Modern Research Software For Fast Multipole Methods

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Declaration

I, Srinath Kailasa, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

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I leave the past five years transformed personally and professionally, the completion of this thesis simply wouldn't have been possible without the strong prevailing wind of emotional support from my family the regularity of fun with my friends, and the sympathetic and dedicated teachers and colleagues I met at UCL and across the world. It's been a pleasure to grow as a person and as a scientist with your support over these years which have been incredibly formative and I will likely carry through the rest of my life. Thank you *all* for giving me this opportunity, I'm excited for what the future brings.

सत्यमेव जयते नानृतं सत्येन पन्था वितितो देवयानः।

UCL Research Paper Declaration Form

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        i. Srinath Kailasa was the lead author and responsible for the direction of this research and the preparation of the manuscript.

        ii. Tingyu Wang offered expert guidance as on fast multipole method implementations, and critical feedback of the manuscript.

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Abstract

Software has come to be a central asset produced during computational science research. Projects that build off the research software outputs of external groups rely on the software implementing proper engineering practice, with code that is well documented, well tested, and easily extensible. As a result research software produced in the course of scientific discovery has become an object of study itself, and successful scientific software projects that operate with performance across different software and hardware platforms, shared and/or distributed memory systems, can have a dramatic impact on the research ecosystem as a whole. Examples include projects such as the SciPy and NumPy projects in Python, OpenMPI for distributed memory computing, or the package manager and build system Spack, which collectively support a vast and diverse ecosystem of scientific research.

This thesis is concerned with the development of a software platform for kernel independent Fast Multipole Methods. These algorithms have emerged in recent decades to optimally apply dense matrices that exhibit a special low-rank structure in their off-diagonal elements. Such matrices arise in numerous areas of science and engineering, for example in the linear system matrices of boundary integral formulations of problems from acoustics and electromagnetics to fluid dynamics, geomechanics and even seismology. In the best case matrices can be stored and applied in $O(N)$, in contrast to $O(N^2)$ for storage and application when computed naively. The diversity of the implementation approaches for these algorithms, as well as their intricacy, makes the development of an ergonomic, unified, software framework, that maximally re-uses data structures, is designed for high performance, distributed memory environments, and works seamlessly across platforms highly challenging.

In Chapter 1 we review the Fast Multipole Method and its kernel independent variant, going over the key challenges in achieving high performance parallel implementations. Chapter 2 reviews the challenges of software engineering in research, documenting our experience with Python as an alternative for achieving low-level performance as well as our chosen platform Rust, a relatively new language emerging

as a contender for performant and productive research software. Chapter 3 describes in detail the engineering approach of our software, and Chapter 4 demonstrates the utility of these techniques with a benchmark study of competing approaches to a critical algorithmic subcomponent enabled by our design. Chapter 5 contains benchmarks of our codes, and we conclude with a reflection on this work in Chapter 6.

Impact Statement

This thesis establishes norms and practices for developing practical implementations of the kernel independent Fast Multipole Method (kiFMM), which will be of significant utility to the developers specialising in this and related algorithms. During this research we re-visited established codes for the kiFMM, identified software construction techniques that can lead to more flexible implementations that allow users to experiment, exchange, and build upon critical algorithmic subcomponents, computational backends, and problem settings - which are often missing from competing implementations which focus achieving specific benchmarks. For example, the flexibility of the software presented in this thesis allows for the critical evaluation of key algorithmic subcomponents, such as the 'multipole to local' (M2L) operator which we presented in [2].

As the primary outputs are open-source software libraries [3, 1] which are embedded within existing open-source efforts, most significantly the Bempp project, with an existing user-base the software outputs of this thesis are likely to have a wide ranging impact in academia and industry influenced by the demand for these softwares. Furthermore, the adoption and promotion of Rust for this project, and within our group, establishes further the utility of this relatively new language for achieving high-performance in scientific codes, which in recent years has been the subject of growing interest in the wider high-performance scientific computing community.

Contents

Introduction and Background

1.1 Fast Multipole Methods

- Introduction to idea and justification of fast multipole methods - origin of idea, and difference with respect to similar ideas, and utility in the era of exascale computing.
- their research context and utility, and reason for why implementing them is still a research question.

- Review of FMM literature for software

- Go through the details of current and past projects, and detail exactly where in this context this thesis fits in.

- open questions on software side addressed by this thesis. How to make a framework that is usable, and open to extension.

- open questions on the algorithm side addressed by this thesis, with a software framework in hand can compare subcomponents of the algorithm.

1.2 Kernel Independent Fast Multipole Method

- Review of the KiFMM and variants.

