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KEMField - an electrostatic and magnetostatic field solving toolkit

A user's guide for KATRIN members

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Abstract

The electrostatic and magnetostatic field solving software KEMField, developed and maintained by the KATRIN simulation group, is introduced. The document provides a detailed explanation of the installation and implementation of KEMField, as well as a general description of the structure of the underlying C++ code.

Contents

1 Introduction

1.1 Overview

KEMField is a toolkit written in C++ for solving electrostatic and magnetostatic fields from user-defined electrode and magnet configurations. The Boundary Element Method (BEM) is used to compute discretized charge densities from continuous potential distributions along electrodes [1],[2], and the field is computed using a combination of zonal harmonic expansions and direct calculations from geometry primitives using the principle of superposition. In addition, adaptive-refinement field maps can be generated for commonly accessed regions with computationally complex electric fields. The techniques employed are adapted from the routines of Dr. Ferenc Glück [3],[4],[5],[1],[6],[7]. KEMField utilizes the GNU Scientific Library (GSL) [8] and ROOT data analysis framework [9] for computation and save/retrieval algorithms, respectively. KEMField employs both MPI [10] and OpenMP [11] for parallel field computation on a computer grid.

1.2 Building the KEMField libraries

In order to build the KEMField libraries, the user must first add the main directory (`KEMField/`) to the `path` environment variable, and the library directory (`KEMField/lib`) to the `LD_LIBRARY_PATH` environment variable. This enables programs to link aginst the KEMField libraries by using the `KEMField-config` command. The user must also have GSL (version 1.12 or newer) and ROOT (version 2.24 or newer) installed, with the executables `gsl_config` and `root_config` correctly identifying the respective library and include paths. To build the libraries and a suite of test programs, the user need only execute the `make` command within the top directory[1] [2]. The included test programs are designed to demonstrate the functionality of different aspects of the KEMField toolkit.

The libraries can be built to use MPI and OpenMP, if they are installed on the user's operating system. To use MPI, the user must first set the environment variable `USE_MPI`, and then recompile. Setting this flag causes Both MPI-enabled and MPI-disabled versions of the libraries to be created (the MPI-enabled libraries and executables have the suffix `_MPI` in the root of the name). To use OpenMP, the user must set the environment variable `USE_OPENMP` and recompile.

1.3 File structure

1.3.1 Source files

The source files for KEMField, located in `KEMField/Source/`, are divided into folders according to the library to which they belong. They are:

- `Geometry`: classes defining the geometry primitives, primitive stores and geometry managers (see Section 3),
- `BEM`: classes used in performing the matrix algebra associated with the Boundary Element Method of solving for charge densities on electrode sub-elements (see Section 4),
- `Direct`: classes used to perform the direct field solving method (see subsection 5.2),
- `ZHExpansion`: classes used to perform the zonal harmonic expansion field solving method (see subsection 5.3),

[1]KEMField has been successfully tested on Mac OS X 10.4, 10.5 and 10.6, as well as several Linux flavors.

[2]Thanks to Daniel Furse for his complete revision of the Makefile, making the build process much more dynamic.

- `FieldMap`: classes used to perform field map generation and field solving using field maps (see subsection 5.4),
- `IO`: classes used to manage the input and output of files and messages for KEMField,
- `Field`: contains the base field solving class (see subsection 5.1), and the metaclass `KEMField` (see Section 2), and
- `Test`[3]: main functions for test programs designed to demonstrate the utility of KEMField.

Within each folder for which there is an associated library, the source code is divided into header files (`include/`), source files (`src/`), and files necessary to link against the ROOT libraries (`LinkDef/`).

1.3.2 Saved files

Although the base folder for saved files may be changed by the user, the default configuration is for saved files to be located within `KEMField/field_data/saved_files/`. Within this folder, ROOT files unique to the electrode and magnet geometry are read and written, and the folder `fieldmap/` contains data pertinent to a generated field map (if one exists). The folder `field_data/` also contains the folder `images/` for storing test images generated by certain test programs, and `input_files/`, where geometry cards are kept (see subsection 3.2.2).

