# Appendix D

# Fast Multipole Methods

A whole range of important problems encountered in mathematical physics are described by linear PDE's that can be cast in the following operator form

$$L\Psi = W\,, \tag{D.1}$$

where $L$ is the given linear differential operator, $\Psi$ is the solution and $W$ the source term. In many cases the solution of this problem can be found by convolving the source term $W$ with the suitable Green's function $G(x,x')$

$$\Psi(x) = \int_\Omega W(x')G(x,x')dx'\,, \tag{D.2}$$

where $\Omega$ denotes the computational domain. When the support of the source term is a collection of points, then the integral in (D.2) reduces to a sum

$$\Psi(x) = \sum_{i=1}^{N} W(x')G(x,x')\,, \tag{D.3}$$

with $N$ standing for the number of points (i.e. the computational elements). This is the origin of the *N-Body Problem*, widely encountered in various areas of astrophysics, electrostatics, heat transfer, hydrodynamics, etc. In the context of our study the general relation (D.1) corresponds to the Poisson equation (4.4), whereas the solution (D.2) is equivalent to formula (4.6). The Green's function for this problem is given by (4.5).

In the literature there are many varieties of Fast Multipole Methods (see the review paper by Strickland and Baty [131]), in our study however we will consider the Greengard-Rokhlin algorithm proposed in [52][1] All FMM's rely

[1] Application of the Greengard-Rokhlin algorithm to solution of boundary integral equations is described by Rokhlin in [115]. Problems posed in spatially periodic settings are addressed by Berman and Greengard in [14] and by Hamilton and Majda in [58].





on the observation that induction of all the particles at a given point can be split into that coming from neighbors and that due to all remaining objects. The former must be evaluated exactly, whereas for the latter approximate formulas can be derived. In these relations multipolar expansions are used to account for the induction of particle clusters. In the derivation we will use complex notation with $z = x + iy$ ($i$ is the imaginary unit), in which the potential (4.5) is given by

$$\Phi(z) = \frac{\Gamma}{2\pi i}\ln(z - z_0)\,, \tag{D.4}$$

where $\Gamma$ is the particle charge (i.e. circulation). Using the well-known expansion formula $\ln(1-\alpha) = -\sum_{k=1}^{\infty}\frac{\alpha^k}{k}$, $(|\alpha|<1)$ we obtain for (D.4)

$$\Phi(z) = \frac{\Gamma}{2\pi i}\left[\ln(z) - \sum_{k=1}^{\infty}\frac{1}{k}\left(\frac{z_0}{z}\right)^k\right],\ \ |z| > |z_0|\,. \tag{D.5}$$

In the algorithm the following four lemmas are essential:

**Lemma D.1** *For a set of particles $z_i$, $i = 1,\dots m$, with circulations $\Gamma_i$ located inside a circle with radius $r$, the induced potential at point $z$ belonging to the exterior of the circle (see Fig.D.1a) is given by*

$$\Phi(z) = Q\ln(z) + \sum_{k=1}^{\infty}\frac{a_k}{z^k}, \tag{D.6}$$
$$Q = \sum_{i=1}^{m} q_i,\ \ q_i = \frac{\Gamma_i}{2\pi i},\ \ a_k = -\sum_{i=1}^{m}\frac{q_i z_i^k}{k}\,.$$

*This is equivalent to finding an expansion centered at the origin.*

**Lemma D.2** *If the complex potential valid in the exterior of a circle centered at $z_0$ and with radius $r$ is given by $\Phi(z) = a_0\ln(z-z_0) + \sum_{k=1}^{\infty}\frac{a_k}{(z-z_0)^k}$ for every $z$ such that $|z| > |z_0| + r$ (see Fig.D.1b), then it can be re-evaluated as*

$$\Phi(z) = a_0\ln(z) + \sum_{l=1}^{\infty}\frac{b_l}{z^l}, \tag{D.7}$$
$$b_l = -\sum_{k=1}^{l}\left[a_k z_0^{l-k}\begin{pmatrix} l-1 \\ k-1\end{pmatrix}\right] - \frac{a_0 z_0^l}{l}\,.$$

