

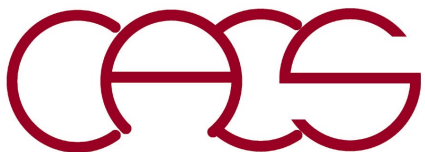
Fast Multipole Method

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Objectives: Space-time multiresolution algorithms
> Tree codes: fast multipole method
> Multiple time stepping



Top 10 Algorithms in History

In putting together this issue of *Computing in Science & Engineering*, we knew three things: it would be difficult to list just 10 algorithms; it would be fun to assemble the authors and read their papers; and, whatever we came up with in the end, it would be controversial. We tried to assemble the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century. Following is our list (here, the list is in chronological order; however, the articles appear in no particular order):

PHYS 516
CSCI 596
CSCI 653

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection

IEEE CiSE 2(1), 22 ('00)

● Fast Multipole Method

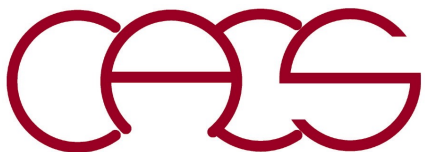
<https://ieeexplore.ieee.org/xpl/tocresult.jsp?isnumber=17639>
<https://aiichironakano.github.io/cs653/Greengard-FMM-JCP87.pdf>

Data Locality in MD

- **Spatial locality:** Atoms closer to each other interact more tightly
- **Temporal locality:** Computations performed in consecutive MD time steps are similar

↓ **Take advantage!**

- **Efficient simulation algorithms**
 - > **Reduced computational complexity**
 - > **Better utilization of hardware memory hierarchy (intranode)**
 - > **Minimized communication overhead (internode)**



Molecular Dynamics: N -Body Problem

- Newton's equations of motion

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = - \frac{\partial E_{\text{MD}}(\mathbf{r}^N)}{\partial \mathbf{r}_i} \quad (i = 1, \dots, N)$$

- Reliable interatomic potential

$$E_{\text{MD}} = \sum_{i < j} u_{ij}(r_{ij}) + \sum_{i, j < k} v_{jik}(\mathbf{r}_{ij}, \mathbf{r}_{ik})$$

- N -body problem

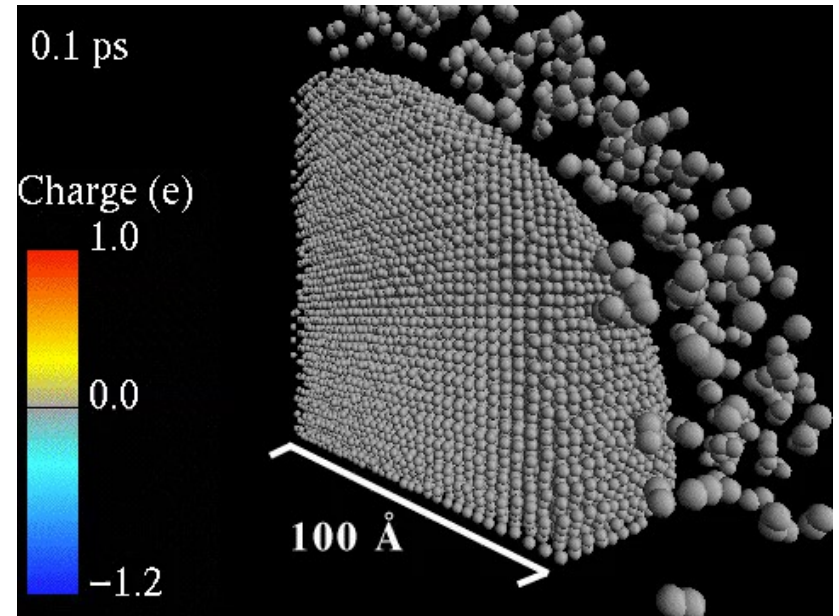
Long-range electrostatic interaction — $O(N^2)$

$$\text{Evaluate } V_{\text{es}}(\mathbf{x}) = \sum_{i=1}^N \frac{q_i}{|\mathbf{x} - \mathbf{x}_i|} \text{ at } \mathbf{x} = \mathbf{x}_j \ (j = 1, \dots, N)$$