1.3.3 Other files

In keeping with commonly accepted UNIX programming standards, generated executables designed to test, validate and demonstrate the utility of KEMField are located in `KEMField/bin/`, generated libraries are located in `KEMField/lib/`, temporary files are stored in `KEMField/tmp/`, and scripts associated to KEMField (document generating scripts and submission scripts for various grids) are kept in `KEMField/scripts/`. The documentation for KEMField (including the document you are reading) is located in `KEMField/doc/`. Finally, the executable shell script `KEMField-config` is designed for use by other programs to link against the libraries of KEMField, in keeping with the standard `*-config` format.

2 Class `KEMField`: the user interface

In addition to being the name of the toolkit described by this document, `KEMField` is also the name of the top-level class through which the user accesses the geometry and field solving classes (to avoid ambiguity, `KEMField`, in this font, will hereafter always refer to the class, and KEMField to the toolkit).

2.1 Adding field solvers

When an instance of `KEMField` is created, it has associated with it an electrode and magnet manager (see subsection 3.3), but by default there are no field solving methods. The user must choose which methods are appropriate to the simulation being performed, and in what order they should be used. An example of adding field solvers to an instance of `KEMField` is demonstrated below:

```
...
// construct an instance of KEMField
```

[3]No library is associated with the Test folder.

```
KEMField* field = new KEMField();

// a general verbosity setting for managers and field solvers
Int_t verbose = 3;

// access the electrode and magnet managers
KElectrodeManager* eManager = field->GetElectrodeManager();
KMagnetManager*    mManager = field->GetMagnetManager();

// add a direct electric field solver to KEMField
field->AddEFieldSolver(new KEDirectFieldSolver(eManager));

if (eManager->CheckForAxialSymmetry())
{
  // if the simulation is axially symmetric, add a zonal harmonic electric
  // field solver to KEMField
  field->AddEFieldSolver(new KEZHFieldSolver(eManager));

  // set the solver to the highest priority (NB: the field solver can be
  // accessed by name or by its index within KEMField)
  field->SetPriority("KEZHFieldSolver",1);

  // set the field solver's verbosity level
  field->SetVerbose("KEZHFieldSolver",verbose);
}

// set the direct field solver's priority level to be lower than that of
// the zonal harmonic electric field solver
field->SetPriority("KEDirectFieldSolver",3);

// set the field solver's verbosity level
field->SetVerbose("KEDirectFieldSolver",verbose);

// add a direct magnetic field solver to KEMField
field->AddBFieldSolver(new KMDirectFieldSolver(mManager));

// add a zonal harmonic magnetic field solver to KEMField
field->AddBFieldSolver(new KMZHFieldSolver(mManager));

// set the magnetic field solver's priorities
field->SetPriority("KMZHFieldSolver",1);
field->SetPriority("KMDirectFieldSolver",2);

// set the field solvers' verbosity levels
field->SetVerbose("KMZHFieldSolver",verbose);
field->SetVerbose("KMDirectFieldSolver",verbose);

// set the electrode and magnet manager's verbosity levels
// (this could also have been done by accessing the managers directly)
field->SetVerbose("KElectrodeManager",verbose);
field->SetVerbose("KMagnetManager",verbose);
  ...
```

Once a field solver is added to an instance of `KEMField`, `KEMField` takes ownership of it. In other words, when the user deletes the instance of `KEMField` that was created above, all of the field solvers (and, naturally, the geometry managers) are deleted with it. While more than one instance of `KEMField` can exist at once, the user must take care when sharing field solvers between distinct instances of `KEMField`.

2.2 Initializing the geometry managers and field solvers

Since the geometry managers both share the same underlying structure, and the field solving classes conform to a base model, it is possible to initialize the instance of KEMField for use in field solving by merely executing the command

```
...
field->Initialize();
...
```

The preparation of the geometry and field solvers is then taken care of by KEMField, and no other user input is necessary. Once the geometry is loaded into the managers and the KEMField instance is initialized, the user is ready to compute electric and magnetic fields and potentials.

