Documentation

`solidfmm`

Version 1.5

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Part I

User Guide

Chapter 1

Quick Start

This chapter is written for people who already have an understanding of the fast multipole method and the expansions it uses. The definition of these expansions alongside with the notational conventions employed by `solidfmm` are given Chapter 2. That chapter also contains an introduction to these topics. A complete reference of the user interface is given in Chapter 3.

We assume that you are familiar with the command line and a POSIX shell, that you have some background in programming in C++, and that you know how to use the standard development toolchain on GNU/Linux systems.

1.1 Licencing and Copyright

I, Matthias Kirchhart, am the sole author and copyright holder of `solidfmm`. `solidfmm` is free software. You may use, modify, and redistribute `solidfmm` under the terms and conditions of the 'GNU General Public License' (GPL) as published by the Free Software Foundation, either version three, or, at your option, any later version. You should have received a copy of this licence document together with `solidfmm`, it can also be found in Appendix B of this book.

The GPL gives you a lot of freedoms. However, it is a copyleft licence. Consider you write your own piece of software that makes use of `solidfmm`. Then, in case you decide to publish or redistribute your software, you *must* distribute it under the terms of the GPL. In particular, the GPL *does not* allow you to incorporate `solidfmm` into closed-source, non-free, commercial software for retail. If you wish to do so, please contact me to negotiate alternative licencing options.

1.2 Installing `solidfmm`

1.2.1 System Requirements

To compile and install `solidfmm` you will need a fairly recent version of the GNU Compiler Collection (`g++`) *or* LLVM (`clang++`) with support for C++20.

The only external library dependency is `hwloc`,[1] which is necessary for the multi-threading functionality. Apart from this, on Unix systems you will only need standard development tools, i. e., a POSIX compatible shell (like `bash`), and `make`. It should also be possible to compile under Windows using Cygwin or MinGW, but I have not tested this. If you downloaded `solidfmm` by cloning the GitHub repository, you will additionally need the GNU Autotools: `autoconf`, `automake`, `libtool`, as well as `pkg-config` and the software they depend on.

The reason for requiring specific compilers is the following. The performance critical parts of the code—the so-called microkernels—are written in assembly language, in the form of *inline assembly* which is directly embedded in the C++ code. Unfortunately, there is no consensus on how to do this, and different compilers have different formats. Even worse, Microsoft's compiler (MSVC) simply does not support inline assembly at all anymore.[1] `solidfmm` uses GCC's syntax, because GCC is available for almost all platforms, it is free software, and fairly up-to-date with current C++ standards. LLVM also uses the same syntax. Additionally, on x86 platforms the code uses GCC's feature `__builtin_cpu_supports()` to detect the availability of AVX and AVX-512 at runtime. This extension is also supported by LLVM.

1.2.2 Download Sources

`solidfmm` is available from GitHub at `https://github.com/vorticle/solidfmm` in two forms

1. *Recommended:* As so-called 'tarballs', i. e., compressed archives of the source code which come with the readily prepared configuration scripts. Additionally, digital signatures are provided to validate the authenticity of the code. You can find these releases under the 'Releases' section on the GitHub project page, a little bit hidden on the right of the page.

2. As a source repository which can be cloned using the `git` versioning tool. This repository does not contain the prepared configuration scripts; you will additionally need the GNU Autotools to generate these scripts from the source code.

We highly recommend the first option, as it is simpler to use and comes with the additional security benefit of digital signatures.

1.2.3 Verification (Optional)

The next step is to verify the authenticity of the downloaded files. For this you will need the GNU Privacy Guard, also known as GnuPG.[2] Its executable is commonly called `gpg`. It comes preinstalled by default on most current GNU/Linux distributions. Here we will only describe how to use this software to verify the authenticity of `solidfmm` on GNU/Linux systems, a detailed user guide of `gpg` is given on its project website. We will only describe the process for the tarball release, which is the recommended download option. For verifying a cloned GitHub repository we assume that you have sufficient familiarity with `git` to perform the verification yourself.

[1]We quote: 'Inline assembly is not supported on the ARM and x64 processors.' `https://docs.microsoft.com/en-us/cpp/assembler/inline/inline-assembler?view=msvc-170`

Setting up GnuPG

GnuPG only needs to be set up once. If you have already done so during installations of previous versions, you can safely skip this section.

You will need your own keypair. If you do not know what this is, you probably do not have one yet. In this case you can easily create one by entering

```
gpg --gen-key
```

and following the instructions on your screen. This a local procedure: no data is submitted to the internet and your privacy is preserved.

Once you have your own keypair, you can import my key into GnuPG. My public key is included in the repository, it can be downloaded individually from GitHub.

```
gpg --import kirchhart_pubkey.gpg
```

You now need to double check if my key itself has not been compromised. This can *only* be achieved by *manually* comparing it to a second, trustworthy source. To do this, first display the key's fingerprint:

```
gpg --fingerprint "Matthias Kirchhart"
```

This command should show something like:

```
pub   rsa4096 2012-11-02 [SC]
      BC55 D501 A8DC 2D9B D2C9  95F3 00D1 76A4 818C 2BCE
uid           [ ultimativ ] Matthias Kirchhart <matthias.kirchhart@rwth-aachen.de>
uid           [ ultimativ ] Matthias Kirchhart <kirchhart@acom.rwth-aachen.de>
sub   rsa4096 2012-11-02 [A]
sub   rsa4096 2012-11-02 [E]
```

The long string of characters 'BC55 D501 A8DC…' is my public key's fingerprint. You have to compare this fingerprint with the one given in the 'About' section on my LinkedIn page: https://www.linkedin.com/in/matthiaskirchhart/. *Only if the two fingerprints match **completely***, you have successfully imported my public key. If they do not match, something strange is going on and you should abort immediately, check your computer for viruses, etc.

Usually, however, things should work out just fine. In this case, you sign this process off by adding your signature:

```
gpg --sign-key "Matthias Kirchhart"
```

This procedure might seem rather tedious, but security comes at a price. Also note that these steps only need to be carried out once. You will never need to do this again, unless you move to a different computer and forget moving your GnuPG data. You do *not* need to set up GnuPG again when installing updates to `solidfmm`.

Verifying the Tarball

Once you set up GnuPG, verifying the tarball is easy. Simply run the following command in the folder into which you downloaded the tarball and the signature file.

```
gpg --verify solidfmm-1.5.tar.xz.asc solidfmm-1.5.tar.xz
```

The output should contain a message stating that the signature is correct. If so, verification is complete. Otherwise you have downloaded compromised files and should abort *immediately*. Replace the version number 1.5 with the version you downloaded in the above command, if necessary.

1.2.4 Unpacking the Tarball

Once you have downloaded and (optionally) verified the tarball, it can be unpacked as follows.

```
tar Jxf solidfmm-1.5.tar.xz
```

For this command to work, you will need `tar`[3] and the XZ utils,[4] which come preinstalled by default on most current GNU/Linux systems. This should create a folder named `solidfmm-1.5`, containing the source code of `solidfmm`. Enter this folder by typing

```
cd solidfmm-1.5
```

1.2.5 Preparing a Cloned Repository

If you instead downloaded `solidfmm` from GitHub by cloning the repository using the `git` versioning tool, you will need the GNU Autotools to generate the build system and the necessary scripts.

```
autoreconf --install
```

After this the compilation and installation instructions in the next subsection also apply to the cloned repository.

1.2.6 Configuring and Compiling

solidfmm uses the GNU Autotools to configure, build, and install the library. These tools give you great flexibility in doing this and are well beyond the scope of this manual. These tools are, for example, described in detail in John Calcote's book.[5] In the simplest setting you can just enter the source directory and configure and compile using:

```
./configure && make
```

The configure script allows you to control many aspects of the process. For example, it is possible to only build the static library, or to only compile the dynamically linked version. You can chose the compiler, linker, optimisation flags, installation directories, and many more using environment variables and options to the script. It is even possible to cross-compile for a different system. If you want to install solidfmm in a non-standard location, you can do so by passing the --prefix option:

```
./configure --prefix=/your/preferred/location && make
```

However, you should only use this option if you know what you are doing: if you install solidfmm to a non-standard location, you will need to configure your compiler and linker such that they know where to look for solidfmm when using the library. A quick overview over some of the options that configure supports can be seen by executing the following command:

```
./configure --help
```

More detailed options are given in the file INSTALL.

One important aspect for solidfmm is the choice of compiler. Only recent versions of the GNU Compiler Collection, i. e., g++,[6] and LLVM, i. e., clang++,[7] are supported. To specify the compiler to use, you can use the environment variable CXX. For example:

```
# To compile using clang++ use:
CXX=clang++ ./configure && make

# To compile using g++ use:
CXX=g++ ./configure && make
```

If you do not specify CXX, your system's default compiler will be used.

1.2.7 Installing

When compilation is complete, you can install solidfmm. Unless you specified a different --prefix when running configure, solidfmm will be installed into your system's default locations for libraries and headers. These directories are protected, and can only be written to by the system administrator. On Unix systems you would thus first change to the administrator's account and install afterwards:

```
su # Changes to the system administrator's account, requires his or her password
make install
exit # Important: leave administrator's account afterwards
```

Some current GNU/Linux distributions do not allow the use of `su` anymore, because they claim it would be unsafe. As so often, when used properly, this is not true; however `su` does have a history of being used incorrectly. For this reason these distributions promote the use of `sudo` instead. If the above command does not work, on these systems, you can try using the following instead:

```
sudo make install
```

This command requires *your* password and not that of the administrator. It will only work if the system administrator has granted you the necessary rights.

1.3 Using the Library

1.3.1 Headers and Linker Flags

The user interface consists of only four header files. Simply `#include` them at the beginning of your source files:

```
#include <solidfmm/solid.hpp>
#include <solidfmm/handles.hpp>
#include <solidfmm/harmonics.hpp>
#include <solidfmm/translations.hpp>
```

All classes and functions of the library lie in the C++ namespace `solidfmm`. When creating your programme, you will need to link against the library. For example, when using `g++`, this can be achieved by adding the flag `-lsolidfmm` as follows:

```
# Compile your programme
g++ -o yourprogramme.o -c yourprogramme.cpp

# Link it into an executable
g++ -o yourprogramme -lsolidfmm yourprogramme.o
```

Since version 1.5, `solidfmm` also supports the `pkg-config` tool to automatically discover the right linkage and preprocessor flags. If you have this tools installed on your system, you can use it to query the correct flags:

```
pkg-config --libs   solidfmm   # Prints Flags for linking against solidfmm
pkg-config --cflags solidfmm   # Flags for the C-preprocessor to find headers
```

1.3.2 Creating Expansions

Suppose we were given N point charges at locations $(x_i, y_i, z_i)^\top \in \mathbb{R}^3$ with associated charges $m_i \in \mathbb{R}$, $i = 0, \dots, N-1$. We now seek to create a multipole expansion of order $P = 15$ around the point $(x_A, y_A, z_A)^\top \in \mathbb{R}^3$. To do this so-called P2M operation in `solidfmm`, one could use the following code.

```
using solidfmm::solid;
using solidfmm::fmadd;
using solidfmm::harmonics::R; // Regular harmonics.

size_t P { 15 };              // The order of the expansion you want to use.
size_t N;                     // Number of point charges, initialised somewhere else.
const double *x, *y, *z, *m; // Coordinates and charges, initialised somewhere else.

// Objects of type solid store coefficients of multipole or local expansions.
// Pass the desired order of the expansion. Initialised with zero coefficients.
// You can also use "float" for single precision.
solid<double> M( P );

// Add the contribution of each point mass to multipole expansion.
for ( size_t i = 0; i < N; ++i )
    fmadd( m[i], R<double>(P,x[i]-xA,y[i]-yA,z[i]-zA), M );
```

After this, the object `M` of type `solid<double>` contains the coefficients $M_n^m \in \mathbb{C}, n = 0, \dots, P-1,\ m = -n, \dots, n$ of the multipole expansion.

Although much less common, local expansions can be created directly from the given point charges (P2L) in almost the exact same way. All we need to do is to replace the regular harmonics with the singular ones. Thus, assume we wanted to create a local expansion for the same charges around the centre $(x_B, y_B, z_B)^\top \in \mathbb{R}^3$. This can be achieved as follows:

```
using solidfmm::solid;
using solidfmm::fmadd;
using solidfmm::harmonics::S; // Singular harmonics.

solid<double> L( P );
for ( size_t i = 0; i < N; ++i )
    fmadd( m[i], S<double>(P,x[i]-xB,y[i]-yB,z[i]-zB), L );
```

We note that `solidfmm` also supports vector-valued expansions. For this we refer the reader to Chapter 3.

1.3.3 Evaluating Expansions

Evaluation of multipole and local expansions can be done using `dot`. Assume we were given the coefficients $M_n^m \in \mathbb{C}, n = 0, \dots, P-1, m = -n, \dots, n$ of a multipole expansion of order P around the centre $(x_A, y_A, z_A)^\top \in \mathbb{R}^3$. To evaluate this expansion at some point $(x, y, z)^\top \in \mathbb{R}^3$, you would do the following:

```
using solidfmm::dot;
using solidfmm::solid;
using solidfmm::harmonics::S; // Singular harmonics.

solid<double> M;    // Given coefficients,     initialised somewhere else.
double xA, yA, zA;  // Given expansion centre, initialised somewhere else.
double x,  y,  z;   // Given evaluation point, initialised somewhere else.

double result { 0 };
dot( M, S<double>(P,x-xA,y-yA,z-zA), &result );
```

Local expansions work similarly: here you need to replace the singular harmonics with the regular ones. Thus, assuming you were given the coefficients $L_n^m \in \mathbb{C}$, $n = 0, \dots, P-1$, $m = -n, \dots, n$ of a local expansion at centre $(x_B, y_B, z_B)^\top \in \mathbb{R}^3$, you would evaluate it as follows:

```
using solidfmm::dot;
using solidfmm::solid;
using solidfmm::harmonics::R; // Regular harmonics.

solid<double> L;    // Given coefficients,     initialised somewhere else.
double xB, yB, zB;  // Given expansion centre, initialised somewhere else.
double x,  y,  z;   // Given evaluation point, initialised somewhere else.

double result { 0 };
dot( L, R<double>(P,x-xB,y-yB,z-zB), &result );
```

Again, we remark that `solidfmm` also supports vector-valued expansions and refer to Chapter 3 for this.