- $O(N)$ space-time multiresolution MD (MRMD) algorithm

1. Fast multipole method (FMM) Greengard & Rokhlin, '87

2. Symplectic multiple time stepping (MTS) Tuckerman *et al.*, '92



Clustering in the Fast Multipole Method

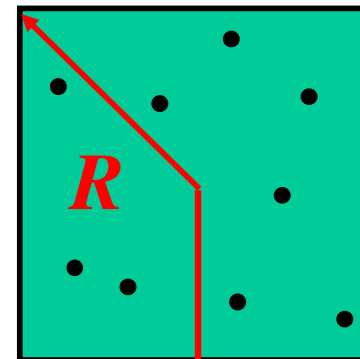
- Encapsulate far-field information in terms of multipoles at the source

$$V(\mathbf{x}) = \sum_{i=1}^N \frac{q_i}{|\mathbf{x} - \mathbf{x}_i|}$$

Spherical harmonics

$$= \sum_{l=0}^{\infty} \sum_{m=-l}^l \left\{ \sum_{i=1}^N q_i r_i^l Y_l^{*m}(\theta_i, \phi_i) \right\} \frac{Y_l^m(\theta, \phi)}{r^{l+1}}$$

multipole



- Well-defined error bound

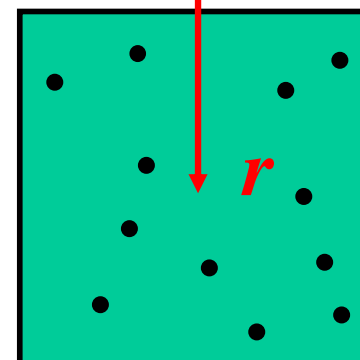
$$\text{Error} \leq \frac{\sum_{i=1}^N |q_i|}{r - R} \left(\frac{R}{r} \right)^{p+1}$$

p : l -sum truncation

- Local expansion at the destination

$$V(\mathbf{x}) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \left\{ \sum_{i=1}^N \frac{q_i Y_l^m(\theta_i, \phi_i)}{r_i^{l+1}} \right\} r^l Y_l^{*m}(\theta, \phi)$$

local term



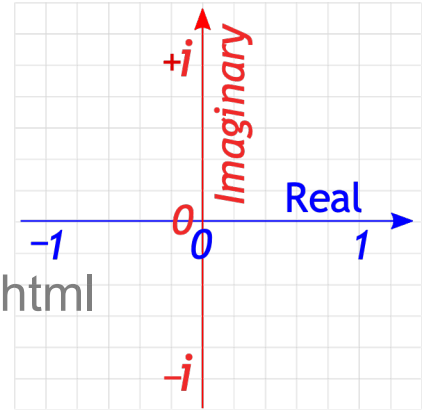
L. Greengard & V. Rokhlin, *J. Comput. Phys.* **73**, 325 ('87)

<https://aiichironakano.github.io/cs653/Greengard-FMM-JCP87.pdf>

FMM Math

{ 3D: Spherical harmonics
2D: Taylor expansion in complex plane

see lecture notes at <https://aiichironakano.github.io/cs653-lecture.html>



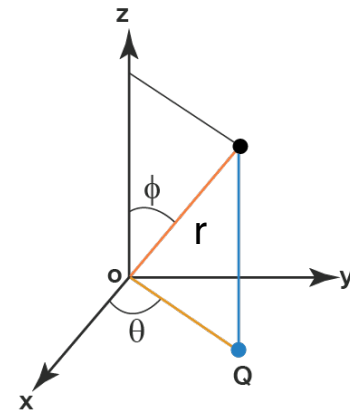
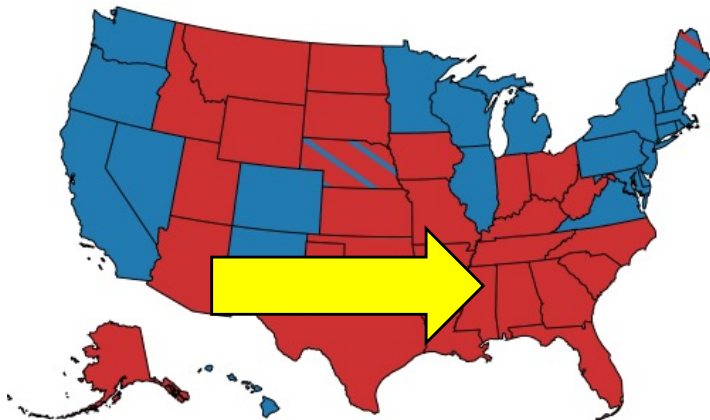
- **Multipole examples**

