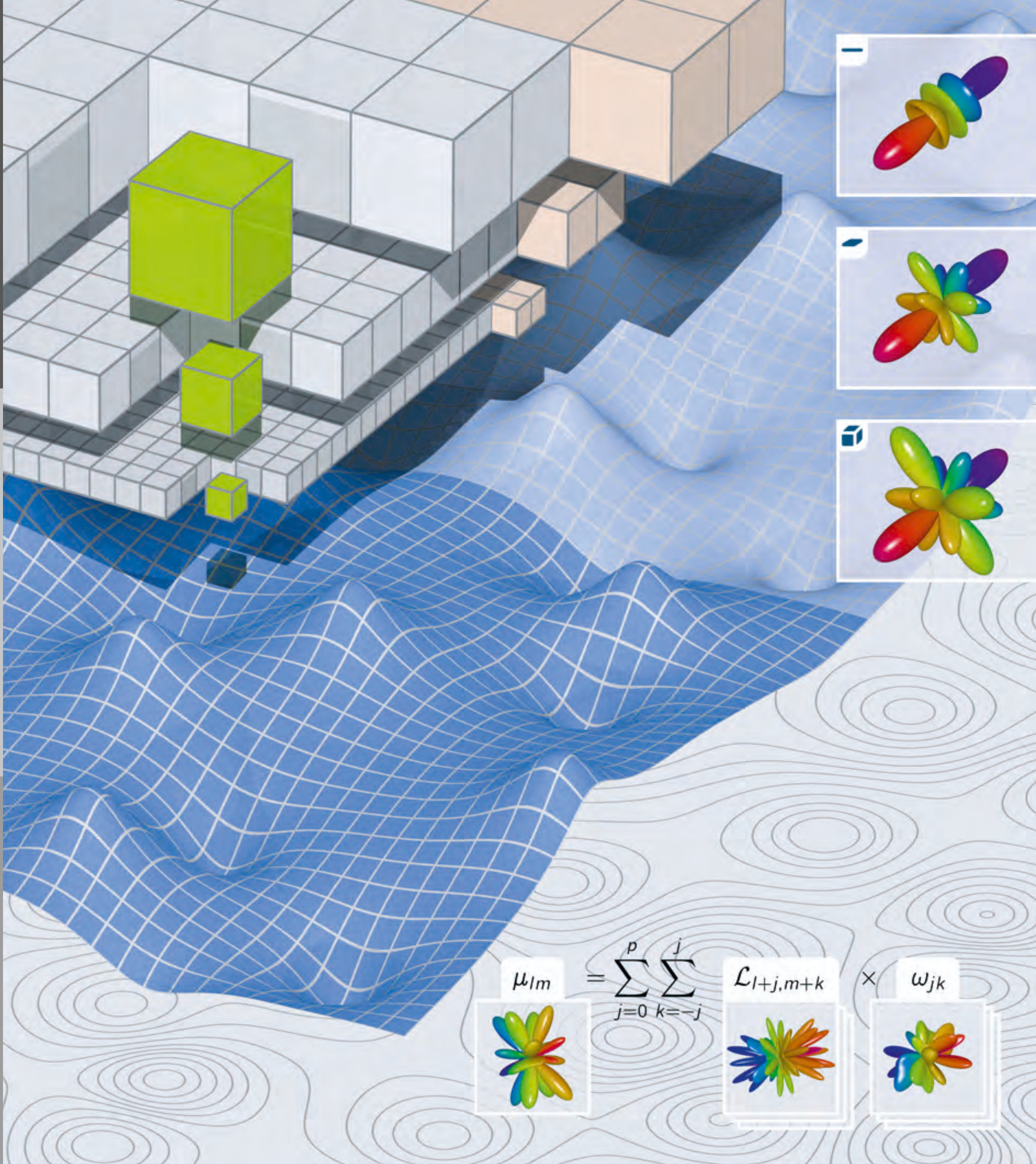

Periodic Boundary Conditions and the Error-Controlled Fast Multipole Method

Ivo Kabadshow

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Schriften des Forschungszentrums Jülich
IAS Series Volume 11

ISSN 1868-8489 ISBN 978-3-89336-770-2

Contents

1. Introduction **1**
1.1. The N-body Problem . . . 1
1.1.1. Simple Schemes to Reduce the Complexity . . . 3
1.1.2. Different Types of Potentials . . . 3
1.2. Fast Summation Techniques . . . 3