1.3.4 Translations

We now come to the main reason for the existence of this library: to provide an efficient implementation of the translation operators M2M, M2L, and L2L. In this section we describe how to use the `multithreaded_scheduler`, as it is most easy to use. If you prefer to do the workbalancing and scheduling of threads yourself, you can use the single threaded functions as discussed in Section 3.5.

In `solidfmm`, a translation is described using a `translation_info` object:

```
template <typename real>
struct translation_info
{
    const solid<real> *source;  // Source coefficients
          solid<real> *target;  // Target coefficients

    real x, y, z;               // Shift vector.
};

extern template class translation_info<float>;
extern template class translation_info<double>;
```

The result of translating the `source` solid is *added* to `target`, making accumulation possible. So in pseudo-code we have:

$$\texttt{target} \quad \texttt{+=} \quad \text{translate}(\texttt{source}, x, y, z);$$

where 'translate' can mean any of M2M, M2L, or L2L. Note that `solidfmm` supports translations of mixed orders, so it is important that you initialise the `target` to the correct order. Also note that vector-valued expansions are also supported. Default-constructed objects of type `solid` are of order zero and dimension 1; so in this case nothing happens. If in doubt, you can explicitly initialise the targets using the `resize()` member function. For example, you could use the following code:

```
// If in doubt if your targets were already initialised to the desired
// output order, you can use the following code.

// Large list of translations, initialised somewhere else
std::vector< translation_info<double> > translations;

for ( auto i = translations.begin(); i != translations.end(); ++i )
{
        i->target->resize(P); // Choose your desired output order here.
        i->target->zeros();   // Initialise target to zero.
}
```

The easiest way to carry out translations is the `multithreaded_translator` class. By default, an instance of this class will use *all available cores* to carry out as many translations in parallel as possible. It takes care of data races, so accumulation will work as expected. However, it does not do dependency checking, so a list of translations where some `solid`s are *both* a source and a target will lead to undefined behaviour. In particular, in the usual workflow of the fast multipole method, it usually works to pass a list of *all* M2L translations; however M2M and L2L translations must be carried out level-wise.

```
// Large list of translations, initialised somewhere else
std::vector< translation_info<double> > translations;
```

```
// Maximum order P that we are going to use, initialised somewhere else.
size_t P;

// Expensive to create! Only create once at program start-up if possible.
// Will by default use all available cores on the system and distribute work
// equally among them.
multithreaded_translator<double> T( P );

// On systems with different kinds of cores, e.g., performance cores
// and efficiency cores, it makes sense to measure the throughput and schedule
// work accordingly. Uncomment the following line for this. Measurement is
// expensive, it should be done only once at program start-up.
//T.schedule_by_measuring_throughput();

// Carry out, e.g., m2l translations. m2m and l2l are called analogously.
T.m2l( translations.data(), translations.data() + translations.size() );
```

By default, the translator class will carry out a check at runtime if the list of translations is valid: does no source or target exceed order P? For vector-valued coefficients: do the dimensions of sources and targets match? If one of these checks fails an exception is thrown and nothing happens (strong exception guarantee).

For maximum performance, you can omit these checks. If you pass data that violates the above criteria, however, the results will be undefined.

```
T.m2l_unchecked(translations.data(),translations.data()+translations.size());
```

Lastly, we would like to point out that it is possible to specify how many threads and which cores the `multithreaded_translator` should use. For this, you need to use `hwloc` and the following constructor:

```
multithreaded_translator( size_t P, hwloc_topology_t topo,
                          hwloc_cpuset_t *begin, hwloc_cpuset_t *end );
```

For each CPU-set that you pass, the `multithreaded_translator` creates and manages a thread and pins it to that set. How to create such sets is described in the `hwloc` documentation.

1.3.5 Computing Minimal Bounding Spheres

Since version 1.4, `solidfmm` provides routines for computing minimal bounding spheres. These are useful in adaptive fast multipole codes to avoid being overly pessimistic in the multipole acceptance criterion. We provide two kinds of routines: one computes the minimal bounding sphere of a set of points; the other routine can be used to compute the minimal bounding sphere of a set of spheres. To use these routines, include the following short, self-explanatory header:

```
#include <solidfmm/sphere.hpp>
```

The routines in this header implement an algorithm by Fischer and Gärtner.[8] The theoretical complexity of this algorithm is rather high. However, just like Fischer and Gärtner, in our experiments we found that the *empirical complexity is linear in the number points or spheres*. This implementation is particularly tuned for three-dimensional space; in our experiments it was faster than the more general CGAL implementation[2] and also provided more accurate results in floating point arithmetic.

[2] https://doc.cgal.org/latest/Bounding_volumes/classCGAL_1_1Min__sphere__d.html

Chapter 2

Mathematical Background

In this chapter we will give a description of some of the mathematical background of the fast multipole method (FMM) and its use of the solid harmonics. If you are already familiar with these topics, this chapter will probably contain nothing new for you, except for maybe sign and notational conventions.

2.1 Motivation: Movement of Planets

Consider we have a set of N planets in space, having location $\mathbf{x}_i = (x_i, y_i, z_i)^\top \in \mathbb{R}^3$ (measured in metres) and mass $m_i \in \mathbb{R}$ (measured in kilogrammes), $i = 1, \dots, N-1$. Throughout this text, we will use a **bold** font to indicate three-dimensional vectors. These planets mutually attract each other through gravity. Thus, let us define the gravimetric potential, following Newton's law of gravity:

$$\varphi(x,y,z) := G \sum_{i=0}^{N-1} \frac{m_i}{\sqrt{(x-x_i)^2 + (y-y_i)^2 + (z-z_i)^2}} = G \sum_{i=0}^{N-1} \frac{m_i}{|\mathbf{x} - \mathbf{x}_i|}, \tag{2.1}$$

where $|\mathbf{x} - \mathbf{x}_i|$ denotes the Euclidean distance between the point $\mathbf{x} = (x,y,z)^\top \in \mathbb{R}^3$ and the location $\mathbf{x}_i$ of planet i, and $G \approx 6.674 \times 10^{-11} \frac{\mathrm{m}^3}{\mathrm{kg\,s}^2}$ is the universal gravitational constant. Then, applying Newton's laws of motion, the planet movements obey the following set of ordinary differential equations (ODEs):

$$\frac{\mathrm{d}^2 \mathbf{x}_i}{\mathrm{d}t^2} = -\nabla\varphi(\mathbf{x}_i) = \sum_{\substack{j=0 \\ j\neq i}}^{N-1} G m_j \frac{\mathbf{x}_j - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|^3}, \qquad i = 0, \dots, N-1. \tag{2.2}$$

If you now consider entire galaxies, the number of planets is large, say $N \approx 1\,000\,000$. In order to solve this set of ODEs, you need to repeatedly evaluate $\nabla\varphi(\mathbf{x})$ at all planet locations $\mathbf{x}_i$. Each evaluation costs $\mathcal{O}(N)$, giving you a total cost of $\mathcal{O}(N^2) = \mathcal{O}(10^{12})$. This cost is prohibitive, even for large super computers. The fast multipole method (FMM) allows you to evaluate *approximations* of $\varphi(\mathbf{x})$ and its gradient and reduces this cost from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$. This results in dramatic speed ups, and it is this speed up alone that makes large scale simulations of galaxies possible.

2.2 Expansions

2.2.1 Expansion of the Kernel Function

Let us denote by $k(\mathbf{x}, \mathbf{y}) \coloneqq |\mathbf{x} - \mathbf{y}|^{-1}$ the so-called *kernel function*. Using this function, the gravimetric potential from equation (2.1) can more compactly be given as

$$\varphi(\mathbf{x}) = G \sum_{i=0}^{N-1} m_i k(\mathbf{x}, \mathbf{x}_i). \tag{2.3}$$

The key to fast multipole methods is that this kernel function can be *expanded* in terms of the *solid harmonics* as follows:

$$k(\mathbf{x}, \mathbf{y}) \approx \sum_{n=0}^{P-1} \sum_{m=-n}^{n} S_n^m(\mathbf{x}) \overline{R_n^m(\mathbf{y})} \qquad \text{whenever } |\mathbf{x}| > |\mathbf{y}|. \tag{2.4}$$

The number $P \in \mathbb{N}$ is called the *order* of the expansion. The functions $S_n^m : \mathbb{R}^3 \setminus \{\mathbf{0}\} \to \mathbb{C}$ and $R_n^m : \mathbb{R}^3 \to \mathbb{C}$ are respectively called the *singular* and *regular solid harmonics*. While these functions are complex-valued—the overline on R_n^m denotes complex conjugation—the expansion always takes real values. We will define these functions precisely in following section. For now it suffices to remember that this expansion is very rapidly converging, it satisfies the following error-bound:[9, Theorem 3.2]

$$\left| k(\mathbf{x}, \mathbf{y}) - \sum_{n=0}^{P-1} \sum_{m=-n}^{n} S_n^m(\mathbf{x}) \overline{R_n^m(\mathbf{y})} \right| \leq \frac{1}{|\mathbf{x}| - |\mathbf{y}|} \left(\frac{|\mathbf{y}|}{|\mathbf{x}|} \right)^P. \tag{2.5}$$

In other words, its accuracy exponentially increases with order P, additionally the approximation gets more accurate as $|\mathbf{x}|$ increases and $|\mathbf{y}|$ decreases.

2.2.2 Multipole Expansions (P2M)

We now again consider the gravimetric potential φ as given in equation (2.3). Furthermore assume the case where planets are clustered around some point $\mathbf{x}_A \in \mathbb{R}^3$, and we would like to evaluate φ at locations $\mathbf{x}$ that are far away from that cluster, i. e., $|\mathbf{x} - \mathbf{x}_A| > |\mathbf{x}_i - \mathbf{x}_A|$ for all $i = 0, \dots, N-1$. We then have, by means of the kernel expansion (2.4):

$$\begin{aligned} \varphi(\mathbf{x}) &= \sum_{i=0}^{N-1} G m_i k(\mathbf{x}, \mathbf{x}_i) = \sum_{i=0}^{N-1} G m_i k(\mathbf{x} - \mathbf{x}_A, \mathbf{x}_i - \mathbf{x}_A) \\ &\overset{(2.4)}{\approx} \sum_{n=0}^{P-1} \sum_{m=-n}^{n} S_n^m(\mathbf{x} - \mathbf{x}_A) \overline{\underbrace{\sum_{i=0}^{N-1} R_n^m(\mathbf{x}_i - \mathbf{x}_A) G m_i}_{=:M_n^m}}. \end{aligned} \tag{2.6}$$

This suggests the following approach:

1. Compute the *multipoles* $M_n^m \in \mathbb{C}$:
$$M_n^m := \sum_{i=1}^{N} Gm_i R_n^m(\mathbf{x}_i - \mathbf{x}_A). \tag{2.7}$$
Cost: $\mathcal{O}(NP^2)$.

2. Evaluate the *multipole expansion* (or, if requested, its gradient) at the desired locations:
$$\varphi(\mathbf{x}) \approx \sum_{n=0}^{P-1} \sum_{m=-n}^{n} \overline{M_n^m} S_n^m(\mathbf{x}-\mathbf{x}_A) \qquad |\mathbf{x}-\mathbf{x}_A| > |\mathbf{x}_i-\mathbf{x}_A|, i = 1\ldots,N-1. \tag{2.8}$$
Cost: $\mathcal{O}\left(P^2\right)$ per evaluation point $\mathbf{x}$.

If we only want to evaluate φ at a single location $\mathbf{x}$, then nothing is gained. However, suppose you want to evaluate φ at M locations, where both $N, M \approx 1\,000\,000$. Then the cost for direct evaluation is $\mathcal{O}(NM) = \mathcal{O}\left(10^{12}\right)$, whereas the approach via the multipole expansion only costs $\mathcal{O}\left(NP^2 + MP^2\right) = \mathcal{O}\left(10^6 P^2\right)$. This results in the aforementioned dramatic speed up, assuming that P is not too large. In practice, choices up to $P = 20$ are common—remember that the kernel expansion (2.4) converges exponentially with P. Only very few calculations require even higher accuracies. Operation (2.7) computes multipole coefficients M_n^m from a given set of planets or particles; it is commonly called P2M: particle-to-multipole.

In summary, a multipole expansion approximates the potential φ of a particle cluster around some centre $\mathbf{x}_A$ *outside of this cluster*. The expansion gets *more accurate as the distance increases.* This is illustrated in Figure 2.1.