2.3 Accessing the electric and magnetic field and potential

In order to get field and potential values from KEMField, the following functions are used:

- `void CalculateBField(const Double_t P[3], Double_t field[6]) const`: computes the magnetic field at `(P[0],P[1],P[2])`. The first 3 components of `field[6]` correspond to the x, y, and z-components of the magnetic field, and the last 3 the electric field (GEANT format).
- `void CalculateEField(const Double_t P[3], Double_t field[6]) const`: computes the electric field at `(P[0],P[1],P[2])`.
- `void CalculateField(const Double_t P[3], Double_t field[6]) const`: computes both the electric and magnetic fields at `(P[0],P[1],P[2])`.
- `void CalculateBPotential(const Double_t P[3], Double_t field[6]) const`: computes the magnetic vector potential at `(P[0],P[1],P[2])`. The first component of `phi[4]` corresponds to the electric potential, and the last 3 the magnetic vector potential $\vec{A} = (A_x, A_y, A_z)$.
- `void CalculateEPotential(const Double_t P[3], Double_t field[6]) const`: computes the electric potential at `(P[0],P[1],P[2])`.
- `void CalculatePotential(const Double_t P[3], Double_t field[6]) const`: computes both the electric potential and the magnetic vector potential at `(P[0],P[1],P[2])`.

A complete demonstration of their use is given in the test program `bin/TestEMField`.

3 Geometry primitives

3.1 Available primitives

Electrodes can be arranged in a general 3-dimensional configuration using wires, rectangles and triangles, but axially symmetric (or approximately axially symmetric) electrode configurations consisting of conic sections and repeated wires, rectangles and triangles about the azimuthal axis are preferable, as they facilitate the use of faster field computation algorithms. Currently supported magnets include wire loops, solenoids and thick coils (electromagnets), each of which can be defined according to its own symmetry axis. A graphical description of the available electrode and magnet primitives can be seen in Table 1.

Depending on their symmetry properties, electrode primitives are either represented as singular instances or as collections of identical sub-elements repeated about the azimuthal axis. For example, a KTConicSectElectrode describes a single conic section electrode with only one placement in the system because it is naturally axially symmetric, whereas a KTWireElectrode can describe a collection of multiply placed wire segments about the azimuthal axis. In addition,

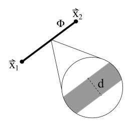
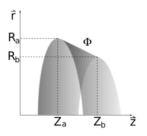
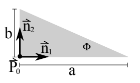
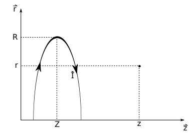
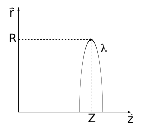
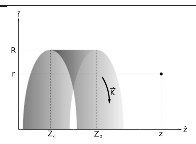
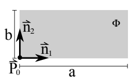
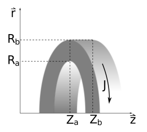
Geometry Primitive	Graphical Description	Geometry Primitive	Graphical Description
`KTWireElectrode` *(collective)*		`KTConicSectElectrode` *(singular)*	
`KTTriangleElectrode` *(collective)*		`KTRingMagnet` *(singular)*	
`KTRingElectrode` *(singular)*		`KTSolenoidMagnet` *(singular)*	
`KTRectangleElectrode` *(collective)*		`KTCoilMagnet` *(singular)*	

Table 1: Available electrode and magnet geometry primitives. Collective primitives can be represented as repeated instances about the azimuthal axis, demonstrating discrete rotational symmetry. Singular primitives inherently have continuous rotational symmetry, and are therefore represented as singular instances.

each electrode type can be placed into a `KTElectrodeGroup`, where the group of electrodes is treated as a single independent electrode primitive during the implementation of the BEM.

Currently, only magnet primitives that have rotational symmetry about one of its axes are represented in KEMField. There are therefore no collective magnet primitives, as all supported magnets are singular primitives. Since the computation of the magnetic field from a magnet description is more straightforward than for its electric counterparts, and because magnet discretization and implementation of the BEM are unnecessary, there is no need to group magnets for the simplification of a BEM calculation. Instead, magnets are grouped that share a common axis of symmetry, allowing for multiple magnet groups that have different symmetry axes. The grouping of coaxial magnets is done in much the same way that electrodes are grouped, using instances of `KTMagnetGroup`. Examples of electrode and magnet groups can be seen in the program `bin/TestGeometry`.