2. FMM in Three Dimensions **7**
2.1. Informal Description of the FMM . . . 7
2.2. Mathematical Preliminaries . . . 10
2.2.1. Expansion of the Inverse Distance . . . 11
2.2.2. Spherical Harmonic Addition Theorem . . . 12
2.2.3. Expansion of Particle-Particle Interactions . . . 15
2.2.4. Addition Theorem for Regular Solid Harmonics . . . 17
2.2.5. Addition Theorem for Irregular Solid Harmonics . . . 18
2.2.6. Formal Double Sum Manipulations . . . 19
2.3. Mathematical Operators . . . 20
2.3.1. Translation of a Multipole Expansion (M2M) . . . 20
2.3.2. Conversion of a Multipole Expansion into a Local Expansion (M2L) . . . 21
2.3.3. Translation of a Local Expansion (L2L) . . . 22
2.3.4. Rotation-Based Operators . . . 25
2.3.5. Further Operator Compression . . . 26
2.4. $\mathcal{O}(N \log N)$ Algorithm . . . 27
2.5. $\mathcal{O}(N)$ Algorithm . . . 30
2.6. Implementation Details . . . 35
2.6.1. Fractional Tree Depth . . . 35
2.6.2. Data Structures . . . 36
2.6.3. Minimization of Near Field and Far Field Computation Time . . . 40
2.6.4. Limitations of the Algorithm . . . 41
2.7. Error Analysis . . . 44
2.7.1. Worst Case Error Bound . . . 45
2.7.2. Improved Workflow / Error Bound . . . 47
2.7.3. Stage I of the Error Estimation Scheme . . . 48
2.7.4. Stage II of the Error Estimation Scheme . . . 54

2.7.5. FMM without Far Field Contributions 67
2.7.6. Further Analysis of the Error Bound 68

3. FMM and Periodic Boundary Conditions **77**
3.1. Minimum Image Convention 77
3.2. Definition of the Boundary Condition 78
3.2.1. Three Dimensional Periodicity 78
3.2.2. Two Dimensional Periodicity 79
3.2.3. One Dimensional Periodicity 79
3.2.4. Periodic Potential and Energy 79
3.3. Convergence of Lattice Sums 80
3.4. Ewald-Based Summation Schemes 81
3.5. Parameter-Free Renormalization Approach 84
3.5.1. Informal Description 84
3.5.2. Mathematical Operators 84
3.5.3. Lattice Sum Algorithm 86
3.6. Implementation Details 90
3.6.1. Additional FMM Pass for the Lattice Operator 91
3.6.2. Modifications of FMM Pass 1–5 91
3.6.3. Fractional Tree Depth and Periodic Boundary Conditions 92
3.6.4. Dipole Correction 92
3.7. Periodic Boundaries and Error Control 92
3.7.1. Stage I of the Error Estimation Scheme 92
3.7.2. Stage II of the Error Scheme 94

4. Performance Details of the FMM Implementation **101**
4.1. Scaling 101
4.2. Precision Verification 102
4.3. Benchmark 105
4.4. Additional Features 108

5. Conclusion and Future Directions **111**
5.1. Conclusion 111
5.2. Future Directions 112

A. Appendix **115**

Bibliography **121**

The simulation of pairwise interactions in huge particle ensembles is a vital issue in scientific research. Especially the calculation of long-range interactions poses limitations to the system size, since these interactions scale quadratically with the number of particles N. Fast summation techniques like the Fast Multipole Method (FMM) can help to reduce the complexity to O(N).

This work extends the possible range of applications of the FMM to periodic systems in one, two and three dimensions with one unique approach. Together with a tight error control, this contribution enables the simulation of periodic particle systems for different applications without the need to know and tune the FMM specific parameters. The implemented error control scheme automatically optimizes the parameters to obtain an approximation for the minimal runtime for a given energy error bound.

This publication was written at the Jülich Supercomputing Centre (JSC) which is an integral part of the Institute for Advanced Simulation (IAS). The IAS combines the Jülich simulation sciences and the supercomputer facility in one organizational unit. It includes those parts of the scientific institutes at Forschungszentrum Jülich which use simulation on supercomputers as their main research methodology.

IAS Series
Volume 11
ISBN 978-3-89336-770-2

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