2.2.3 Local Expansions (P2L)

Local expansions in some ways consider the opposite case, as illustrated in Figure 2.2. Here we want to evaluate φ at a cluster of locations $\mathbf{x}$ around some centre $\mathbf{x}_B$, where the particles lie *outside* of this cluster. In other words, we have $|\mathbf{x} - \mathbf{x}_B| < |\mathbf{x}_i - \mathbf{x}_B|$ for all $i = 1, \ldots, N-1$, and thus:

$$\begin{aligned}\varphi(\mathbf{x}) &= \sum_{i=0}^{N-1} Gm_i k(\mathbf{x}, \mathbf{x}_i) = \sum_{i=0}^{N-1} Gm_i k(\mathbf{x}_i - \mathbf{x}_B, \mathbf{x} - \mathbf{x}_B) \\ &\overset{(2.4)}{\approx} \sum_{n=0}^{P-1} \sum_{m=-n}^{n} \overline{R_n^m(\mathbf{x} - \mathbf{x}_B)} \underbrace{\sum_{i=0}^{N-1} S_n^m(\mathbf{x}_i - \mathbf{x}_B) Gm_i}_{=:L_n^m}.\end{aligned} \tag{2.9}$$

After computing the *local coefficients* $L_n^m \in \mathbb{C}$, the potential φ can be approximated near $\mathbf{x}_B$ using the local expansion:

$$\varphi(\mathbf{x}) \approx \sum_{n=0}^{P-1} \sum_{m=-n}^{n} L_n^m \overline{R_n^m(\mathbf{x} - \mathbf{x}_B)} \qquad |\mathbf{x} - \mathbf{x}_B| < |\mathbf{x}_i - \mathbf{x}_B|,\ i = 1, \ldots, N-1. \tag{2.10}$$

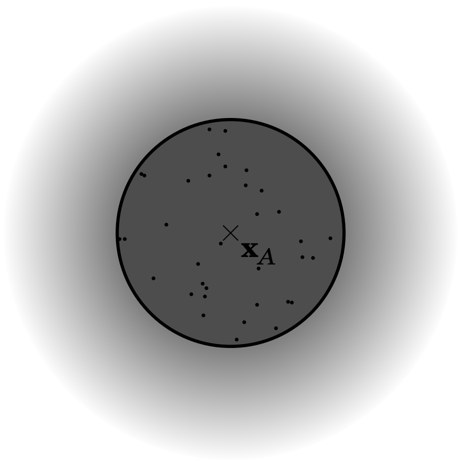


Figure 2.1: Multipole expansions converge outside of the smallest ball around their centre that contains all particles. Here, the cluster of planets near the centre $\mathbf{x}_A$ is contained within the drawn circle. Outside this region the expansion converges and gets more accurate as the distance increases, indicated by grey fading into white. The accuracy increases faster for expansions of higher order P. The expansion does not converge within the circle and gives large errors there, indicated by a dark grey colour.

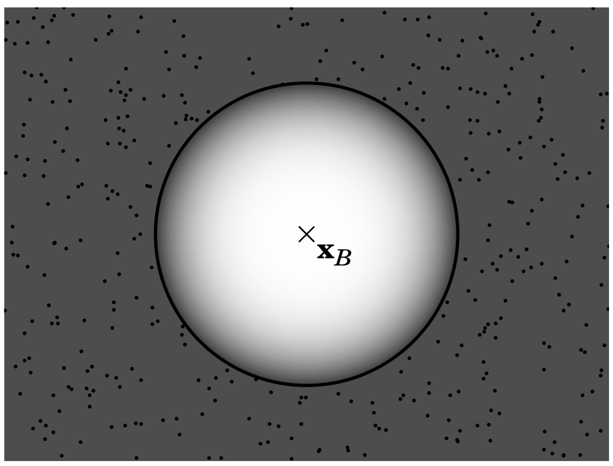


Figure 2.2: Local expansions converge in the largest ball around their centre that contains no particles. The error of a local expansion is zero at its centre $\mathbf{x}_B$, indicated by a shade of white in this figure. It then gradually increases when approaching the boundary of the ball (white fading to grey). This increase is slower for expansions of higher order P. Outside of this ball, the local expansion does not converge and gives large errors (dark grey).

The operation of computing the local coefficients directly from the particles is called particle-to-local (P2L):

$$L_n^m := \sum_{i=0}^{N-1} S_n^m(\mathbf{x}_i - \mathbf{x}_B) G m_i. \tag{2.11}$$

However, most FMM implementations do not compute local coefficients via P2L; those that do only use it in rare circumstances. The usual way to obtain local coefficients is the so-called M2L translation and will be discussed later.

2.2.4 Remarks on the Derivation of Expansions

Key to all fast multipole methods is the availability of rapidly converging series expansions of the underlying kernel function $k(\mathbf{x}, \mathbf{y})$, such as in Equation (2.4). Generic expansions, such as Taylor series, can in principle be applied to any kind of kernel k. For example, the Taylor expansion of order P of some kernel $k(\mathbf{x}, \mathbf{y})$ for a fixed $\mathbf{x}$ around $\mathbf{y} = \mathbf{0}$ reads:

$$k(\mathbf{x}, \mathbf{y}) \approx \sum_{|\boldsymbol{\alpha}|<P} \underbrace{\partial_{\mathbf{y}}^{\boldsymbol{\alpha}} k(\mathbf{x}, \mathbf{0})}_{=:\widetilde{S}_{\boldsymbol{\alpha}}(\mathbf{x})} \underbrace{\frac{\mathbf{y}^{\boldsymbol{\alpha}}}{\boldsymbol{\alpha}!}}_{=:\widetilde{R}_{\boldsymbol{\alpha}}(\mathbf{y})}, \tag{2.12}$$

where $\boldsymbol{\alpha} \in \mathbb{N}_0^3$ is a multi-index. The key point is that this expansion is a sum of products, where one factor only depends on $\mathbf{x}$ and the other factor only depends on $\mathbf{y}$. In this way the simultaneous dependence of k on both $\mathbf{x}$ and $\mathbf{y}$ *decouples*.

The Taylor expansion consists of $\mathcal{O}(P^3)$ terms, where the functions $\widetilde{S}_{\boldsymbol{\alpha}}$ and $\widetilde{R}_{\boldsymbol{\alpha}}$ take similar roles as the S_n^m and R_n^m in Equation (2.4). Thus, assuming sufficient regularity of k, Taylor's theorem is all we need to to construct multipole and local expansions and it also provides us with error bounds. Without additional knowledge about k, this is essentially already the best we can do. However, also note that the Taylor expansion has $\mathcal{O}(P^3)$ terms, while Equation (2.4) requires only $\mathcal{O}(P^2)$. Why is this so?

With the particular choice $k(\mathbf{x}, \mathbf{y}) = |\mathbf{x} - \mathbf{y}|^{-1}$ and fixed $\mathbf{x}$, the Taylor polynomials (2.12) are always *harmonic*. In other words, the exact kernel function satisfies $-\Delta_{\mathbf{y}} k(\mathbf{x}, \mathbf{y}) = 0$, where $-\Delta_{\mathbf{y}}$ is the Laplace operator with respect to the $\mathbf{y}$-variable. This property is inherited by the Taylor polynomials. There are only $\mathcal{O}(P^2)$ linearly independent harmonic polynomials, so it suffices to use a basis for this *sub*space. The regular solid harmonics R_n^m, $|m| \leq n$, are exactly that: they are a basis of the space of homogeneous harmonic polynomials of degree n. Expansion (2.4) achieves better compression because only basis functions for the proper subspace are used. The Taylor expansion (2.12), on the other hand, uses the generic monomial basis for *all* polynomials, not just the harmonic ones.

Only for the particular kernel $k(\mathbf{x}, \mathbf{y}) = |\mathbf{x} - \mathbf{y}|^{-1}$ the solid harmonics are the correct choice. `solidfmm` only considers this kernel function and the solid harmonics. For other kernel functions one can either use the more expensive, but more general Taylor expansion (2.12), or other generic $\mathcal{O}(P^3)$ approaches like Chebyshev interpolation.

Alternatively, if performance is critical, it might be worthwhile to develop more efficient expansions specific to the particular kernel at hand.

2.3 Solid Harmonics

The solid harmonics can be motivated and derived in many different ways. We refer the interested reader to the literature for this. Often they are given in spherical coordinates. When restricting the solid harmonics to the surface of the unit sphere, one obtains the more well-known *spherical* harmonics $Y_n^m(\theta,\varphi)$, i. e., $Y_n^m(\theta,\varphi) = R_n^m(r=1,\theta,\varphi)$. This explains their name: unlike the spherical harmonics Y_n^m, the solid harmonics S_n^m and R_n^m are defined not only on the sphere's surface, but also on the volume it encloses, i. e., on the entire solid sphere. They are called *harmonic* because $-\Delta S_n^m(\mathbf{x}) = 0$ for $\mathbf{x} \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$ and $-\Delta R_n^m(\mathbf{x}) = 0$ for $\mathbf{x} \in \mathbb{R}^3$. The functions S_n^m are called singular solid harmonics because of their singularities at $\mathbf{x} = \mathbf{0}$. The functions R_n^m are polynomials, hence they are called regular solid harmonics.

While spherical coordinates have certain benefits for analysis, these functions can more easily evaluated in Cartesian coordinates. There are countless conventions concerning signs and normalisations. `solidfmm` follows the convention given by Dehnen.[10] For computational purposes, the solid harmonics are best defined recursively. Let $\mathbf{x} = (x,y,z)^\top \in \mathbb{R}^3$ be given, and let $|\mathbf{x}| = \sqrt{x^2+y^2+z^2}$ denote its Euclidean length. Starting with $S_0^0(\mathbf{x}) = |\mathbf{x}|^{-1}$ and $R_0^0(\mathbf{x}) = 1$, one continues with the diagonal $n = m$:

$$S_n^n = (2n-1)\frac{x+Iy}{|\mathbf{x}|^2}S_{n-1}^{n-1}, \qquad R_n^n = \frac{x+Iy}{2n}R_{n-1}^{n-1}, \tag{2.13}$$

where I denotes the imaginary unit $I^2 = -1$. For the remaining non-negative $m = 0,\dots,n-1$, they can be computed via:

$$\begin{aligned} |\mathbf{x}|^2 S_n^m &= (2n-1)zS_{n-1}^m - ((n-1)^2-m^2)S_{n-2}^m, \\ (n^2-m^2)R_n^m &= (2n-1)zR_{n-1}^m - |\mathbf{x}|^2 R_{n-2}^m. \end{aligned} \tag{2.14}$$

Here, it is implicitly assumed that $R_{n-2}^m = S_{n-2}^m = 0$ whenever $m = n-1$.

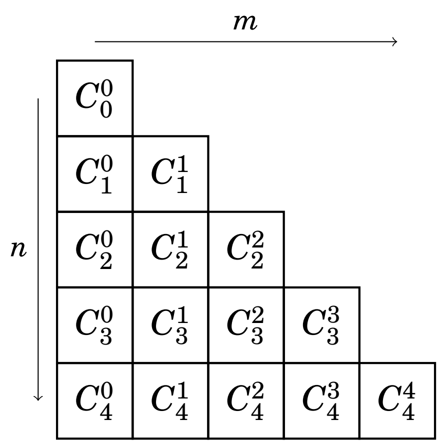
For the negative values of m, i. e., $m = -n,\dots,-1$, they are defined *implicitly* via

$$S_n^m(\mathbf{x}) = (-1)^m\overline{S_n^{-m}(\mathbf{x})} \quad \text{and} \quad R_n^m(\mathbf{x}) = (-1)^m\overline{R_n^{-m}(\mathbf{x})}. \tag{2.15}$$

This property therefore also holds for the coefficients of the multipole and local expansions:

$$M_n^m = (-1)^m\overline{M_n^{-m}} \quad \text{and} \quad L_n^m = (-1)^m\overline{L_n^{-m}}. \tag{2.16}$$

Thus, to even further increase compression, in a computer implementation neither the solid harmonics R_n^m and S_n^m, nor the multipole and local coefficients L_n^m and M_n^m should be explicitly stored for negative m. Taking these symmetries into account,



m
n
C_0^0
C_1^0 C_1^1
C_2^0 C_2^1 C_2^2
C_3^0 C_3^1 C_3^2 C_3^3
C_4^0 C_4^1 C_4^2 C_4^3 C_4^4

Figure 2.3: The coefficients $C_n^m \in \mathbb{C}$, $C \in \{S, R, M, L\}$ of both multipole and local expansions, as well as the values of the solid harmonics S_n^m and R_n^m can be stored using $P(P+1)/2$ complex numbers. In this example we have $P = 5$. They can be arranged in a triangular pattern according to their indices $n = 0, \ldots, 4$ and $m = 0, \ldots, n$, where the values for negative m are given implicitly by $C_n^m = (-1)^m \overline{C_n^{-m}}$.

a local or multipole expansion of order P consists of $P(P+1)/2$ complex numbers, which can be arranged in a triangular pattern as shown in Figure 2.3.

At the same time, this property guarantees that the expansion (2.4) always is real-valued: for $m = 0$ we have $R_n^0 \in \mathbb{R}$ and $S_n^0 \in \mathbb{R}$. For $m \neq 0$ the imaginary parts for $\pm m$ cancel each other out:

$$\sum_{n=0}^{P-1} \sum_{m=-n}^{n} S_n^m \overline{R_n^m} = \sum_{n=0}^{P-1} S_n^0 R_n^0 + \sum_{n=0}^{P-1} \sum_{m=1}^{n} \left(S_n^m \overline{R_n^m} + S_n^{-m} \overline{R_n^{-m}} \right)$$
$$\overset{(2.15)}{=} \sum_{n=0}^{P-1} \underbrace{S_n^0 R_n^0}_{\in \mathbb{R}} + \sum_{n=0}^{P-1} \sum_{m=1}^{n} \underbrace{\left(S_n^m \overline{R_n^m} + \overline{S_n^m} R_n^m \right)}_{\in \mathbb{R}}. \qquad (2.17)$$

2.4 Translations

Translation operators take in one expansion around centre $\mathbf{x}_A$ and produce another around some centre $\mathbf{x}_B$. When both in- and output expansions are of the same order P, the translation operators map $\mathcal{O}(P^2)$ input coefficients to $\mathcal{O}(P^2)$ output coefficients at the cost of $\mathcal{O}(P^4)$ arithmetic operations. The so-called M2L-translation is particularly important for FMMs, and a significant portion of the computational time is spent on performing these translations. They are the main reason for the existence of this library: it provides highly efficient, vectorised implementations of the translation operators. Additionally, `solidfmm`'s implementation is based on the approach outlined by Dehnen,[10] which reduces the complexity from $\mathcal{O}(P^4)$ to $\mathcal{O}(P^3)$ in theory and even $\mathcal{O}(P^2)$ in practice.