- Motivation for use from a software engineering and computational performance perspective.

- Data flow during the KiFMM.

- Performance characteristics and features of the kiFMM.

- Reflection on the kiFMM and modern software and hardware

1.2.1 Laplace

1.2.2 Helmholtz

1.2.3 Shared vs Distributed Memory

Modern Programming Environments for Science

2.1 Requirements for Research Software Engineering

- Requirements and constraints on research software development.

- Hardware and software complexity, and gap between a one-off coding project and extensible maintainable software tooling.

- Review developments in computer hardware and software that make this easier to be more productive, but also more challenging to wrap together over time

- Emerging and future trends.

2.2 Python for Scientific Computing

- Summary of Python paper results

- Review of why this was thought to be a good idea, and why it might be worth trying again in the future.

- What problems does this paper address, wrt to the literature?

2.3 Rust for Scientific Computing

- Brief review of motivation and reasoning behind Rust, and which features we take advantage of

    - Review of data oriented design, how this can be enabled with traits.

Designing Software for The Fast Multipole Method

3.1 Data Oriented Design with Rust Traits

- Motivation, and review

    - How do traits enable data oriented design.

3.2 FMM Software As A Framework

- Code generation for multiple targets

    - Flexible backends

3.3 High Performance Trees

Bottlenecks in shared and distributed memory

Tree Construction approach and algorithms

Important implementation details - construction of interaction lists, neighbour finding. - construction of Morton encodings. - trade-offs of approach in shared and distributed memory - e.g. adaptive vs weakly adaptive trees. - problems with load balancing approach etc - justification - simplicity/works vs complex/private

3.4 High Performance FMM Operators

- Go through each operator of kiFMM and how it's been optimised, at a high level for M2L operators.

Comparing Field Translation Approaches for Kernel Independent Fast Multipole Method

- Review of approaches, success and failures, and what works in the context of modern software and hardware systems.

- What are important trends, and what have we actually done.

Experiments

5.1 Single Node

5.2 Multi Node

Conclusion

In this subsidiary thesis we've presented progress on the development of a new software infrastructure for fast algorithms. We've documented recent outputs towards this goal including foundational software as well as algorithmic techniques. The main outputs being an investigation into programming languages and environments most suitable for scientific computing, investigations to ensure an ergonomic design for our software, a distributed load balanced octree library designed for high-performance, as well as significant inroads to a distributed FMM based on this by studying sparsification schemes for the multipole-to-local translation operator T^{M2L}.

The immediate next steps of this project will be to publish our recent software results on octrees and the parallel FMM in an appropriate scientific journal, and release a first version of our software. The final stages of this project will focus on completing the outlined improvements to our translation operator library to achieve, and hopefully supersede the current state of the art, creating a new benchmark distributed FMM library that is open to extension to other fast algorithms.

The Adaptive Fast Multipole Method Algorithm

FMM literature distinguishes between types of relationships between neighbouring nodes with the concept of *interaction lists*. There are four such lists for a given node B, called V, U, W and X. For a leaf node B, the U list contains B itself and leaf nodes adjacent to B. and the W list consists of the descendants of B's neighbours whose parents are adjacent to B. For non-leaf nodes, the V list is the set of children of the neighbours of the parent of B which are not adjacent to B, and the X list consists of all nodes A such that B is in their W lists. The non-adaptive algorithm is similar, however the W and X lists are empty

Algorithm 1 Adaptive Fast Multipole Method.

N is the total number of points
s is the maximum number of points in a leaf node.

Step 1: Tree construction
for each node B in *preorder* traversal of tree, i.e. the nodes are traversed bottom-up, level-by-level, beginning with the finest nodes. **do**
  subdivide B if it contains more than s points.
end for
for each node B in *preorder* traversal of tree **do**
  construct *interaction lists*, U, V, X, W
end for

Step 2: Upward Pass
for each leaf node B in *postorder* traversal of the tree, i.e. the nodes are traversed top-down, level-by-level, beginning with the coarsest nodes. **do**
  P2M: compute multipole expansion for the particles they contain.
end for
for each non leaf node B in *postorder* traversal of the tree **do**
  M2M: form a multipole expansion by translating the expansion centre of its children to its centre and summing their multipole expansion coefficients.
end for