3.2 Adding primitives to the simulation

3.2.1 Manually adding primitives

An example of manually creating geometry primitives and adding them to the simulation is displayed below:

```
#include <cstdlib>
#include <iostream>

#include "KElectrodeManager.hh"

#include "KTConicSectElectrode.hh"
```

```
#include "KTWireElectrode.hh"

int main(Int_t argc, char* argv[])
{
  // Construct a single conic section electrode.
  KTConicSectElectrode* c = new KTConicSectElectrode(0,        // z_A (m)
                                                     .5,       // r_A (m)
                                                     1,        // z_B (m)
                                                     .5,       // r_B (m)
                                                     1,        // potential (V)
                                                     5);       // numDisc

  // Construct fifty wires with discrete rotational symmetry about the
  // azimuthal axis.
  Double_t a[3] = {1,1,1}; // x,y,z of 1st endpoint of 1st copy (m)
  Double_t b[3] = {3,1,2}; // x,y,z of 2nd endpoint of 1st copy (m)

  KTWireElectrode* w = new KTWireElectrode(a,
                                           b,
                                           .05,// diameter of the wire (m)
                                           10, // potential of the wire (V)
                                           50, // # of wires about the azi. axis
                                           10);// numDisc

  // Construct a new electrode manager.
  KElectrodeManager* eManager = new KElectrodeManager();

  // Add the conic section electrode to the manager.
  eManager->Add(c);

  // Add the wire electrodes to the manager.
  eManager->Add(w);

  // When a primitive is added to the manager, a copy of the primitive is
  // constructed as an object within the manager's storage classes.  The
  // original primitive is no longer needed, and can be deleted by the user.
  delete c;
  delete w;
  ...
```

Note that, when an electrode is added to the simulation, a copy of its parameters is passed to the appropriate storage classes. This means that the same electrode can be modified and added to the simulation multiple times, reducing the number of times the user must call `new` and `delete`.

3.2.2 Card readers

Alternatively, geometry primitives can be loaded into a simulation via `Elcd3_2`, `Elcd3_3`, and `Magfield3`-style cards. Card readers exist for conic section, rectangle, triangle and wire electrodes, and for coil magnets. Cards that are read into the simulation can be commented by using the escape character "#". Card readers can be used independently (see test program `bin/TestCardInput`), or in conjunction with `KEMField` with the function

```
    void KEMField::ReadGeometryFromCards(std::string ConicSectFileName,
                                         std::string CoilFileName,
                                         std::string RectangleFileName,
                                         std::string WireFile,
                                         std::string TriangleFileName);
```