2.4.1 Multipole-to-Multipole (M2M)

M2M may be interpreted just like P2M, with the difference that the input is not a planet with mass m_i at location $\mathbf{x}_i$, but a multipole expansion of order P_i with coefficients $M_{n,i}^m$ and centre $\mathbf{x}_i$. Thus, in M2M, both the input and output are multipole expansions. We again denote by $\mathbf{x}_A$ and P the centre and order of the output expansion. We furthermore introduce the *shift vector* $\mathbf{r} = \mathbf{x}_A - \mathbf{x}_i$, pointing from the old to the new expansion centre.

Instead of expanding the kernel $k(\mathbf{x}, \mathbf{y}) = S_0^0(\mathbf{x} - \mathbf{y})$, we now expand the singular solid harmonics $S_n^m(\mathbf{x} - \mathbf{y})$, analogously to expansion (2.4):[10, Equation (49)]

$$S_n^m(\mathbf{x} - \mathbf{y}) = \sum_{k=0}^{\infty} \sum_{l=-k}^{k} S_{n+k}^{m+l}(\mathbf{x}) \overline{R_k^l(\mathbf{y})} \qquad |\mathbf{x}| > |\mathbf{y}|. \tag{2.18}$$

Thus, whenever $|\mathbf{x} - \mathbf{x}_A| > |\mathbf{x}_i - \mathbf{x}_A|$, the input multipole expansion with centre $\mathbf{x}_i$ can itself be expanded around $\mathbf{x}_A$ as follows:

$$\begin{aligned}
&\sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m(\mathbf{x} - \mathbf{x}_i) \\
&\qquad = \sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m((\mathbf{x} - \mathbf{x}_A) - (\mathbf{x}_i - \mathbf{x}_A)) \\
&\qquad \overset{(2.18)}{=} \sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \sum_{k=0}^{\infty} \sum_{l=-k}^{k} \overline{M_{n,i}^m R_k^l(-\mathbf{r})} S_{n+k}^{m+l}(\mathbf{x} - \mathbf{x}_A).
\end{aligned} \tag{2.19}$$

All that remains is a change of indices and rearranging the sums. To simplify the summation limits, we will implicitly assume that we have $R_{n-k}^{m-l}(-\mathbf{r}) = 0$ whenever $|m - l| > n - k$ or $n - k < 0$. This finally results in:

$$\begin{aligned}
&\sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m(\mathbf{x} - \mathbf{x}_i) \\
&\qquad = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} S_n^m(\mathbf{x} - \mathbf{x}_A) \left(\sum_{k=0}^{P_i-1} \sum_{l=-k}^{k} \overline{M_{k,i}^l R_{n-k}^{m-l}(-\mathbf{r})} \right).
\end{aligned} \tag{2.20}$$

We may thus define the new multipoles M_n^m via:

$$M_n^m := \sum_{k=0}^{P_i-1} \sum_{l=-n}^{n} M_{k,i}^l R_{n-k}^{m-l}(-\mathbf{r}). \tag{2.21}$$

This is the general M2M-translation formula. We then have, after truncating at the given output order P:

$$\sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m(\mathbf{x} - \mathbf{x}_i) \approx \sum_{n=0}^{P-1} \sum_{m=-n}^{n} \overline{M_n^m} S_n^m(\mathbf{x} - \mathbf{x}_A) \qquad |\mathbf{x} - \mathbf{x}_A| > |\mathbf{x}_i - \mathbf{x}_A|. \tag{2.22}$$

While P2M allows us to combine several 'particles' or 'planets' into a single multipole expansion with centre $\mathbf{x}_A$, M2M allows us to combine several multipole expansions into one. Suppose we were given N multipole expansions with centres $\mathbf{x}_i$ and orders P_i, $i = 0, \dots, N-1$. The potential approximated by these expansions:

$$\varphi(\mathbf{x}) \approx \sum_{i=0}^{N-1} \sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m(\mathbf{x} - \mathbf{x}_i) \tag{2.23}$$

can then in turn be approximated as follows:

1. Compute the combined multipole moments around $\mathbf{x}_A$ using M2M:

$$M_n^m \overset{(2.21)}{=} \sum_{i=0}^{N-1} \sum_{k=0}^{P_i-1} \sum_{l=-k}^{k} M_{k,i}^l R_{n-k}^{m-l}(\mathbf{x}_i - \mathbf{x}_A). \tag{2.24}$$

   Cost, assuming $P_i = P$ for all $i = 0, \dots, N-1$: $\mathcal{O}\left(NP^4\right)$. `solidfmm` reduces this cost to $\mathcal{O}\left(NP^3\right)$ for large P. For all practically relevant choices of P, however, the empirically measured timings behave even better, namely optimally as $\mathcal{O}\left(NP^2\right)$.

2. Evaluate the new expansion at the desired output locations:

$$\varphi(\mathbf{x}) \approx \sum_{n=0}^{P-1} \sum_{m=-n}^{n} \overline{M_n^m} S_n^m(\mathbf{x} - \mathbf{x}_A). \tag{2.25}$$

   Cost: $\mathcal{O}\left(P^2\right)$ per evaluation point $\mathbf{x}$.

The resulting approximation now contains *two sources of error*:

1. The error of the original approximation (2.23).
2. The error from the M2M translation.

The additional error behaves just like the error for an individual expansion obtained via P2M. In particular, Figure 2.1 also describes this additional error and area of convergence, where the 'dots' in this figure now correspond to the multipole expansions $M_{n,i}^m$ and their centres $\mathbf{x}_i$.

2.4.2 Multipole-to-Local (M2L)

M2L is to P2L what M2M is to P2M: we can again treat a given multipole expansion just like a planet or particle. While P2L allows us to locally approximate the potential induced by several planets, M2L allows us to approximate the potential given by multipole expansions. Thus, suppose we were given a multipole expansion with coefficients $M_{n,i}^m$ and order P_i around some centre $\mathbf{x}_i$. We now wish to locally approximate this expansion near $\mathbf{x}_B$ using a local expansion. Again, we denote by $\mathbf{r} = \mathbf{x}_B - \mathbf{x}_i$ the *shift vector*, pointing from the old to the new expansion centre.

We will make use of the fact that we can flip signs via $S_n^m(-\mathbf{x}) = (-1)^n S_n^m(\mathbf{x})$. For $|\mathbf{x} - \mathbf{x}_B| < |\mathbf{x} - \mathbf{x}_i|$ we then have:

$$\begin{aligned}
&\sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m(\mathbf{x} - \mathbf{x}_i) \\
&\quad= \sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m\left((\mathbf{x} - \mathbf{x}_B) - (\mathbf{x}_i - \mathbf{x}_B)\right) \\
&\quad\overset{\text{sign flip}}{=} \sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} (-1)^n \overline{M_{n,i}^m} S_n^m\left((\mathbf{x}_i - \mathbf{x}_B) - (\mathbf{x} - \mathbf{x}_B)\right) \\
&\quad\overset{(2.18)}{=} \sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \sum_{k=0}^{\infty} \sum_{l=-k}^{k} (-1)^n \overline{M_{n,i}^m} S_{n+k}^{m+l}(-\mathbf{r}) \overline{R_k^l(\mathbf{x} - \mathbf{x}_B)} \\
&\quad\overset{\text{sign flip}}{=} \sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \sum_{k=0}^{\infty} \sum_{l=-k}^{k} (-1)^k \overline{M_{n,i}^m} S_{n+k}^{m+l}(\mathbf{r}) \overline{R_k^l(\mathbf{x} - \mathbf{x}_B)}. \qquad (2.26)
\end{aligned}$$

It again remains to rearrange the sums and change the indices to obtain:

$$\begin{aligned}
&\sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_{n,i}^m} S_n^m(\mathbf{x} - \mathbf{x}_i) \\
&\quad= \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \overline{R_n^m(\mathbf{x} - \mathbf{x}_B)} \left((-1)^n \sum_{k=0}^{P_i-1} \sum_{l=-k}^{k} \overline{M_{k,i}^l} S_{n+k}^{m+l}(\mathbf{r}) \right). \qquad (2.27)
\end{aligned}$$

Thus, the general M2L-translation formula is as follows:

$$L_n^m := (-1)^n \sum_{k=0}^{P_i-1} \sum_{l=-k}^{k} \overline{M_{k,i}^l} S_{n+k}^{m+l}(\mathbf{r}). \qquad (2.28)$$

After truncating at the output order P, the resulting local expansion then approximates the original multipole expansion near $\mathbf{x}_B$:

$$\sum_{n=0}^{P_i-1} \sum_{m=-n}^{n} \overline{M_n^m} S_n^m(\mathbf{x} - \mathbf{x}_i) \approx \sum_{n=0}^{P-1} \sum_{m=-n}^{n} L_n^m \overline{R_n^m(\mathbf{x} - \mathbf{x}_B)} \qquad |\mathbf{x} - \mathbf{x}_B| < |\mathbf{x}_i - \mathbf{x}_B|. \qquad (2.29)$$

The remarks on the error of M2M analogously carry over to M2L. Several multipole expansions can be combined into a single local expansion. There are then two sources of error: the error from the original expansions plus the error from M2L. The second error contribution behaves just like in Figure 2.2: it is zero at $\mathbf{x}_B$, and then gradually increases as one approaches the perimeter of the largest sphere around $\mathbf{x}_B$ that contains none of the $\mathbf{x}_i$.

2.4.3 Local-to-Local (L2L)

L2L differs from the previous translation operators in that it does not make sense to choose the output's order P higher than that of the input expansion P_i. In L2L, the input is a local expansion of order P_i, i. e., a harmonic polynomial of total degree less than P_i. The space of harmonic polynomials is invariant under translation, i. e., polynomials can be translated exactly. Thus, when $P = P_i$, L2L is an error-free operation. Errors are only introduced when $P < P_i$, in which case they are zero at the new expansion centre $\mathbf{x}_B$ and gradually increase from there.

The derivation is similar to that of M2M and M2L. We begin by expanding the regular solid harmonics:[10, Equation (48)]

$$R_n^m(\mathbf{x}-\mathbf{y}) = \sum_{k=0}^{n}\sum_{l=-k}^{k} R_k^l(\mathbf{x})R_{n-k}^{m-l}(-\mathbf{y}) \qquad \text{(exact for any } \mathbf{x},\mathbf{y}\in\mathbb{R}^3\text{)}. \tag{2.30}$$

Here, to simplify notation, we again implicitly assume that $R_n^m = 0$ whenever $|m| > n$.

Thus, for a given input expansion $L_{n,i}^m$ around $\mathbf{x}_i$ and of order P_i, and shift vector $\mathbf{r} = \mathbf{x}_B - \mathbf{x}_i$, one obtains:

$$\begin{aligned}\sum_{n=0}^{P_i-1}\sum_{m=-n}^{n} L_{n,i}^m\overline{R_n^m(\mathbf{x}-\mathbf{x}_i)} &= \sum_{n=0}^{P_i-1}\sum_{m=-n}^{n} L_{n,i}^m\overline{R_n^m((\mathbf{x}-\mathbf{x}_B)-(\mathbf{x}_i-\mathbf{x}_B))}\\ &\overset{(2.30)}{=} \sum_{n=0}^{P_i-1}\sum_{m=-n}^{n}\sum_{k=0}^{n}\sum_{l=-k}^{k} L_{n,i}^m\overline{R_k^l(\mathbf{x}-\mathbf{x}_B)R_{n-k}^{m-l}(\mathbf{r})}\\ &\overset{\text{rearranging}}{=} \sum_{n=0}^{P_i-1}\sum_{m=-n}^{n}\overline{R_n^m(\mathbf{x}-\mathbf{x}_B)}\left(\sum_{k=n}^{P_i-1}\sum_{l=-k}^{k} L_{k,i}^l\overline{R_{k-n}^{l-m}(\mathbf{r})}\right).\end{aligned} \tag{2.31}$$

Thus, we may define new local moments via:

$$L_n^m = \sum_{k=n}^{P_i-1}\sum_{l=-k}^{k} L_{k,i}^l\overline{R_{k-n}^{l-m}(\mathbf{r})} \tag{2.32}$$

resulting in

$$\sum_{n=0}^{P_i-1}\sum_{m=-n}^{n} L_{n,i}^m\overline{R_n^m(\mathbf{x}-\mathbf{x}_i)} = \sum_{n=0}^{P_i-1}\sum_{m=-n}^{n} L_n^m\overline{R_n^m(\mathbf{x}-\mathbf{x}_B)} \qquad \text{exactly.} \tag{2.33}$$

The output expansion may be truncated ($P < P_i$). Choosing ($P > P_i$) will only result in adding zero coefficients $L_n^m = 0$ for $n \geq P_i$.

2.4.4 Summary of the Translation Formulæ

All of the translation operators take an input expansion of order P_i around some centre $\mathbf{x}_i$ and produce a new expansion of order P around centre $\mathbf{x}_i + \mathbf{r}$, where $\mathbf{r}$ is the so-called *shift vector*. Depending on the type of translation, the output expansion may coincide with the input expansion, or just be an approximation of it. The formulæ for computing the output coefficients are as follows.

M2M:

$$M_n^m = \sum_{k=0}^{P_i-1} \sum_{l=-n}^{n} M_{k,i}^l R_{n-k}^{m-l}(-\mathbf{r}). \tag{2.34}$$

M2L:

$$L_n^m = (-1)^n \sum_{k=0}^{P_i-1} \sum_{l=-k}^{k} \overline{M_{k,i}^l} S_{n+k}^{m+l}(\mathbf{r}). \tag{2.35}$$

L2L:

$$L_n^m = \sum_{k=n}^{P_i-1} \sum_{l=-k}^{k} L_{k,i}^l \overline{R_{k-n}^{l-m}(\mathbf{r})}. \tag{2.36}$$

In these sums it is implicitly assumed that $R_n^m = 0$ whenever $n < 0$ or $|m| > n$. When in- and output order $P = P_i$ coincide, computing all output coefficients using these forumulæ costs $\mathcal{O}(P^4)$. `solidfmm` uses acceleration techniques to reduce this cost to $\mathcal{O}(P^3)$ in theory, but measurements have shown that in practice it performs even better as $\mathcal{O}(P^2)$.