Step 3: Downward Pass
for each non-root node B in *preorder* traversal of the tree **do**
  M2L: translate multipole expansions of nodes in B's V list to a local expansion at B.
  P2L: translate the charges of particles in B's X to the local expansion at B.
  L2L: translate B's local expansion to its children by translating its expansion centre to the centre of its children, and assigning the same coefficients.
end for
for each leaf node B in *preorder* traversal of the tree **do**
  P2P: directly compute the local interactions using the kernel between the particles in B and its U list.
  L2P: translate local expansions for nodes in B's W list to the particles in B.
  M2P: translate the multipole expansions for nodes in B's W list to the particles in B.
end for

Hyksort

The parallel splitter selection and HykSort algorithms are provided below. In terms of complexity analysis, we adapt the analysis provided in section 3.4 of [4]. The main costs of SampleSort is sorting the splitters and the MPI collectives for data reshuffling. This can lead to a load imbalance and network congestion, represented by a constant c below,

$$T_{ss} = t_c c \frac{N}{p} \log \frac{N}{p} + (t_s + t_w p) \log^2 p + t_w c \frac{N}{p}$$

Where t_c is the intranode memory slowness (1/RAM bandwidth), t_s interconnect latency, t_w is the interconnect slowness (1/bandwidth), p is the number of MPI tasks in *comm*, and N is the total number of keys in an input array A, of length N.

The parallel splitter selection algorithm for determining k splitters uses MPI collectives, `All_Gather`() and `All_Reduce`(). The main cost is in determining the local ranks of the samples using a binary search. The number of iterations η depends on the input distribution, the required tolerance N_ϵ/N and the parameter β. The expected value of η varies as $\log(\epsilon)/\log(\beta)$ and β is chosen experimentally to minimise the running time, leading to a complexity of,

$$T_{ps} = \eta t_c \beta k \log \frac{N}{p} + \eta (t_s + t_w \beta k) \log p$$

HykSort relies on a specialised `All_to_all_kway`() collective, we defer to the

original paper for details. It uses only point to point communications with staged message sends and receives, allowing HykSort to minimise network congestion. It has $\log p / \log k$ stages with $O(N/p)$ data transfer and k messages for each task in every stage. This leads to a complexity of,

$$T_{a2a} = \left(t_s k + t_w \frac{N}{p} \right) \frac{\log p}{\log k}$$

Finally, HykSort has the same communication pattern as `All_to_all_kway`(). In addition it relies on the parallel splitter selection algorithm to determine splitters. The main computational cost is the initial local sort, and merging k arrays during each iteration.

$$T_{Hk} = t_c \frac{N}{p} \log \frac{N}{p} + \left(t_c \frac{N}{p} + T_{ps} \right) \frac{\log p}{\log k} + T_{a2a} \tag{B.1}$$

Unlike SampleSort, the complexity of HykSort doesn't involve any $O(p)$ terms. This is the term that can lead to network congestion for higher core counts.

Algorithm 2 Parallel Select

Input: A_r - array to be sorted (local to each process), n - number of elements in A_r, N - total number of elements, $R[0, ..., k-1]$ - expected global ranks, N_ϵ - global rank tolerance, $\beta \in [20, 40]$,
Output: $S \subset A$ - global splitters, where A is the global array to be sorted, with approximate global ranks $R[0, ..., k-1]$
$R^{\text{start}} \leftarrow [0, ..., 0]$ - Start range of sampling splitters
$R^{\text{end}} \leftarrow [n, ..., n]$ - End range of sampling splitters
$n_s \leftarrow [\beta/p, ..., \beta/p]$ - Number of local samples, each splitters
$N_{\text{err}} \leftarrow N_\epsilon + 1$
while $N_{\text{err}} > N_\epsilon$ **do**
  $Q' \leftarrow A_r[\texttt{rand}(n_s, (R^{\text{start}}, R^{\text{end}}))]$
  $Q \leftarrow \texttt{Sort}(\texttt{All\_Gather}(\hat{Q}'))$
  $R^{loc} \leftarrow \texttt{Rank}(Q, A_r)$
  $R^{glb} \leftarrow \texttt{All\_Reduce}(R^{loc})$
  $I[i] \leftarrow \text{argmin}_j |R^{glb} - R[I]|$
  $N_{err} \leftarrow \max |R^{glb} - RI|$
  $R^{\text{start}} \leftarrow R^{loc}[I-1]$
  $R^{\text{end}} \leftarrow R^{loc}[I+1]$
  $n_s \leftarrow \beta \frac{R^{\text{end}} - R^{\text{start}}}{R^{glb}[I+1] - R^{glb}[I-1]}$
end while
return $S \leftarrow Q[I]$