Example Cards: The following are sample cards for conic sections, rectangles, wires and magnets.

```
# inputfull.dat

# total number of conic sections described by the file

2

# the following 6 parameters are described as follows:
#      1: z-coordinate of the 1st endpoint of the generating line (m)
#      2: r-coordinate of the 1st endpoint of the generating line (m)
#      3: z-coordinate of the 2nd endpoint of the generating line (m)
#      4: r-coordinate of the 2nd endpoint of the generating line (m)
#      5: Potential at which the electrode is held (V)
#      6: the number of conic sections into which the conic section
#          will be discretized (0 if no discretization)

1.5      1        3        1        50       10

# the next 6 parameters are identical in meaning to the previous line,
# for the second conic section

3    0    3        1        0        5
```

```
# inputrectangle.dat

# total number of rectangles described by this file

2

# the following 16 parameters are described as follows:
# 1: The index is the number of the rectangle in the file. It starts
#    at 1 for the first rectangle, and increments by one for each
#    subsequent rectangle.
# 2: This parameter indicates to which KTElectrodeGroup the rectangle
#    belongs. Rectangles that are in the same group must be placed
#    together in the file, and the group parameter must start at one and
#    increment by only one (for rectangles within the same group, it does
#    not increment at all). Alternatively, the group parameter can be set
#    to -1 for all of the rectangles, indicating that the rectangles are
#    not grouped.
# 3: This parameter is not used by the card reader.
# 4: For repeated rectangles about the azimuthal axis, this parameter
#    sets the number of repeated instances of the rectangle the program
#    should create. The # of replicas must be greater than or equal to
#    one; if a rectangle is not repeated about the azimuthal axis, the
#    parameter should be set to one.
# 5,6,7: The x, y, and z-coordinates of a corner of the rectangle (m)
# 8,9,10: the unit vector pointing from P0 along the longer side of
#          the rectangle (side A)
# 11,12,13: the unit vector pointing from P0 along the shorter side of
#             the rectangle (side B)
# 14: the magnitude of the longer side (A) of the rectangle (m)
# 15: the magnitude of the shorter side (B) of the rectangle (m)
# 16: the potential of the electrode (V)

1  1  0  10  0  10.  0  1  0  0  0  1  0  .05  .05  10
```

```
# the next 16 parameters are identical in meaning to the previous
# line, for the second rectangle

2 2 0 1 0 0 1 1 0 0 0 1 0 1 1 1
```

```
# inputwire.dat

# total number of wires described by this file

1

# the following 16 parameters are described as follows:
# 1: The index is the number of the wire in the file. It starts at 1
#    for the first wire, and increments by one for each subsequent
#    wire.
# 2: This parameter indicates to which KTElectrodeGroup the wire
#    belongs. Wires that are in the same group must be placed together in
#    the file, and the group parameter must start at one and increment by
#    only one (for wires within the same group, it does not increment at
#    all). Alternatively, the group parameter can be set to -1 for all of
#    the wires, indicating that the wires are not grouped.
# 3: This parameter is not used by the card reader.
# 4: For repeated wires about the azimuthal axis, this parameter sets
#    the number of repeated instances of the wire the program should
#    create. The # of replicas must be greater than or equal to one; if a
#    wire is not repeated about the azimuthal axis, the parameter should
#    be set to one.
# 5,6,7: These three parameters describe the x, y, and z-coordinates
#        of one end of the wire (m).
# 8,9,10: These three parameters describe the x, y, and z-coordinates of
#         the other end of the wire (m).
# 11: Describes the diameter of the wire (m).
# 12,13,14,15: These parameters are not used by the card reader.
# 16: Describes the potential of the electrode (V).

1 -1 0 10 .5 .5 -.15 .5 .5 .15 .05 0 0 0 0 100
```

```
# inputcoil.dat

# total number of magnets described by the file

2

# the following 13 parameters are described as follows:
#     1,2,3:     global (x,y,z) of local origin
#     4,5,6:     global (x,y,z) of local (1,0,0)
#     7,8,9:     global (x,y,z) of local (0,1,0)
#     10,11,12: global (x,y,z) of local (0,0,1)
#     13:        number of magnets defined within this cooridnate frame
#
# numbers may be separated by tabs or spaces (or both)

0   0   0   1.   0   0   0   1.   0   0   0   1.   2

# the following 5 parameters are described as follows:
#     1: the z-coordinate of the middle of the magnet (m)
#     2: the minimum r-coordinate of the magnet  (m)
#     3: the thickness of the magnet in the r-direction  (m)
#      4: the length of the magnet in the z-direction  (m)
#      5: the total current in the magnet (A)

-2.15     0.227   0.043    0.320    2120000.

# the next 5 parameters are identical in meaning to the previous line,
# for the second magnet defined within this coordinate frame

2.15      0.227   0.043    0.320    2120000.
```

3.2.3 KXML, other interfaces

Alternative methods for adding geometry primitives to KEMField, including KXML[12] and direct inputs from the KATRIN database, are currently being developed.

3.3 Managing geometry primitives

The interfaces between electrode and magnet primitives created by the user and the field solving routines employed in KEMField are `KElectrodeManager` and `KMagnetManager`, respectively. By interacting with the electrode and magnet managers, the user is able to:

- Add and retrieve electrodes/magnets
- Set the reflectional symmetry of the simulation (electrodes only)
- Discretize electrodes (used for constant charge density approximation)
- Save and retrieve electrode/magnet geometries from file

The electrode and magnet managers contain methods that automate the preparation of a geometry configuration for use in field computation. Once the geometry primitives have been loaded into their respective managers, the user need only execute the commands

```
 ...
 eManager->Initialize();
 mManager->Initialize();
 ...
```

and the requisite steps are taken to enable field computation[4]. Feedback from the manager classes can be printed to the screen by setting the verbosity of each class (`e/mManager->SetVerbose(#)`) from 0 (silent) to 5 (most verbose). The general steps of the initialization methods are outlined below.

3.3.1 Save and retrieval of geometry configurations

When a geometry configuration is inputted into the simulation, a check is performed to determine whether or not a similar configuration has been processed during a prior simulation. The default locations and names for file saving/retrieving is `KEMField/field_data/saved_files/electrodes.root` and `KEMField/field_data/saved_files/magnets.root`, but can be changed prior to initialization by executing the commands

```
 ...
 eManager->SetSaveFileName(filename);
 eManager->SetRetrieveFileName(filename);
```

[4]When used within the context of the class `KEMField`, the managers are automatically initialized as part of `KEMField::Initialize()`.

```
mManager->SetSaveFileName(filename);
mManager->SetRetrieveFileName(filename);
...
```

The manager classes determine if the loaded configuration is

- identical to a previous simulation,
- geometrically equivalent to a previous simulation, but with electrodes held at different potential values,
- geometrically similar to a previous simulation, with identical potential values, or
- completely different from all previous simulations.