$$l = 0 \quad Q = \sum_{i=1}^N q_i$$

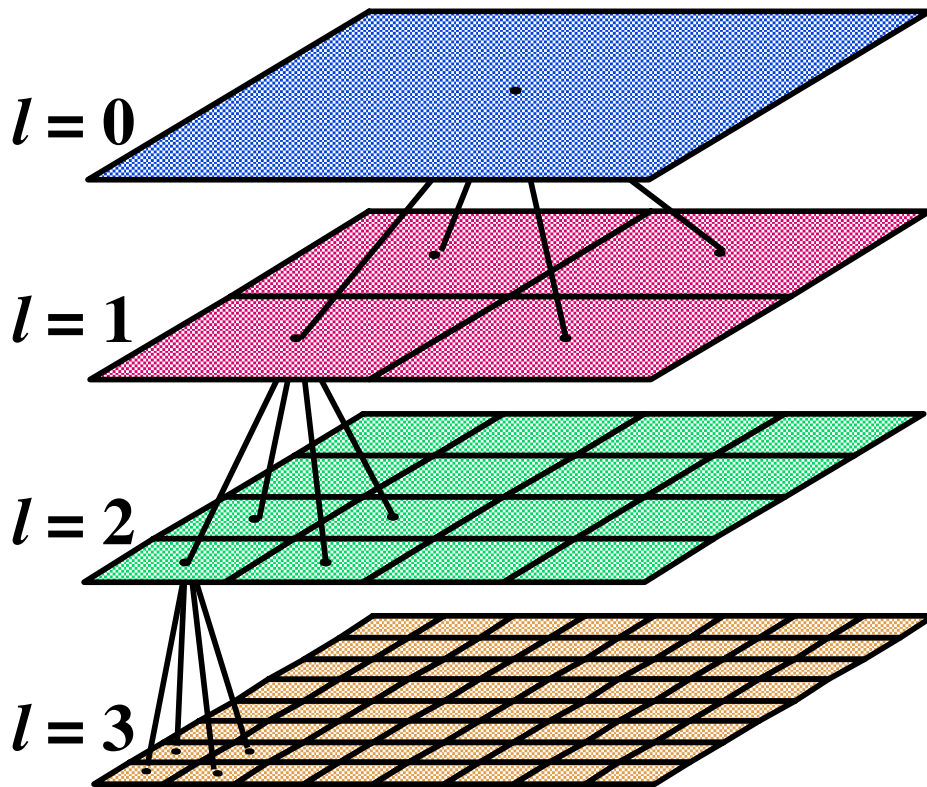
monopole

$$l = 1 \quad \vec{P} = \sum_{i=1}^N q_i r_i \cos \theta_i \begin{cases} e^{i\phi_i} \\ 1 \\ e^{-i\phi_i} \end{cases}$$