*This is equivalent to shifting the expansion center from $z_0$ to the origin.*

**Lemma D.3** *If the complex potential valid in the exterior of the circle $K_1$ (see Fig.D.1c) with radius cr and centered at $z_0$ ($|z_0| > (c+1)r$) is again given by $\Phi(z) = a_0 \ln(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z-z_0)^k}$, then inside the circle $K_2$ (Fig.D.1c) centered at the origin and with radius r the complex potential can be recomputed as*

$$\Phi(z) = \sum_{l=1}^{\infty} b_l z^l, \quad b_0 = \sum_{k=1}^{\infty} (-1)^k \frac{a_k}{z_0^k} + a_0 \ln(-z_0), \tag{D.8}$$

$$b_l = \frac{1}{z_0^l} \left[ \sum_{k=1}^{\infty} \left[ (-1)^k \begin{pmatrix} l+k-1 \\ k-1 \end{pmatrix} \frac{a_k}{a_0^k} \right] - \frac{a_0}{l} \right], \quad l \geq 1 \, .$$

*This is equivalent to changing from Laurent to Taylor series expansions with different, though overlapping, ranges of validity.*

**Lemma D.4** *If $\Phi(z) = \sum_{k=1}^{n} a_k (z - z_0)^k$ represents complex potential valid inside the circle $K_1$ (see Fig.D.1d) centered at $z_0$ and with radius $|z_0| + r$, then in the interior of a circle $K_2$ with radius r and centered at the origin this potential can be recomputed as*

$$\Phi(z) = \sum_{l=1}^{\infty} b_l z^l, \quad b_l = \sum_{k=1}^{n} a_l \begin{pmatrix} k \\ l \end{pmatrix} (-z_0)^{k-1} \, . \tag{D.9}$$

*This transformation represents the shift of the expansion center from $z_0$ to the origin.*

In all of the above lemmas infinite series were used, hence the expansions are exact. Nevertheless, in numerical computations only finite numbers of terms can be used which unavoidably introduces errors. In [52] suitable error bounds were derived which are used to determine the number of terms required to achieve desired accuracy.

In the algorithm it is assumed that all the particles are located within a unit square in which an $(H + 1)$-level hierarchy of meshes is introduced. Every cell at level $i$ consists of four cells at level $(i + 1)$ (Fig.D.2a). At the center of every cell we introduce a local coordinate system in which the corresponding expansions will be computed. Below we will make use of the following definitions:

- every cell located at the level $i = \{0, \ldots, H\}$ will be regarded as the *parent* of the four *children* cells at the level $i + 1$ and contained in it (Fig.D.2a),



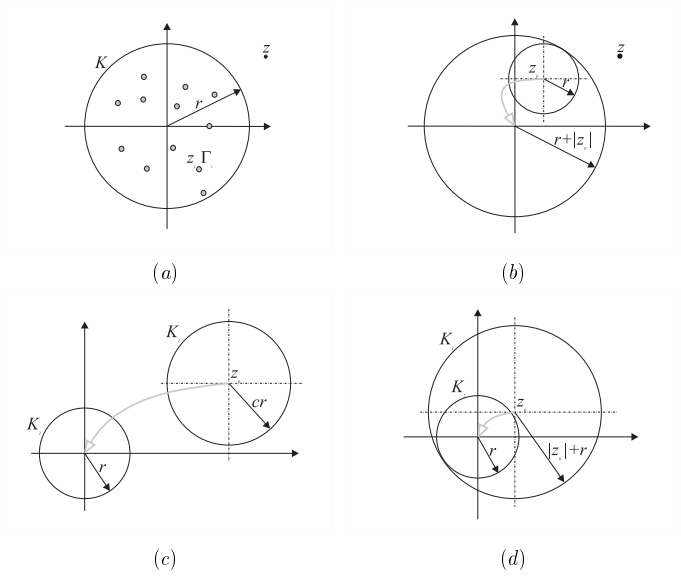
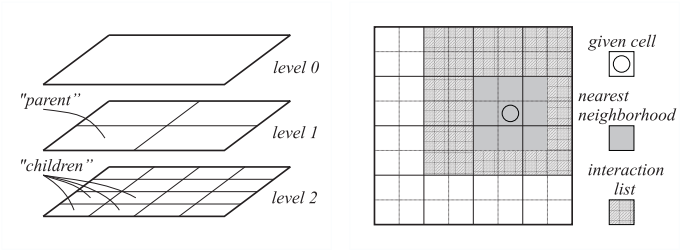



Figure D.1: Figures illustrating the four expansion lemmas (D.6)-(D.9) .