2.5 Outlook

The concepts described in this chapter form the main building blocks of fast multipole methods. With the mathematical background presented here, it should be possible to understand the library functionality described in Chapter 1. At the moment, `solidfmm` does not provide a full implementation of the fast multipole method, but only an efficient, optimised implementation of these building blocks. This is intentional, so that the library remains slim can be used in existing implementations of the FMM. For this reason we do not give a full description of the algorithm, of which there exist many variations.

The original FMM is due to Greengard and Rokhlin.[11] Since then the algorithm has developed into more simple, adaptive, parallelisable variants. A description of the 'dual tree traversal' by Dehnen[12] and a comparison to other variants was given by Yokota.[13] We find this version of the FMM particularly intuitive. He also compares different series expansions and mentions the lack of efficient implementations for the solid harmonics, even though they are the most efficient expansions available for the important kernel function $k(\mathbf{x},\mathbf{y}) = |\mathbf{x}-\mathbf{y}|^{-1}$. `solidfmm`'s aim is to provide such an implementation.

Chapter 3

User Reference

This chapter considers `solidfmm`'s API for users. The implementation details are covered in Part II of this book. All components of the library are in the `solidfmm` namespace. For brevity, we will omit the explicitly stating namespace in the discussion that follows. For example we will simply write `solid` instead of `solidfmm::solid`.

3.1 Overview

`solidfmm` exposes its interface through four header files, each of which will be described in a separate section below:

- `solidfmm/solid.hpp` Contains the `solid` data structure for storing the coefficients of expansions and values of the solid harmonics. Also contains the `dot` and `fmadd` operations.
- `solidfmm/harmonics.hpp` Evaluation of the solid harmonics and their gradients.
- `solidfmm/handles.hpp` Handle classes for creating buffers and shared data which are needed for the translation operations.
- `solidfmm/translations.hpp` The actual translation operations.

Most operations are templates and take a type parameter which is commonly called `real`. This type specifies which fundamental arithmetic type should be used to represent a real number. `solidfmm` supports single and double precision, i. e., `float` and `double` for this parameter. It is illegal to use other types for `real`.

3.2 `solidfmm/solid.hpp`

Objects of type `solid` are used to store the coefficients of both local and multipole expansions. Additionally, when evaluating the solid harmonics $S_n^m(\mathbf{x})$ and $R_n^m(\mathbf{x})$ at some given point $\mathbf{x} \in \mathbb{R}^3$, the resulting values are also stored in objects of this type. Instances can either hold scalar or vector-valued data. For example, the solid harmonics $S_n^m(\mathbf{x}), R_n^m(\mathbf{x}) \in \mathbb{C}$ are scalars. Their gradients are vector-valued: $\nabla S_n^m(\mathbf{x}), \nabla R_n^m(\mathbf{x}) \in \mathbb{C}^3$. For these reason most operations additionally take a parameter called `dim`, which, however, can be omitted when working with scalars. Similarly, it is possible to use vector-valued multipole and local expansions.

```
template <typename real>
class solid
{
public:
    solid() = default;
    solid( size_t P, size_t dim = 1 );
    solid( const solid  &rhs );
    solid(       solid &&rhs ) noexcept;
    solid& operator=( const solid  &rhs );
    solid& operator=(       solid &&rhs ) noexcept;
   ~solid();

    void resize( size_t P, size_t dim = 1 );
    void reinit( size_t P, size_t dim = 1 );
    void zeros() noexcept;

    const real& re( size_t n, size_t m, size_t d = 0 ) const noexcept;
          real& re( size_t n, size_t m, size_t d = 0 )       noexcept;
    const real& im( size_t n, size_t m, size_t d = 0 ) const noexcept;
          real& im( size_t n, size_t m, size_t d = 0 )       noexcept;

    size_t order    () const noexcept;
    size_t dimension() const noexcept;

    const real*  memptr() const noexcept;
          real*  memptr()       noexcept;

private:
        // …
};
```

Listing 3.1: Public interface of the `solid` class.

3.2.1 Construction and Resizing

The default constructor creates instances of order $P = 0$, i. e., empty objects which do not contain any coefficients or values. When creating a fresh object using the second constructor, or when calling `reinit` with the desired order and dimension, one obtains a `solidfmm::solid` containing only zero values. Calling the member `resize`, on the other hand, will result in object of the desired order and dimension, but with *undefined* contents. `zeros` can be used to set all members to zero. Thus, `reinit` is equivalent to calling `resize` and `zeros` immediately afterwards. The copy and move constructors, as well as the assignment operators have the usual semantics. All these operations either come with a no-throw guarantee, or the strong exception guarantee. In particular, functions like `resize` can only throw exceptions of type `std::bad_alloc`, but in case they do, they leave the object unchanged.

3.2.2 Accessing Elements

The contents of a solid can be accessed using the member functions re and im, which respectively return the real and imaginary parts of the specified element.

```
solid<double> M; // Given multipole coefficients, initialised somewhere else.

double a = M.re(4,2);
M.im(2,1) = 42;
```

Under the assumption that M.order() > 4, this code stores the value of $\Re M_4^2$ in the variable a and assigns the value 42 to $\Im M_2^1$. For vector-valued a solid, the above code would access the zeroth component of the respective vectors; dimensions are counted beginning with zero. For example, to access the 'y-component' of the real part of some $\mathbf{M}_4^2 \in \mathbb{C}^3$, one would instead use:

```
double a = M.re(4,2,1);
```

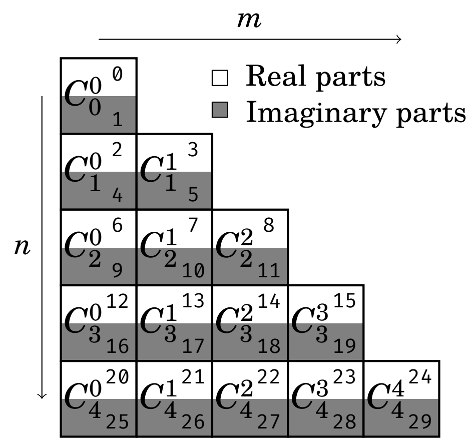
The indices n, m, and d (default value $d = 0$) must be valid. No range checks are performed; passing invalid arguments will result in undefined behaviour. As discussed in Section 2.3, it is not necessary to store the values of M_n^m for the negative values of m, as they are given implicitly. For this reason, for a given solid of order P and dimension D, the valid range of parameters is $0 \leq n < P$, $0 \leq m \leq n$, and $0 \leq d < \mathrm{D}$.

3.2.3 Direct Memory Access

The member function memptr() gives direct memory access to the data that a solid is holding. The indexing scheme is best illustrated graphically, see Figure 3.1. Assume we were given a solid of order P and dimension D. Then the real and imaginary parts of the dth vector-component of some $\mathbf{M}_n^m \in \mathbb{C}^{\mathrm{D}}$, $0 \leq n < P$, $0 \leq m \leq n$, $0 \leq d < \mathrm{D}$ can be accessed via:

```
double real_part = M.memptr()[ d*P*(P+1) + (n  )*(n+1) + m ];
double imag_part = M.memptr()[ d*P*(P+1) + (n+1)*(n+1) + m ];
```

Don't even think about calling delete, delete [], free(), realloc(), or the like on this pointer—unless, of course, you are keen on causing undefined behaviour and crashing your programme.



$$\begin{aligned}\texttt{pos}(\Re(C_n^m)) &= (n+0)(n+1)+m,\\ \texttt{pos}(\Im(C_n^m)) &= (n+1)(n+1)+m.\end{aligned}$$

Figure 3.1: A generic `solid` C may contain coefficients of local or multipole expansions, as well as the values of regular or singular harmonics. The memory layout of a *scalar* `solid` of order 5 is illustrated above. Only the values C_n^m for $m \geq 0$ need to be stored, as the values for negative m are given implicitly. The array position `pos` of the respective values is indicated by the numbers in the upper and lower right corners of the boxes. A vector-valued `solid` first stores all values for dimension $d = 0$ as shown above. Then all elements for dimension $d = 1$ follow using the same layout, then those of dimension $d = 2$, and so forth.

3.2.4 Evaluating Expansions using dot

Consider the task of evaluating a given multipole expansion around some centre $\mathbf{x}_A$:

$$\sum_{n=0}^{P-1} \sum_{m=-n}^{n} \overline{M_n^m} S_n^m(\mathbf{x} - \mathbf{x}_A) \tag{3.1}$$

as discussed in Chapter 2. This operation is essentially the dot-product on two complex-valued vectors $M, S \in \mathbb{C}^{P^2}$ which are indexed in a non-standard way. Additionally, as discussed before, this sum always takes real values, so the roles of M and S can be swapped without changing the result. For this reason, `solidfmm` implements such operations using the function `dot`.

```
void dot( const solid<float>  &A, const solid<float>  &B, float  *result ) noexcept;
void dot( const solid<double> &A, const solid<double> &B, double *result ) noexcept;
```

This function supports inputs of differing orders and dimensions, i. e., it is legal to have `A.order()` $\neq$ `B.order()` and `A.dimension()` $\neq$ `B.dimension()`. The semantics of these cases are as follows.

1. In case we have `A.order()` $\neq$ `B.order()`, the `solid` of lower order is padded with zeros to match the other `solid`'s order.

2. In case we have `A.dimension()`$\neq$`1` or `B.dimension()`$\neq$`1`, all combinations of components are dotted together, i. e., the result is a matrix of dimension

   $$\texttt{A.dimension()} \times \texttt{B.dimension()}$$

   that is stored in row-major order. The entry at position (i,j) then contains the value

   $$\sum_{n=0}^{P-1} \sum_{m=-n}^{n} \overline{A_{n,i}^m} B_{n,j}^m.$$

   If you prefer column-major order, you can just swap `A` and `B` when calling `dot`.

For this reason, `dot` does not simply return a floating point value, but takes a pointer to the first element where the result should be stored. It is the duty of the user to ensure that these pointers point to a region of memory which is sufficiently large to store the result.

Assume you were given a vector-valued local expansion of order P with coefficients $\mathbf{L}_n^m \in \mathbb{C}^3$ around expansion centre $\mathbf{x}_B = (\texttt{xB}, \texttt{yB}, \texttt{zB})^\top \in \mathbb{R}^3$. To evaluate this expansion at some location $\mathbf{x} = (\texttt{x}, \texttt{y}, \texttt{z})^\top \in \mathbb{R}^3$, you would use the following code:

```
double result[3];
dot( L, harmonics::R<double>(P,x-xB,y-yB,z-zB), result );
```

To evaluate its derivative, i. e., its Jacobian matrix of dimension $\mathbb{R}^{3\times 3}$, you would then use the following code and replace the regular harmonics `R` with their gradients `dR`:

```
double jacobian[9];
dot( L, harmonics::dR<double>(P,x-xB,y-yB,z-zB), jacobian );
```

Note that calling `harmonics::R` or `harmonics::dR` requires you to `#include` the `solidfmm/harmonics.hpp` header, which is described in Section 3.3.

3.2.5 Creating Expansions using `fmadd`

We recall the P2M and P2L operations from Chapter 2. Given a set of 'particles' with location $\mathbf{x}_i$ and mass m_i, $i = 0, \dots, N-1$, we desire to compute multipole or local expansions around respective centres $\mathbf{x}_A$ and $\mathbf{x}_B$:

$$M_n^m = \sum_{i=0}^{N-1} m_i R_n^m(\mathbf{x}_i - \mathbf{x}_A), \qquad L_n^m = \sum_{i=0}^{N-1} m_i S_n^m(\mathbf{x}_i - \mathbf{x}_B). \tag{3.2}$$

This operation thus always takes multiples of a `solid` containing the values of the regular or singular harmonics, and accumulates them into a `solid` that contains the expansion coefficients. There also is support for vector-valued expansions:

```
void fmadd( const float   fac, const solid<float > &A, solid<float > &B );
void fmadd( const float  *fac, const solid<float > &A, solid<float > &B );
void fmadd( const double  fac, const solid<double> &A, solid<double> &B );
void fmadd( const double *fac, const solid<double> &A, solid<double> &B );
```

In all of these operations one must have both `A.dimension() == B.dimension()` and `A.order() == B.order()`, because it is not clear how to meaningfully define those operations otherwise. These functions throw exceptions of type `std::logic_error` if one of these conditions is violated. Again, the strong exception guarantee is given: in case an exception is thrown, the function's arguments are not changed.

The functions taking a *value* `fac` essentially perform `B += fac*A`; but note that `solidfmm` does not implement `operator+=`. The operations taking a *pointer* `fac` assume that it points to an array of size `A.dimension() == B.dimension()`; the d'th component is then scaled by `fac[d]`.

We are still not sure how to devise a more flexible interface, we are open for suggestions!

3.3 `solidfmm/harmonics.hpp`

This header contains the function declations for evaluating the regular and singular harmonics, as well as their gradients, as they are defined in Section 2.3. The interface should be pretty self-explanatory:

```
namespace harmonics
{

template <typename real> solid<real>  R( size_t P, real x, real y, real z );
template <typename real> solid<real>  S( size_t P, real x, real y, real z );
template <typename real> solid<real> dR( size_t P, real x, real y, real z );
template <typename real> solid<real> dS( size_t P, real x, real y, real z );

}
```

The parameter `P` specifies the order up to which you wish to evaluate the harmonics. The parameters `x`,`y`, and `z` are the respective components of the position vector $\mathbf{x} = (x, y, z)^\top \in \mathbb{R}^3$ at which you want to evaluate the harmonic functions. Only `double` and `float` are supported for the template parameter `real`. These functions may throw exceptions of type `std::bad_alloc`.