Algorithm 3 HykSort

Input: A_r - array to be sorted (local to each process), *comm* - MPI communicator, p - number of processes, p_r - rank of current task in *comm*
Output: globally sorted array B.
while $p > 1$, Iters: $O(\log p / \log k)$ **do**
  $N \leftarrow$ `MPI_AllReduce`$(|B|, comm)$
  $s \leftarrow$ `ParallelSelect`$(B, \{iN/k; i = 1, ..., k-1\})$
  $d_{i+1} \leftarrow$ `Rank`(s_i, B), $\forall i$
  $[d_0, d_k] \leftarrow [0, n]$
  $color \leftarrow \lfloor kp_r/p \rfloor$
  parfor $i \in 0, ..., k-1$ **do**
    $p_{recv} \leftarrow m((color - i) \mathrm{mod} k) + (p_r \mathrm{mod} m)$
    $R_i \leftarrow$ `MPI_Irecv`$(p_{recv}, comm)$
  end parfor
  for $i \in 0, ..., k-1$ **do**
    $p_{recv} \leftarrow m((color - i) \mathrm{mod} k) + p_r \mathrm{mod} m$
    $p_{send} \leftarrow m((color + i) \mathrm{mod} k) + p_r \mathrm{mod} m$
    $j \leftarrow 2$
    while $i > 0$ and $i \mathrm{mod} j = 0$ **do**
      $R_{i-j} \leftarrow$ `merge`$(R_{i-j}, R_{i-j/2})$
      $j \leftarrow 2j$
    end while
    `MPI_WaitRecv`(p_{recv})
  end for
  `MPI_WaitAll`()
  $B \leftarrow$ `merge`$(R_0, R_{k/2})$
  $comm \leftarrow$ `MPI_Comm_splitt`(color, comm)
  $p_r \leftarrow$ `MPI_Comm_rank`$(comm)$
end while
return B

Distributed Octrees

C.1 Useful Properties of Morton Encodings

These properties are taken from Appendix A in [5]

1. Sorting the leaves by their Morton keys is equivalent to pre-order traversal of an octree. If one connects the centers of the boxes in this order we observe a 'Z'-pattern in Cartesian space. Nearby octants in Morton order are clustered together in Cartesian space.

2. Given three octants $a < b < c$ and $c \notin$ Descendants(b)

$$a < d < c \forall d \in \{\text{Descendants(b)}\}$$

3. The Morton key of any box is less than those of its descendants.

4. Two distinct octants overlap only if and only if one is an ancestor of another.

5. The Morton key of any node and its first child are consecutive.

6. The first descendant at level l, FirstDescendant(N, l) of any box N is the descendant at that level with the least Morton key.

7. The range $(N, \text{DeepestFirstDescendent}(N)]$ contains only the first descendants of N at different levels, and hence there can be no more than one leaf in this range in the entire linear octree.

8. The last descendant at level l of N, LastDescendant(N, l) of any node N is the descendant at that level with the greatest Morton key.

9. Every octant in the range $(N, \text{DeepestLastDescendant}(N)]$ is a descendant of N.

C.2 Algorithms Required for Constructing Distributed Linear Octrees

These listings are adapted from [5].

Algorithm 4 Remove Overlaps From Sorted List of Octants (Sequential) - `Linearise`. Favour smaller octants over larger overlapping octants.

Input: A sorted list of octants, W.
Output: R, an octree with no overlaps.
Work: $O(n)$, where n=len(W).
Storage: $O(n)$, where n=len(W).
for i $\leftarrow$ 1 to len(W) **do**
  if $W[i] \notin \{\text{Ancestors}(W[i+1]), W[i+1]\}$ **then**
    $R \leftarrow R + W[i]$
  end if
end for
$R \leftarrow R + W[\text{len}(i)]$

Algorithm 5 Construct a Minimal Linear Octree Between Two Octants (Sequential) - `CompleteRegion`.

Input: Two octants a and b, where $a > b$ in Morton order.
Output: R, minimal linear octree between a and b.
Work: $O(n \log n)$, where n=len(R).
Storage: $O(n)$, where n=len(R).
for $w \in W$ **do**
  if $a < w < b$ **and** $w \notin \{\text{Ancestors}(b)\}$ **then**
    $R \leftarrow R + w$
  else if $w \notin \{\text{Ancestors}(a), \text{Ancestors}(b)\}$ **then**
    $W \leftarrow W - w + \text{Children}(w)$
  end if
end for
Sort(R)

Algorithm 6 Balance a Local Octree (Sequential) - `Balance`. A 2:1 balancing is enforced, such that adjacent octants are at most twice as large as each other.