Each of these situations is handled differently during the computation of charge densities, which is explained in Section 4. When a new file is to be created, its name is the chosen (or default) save name root, appended with `_#.root` when a file with that name already exists. During the comparsion against preexisting files, all files with the same name root are compared against the current geometry.

3.3.2 Electrode discretization

One of the approximations of the BEM is the assumption of constant charge density across an electrode. It is therefore necessary to discretize the electrode primitives added to the simulation into smaller sub-elements, so the approximation can be held valid. Each electrode primitive in KEMField has a method associated with it that automates this process, discretizing itself into smaller electrodes according to an associated discretization parameter (passed to the electrode in its constructor), as well as a static parameter associated with each primitive type. The discretization of electrodes is performed once all of the electrodes are added into the simulation.

3.3.3 Computation of electrode charge densities

The computation of electrode charge densities is performed using the BEM. A more detailed explanation of this procedure is given in Section 4.

3.3.4 Axially symmetric and asymmetric approximations

Once the electrodes are discretized and the charge densities for each electrode have been computed, symmetry-related approximations can be made. For electrode configurations that are nearly axially symmetric, primitives with discrete rotational symmetry can be approximated as axially symmetric electrodes. The approximated electrode will be used in lieu of the original electrode when the field point to be computed is sufficiently far from the electrode (scalable by a user-defined parameter). Each collective electrode class contains a method for performing this approximation.

Additionaly, electrode configurations that contain axially symmetric electrodes but in general are *not* axially symmetric must be converted into a completely asymmetric configuration, in order to allow for a varying charge density about the aximuthal axis. Each singular electrode class contains a method for performing this approximation.

4 The Boundary Element Method

4.1 Overview

The theory behind the computation of the charge densities on electrode sub-elements via the BEM is explained in [7], [13]. Procedurally, the task of the BEM classes is to solve the linear algebraic equation

$$U_i = W_{ij} \cdot \sigma_j \tag{1}$$

for σ_j, where U_i is the electric potential of electrode i, W_{ij} is the geometric component of the electric potential at a point centered on electrode i due to electrode j, and σ_j is the charge density on electrode j. KEMField employs three methods for solving this equation:

- Gaussian elimination,
- inversion of the matrix W_{ij}, and
- Gauss-Seidel method of successive displacement.

The BEM is employed automatically during the initialization method of the electrode manager.

4.2 Gaussian elimination and matrix inversion

For electrode configurations that are entirely dissimliar to those of previously computed simulations, one of the first two methods (selected by a user-defined parameter) is employed to solve for the components of the σ_j vector. While Gaussian elimination is faster than complete matrix inversion, the latter method has the benefit of facilitating the speed of future computations, where a geometry configuration differs from the current one only by differences in the potential values on the electrodes. When it is used, the method of matrix inversion saves the computed inverted matrix to file. Future simulations that vary in potential only can then be rapidly solved by simply multiplying this matrix with the new potential values. Both methods are written for serial computation and for MPI-enabled parallel computation using techniques from [14] for use in distributed computing.

4.3 Gauss-Seidel method of successive displacement

The third method is used when a previously computed simulation differs geometrically only slightly from the current configuration, and the initial approximate values for the charge densities can be taken from the previous simulation. When the conditions for its use are appropriate, the Gauss-Seidel method is the fastest method for solving the linear algebraic equation. However, the method is not readily transferrable into parallel computation, and must be performed serially.

5 Field Solvers

5.1 General Properties

Once the geometry is prepared (electrodes and magnets inputted into their respective managers, electrodes discretized and charge densities computed, symmetry approximations made, and files saved), the user then selects the field solvers to be used in the simulation. All field solvers inherit from the parent class `KEMFieldSolver`, and can perform the following basic tasks:

- `std::string GetName()`: returns the name of the field solver.
- `void Initialize()`: prepares the field solver for use in simulation.