3.4 solidfmm/handles.hpp

The handle classes encapsulate resources that are implementation details but are needed to carry out the single-threaded versions of the translation operations M2M, M2L, and L2L. You do not need these if you use the `multithreaded_translator` as described in Section 1.3.4.

There are two kinds of handles:

1. `operator_handle`. Only one of these handles is needed, it can and *should be shared* among threads. It is a wrapper to an implementation detail, which essentially stores the so-called Wigner matrices, which are needed for the efficient implementation of the translation operators. This class also automatically determines the available CPU features at runtime and chooses the most efficient implementation available.

2. `buffer_handle`. *Each thread needs its own handle.* These handles need to be created for a given `operator_handle`. As the name implies, a `buffer_handle` encapsulates buffers which a thread can use as its workspace when performing translations.

Handles can be copied, default constructed, and also support assignment operations. In a typical scenario, however, a user would create these handles *only once* at program start-up and then pass them around by reference. The relevant parts of the user-interface are as follows:

```
template <typename real>
class operator_handle
{
public:
        // …
    operator_handle( size_t P );
    buffer_handle<real> make_buffer() const;
        // …
};

template <typename real>
class buffer_handle
{
public:
        // …
    buffer_handle( const operator_data<real> &op );
        // …
};
```

In other words, a `buffer_handle` needs to be created specifically for a particular `operator_handle`. This can for example be achieved as follows:

```
// The maximum number of concurrent threads you are going to use.
// For example, on a CPU with 8 cores:
const size_t nthreads { 8 };

// Only one such object is necessary; it can and should be shared among threads.
// For exmaple, if you never need expansion orders beyond P = 30:
operator_handle<double> op  { 30 };

// Each thread needs its own buffer; it must not be shared.
std::vector<buffer_handle<double>> buffers(nthreads,op.make_buffer());
```

These routines may throw exceptions of type `std::bad_alloc`. Again, it is illegal to use other types than `double` and `float` for the template parameter `real`.

The translation operations make use of faculties up to $2P - 2$. For this reason, for `float` the maximum supported order is 18: for higher orders the number $(2P - 2)!$ is out of the range of this type. For double precision calculations the corresponding limit is 86. In both cases, the accuracies achieved by expansions of such high order are usually already exceeding the precision of the respective floating point numbers. In this case the constructors throw exceptions of type `std::overflow_error`. Passing $P = 0$ will case an exception of type `std::logic_error` to be thrown.

3.5 solidfmm/translations.hpp

This header contains methods for carrying out the translation operations M2M, M2L, and L2L. The mathematical background and details of these operations are discussed in Chapter 2. The `translation_info` and `multithreaded_translator` classes were already described in Section 1.3.4. Additionally this header contains the single threaded functions. To use these, you will need to create handles as described in Section 3.4.

3.5.1 Single-threaded Translation Routines

```
void           m2l( const operator_data<double> &op,
                          threadlocal_buffer<double> &buf,
                    const translation_info<double> *begin,
                    const translation_info<double> *end );

void m2l_unchecked( const operator_data<double> &op,
                          threadlocal_buffer<double> &buf,
                    const translation_info<double> *begin,
                    const translation_info<double> *end ) noexcept;

// Analogous for m2m, l2l, and single precision (float).
```

Just like the `multithreaded_translator`, these operations also support vector-valued `solids`. In this case, the translations are carried out component-wise along the specified shift vector. For this to work, the target `solids` must match the dimension of the input expansion.

The functions come in two variants. The default variants perform some simple runtime checks to ensure that the operations are well-defined. First of all, they check if the `operator_handle` and `buffer_handle` are compatible with each other. They then check that none of the coefficients exceed the maximum order P of the supplied handles. In the case of vector-valued coefficients, they check that dimensions of source and target expansions match. If one of these checks fails, an exception is thrown and the arguments are left unchanged (strong exception guarantee). In summary, the following exceptions can be thrown:

- `std::logic_error` If input and output dimensions of the passed `solids` differ. This also is thrown if you pass a `buffer_handle` that was created for a different `operator_handle`.
- `std::out_of_range` if the order of one of the passed `solids` exceeds the order of the given `operator_handle`.

The unchecked variants omit these checks, never throw and exception and lead to *undefined behaviour* when invalid data is supplied.

The types `operator_data` and `threadlocal_buffer` are the implementation details that are encapsulated by the handle classes in Section 3.4. Thus, a user should pass the corresponding handles instead, and *never* use the internal classes `operator_data` and `threadlocal_buffer` directly.

Just like the `multithreaded_translator` class, these functions *add* and accumulate the translation results into the corresponding targets:

$$\text{target} \quad \texttt{+=} \quad \text{translate}(\text{source}, x, y, z).$$

These functions do not create any threads, they operation is carried out by the calling thread of execution. You may call `m2m`, `l2l`, and `m2l` simultaneously from several threads. In this case, each thread needs its own buffer. You cannot have different threads write to the same output, this will cause a race condition and undefined results.

3.5.2 Single-threaded Methods using the Classic Interface

The classic interface only comes in the ‘checked’ variant and behaves identically to the interface using the `translation_info` class described in the previous subsection.

```
void m2m( const operator_data<double> &op, threadlocal_buffer<double> &buf,
          size_t howmany, const solid<double> *const *const Min,
                                solid<double> *const *const Mout,
          const double *x, const double *y, const double *z );

void m2l( const operator_data<double> &op, threadlocal_buffer<double> &buf,
          size_t howmany, const solid<double> *const *const M,
                                solid<double> *const *const L,
          const double *x, const double *y, const double *z );


void l2l( const operator_data<double> &op, threadlocal_buffer<double> &buf,
          size_t howmany, const solid<double> *const *const Lin,
                                solid<double> *const *const Lout,
          const double *x, const double *y, const double *z );
```

and the corresponding functions for single precision calculations using `float`.

Again, the types `operator_data` and `threadlocal_buffer` are the implementation details that are encapsulated by the handle classes in Section 3.4. Thus, a user should pass the corresponding handles instead, and *never* use the internal classes `operator_data` and `threadlocal_buffer` directly.

Assume we were given the following data, initialised somewhere else:

```
// Number of translations you want to carry out.
size_t howmany;

// Arrays of size howmany, containing *pointers* to coefficients.
solidfmm::solid<double> *input [howmany];
solidfmm::solid<double> *output[howmany];

// Shift vectors for the translations. That is, if the input coefficients
// represent expansions about a point (xA,yA,zA), and the output coefficients
// should be around another centre (xB,yB,zB), the shift-vectors would be
// (xB-xA,yB-yA,zB-zA).
double xshift[howmany];
double yshift[howmany];
double zshift[howmany];
```

We also assume that you already have created operator and buffer handles as described in Section 3.4. To perform the actual translation, you just need to call M2L, or, respectively m2m and l2l, as follows:

```
solidfmm::m2l(op_handle,buf_handle,howmany,input,output,xshift,yshift,zshift);
```

Part II

Developer Guide

Chapter 4

Microkernels

At their core, the translations M2M, M2L, and L2L break down to certain copy operations and dense matrix–matrix products. However, every CPU architecture is different, hence each requires its own specific, optimised implementation of these operations to obtain maximum performance. This leads to the question: 'How can we write *one* library that achieves high performance on *many* platforms?'

To answer this question, `solidfmm` follows the approach taken the BLIS developers and uses the concept of microkernels.[14],[15] While each CPU requires its own implementation, microkernels encapsulate the key operations behind a unified interface. The 'driver code' then can remain machine independent, while the machine specific code is reduced to a well-defined, isolated, small set of functions. Due to this localisation, the library can be quickly adapted to new architectures.

In C++, the most natural choice to represent such an interface is an abstract base class gives this interface in the form of `virtual` functions. For each new CPU architecture optimised implementations can then be provided by deriving from this base class and overriding the generic default routines. The driver routines only make use of the base class, and through run-time polymorphism the optimised, machine specific routines get called.

In this chapter we describe `solidfmm`'s microkernel interface. We specify the functionality that these functions must implement, how to include such a new microkernel into `solidfmm`, and how to test that it is working. How to achieve maximum performance on your computer is, of course, machine dependent. However, many routines are similar to general matrix–matrix products. As a starting point, we thus suggest to take a look at the BLIS,[16] which comes with highly efficient microkernels for a variety of platforms. These can serve as an inspiration when writing your own microkernels for `solidfmm`. Their authors furthermore created an excellent lecture series in which they share their expertise.[15]

4.1 Overview

The `microkernel` class is declared in its own header file:

```
#include <solidfmm/microkernel.hpp>
```

Its interface is given in the following listing. As usual, the only permissible values for the template parameter `real` are `float` and `double`.

```
template <typename real>
class microkernel
{
public:
    const size_t rows;
    const size_t cols;
    const size_t alignment;

    microkernel( size_t p_rows, size_t p_cols, size_t p_alignment ) noexcept:
    rows { p_rows }, cols { p_cols }, alignment { p_alignment } {}

    virtual ~microkernel() = default;

    virtual void euler( const real *x,   const real *y, const real *z,
                              real *r,         real *rinv,
                              real *cos_alpha, real *sin_alpha,
                              real *cos_beta,  real *sin_beta,
                        size_t k ) const noexcept = 0;

    virtual void rotscale( const real *cos, const real *sin, const real *scale,
                           const real *real_in,  const real *imag_in,
                                 real *real_out,       real *imag_out,
                           size_t k, bool forward ) const noexcept = 0;

    virtual void swap( const real *mat, const real *in,
                       real *out, size_t k, bool pattern ) const noexcept = 0;

    virtual void zm2l( const real *mat, const real *in,
                       real *out, size_t k, bool pattern ) const noexcept = 0;

    virtual void zm2m( const real *mat, const real *in,
                       real *out, size_t k ) const noexcept = 0;

    virtual void swap2trans_buf( const real  *real_in,  const real  *imag_in,
                                       real **real_out,       real **imag_out,
                                 size_t n ) const noexcept = 0;

    virtual void trans2swap_buf( const real *const *const real_in,
                                 const real *const *const imag_in,
                                       real *real_out, real *imag_out,
                                 size_t n, size_t Pmax ) const noexcept = 0;

    virtual void solid2buf( const real *const *solids,
                  const real *const  zeros, const size_t *P,
                  real *real_out, real *imag_out, size_t n ) const noexcept = 0;

    virtual void buf2solid( const real *real_in, const real *imag_in,
                            real **solids, real *trash,
                            const size_t *P, size_t n ) const noexcept = 0;
};
```

Listing 4.1: Interface of the `microkernel` class.

4.1.1 Data Members

Block Size. As described before, in the course of a translation operation, certain matrix–matrix products $C = AB$ need to be computed. `solidfmm` computes such products in a block-wise fashion: the matrix C is sub-divided into blocks of size `rows` × `cols` and then calls the necessary microkernel routines. Together these two parameters are called *block size*. The block size should be chosen according to the following guidelines:

- Even number of rows. The parameter `rows` *must* be a multiple of two.
- Register space. The block-size should be as large as possible such that it can still fit into the processor's registers, and such that enough spare registers remain for forming the matrix–matrix products. Ideally you use exactly all available registers and leave no un-used registers behind.
- Ratio. The parameters should fulfil `rows` ≈ `cols`, yielding approximately square blocks. This ensures optimal data reuse and avoids unnecessary memory transfers.

For the rest of this chapter we will write μ ≔ `rows` and ν ≔ `cols`.

Alignment. The `alignment` parameter causes `solidfmm` to ensure that the first entry of the matrices B and C (but *not* A) will be aligned as specified. A k byte alignment means that the memory address is a multiple of k. For example, 32 byte alignment causes the addresses of the respective first entries of B and C to be divisible by 32. Many processors offer extra fast instructions for aligned memory access. Use this parameter to be able to make use of these optimisations. There are certain restrictions that this parameter must fulfil:

- It must be a power of two, i. e., `alignment` $= 2^l$ for some integer $l \in \mathbb{N}_0$.
- On POSIX systems, it must be a power of two multiple of `sizeof(void*)`, i. e., on these systems there must exist some $k \in \mathbb{N}$ such that

  $$\texttt{alignment} = 2^k \times \texttt{sizeof(void*)}.$$

- The size of one row needs to be a fixed multiple of `alignment`:

  $$\texttt{sizeof(real)} \times \texttt{cols} = 0 \pmod{\texttt{alignment}},$$

  or, equivalently, in C++ syntax, one must have:

  ```
  (sizeof(real)*cols) % alignment == 0
  ```

  This ensures that the beginning of every row of B and C has the same alignment.

4.1.2 Function Members

There are three kinds of routines in a `microkernel`:

- Copy routines: `solid2buf`, `buf2solid`, `swap2trans_buf`, and `trans2swap_buf`. These operations copy and rearrange data between different locations.
- Matrix–matrix products: `swap`, `m2m`, and `m2l`. These routines carry out specialised matrix–matrix products $C = AB$, where C is of dimension `rows` × `cols`. The remaining dimension of these matrices is called `k` and given as a parameter at run-time.
- Other: `euler` and `rotscale` will be described separately.

We will describe each of these routines in greater detail below.