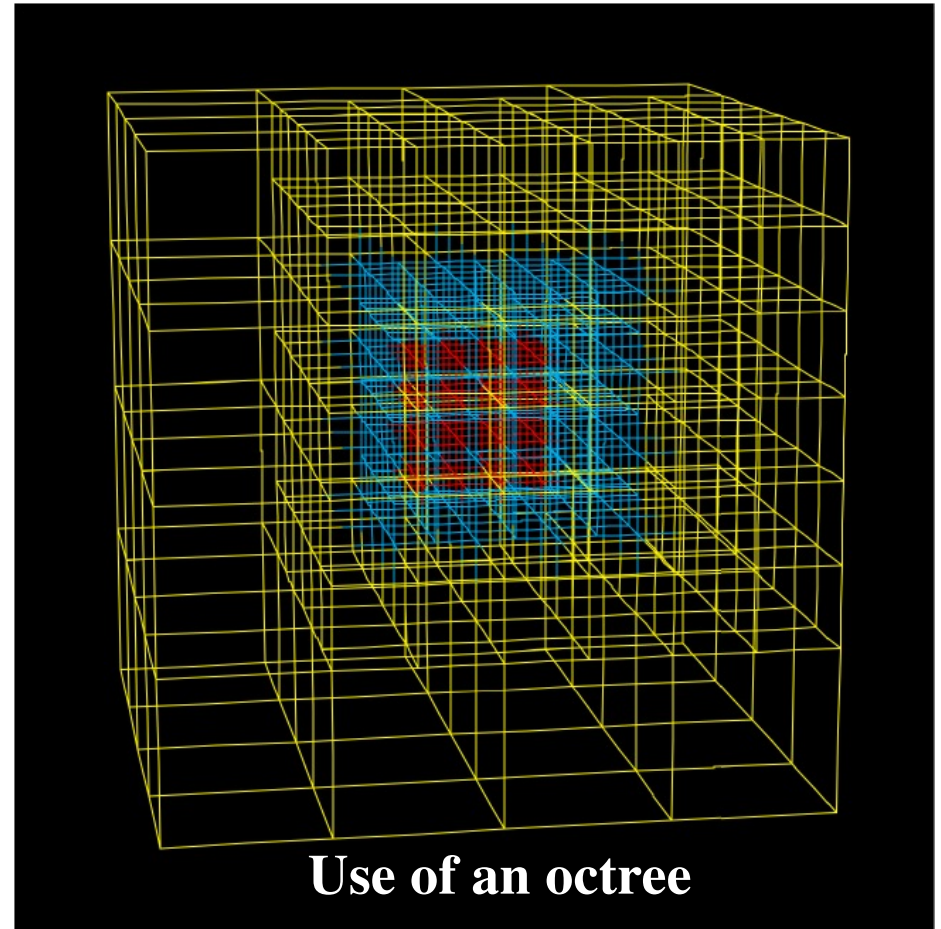
dipole



Hierarchical Abstraction



2D example

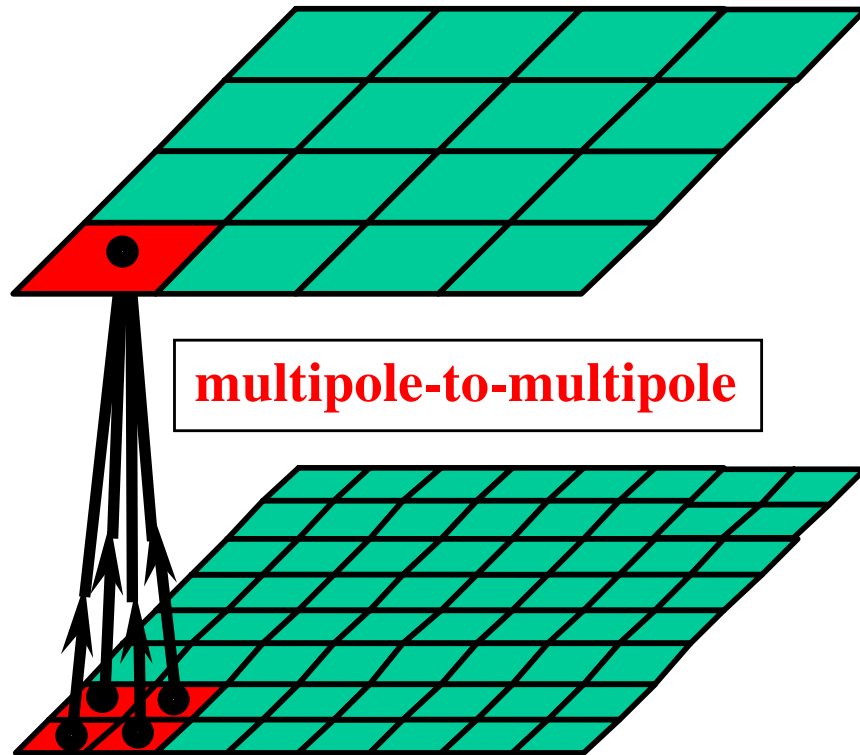


Use of an octree

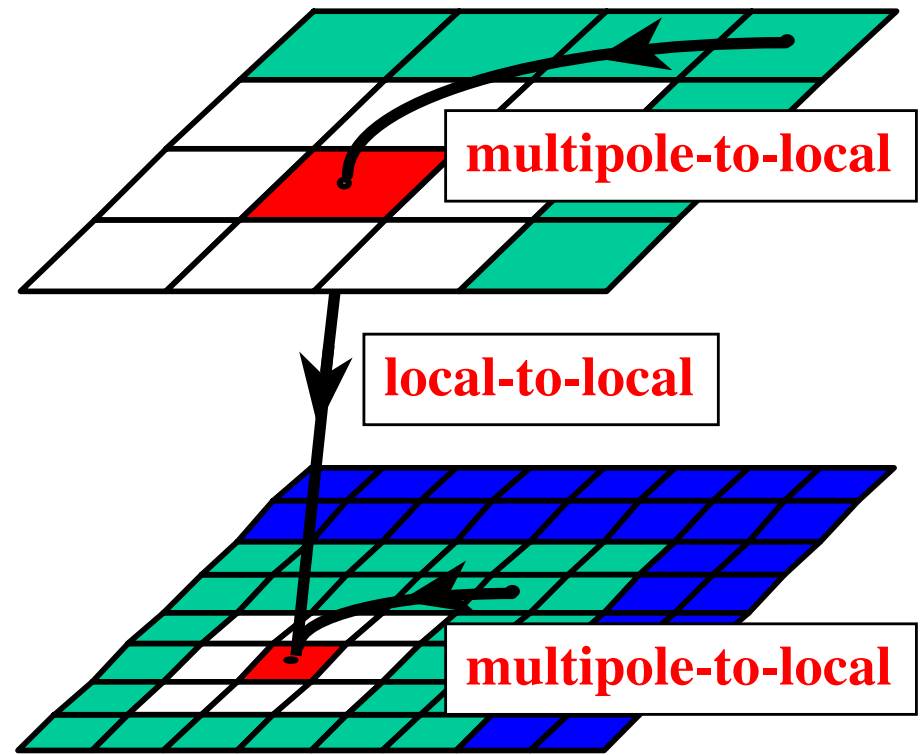
- Larger clusters for longer distances to keep the error constant
- Recursively subdivide the simulation box to form an octree in 3D or quadtree in 2D