$(a)$ $(b)$

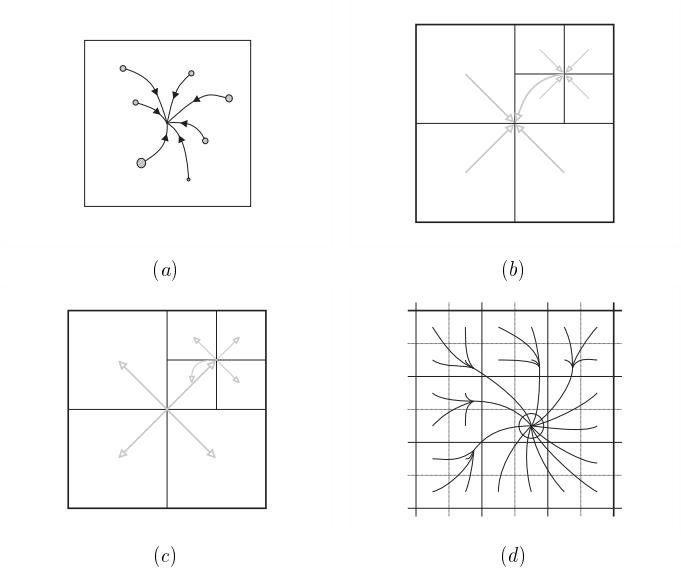
Figure D.2: Figures illustrating the definitions used in the description of the algorithm.

- the *nearest neighborhood* will denote the given cell with the eight adjacent cells located at the same level (see Fig.D.2b),
- the *interaction list* will be the set of *children* whose *parents* belong to the *nearest neighborhood* of the *parent* of the given cell and which are not adjoining to it (see Fig.D.2b),
- *close induction* will refer to the potential due to the particles in the *nearest neighborhood*, whereas *far induction* to those outside of it; at every point the complex potential is the sum of the *close* and *far induction*.

We now describe a method for fast evaluation of the *far induction*. The objective is to construct Taylor series expansions in every cell at the level $H$, so that they could be used to calculate the potential. Basically, the algorithm consists of the three following phases:

1. for every cell located at the level $H$ the Laurent series expansions (D.6) are determined for particles belonging to the given cell; the expansions are computed in the local coordinate system coinciding with the cell's center (Fig.D.3a),
2. expansions analogous to obtained in the previous step are computed for cells at the levels from $(H-1)$ to 1; this is accomplished by using formula (D.7) to shift the expansions computed in the *children* cells to the center of the *parent* cells where they are all summed up (Fig.D.3b); as a result, in every cell we will have multipolar expansions due to all





$(a)$ $(b)$ $(c)$ $(d)$

Figure D.3: Figures describing the consecutive phases of the algorithm.

the particles present in it; every expansion remains valid in the exterior of the *nearest neighborhood* of the given cell; this phase is called the *upward move*,

3. in this phase we compute local Taylor series expansions for induction due to particles located outside the *nearest neighborhood* of a given cell; at the levels 0 and 1 they vanish identically, and at the levels $2, \ldots, H$ the following two sub-steps are required:

   (a) the Taylor series expansions of the *parents* are shifted (using (D.9)) to the centers of the *children* cells (Fig.D.3c); this phase is thus called the *downward move*,

   (b) induction of the particles in the cells belonging to the *interaction list* is accounted for by changing from Laurent to Taylor series expansions (D.8) which are then added to the expansion coefficients obtained in the given cell during the previous substep (Fig.D.3d).

The overall cost of the algorithm depends on $N$ and the number of the expansion terms $p$, and scales as $N\log(N)$. In the original paper [52] it was shown that if the required accuracy is $\epsilon$, then $p \approx |\log_2(\epsilon)|$. The number of levels $H$ does not influence accuracy and is adjusted so as to maximize performance. In the present study we normally use $p = 20$ and $H$ varying from 7 to 9. When the number of particles is around $10^4 - 10^5$, the computational cost of our algorithm is smaller by approximately two orders of magnitude than that required for direct evaluation of interactions.

The present Fast Multipole Method is also used to compute induction of the boundary vortex sheet. Here induction is usually evaluated sufficiently far from the obstacle, where Laurent-type expansions can be used. Consequently, only the *upward move* is needed. When induction must be determined in the close proximity of the boundary, then the influence of the nearby panels is computed using exact formulas (4.75) and (4.76), whereas the remaining panels are accounted for by using Laurent-type expansions at intermediate levels.