4.2 Copy Routines

4.2.1 `solid2buf()`

```
virtual void solid2buf( const real *const *solids,
                        const real *const  zeros, const size_t *P,
                        real *real_out, real *imag_out, size_t n ) const noexcept;
```

This method copies the line n of given solids into buffers for further processing.
We are given ν *scalar* solids $C_n^m[0]$, $C_n^m[1]$, …, $C_n^m[\nu-1]$ of respective orders $P[0], P[1], \ldots, P[\nu-1]$. The parameter `solids` is an array of pointers to these solids. Each of these solids is stored as described in Figure 3.1. In other words, to access $\Re C_n^m[k]$ for some n, m, and k you would write:

```
solids[k][ (n+0)*(n+1) + m ]
```

Here we assumed $n, m, k \in \mathbb{N}_0$ and that $k < \nu$, $n < P[k]$, $m \leq n$. Whenever $n \geq P[k]$ it is implicitly assumed that $C_n^m[k] = 0$. Thus, more correctly, to access the value of, e. g., $\Im C_n^m[k]$, the complete code snippet would be:

```
real value = (n<P[k]) ? solids[k][ (n+1)*(n+1) + m ] : 0;
```

In the method `solid2buf()` the value of n is fixed and given as a parameter. The task is now to copy row n of each solid into the matrices `real_out` and `imag_out`, that respectively hold the real and imaginary parts of the solids. These matrices are stored in *row-major* order and look as follows:

$$\begin{pmatrix} \Re C_n^0[0] & \Re C_n^0[1] & \cdots & \Re C_n^0[\nu-1] \\ \Re C_n^1[0] & \Re C_n^1[1] & \cdots & \Re C_n^1[\nu-1] \\ \vdots & \vdots & \ddots & \vdots \\ \Re C_n^n[0] & \Re C_n^n[1] & \cdots & \Re C_n^n[\nu-1] \end{pmatrix} \begin{pmatrix} \Im C_n^0[0] & \Im C_n^0[1] & \cdots & \Im C_n^0[\nu-1] \\ \Im C_n^1[0] & \Im C_n^1[1] & \cdots & \Im C_n^1[\nu-1] \\ \vdots & \vdots & \ddots & \vdots \\ \Im C_n^n[0] & \Im C_n^n[1] & \cdots & \Im C_n^n[\nu-1] \end{pmatrix} \tag{4.1}$$

Thus, the behaviour of this function is equivalent to the following snippet:

```
for ( size_t m = 0; m <= n;    ++m )
for ( size_t k = 0; k <= cols; ++k )
{
    real_out[ m*cols + k ] = (n<P[k]) ? solids[k][ (n+0)*(n+1) + m ] : 0;
    imag_out[ m*cols + k ] = (n<P[k]) ? solids[k][ (n+1)*(n+1) + m ] : 0;
}
```

The parameter `zeros` points to a memory location containing zero values, that may be used to avoid repeatedly checking if we have `n<P[k]`. This can be done by creating a local pointer array, leading to the following solution of the task:

```
const real* tmp_solids[ cols ];
for ( size_t k = 0; k < cols; ++k )
{
    if ( n < P[k] )
        tmp_solids[ k ] = const_cast<real*>(solids[k]);
    else
        tmp_solids[ k ] = const_cast<real*>(zeros);
}

for ( size_t m = 0; m <= n;    ++m )
for ( size_t k = 0; k <= cols; ++k )
{
    real_out[ m*cols + k ] = tmp_solids[k][ (n+0)*(n+1) + m ];
    imag_out[ m*cols + k ] = tmp_solids[k][ (n+1)*(n+1) + m ];
}
```

This way the condition `n < P[k]` only needs to be checked once per solid.

The matrices `real_out` and `imag_out` are aligned according to the `alignment` member of the microkernel object. The solids will usually be unaligned. Additionally, the solids may alias, i. e., `solid[i]` may point to the same location as `solid[j]`. Keep this in mind when trying to optimise this operation.

4.2.2 buf2solid()

```
virtual void buf2solid( const real *real_in, const real *imag_in,
                        real **solids, real *trash, const size_t *P, size_t n )
                        const noexcept;
```

In essence, this is the inverse to the routine `solid2buf()`, which we described in the previous subsection. In other words, the data from the given buffers is copied to the target solids. If the order of the target solid is below `n`, the data gets discarded. The `trash` parameter can be used to write data in this case. This prevents frequent rechecking if we have `P[k]<n`, similar to the `zeros` parameter from `solid2buf()`.

However, unlike in `solid2buf()`, the data is *added* to the output solids. This enables the users to accumulate several input expansions into a single output expansion. It is thus crucial to keep in mind that the pointers from the `solids` array *may and often do alias*. Thus, after adding to `solids[i]` for some i, it is important to keep in mind that `solid[j]` might also have been changed, as we might have `solid[i]==solid[j]` even when $i \neq j$. In an assembly language implementation this means that `solid[i+1]` can only be read from memory *after writing* `solid[i]`. A simple default implementation in C++ looks as follows:

```
real* tmp_solids[ cols ];
for ( size_t k = 0; k < cols; ++k )
    tmp_solids[ k ] = ( n < P[k] ) ? solids[k] : trash;

for ( size_t m = 0; m <= n;    ++m )
for ( size_t k = 0; k <= cols; ++k )
{
    tmp_solids[k][ (n+0)*(n+1) + m ] += real_in[ m*cols + k ];
    tmp_solids[k][ (n+1)*(n+1) + m ] += imag_in[ m*cols + k ];
}
```

Note that both `solid2buf()` and `buf2solid()` are similar to transposing a matrix in memory. When creating high-performance implementations of this operation, you can try using tricks for matrix transposition to obtain higher performance. Also note that `real_in` and `imag_in` are aligned according to the `alignment` member, but the individual solids are usually not aligned.

4.2.3 `swap2trans_buf()`

```
virtual void swap2trans_buf( const real  *real_in,  const real  *imag_in,
                                   real **real_out,       real **imag_out,
                                   size_t n ) const noexcept;
```

There are two kinds of buffers in `solidfmm`: swap and translation buffers. Swap buffers hold *some row n* of ν solids $C[0], C[1], \dots, C[\nu-1]$, i. e., they are matrices of the shape

$$\begin{pmatrix} \Re C_n^0[0] & \Re C_n^0[1] & \dots & \Re C_n^0[\nu-1] \\ \Re C_n^1[0] & \Re C_n^1[1] & \dots & \Re C_n^1[\nu-1] \\ \Re C_n^2[0] & \Re C_n^2[1] & \dots & \Re C_n^2[\nu-1] \\ \vdots & \vdots & \ddots & \vdots \\ \Re C_n^n[0] & \Re C_n^n[1] & \dots & \Re C_n^n[\nu-1] \end{pmatrix} \quad \begin{pmatrix} \Im C_n^0[0] & \Im C_n^0[1] & \dots & \Im C_n^0[\nu-1] \\ \Im C_n^1[0] & \Im C_n^1[1] & \dots & \Im C_n^1[\nu-1] \\ \Im C_n^2[0] & \Im C_n^2[1] & \dots & \Im C_n^2[\nu-1] \\ \vdots & \vdots & \ddots & \vdots \\ \Im C_n^n[0] & \Im C_n^n[1] & \dots & \Im C_n^n[\nu-1] \end{pmatrix},$$

and are stored in row-major format. Conversely, a translation buffer stores *some column* m of ν different solids. For example, for a fixed m, the real-part of a translation buffer looks like follows:

$$\begin{pmatrix} \Re C_m^m[0] & \Re C_m^m[1] & \dots & \Re C_m^m[\nu-1] \\ \Re C_{m+1}^m[0] & \Re C_{m+1}^m[1] & \dots & \Re C_{m+1}^m[\nu-1] \\ \Re C_{m+2}^m[0] & \Re C_{m+2}^m[1] & \dots & \Re C_{m+2}^m[\nu-1] \\ \vdots & \vdots & \ddots & \vdots \end{pmatrix},$$

where the matrix is stored in row-major format and the imaginary parts are stored analogously.

This method takes the content of the swap buffers given as `real_in` and `imag_in` of the given row `n` and copies it to the corresponding positions in the translation buffers. A simple C++ implementation would look like follows.

```
for ( size_t m = 0; m ⩽  n;    ++m )
for ( size_t k = 0; k <  cols; ++k )
{
    real_out[m][ (n-m)*cols + k ] = real_in[ m*cols + k ];
    imag_out[m][ (n-m)*cols + k ] = imag_in[ m*cols + k ];
}
```

All of the buffers are aligned according to the `alignment` member. This enables the use of fast, aligned copy instructions on certain machines.

4.2.4 trans2swap_buf()

```
virtual void trans2swap_buf( const real *const *const real_in,
                             const real *const *const imag_in,
                                   real *real_out, real *imag_out,
                             size_t n, size_t Pmax ) const noexcept;
```

This is the inverse operation to `swap2trans_buf`, as described above. The parameter `Pmax` indicates that values $C_n^m[k]$ with $m \geq P_{\max}$ are considered to be zero. A simple C++ implementation could thus look as follows:

```
// First the entries where m < Pmax
for ( size_t m = 0; m < min(Pmax,n+1); ++m )
for ( size_t k = 0; k < cols;          ++k )
{
    real_out[ m*cols + k ] = real_in[m][ (n-m)*cols + k ];
    imag_out[ m*cols + k ] = imag_in[m][ (n-m)*cols + k ];
}

// Now the remaining entries, if any.
for ( size_t m = Pmax; m ⩽  n;    ++m )
for ( size_t k = 0;    k <  cols; ++k )
{
    real_out[ m*cols + k ] = 0;
    imag_out[ m*cols + k ] = 0;
}
```

4.3 Matrix–matrix Product Routines

The methods of this section compute matrix–matrix products $C = AB$, where $C \in \mathbb{R}^{\mu\times\nu}$, $A \in \mathbb{R}^{\mu\times k}$, and $B \in \mathbb{R}^{k\times\nu}$. For convenience we abbreviate μ ≔ `rows` and ν ≔ `cols`. We will denote the mathematical matrices with capital letters; pointers to the corresponding data will be denoted by denoted by lower case letters.

The matrices C and B are stored in row-major format, e. g., C_{ij} can be accessed via `c[i*cols + j]`, where $i = 0, \dots, \mu - 1$ and $j = 0, \dots, \nu - 1$. Similarly, B_{ij} can be accessed via `b[i*cols+j]`, where $i = 0, 1, \dots, k - 1$ and $j = 0, 1, \dots, \nu - 1$. Both `c` and `b` will be aligned according to the `alignment` class member.

The pointer `a` will usually not be aligned. The matrix A is stored in special formats, depending on the particular routine.

4.3.1 `swap()`

```
virtual void swap( const real *a, const real *b, real *c, size_t k,
                   bool pattern ) const noexcept;
```

This routine is called `swap`, because it is used in coordinate transformations that correspond to swapping the x- and z-axis. The matrix A here has one of two possible chequerboard patterns. Only half of A's entries are non-zero. Only these non-zero entries are stored in `a`, using a compressed column major format. In particular, if the `pattern` parameter is true, A's first entry is non-zero. For example, when $\mu = 6$, the matrix A then is given by:

$$A = \underbrace{\begin{pmatrix} a[0] & 0 & a[6] & 0 & \cdots \\ 0 & a[3] & 0 & a[9] & \cdots \\ a[1] & 0 & a[7] & 0 & \cdots \\ 0 & a[4] & 0 & a[10] & \cdots \\ a[2] & 0 & a[8] & 0 & \cdots \\ 0 & a[5] & 0 & a[11] & \cdots \end{pmatrix}}_{k \text{ columns}} \qquad \text{if } \texttt{pattern==true}. \tag{4.2}$$

Otherwise, if `pattern==false`, the matrix A is given by:

$$A = \underbrace{\begin{pmatrix} 0 & a[3] & 0 & a[9] & \cdots \\ a[0] & 0 & a[6] & 0 & \cdots \\ 0 & a[4] & 0 & a[10] & \cdots \\ a[1] & 0 & a[7] & 0 & \cdots \\ 0 & a[5] & 0 & a[11] & \cdots \\ a[2] & 0 & a[8] & 0 & \cdots \end{pmatrix}}_{k \text{ columns}} \quad \text{if } \texttt{pattern==false}. \tag{4.3}$$

4.3.2 `zm2l()`

```
virtual void zm2l( const real *a, const real *b, real *c, size_t k,
                   bool pattern ) const noexcept;
```

This operation is needed when performing an M2L translation along the z-axis. Actually, two operations are carried out. First, the matrix–matrix product $C = AB$ is formed, where $A \in \mathbb{R}^{\mu\times k}$ is given as follows:

$$A = \underbrace{\begin{pmatrix} a[0] & a[1] & a[2] & a[3] & \cdots \\ a[1] & a[2] & a[3] & a[4] & \cdots \\ a[2] & a[3] & a[4] & a[5] & \cdots \\ a[3] & a[4] & a[5] & a[6] & \cdots \\ \vdots & \vdots & \vdots & \vdots & \\ a[\mu-1] & a[\mu] & a[\mu+1] & a[\mu+2] & \cdots \end{pmatrix}}_{k \text{ columns}}. \tag{4.4}$$

In other words, the value of A_{ij} can be accessed via `a[i+j]`, where $i = 0, 1, \dots, \mu - 1$ and $j = 0, 1, \dots, k - 1$.

Once the product C has been formed, we apply a sign pattern to the result:

- If `pattern==true`: rows 0, 2, 4, …, μ-2 of the result matrix C are multiplied by (-1).
- If `pattern==false`: rows 1, 3, 5, …, μ-1 of the result matrix C are multiplied by (-1).

4.3.3 `zm2m()`

```
virtual void zm2m( const real *a, const real *b, real *c, size_t k ) const noexcept;
```

This operation is needed when performing M2M or L2L translations along the z-axis.

It carries out a matrix–matrix product $C = AB$, where $A \in \mathbb{R}^{\mu\times k}$ is given as follows:

$$A = \underbrace{\begin{pmatrix} a[\mu-1] & a[\mu] & a[\mu+1] & a[\mu+2] & \cdots \\ a[\mu-2] & a[\mu-1] & a[\mu] & a[\mu+1] & \cdots \\ \vdots & \vdots & \vdots & \vdots & \\ a[1] & a[2] & a[3] & a[4] & \cdots \\ a[0] & a[1] & a[2] & a[3] & \cdots \end{pmatrix}}_{k \text{ columns}}. \tag{4.5}$$

In other words, the matrix A corresponds to that of `zm2l()`, but with the order of the rows reversed.