Input: A local octree W, on a given node.
Output: R, a 2:1 balanced octree.
Work: $O(n \log n)$, where n=len(R).
Storage: $O(n)$, where n=len(W).
R = Linearize(W)
for $l \leftarrow$ Depth to 1 **do**
  $Q \leftarrow \{x \in W | \text{Level}(x) = l\}$
  for $q \in Q$ **do**
    for $n \in \{\text{Neighbours}(q), q\}$ **do**
      if $n \notin R$ and Parent(n) $\notin R$ **then**
        $R \leftarrow R + \text{Parent}(n)$
        $R \leftarrow R + \text{Siblings}(\text{Parent}(n))$
      end if
    end for
  end for
end for

Algorithm 7 Construct Distributed Octree (Parallel)

Input: A distributed list of points L, and a parameter n_{crit} specifying the maximum number of points per octant.
Output: A complete linear octree, B.
Work: $O(n \log n)$, where n=len(L).
Storage: $O(n)$, where n=len(L).
$F \leftarrow$ [Octant(p, MaxDepth), $\forall p \in L$]
ParallelSort(F)
$B \leftarrow$ BlockPartition(F), using algorithm (8)
for $b \in B$ **do**
  if NumberOfPoints(b) $> n_{\text{crit}}$ **then**
    $B \leftarrow B - b +$ Children(b)
  end if
end for

# Optional Balancing over subtrees, f.
if Balance = True **then**
  for $f \in F$ **do**
    Balance(f), using algorithm (6)
  end for
  ParallelSort(F)
  for $f \in F$ **do**
    Linearise(f), using algorithm (4)
  end for
end if

Algorithm 8 Partitioning Octants Into Coarse Parallel Blocks (Parallel) - `BlockPartition`.

Input: A distributed list of octants F.
Output: A list of blocks G, F redistributed but the relative order of the octants is preserved.
Work: $O(n)$, where n=len(F).
Storage: $O(n)$, where n=len(F).
$T \leftarrow$ CompleteRegion(F[1], F[len(F)]), using algorithm (5)
$C \leftarrow \{x \in T | \forall y \in T, \text{Level}(x) \leq \text{Level}(y)\}$
$G \leftarrow$ CompleteOctree(C), using algorithm (9)
for $g \in G$ **do** weight(g) $\leftarrow$ len($F_{global} \cap \{g, \{\text{Descendents (g)}\}\}$)
end for
$F \leftarrow F_{global} \cap \{g, \{\text{Descendants}(g)\} \forall g \in G\}$

Algorithm 9 Construct a Complete Linear Octree From a Set of Seed Octants Spread Across Processors (Parallel) - `CompleteOctree`

Input: A distributed sorted list of seeds L.
Output: R, a complete linear octree.
Work: $O(n \log n)$, where n=len(R).
Storage: $O(n)$, where n=len(R).
$L \leftarrow$ Linearise(L), using algorithm (4).
if rank = 0 **then**
L.push_front(FirstChild(FinestAncestors(DeepestFirstDescendent(root), L[1])))
end if
if rank = $n_p - 1$ **then**
L.push_back(LastChild(FinestAncestors(DeepestLastDescendent(root), L[len(L)])))
end if
if rank ¿ 0 **then**
Send(L[1], (rank-1))
end if
if rank ¡ ($n_p - 1$) **then**
L.push_back(Receive())
end if
for $i \leftarrow 1$ to (len(L)-1) **do**
$A \leftarrow$ CompleteRegion($L[i]$, $L[i+1]$), using algorithm (5)
end for
if rank = $n_p - 1$ **then**
$R \leftarrow R + L$[L]
end if

Bibliography

[1] Srinath Kailasa. "kifmm-rs: A Kernel-Independent Fast Multipole Framework in Rust". Submitted to Journal of Open Source Software. 2024.

[2] Srinath Kailasa, Timo Betcke, and Sarah El Kazdadi. "M2L Translation Operators for Kernel Independent Fast Multipole Methods on Modern Architectures". Submitted to SIAM Journal on Scientific Computing. 2024.

[3] Srinath Kailasa et al. "PyExaFMM: an exercise in designing high-performance software with Python and Numba". In: *Computing in Science & Engineering* 24.5 (2022), pp. 77–84.

[4] Hari Sundar, Dhairya Malhotra, and George Biros. "Hyksort: a new variant of hypercube quicksort on distributed memory architectures". In: *Proceedings of the 27th international ACM conference on international conference on supercomputing*. 2013, pp. 293–302.

[5] Hari Sundar, Rahul S Sampath, and George Biros. "Bottom-up construction and 2: 1 balance refinement of linear octrees in parallel". In: *SIAM Journal on Scientific Computing* 30.5 (2008), pp. 2675–2708.