$O(N)$ Algorithm

Upward Pass



Downward Pass

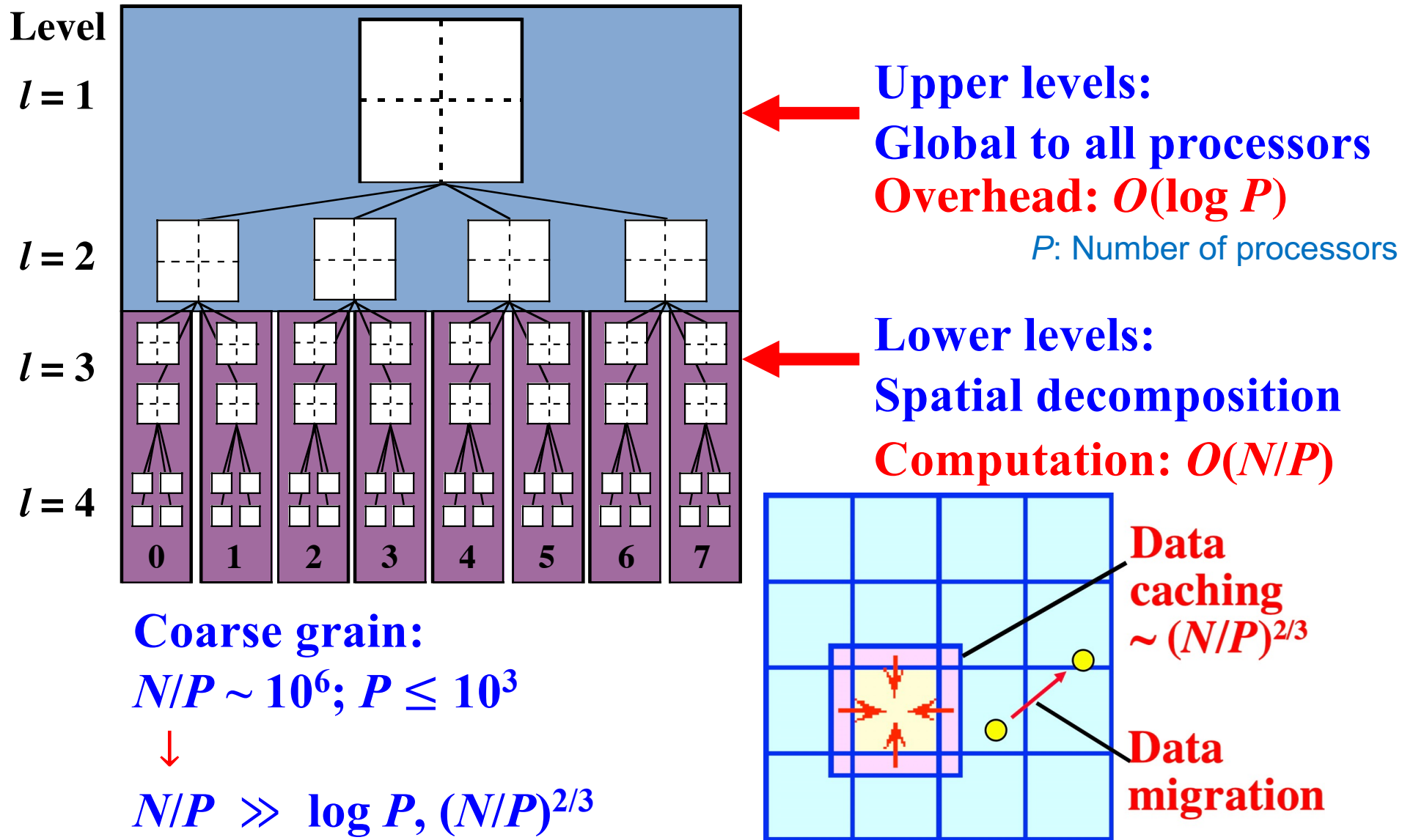


1. **Upward pass** computes multipoles for all cells: M-to-M translation
2. **Downward pass** translates multipoles to local terms for all cells
 - **Constant (189 in 3D) interactive (cousin) cells** per destination cell contribute to M-to-L translation Within parent's neighbor but not my neighbor
 - **Inheritance** from the parent cell: L-to-L translation (& **delegation**)
3. **Direct interactions** for the nearest-neighbor leaf cells

$$6^3 - 3^3$$

See lecture notes for the MM, ML & LL formula in 2D

Parallel Implementation of FMM



S. Ogata et al., *Comput. Phys. Commun.* **153**, 445 ('03)

<https://aiichironakano.github.io/cs653/Ogata-FMM-CPC03.pdf>

FMMP Code Dissemination



CPC

Program Library

Computer programs in physics and physical chemistry

[\[ADRX Licence\]](#) | [Download ADRX](#) | [E-mail ADRX](#) | (16 Kbytes)

**SCALABLE AND PORTABLE IMPLEMENTATION OF THE FAST
MULTIPOLE METHOD ON PARALLEL COMPUTERS.**

**S. OGATA, T.J. CAMPBELL, R.K. KALIA, A. NAKANO, P. VASHISHTA, S.
VEMPARALA.**

PROGRAM SUMMARY

Title of program: FMMP

Catalogue identifier: ADRX

Journal reference: Comput. Phys. Commun. 153(2003)445 [\[Article index\]](#)

Distribution format: tar gzip file

Operating system: LINUX with MPICH, IBM SP, SGI Origin

Number of lines in distributed program, including test data, etc: 3179

Keywords: Fast multipole method, Parallel computation, Stress calculation, Periodic boundary condition, Coulomb interaction, Electrostatics.