4.4 euler and rotscale

4.4.1 euler()

```
virtual void euler( const real *x,   const real *y, const real *z,
                          real *r,         real *rinv,
                          real *cos_alpha, real *sin_alpha,
                          real *cos_beta,  real *sin_beta,
                    size_t k ) const noexcept;
```

Given ν shift vectors with coordinates $(x[i], y[i], z[i])^\top$, $i = 0, \dots, \nu-1$, this method computes data that is related to the Euler angles of a certain coordinate transform.

This method fills the matrix `r` powers of the lengths of these vectors and is stored in row-major format:

$$\mathtt{r} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ r[0] & r[1] & \dots & r[\nu-1] \\ r[0]^2 & r[1]^2 & \dots & r[\nu-1]^2 \\ \vdots & \vdots & \ddots & \vdots \\ r[0]^{k-1} & r[1]^{k-1} & \dots & r[\nu-1]^{k-1} \end{pmatrix},$$

where $r[i] := \sqrt{x[i]^2 + y[i]^2 + z[i]^2}$.

The matrix `rinv` is filled with inverse powers thereof:

$$\mathtt{rinv} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ r[0]^{-1} & r[1]^{-1} & \dots & r[\nu-1]^{-1} \\ r[0]^{-2} & r[1]^{-2} & \dots & r[\nu-1]^{-2} \\ \vdots & \vdots & \ddots & \vdots \\ r[0]^{-(k-1)} & r[1]^{-(k-1)} & \dots & r[\nu-1]^{-(k-1)} \end{pmatrix}.$$

The matrices `cos_alpha` and `sin_alpha` respectively store the real and imaginary parts powers of $e^{I\alpha[i]}$, $i = 1, \dots, \nu-1$, where $I^2 = -1$ is the imaginary unit and:

$$\Re e^{I\alpha[i]} := \frac{y[i]}{\sqrt{x[i]^2 + y[i]^2}}, \quad \Im e^{I\alpha[i]} := \frac{x[i]}{\sqrt{x[i]^2 + y[i]^2}},$$

with one special exception: if $\sqrt{x[i]^2 + y[i]^2} = 0$, one sets $\Re e^{I\alpha[i]} := 1$ and $\Im e^{I\alpha[i]} := 0$. Powers of these numbers can be computed using the complex product of two numbers alone, no trigonometry is needed. However, as $e^{Ik\alpha[i]} = \cos(k\alpha[i]) + I\sin(k\alpha[i])$, the matrices `cos_alpha` and `sin_alpha` shall be filled by `euler()` with the respective real and imaginary parts of $e^{Ik\alpha[i]}$ as follows:

$$\texttt{cos\_alpha} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ \cos(\alpha[0]) & \cos(\alpha[1]) & \dots & \cos(\alpha[\nu-1]) \\ \cos(2\alpha[0]) & \cos(2\alpha[1]) & \dots & \cos(2\alpha[\nu-1]) \\ \cos(3\alpha[0]) & \cos(3\alpha[1]) & \dots & \cos(3\alpha[\nu-1]) \\ \vdots & \vdots & \ddots & \vdots \\ \cos(k\alpha[0]) & \cos(k\alpha[1]) & \dots & \cos(k\alpha[\nu-1]) \end{pmatrix},$$

$$\texttt{sin\_alpha} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \sin(\alpha[0]) & \sin(\alpha[1]) & \dots & \sin(\alpha[\nu-1]) \\ \sin(2\alpha[0]) & \sin(2\alpha[1]) & \dots & \sin(2\alpha[\nu-1]) \\ \sin(3\alpha[0]) & \sin(3\alpha[1]) & \dots & \sin(3\alpha[\nu-1]) \\ \vdots & \vdots & \ddots & \vdots \\ \sin(k\alpha[0]) & \sin(k\alpha[1]) & \dots & \sin(k\alpha[\nu-1]) \end{pmatrix}.$$

Finally, the matrices `cos_beta` and `sin_beta` are defined analogously, where $e^{I\beta[i]}$ is given as follows:

$$\Re e^{I\beta[i]} := \frac{z[i]}{\sqrt{x[i]^2 + y[i]^2 + z[i]^2}}, \quad \Im e^{I\beta[i]} := -\frac{\sqrt{x[i]^2 + y[i]^2}}{\sqrt{x[i]^2 + y[i]^2 + z[i]^2}},$$

and, if $x[i] = y[i] = z[i] = 0$: $\Re e^{I\beta[i]} := 1$, $\Im e^{I\beta[i]} := 0$.

4.4.2 rotscale()

```
virtual void rotscale( const real *cos,      const real *sin, const real *scale,
                       const real *real_in,  const real *imag_in,
                             real *real_out,       real *imag_out,
                       size_t k, bool forward ) const noexcept;
```

This operation performs an element-wise, complex multiplication $C = A \odot B$ of matrices of the same size $\mathbb{C}^{k\times\nu}$, and stores the resulting real and imaginary parts of the matrix C respectively in `real_out` an `imag_out`.

The matrices of `cos` and `sin` contain the real and imaginary parts of powers of $e^{I\gamma}$, where $\gamma \in \{\alpha, \beta\}$, and α and β are defined in the method `euler()` above. If `forward`=`true`, then the products are formed with powers of $e^{I\gamma}$, otherwise with its conjugate $e^{-I\gamma}$.

Finally, each row of the result gets scaled element-wise with the values in `scale`. A simple C++ implementation of this method is as follows:

```
if ( forward )
{
    for ( size_t i = 0; i < k;    ++i )
    for ( size_t l = 0; l < cols; ++l )
    {
        real c   = cos    [ i*cols + l ];
        real s   = sin    [ i*cols + l ];
        real re  = real_in[ i*cols + l ];
        real im  = imag_in[ i*cols + l ];
        real fac = scale  [          l ];

        real_out[ i*cols + l ] = fac*(c*re - s*im);
        imag_out[ i*cols + l ] = fac*(s*re + c*im);
    }
}
else
{
    for ( size_t i = 0; i < k;    ++i )
    for ( size_t l = 0; l < cols; ++l )
    {
        real c   = cos    [ i*cols + l ];
        real s   = sin    [ i*cols + l ];
        real re  = real_in[ i*cols + l ];
        real im  = imag_in[ i*cols + l ];
        real fac = scale  [          l ];

        real_out[ i*cols + l ] = fac*( c*re + s*im);
        imag_out[ i*cols + l ] = fac*(-s*re + c*im);
    }
}
```

All matrices are aligned according to the `alignment` member, the `scale` array usually is not aligned.

4.5 Writing your own Microkernel

In this section we suppose that you want to write optimised routines for a fictional new processor called ‘aicpu’, whose name is based on a currently severely overhyped research topic.

4.5.1 Preparation

Before you start writing your own microkernel, you should be familiar with the basics of high performance dense linear algebra. A very detailed guide is given on the LAFF website.[15]

You will need to determine a suitable block size for your processor. The computationally most expensive routines of solidfmm are specialised dense matrix–matrix products; it is these routines which should determine the block size of your microkernel. For many current architectures, you can find microkernels for the *general* matrix–matrix multiplication (GEMM) in the BLIS library.[16] These are high-quality kernels and form a good starting point for the specialised kernels of solidfmm. Usually, their block size already fulfils the requirements described in Section 4.1.1.

Naturally, you should familiarise yourself with the programming guides of your processor manufacturer. These usually contain detailed information on how to achieve high performance and on important details such as alignment requirements and the sizes of caches and cache lines.

Finally, to develop solidfmm, on top of a current C++ compiler, you will need the GNU Autotools autoconf, automake, libtool, and the autoconf macro library.

4.5.2 Creating Files

You need to create two new files in the solidfmm subfolder of the source code distribution:

- microkernel_aicpu.hpp, containing the class defintition of your microkernel(s). If you want to support both single and double precision, i. e., float and double, this header should contain two classes, one for each floating point type.
- microkernel_aicpu.cpp, containing the microkernel's actual implementation.

For example, when implementing both single and double precision, the header file microkernel_aicpu.hpp could look as follows.

```
#include <solidfmm/microkernel.hpp>

namespace solidfmm
{

class microkernel_aicpu_float: public microkernel<float>
{
public:
    microkernel_aicpu_float();
    virtual ~microkernel_aicpu_float() = default;

    virtual void euler( const float *x,   const float *y, const float *z,
                              float *r,         float *rinv,
                              float *cos_alpha, float *sin_alpha,
                              float *cos_beta,  float *sin_beta,
                        size_t k ) const noexcept override;

    // Similarly, override all the other members of the microkernel base class.

    // Consider adding a static routine that checks at runtime whether the
    // kernel can run on the currently used CPU.
    static bool available() noexcept;
};

class microkernel_aicpu_double: public microkernel<double>
{
public:
    microkernel_aicpu_double();
    virtual ~microkernel_aicpu_double() = default;

    virtual void euler( const double *x,   const double *y, const double *z,
                              double *r,         double *rinv,
                              double *cos_alpha, double *sin_alpha,
                              double *cos_beta,  double *sin_beta,
                        size_t k ) const noexcept override;

    // Similarly, override all the other members of the microkernel base class.

    // Consider adding a static routine that checks at runtime whether the
    // kernel can run on the currently used CPU.
    static bool available() noexcept;
};

}
```

On certain platforms, it makes sense to add static routines called `available()` that perform runtime checks whether the kernel is available on the currently running CPU. The constructors should call this routine and throw an exception if the currently running CPU is not compatible with the 'aicpu'.

4.5.3 Writing the Actual Code

Next you need to write the actual implementation of your microkernel in the freshly created `microkernel_aicpu.cpp` file. For this, we refer to the specification of the individual routines in the previous sections.

It is a good strategy to start with the generic implementations from `microkernel_generic.cpp` and start replacing the individual routines with optimised versions one by one. It is also worth looking at or the other optimised implementations for an inspiration.

4.5.4 Modifying the Build System

Once you have finished writing your code, you need to inform the build system about its existence. For this you need to edit the file `Makefile.am`. Look for the line starting with `noinst_HEADERS` and add the header `solidfmm/microkernel_aicpu.hpp` to the list. Next, add the file `solidfmm/microkernel_aicpu.cpp` to the line beginning with `libsolidfmm_la_SOURCES`. Lastly, you should increase the first and last digits of the 'version-info' of the library. The result should look similar to the following.

```
# Do not touch these lines.
ACLOCAL_AMFLAGS = -I m4
EXTRA_DIST = doc/README doc/solidfmm.tex doc/literature.bib doc/solidfmm.pdf   \
             m4/ax_cxx_compile_stdcxx.m4 m4/ax_pthread.m4 m4/pkg.m4            \
             kirchhart_pubkey.gpg solidfmm.pc.in

pkgconfig_DATA = solidfmm.pc

lib_LTLIBRARIES = solidfmm/libsolidfmm.la

pkginclude_HEADERS = solidfmm/solid.hpp solidfmm/harmonics.hpp                 \
    solidfmm/translations.hpp solidfmm/handles.hpp solidfmm/sphere.hpp         \

# Add your header here
noinst_HEADERS = solidfmm/random.hpp solidfmm/stopwatch.hpp                    \
    solidfmm/swap_matrix.hpp solidfmm/microkernel.hpp                          \
    solidfmm/microkernel_avx.hpp solidfmm/microkernel_avx512f.hpp              \
    solidfmm/microkernel_generic.hpp solidfmm/microkernel_test.hpp             \
    solidfmm/microkernel_armv8a.hpp solidfmm/operator_data.hpp                 \
    solidfmm/threadlocal_buffer.hpp solidfmm/microkernel_aicpu.hpp

# Add your implementation file here
solidfmm_libsolidfmm_la_SOURCES = solidfmm/solid.cpp solidfmm/harmonics.cpp    \
    solidfmm/handles.cpp solidfmm/sphere.cpp  solidfmm/swap_matrix.cpp         \
    solidfmm/operator_data.cpp solidfmm/threadlocal_buffer.cpp                 \
    solidfmm/microkernel.cpp solidfmm/microkernel_avx.cpp                      \
    solidfmm/microkernel_avx512f.cpp solidfmm/microkernel_generic.cpp          \
    solidfmm/microkernel_armv8a.cpp solidfmm/microkernel_test.cpp              \
    solidfmm/translations.cpp solidfmm/multithreaded_translator.cpp            \
    solidfmm/microkernel_aicpu.cpp

# Increase version, e.g., from 4:0:4 to 5:0:5
solidfmm_libsolidfmm_la_LDFLAGS = -version-info 5:0:5

# No need to modify the file below here.
```

More information about the version info can be found in the `libtool` documentation.

Once you have completed these steps, you can compile your code by entering `make` on the command shell. The build system will compile your code and perform the necessary steps to link the new library.

4.5.5 Testing and Benchmarking

Once you have managed to get rid of all compile time errors, it is time to test whether your kernel behaves as expected. For this purpose a testing programme was written that can be found in the `tests` subfolder. Edit the code on the top of the file `tests/test_microkernel.cpp` to compare your implementation against a generic, slow reference implementation. Running the programme will check each routine on a set of random data and test whether it produces the expected results.

You can then finally modify the file `tests/benchmark_microkernel.cpp`. After compiling, you can run the corresponding programme to benchmark your microkernel against a generic implementation.

4.5.6 Enabling the Microkernel for the Library

The final step is to enable the microkernel for the library. For this, you need to edit the methods `get_microkernel<float>()` and `get_microkernel<double>()` in the file `solidfmm/microkernel.cpp`. Edit these functions such that they return your microkernels on the corresponding devices. How to detect a device type at compile- or run-time depends on the specific machine and goes beyond the scope of this book.

Appendices

Appendix A

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