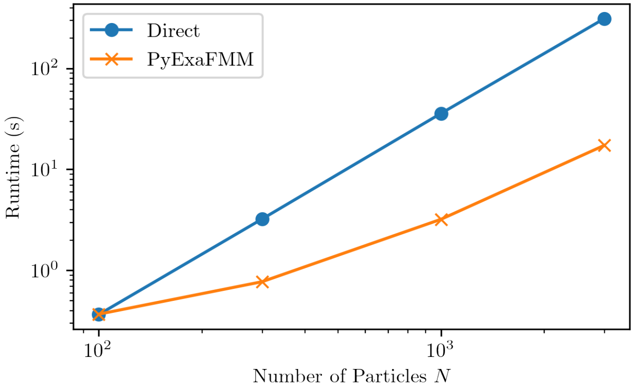
$$\hat{K}_{\text{concatenated}} = \sum_{j=1}^{k} \sigma_j u_j v_j^* \tag{11}$$

UCL

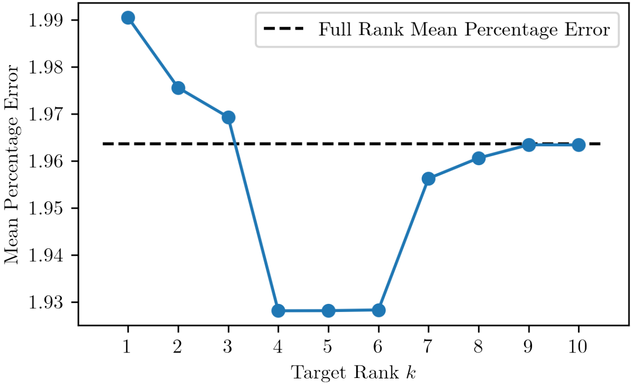
Outcomes - Extensible Software Design

- Full unit tests
- Implements dependency inversion for operator loading
- Implements separation of concerns, between optimisation and logic

Outcomes - Complexity Achieved



Outcomes - Optimum Target Rank Investigated



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Modern Architectures

- Program for shared and distributed memory paradigms [5, 4, 6]
- Take advantage of heterogenous architectures (GPU/CPU) [4, 6]

Randomised SVD Compression

- Reduce cost of wastefully computing full-rank SVD, only to discard all but first k singular values/vectors
- Can be programmed with shared memory paradigm [1, 5]

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