Programming language used: Fortran, C

Computer: IBM SP3 .

Nature of problem:

Parallel computations of Coulomb potentials, forces, and stress tensors for a collection of charged particles.

Method of solution:

The fast multipole method.

Typical running time:

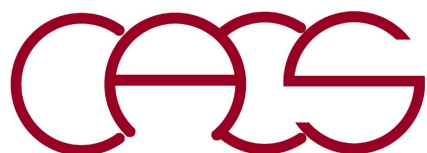
Proportional to the number of charged points.

Unusual features:

None

Additional comments:

The code has been parallelized using MPI Standard.



$O(N)$ Psuedo-charge Method for Calculating Stresses in Coulombic Systems

Microscopic stress tensor: $\vec{\pi}_i = \sum_{j \neq i} \vec{r}_{ij} \vec{f}_{ij}^T = q_i \sum_{j \neq i} q_j \frac{\vec{r}_{ij} \vec{r}_{ij}^T}{r_{ij}^3}$

Attach information of particle position to the particle charge:

$$\vec{C}(\vec{r}_i, \vec{k}) = - \sum_{j \neq i} \frac{\vec{r}_{ij}}{r_{ij}^3} q_j \exp(i\vec{k} \cdot \vec{r}_j)$$

Stress tensor is obtained by numerical differentiation:

$$\frac{\partial}{\partial k_\alpha} \{C_\beta(\vec{r}_i, \vec{k}) \exp(-i\vec{k} \cdot \vec{r}_i)\} \xrightarrow{k_\alpha \rightarrow 0} = i \sum_{j \neq i} q_j \frac{r_{ij}^\alpha r_{ij}^\beta}{r_{ij}^3}$$

No need for multipole translation operators for the stress tensor, which are unknown

S. Ogata *et al.*, *Comput. Phys. Commun.* **153**, 445 ('03)

<https://aiichironakano.github.io/cs653/Ogata-FMM-CPC03.pdf>

Example Run

Random positions in $[0,1]^2$; random charges in $[0,1]$

Npar = 1000: Number of particles
L = 4: Quadtree height
P = 6: Number of multipole terms

```
$ cc -o fmm2d fmm2d.c -lm
```

```
$ ./fmm2d
```

```
===== Max potential difference = 5.363006e-06 =====
```

```
===== Total FMM vs. direct energies & error =
```

```
-1.008232e+05 -1.008232e+05 -7.271538e-08 =====
```

```
===== FMM & direct CPU times = 7.047000e-03 8.541000e-03 =====
```