- `Bool_t FieldCanBeComputedAtPoint(const Double_t P[3])`: returns true if the field solver is valid at `(P[0],P[1],P[2])`, false if it is not.
- `void CalculateField(const Double_t P[3], Double_t field[6])`: computes the field at `(P[0],P[1],P[2])`. The first 3 components of `field[6]` correspond to the x, y, and z-components of the magnetic field, and the last 3 the electric field (GEANT format).
- `void CalculatePotential(const Double_t P[3], Double_t phi[4])`: computes the electric potential and magnetic vector potential at `(P[0],P[1],P[2])`. The first component of `phi[4]` corresponds to the electric potential, and the last 3 the magnetic vector potential $\vec{A} = (A_x, A_y, A_z)$.
- `void SetVerbose(Int_t i)`: like the manager classes, sets the verbosity of the solver.
- `void SetPriority(Int_t i)`: Sets the priority of the solver. This is explained in more detail in Section 2.

5.2 Direct calculation method

```
...
KEDirectFieldSolver* dESolver = new KEDirectFieldSolver(eManager);
KMDirectFieldSolver* dMSolver = new KMDirectFieldSolver(mManager);
...
```

Direct field solvers (`KEDirectFieldSolver`, `KMDirectFieldSolver`) are so named because they compute the electric potential, magnetic vector potential, and electric and magnetic fields using techniques based on analytic forms specific to each geometry primitive. Derivations of the formulae used to perform these calculations can be found in [1], [6], [7], [13].

When possible, analytic techniques for determining the electric field from a geometry primitive are used. If an analytic form has not been derived, the electric field is computed using numeric differentiation of the electric potential. Using the law of superposition, the field values are computed as merely the sum of the contributions from each sub-element. If OpenMP is enabled, these sums are performed in parallel.

5.3 Zonal harmonic expansion method

Geometry configurations that are axially symmetric (or approximately axially symmetric) can be solved using the method of zonal harmonic expansion by envoking the classes `KEZHFieldSolver` and `KMZHFieldSolver`. The method solves for the electric and magnetic field and potential by computing series similar to the following forms:

$$\Phi_{cen}(r_{cyl}, z_{cyl}) = \sum_{n=0}^{\infty} \Phi_n^{cen}|_{z_0} \left(\frac{\rho}{\rho_{cen}}\right)^n P_n(\cos\theta), \tag{2}$$

$$\Phi_{rem}(r_{cyl}, z_{cyl}) = \sum_{n=0}^{\infty} \Phi_n^{rem}|_{z_0} \left(\frac{\rho}{\rho_{rem}}\right)^{-(n+1)} P_n(\cos\theta), \tag{3}$$

for multiple z_0 source points along the axis of rotational symmetry. This method is explained in detail in [4], [5], [13].

Prior to initialization, parameters that characterize the zonal harmonic expansion technique can be set as follows:

```
...
KEZHFieldSolver* zhEFieldSolver = new KEZHFieldSolver(eManager);
zhEFieldSolver->SetZHParameters((Double_t) prox_to_sp,
                                (Double_t) convergenceParam,
                                (Double_t) spSpacing,
                                (Double_t) convergenceRatio,
                                (Int_t)    nCenCoeffs,
                                (Int_t)    nRemCoeffs,
                                (Int_t)    nBifurcations);

KMZHFieldSolver* zhMFieldSolver = new KMZHFieldSolver(eManager);
zhMFieldSolver->SetZHParameters((Double_t) prox_to_sp,
                                (Double_t) convergenceParam,
                                (Double_t) spSpacing,
                                (Double_t) convergenceRatio,
                                (Int_t)    nCenCoeffs,
                                (Int_t)    nRemCoeffs,
                                (Int_t)    nBifurcations);
...
```

where the paramaters are defined as:

- `Double_t prox_to_sp`: if the distance between a field point and a source point is less than this tolerance, only the first terms of the series are used,
- `Double_t convergenceParam`: when the last term in the series is smaller than the former term by this parameter, the summation ends,
- `Double_t spSpacing`: the distance along the z-axis between source points,
- `Double_t convergenceRatio`: when $\frac{\rho}{\rho_{cen}}$ or $\frac{\rho_{rem}}{\rho}$ is less than this ratio, the expansion method is valid for use,
- `Int_t nCenCoeffs`: the maximum number of terms used in each central expansion,
- `Int_t nRemCoeffs`: the maximum number of terms used in each remote expansion, and
- `Int_t nBifurcations`: the maximum number of subdivided geometry collections. This is explained in further detail in 5.3.1.