Try

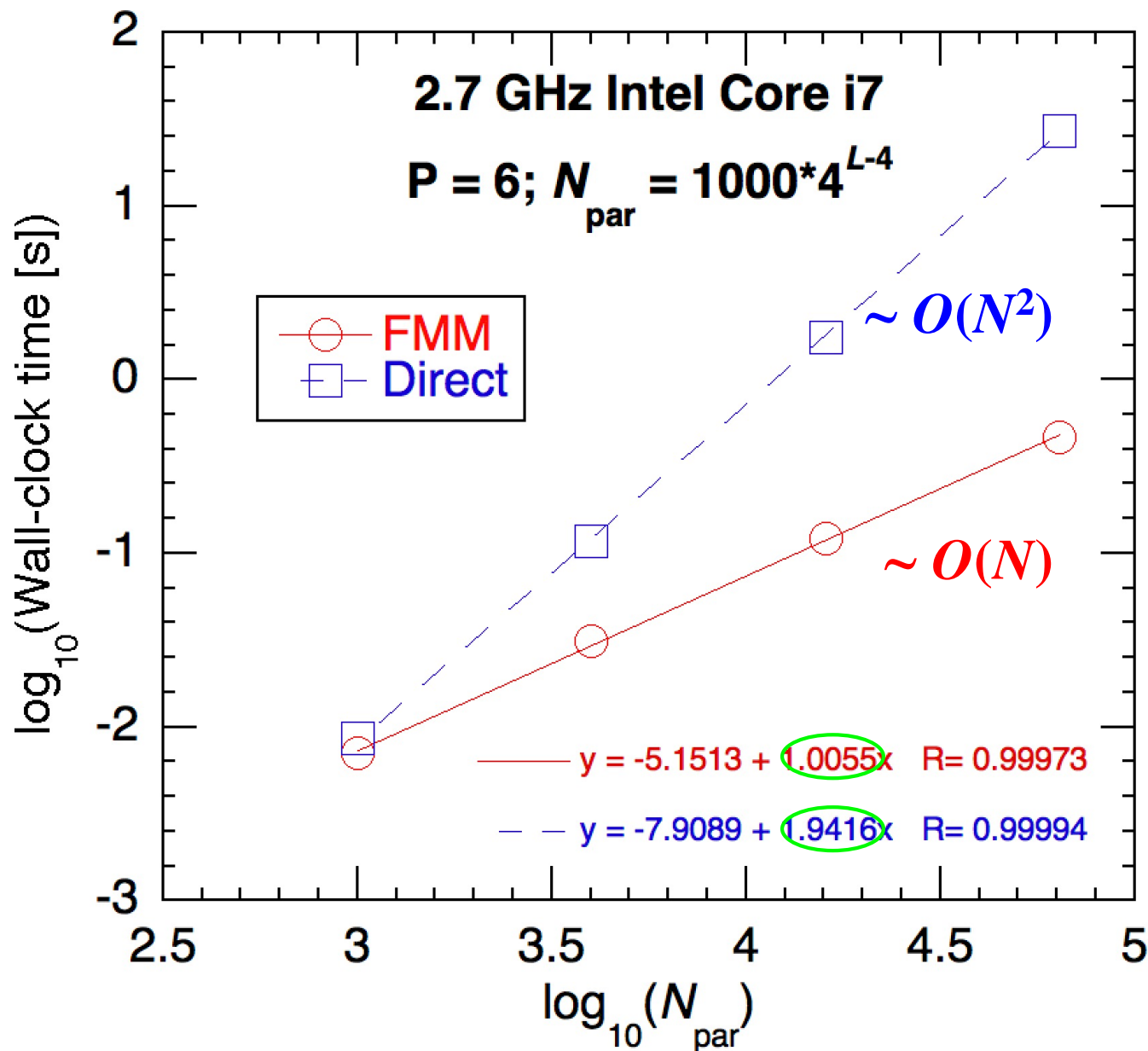
Npar = 4000/16000/64000

L = 5/6/7

P = 6

<https://aiichironakano.github.io/cs653/src/FMM/>

Time-Complexity Measurement



$$T = CN^p$$
$$\overbrace{\log T}^y = \log C + \log N^p$$
$$= \log C + p \overbrace{\log N}^x$$

Fast Multipole Method: Bottom Line

- FMM algorithm evaluates electrostatic potential $\phi(z_j)$ at all particle positions z_j ($j = 0, \dots, N_{\text{par}} - 1$).
- The whole purpose of the algorithm is to compute the local expansion coefficients, $\Psi_c^{(l)}$, of the electrostatic potential for all destination cells c at the leaf level, $l = L$, which arise from particles in non-nearest-neighbor (n.n.n.) leaf cells; they are computed *via* multipoles $\Phi_c^{(l)}$ of source cells (larger cells are used at upper tree levels for longer distances).
- The n.n.n contribution to $\phi(z_j)$ is computed using local expansion, whereas that from the nearest-neighbor (n.n.) leaf cells is computed by direct particle sum.

$$\phi(z_j) = \sum_{\alpha=0}^P \Psi_{c(j)}^{(L)}(\alpha)(z_j - z_{c(j)})^\alpha + \sum_{\substack{k \in \text{n.n.}(c(j)) \\ k \neq j}} q_k \log(z_j - z_k)$$

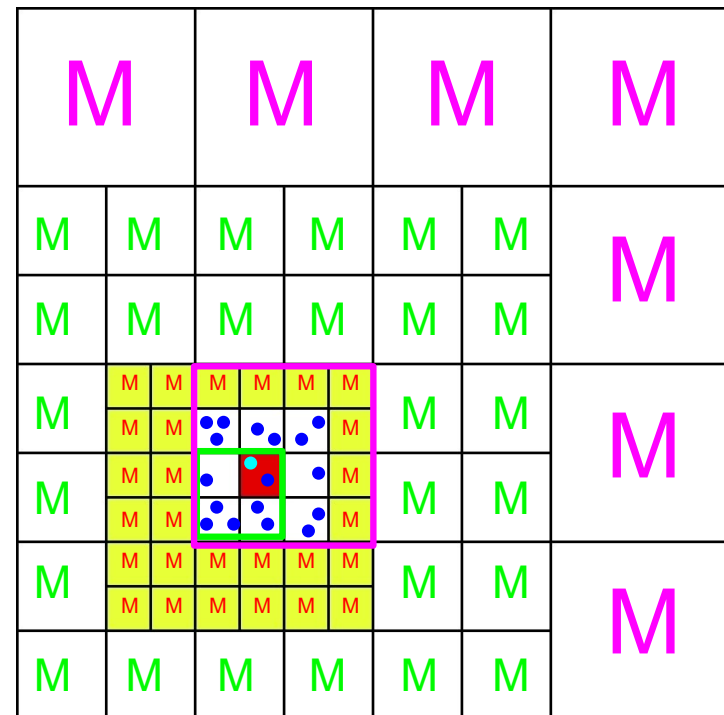
n.n.n. contribution via multipole-derived local expansion
n.n. contribution via direct particle sum

P : Truncation order of local expansion

$\Psi_c^{(l)}(\alpha)$: α -th order local expansion coefficient for cell c at level l

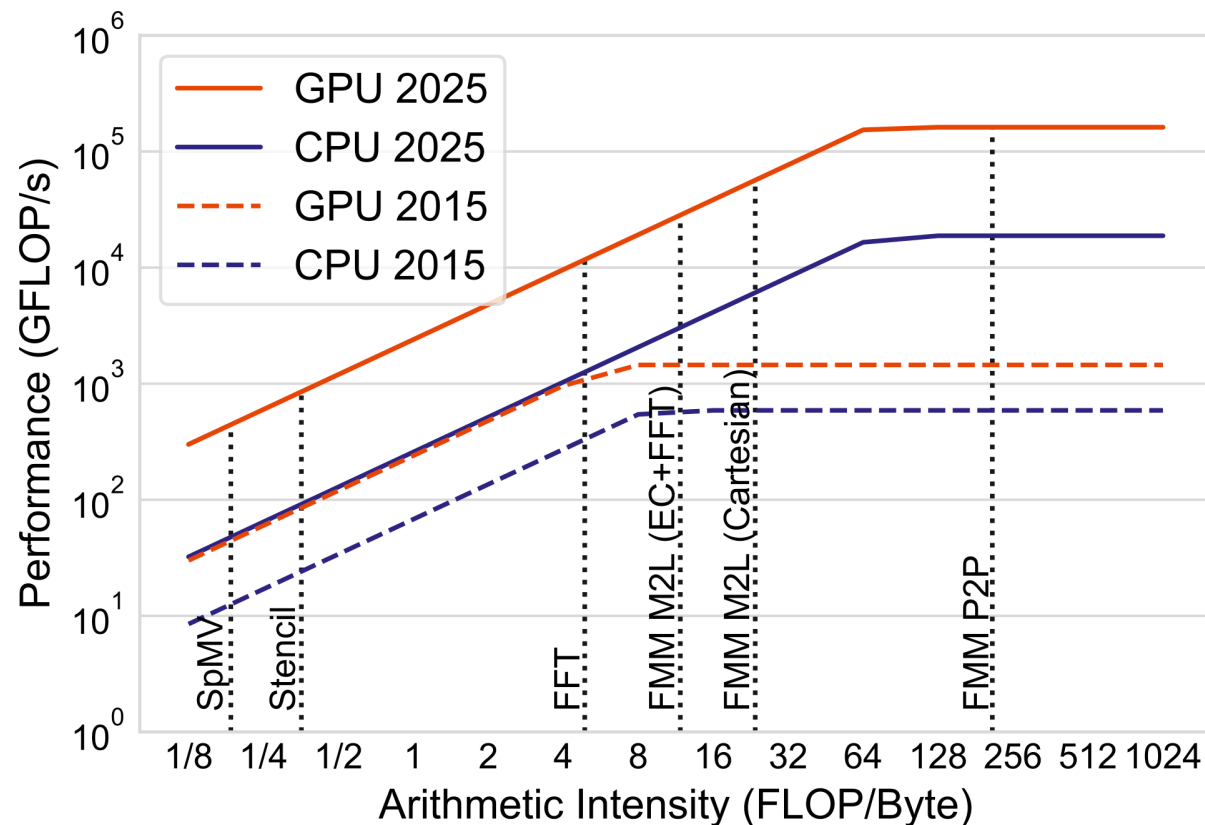
$c(j)$: The leaf cell that j -th particle belongs to

$z_{c(j)}$: The center position of cell $c(j)$



Smart vs. Brute-force Computations

- While the tree algorithm drastically reduces the computational complexity, it does not fully utilize computational resources due to low computation/communication intensity
- Time to rethink computational architectures to embrace smart (sparse) algorithms?



H. Ibeid *et al.*, *J. Par. Distrib. Comput.* **136**, 63 ('20)

cf. Quantum speedup: Q. T. Nguyen *et al.*, *Quantum* **6**, 876 ('22)

Rethinking far-field: A. Langvenis *et al.*, *IPDPS* ('25)