5.3.1 Collections

Both electric and magnetic geometry primitives are grouped into *collections* in order to extend the utility of the method of zonal harmonic expansion. Geometry primtives are gouped according to spacial proximity, allowing for a partial zonal harmonic calculation of fields even if the field point is close to one of the collections of primitives. The grouping of electrodes is performed by repeatedly bifurcating the electrode geometry along the z-axis (the number of bifurcations is set by the user). For magnetic geometry primitives, collections are used to group magnets with a common axis of symmetry, and these groups are subdivided [`nBifurcations`] times. If OpenMP is enabled, the series expansions for different collections are performed in parallel.

5.4 Interpolation from field maps

For regions in which the computation of electric fields is computationally expensive, adaptive-refinement field maps spanning the region can be constructed beforehand. Once the field maps are generated, a fourth order reduced multivariate Hermite interpolator is used to compute the electric potential and electric field to a user-defined tolerance. The technique is discussed in more detail in [13].

5.4.1 Constructing field maps

Field maps may be constructed in serial for both axially symmetric and asymmetric electrode configurations as follows:

```
...
// construct an instance of KEMField
KEMField* field = new KEMField();

...
// add field solvers to the instance of KEMField
...

// create a pointer to a general (2-dimensional or 3-dimensional) field map
KFieldMap_base* fm;

Double_t tolerance   = 1.e-3; // tolerance across the field map
Double_t maxCubeSize = 1.;  // size of a side of the largest cube (m)
Int_t  nLevel      = 3;  // # of times the largest cube can be subdivided

// ...to make the tolerance better reflect the accuracy...
tolerance*=.1;

if (eManager->CheckForAxialSymmetry())
{
  // construct a 2-dimensional field map for the axially symmetric field
  fm = new KFieldMap_2D(field,tolerance,maxCubeSize,nLevel);
  // Set the (r_min, r_max, z_min, z_max) dimensions of the map (in meters)
  fm->SetDimensions(0,3,1.5,5.5);
}
else
{
  // construct a 3-dimensional field map for the asymmetric field
  fm = new KFieldMap_3D(field,tolerance,maxCubeSize,nLevel);
  // set the (x_min,x_max,y_min,y_max,z_min,z_max) dimensions
  // of the map (in meters)
  fm->SetDimensions(-3,3,-3,3,-3,3);
}

// construct the primary grid, save the header information
fm->InitializeFieldMap();

for (Int_t i=0;i<fm->GetNMetaCubes();i++)
{
  // fill each cube in the primary grid
  fm->FillMetaCube(i);
}
  ...
```

The user-defined parameters that characterize a field map are:

- `Double_t tolerance`: the average error of the interpolated value computed from the field map
- `Double_t maxCubeSize`: the length of a side of the top-level cube. The initial map is formed by dividing the region into cubes with this side length, and subsequent cubes are formed

by subdividing these cubes. Top-level cubes that contain an electrode are removed from the map, as a uniform tolerance cannot be guaranteed in this region.

- `Int_t nLevel`: the maximum number of times a top-level cube is subdivided in order to attain the appropriate tolerance.
- `Double_t dimensions[4 or 6]`: the 2- (or 3-) dimensional coordinates of the field map.

While the methods for computing a field map in serial produce the same results as their parallel counterpart, the preferred method for field map construction is in parallel on an MPI-enabled computer grid. An example program that performs exactly this task, `bin/TestFieldMap_MPI`, and its source are provided for the user.

5.4.2 Implementing field maps for use in computation

As they inherit from `KEMFieldSolver`, the classes `KFieldMap_2D` and `KFieldMap_3D` are implemented in much the same way as the other field solvers. However, since a field map used for computing fields must already be generated, the user-defined parameters that characterize the map are taken from the saved configuration of the map itself, rather than set by the user. An example of their implementation is given below:

```
...
// create a pointer to a general (2-dimensional or 3-dimensional) field map
KFieldMap_base* fm;

if (eManager->IsAxiallySymmetric())
  fmEFieldSolver = new KFieldMap_2D((KEMPrimitiveManager*)eManager);
else
  fmEFieldSolver = new KFieldMap_3D((KEMPrimitiveManager*)eManager);
...
```

References

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