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Chapter 1

Main Page

oep-dev

Generalized One-Electron Potentials: Development Platform.

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Overview

Test various models of the intermolecular interaction that is based on the application of the **One-Electron Potentials (OEP's)** technique.

Currently, the interaction between two molecules described by the Hartree-Fock-Roothaan-Hall theory or the configuration interaction with singles theory is considered. In particular, the plugin tests the models of:

1. the Pauli exchange-repulsion interaction energy (Project II)
2. the Induction interaction energy (Project III)
3. the excitation energy transfer couplings (Project I)

against reference solutions (exact or other approximations).

Places to go:

- https://github.com/globulion/oepdev/blob/master/doc/git/doc_oep_design.md "OEP Design"
- https://github.com/globulion/oepdev/blob/master/doc/git/doc_implemented_models.md "Implemented Models"
- https://github.com/globulion/oepdev/blob/master/doc/git/doc_programming_etiquette.md "Programming Etiquette"
- [Current Issues](#)

References

Chapter 2

Introduction

This page introduces the user to the topic.

Now you can proceed to the [advanced section](#).

Chapter 3

OEP Design.

OEP (One-Electron Potential) is associated with certain quantum one-electron operator \hat{v}^A that defines the ability of molecule A to interact in a particular way with other molecules.

Technically, OEP can be understood as a **container object** (associated with the molecule in question) that stores the information about the above mentioned quantum operator. Here, it is assumed that similar OEP object is also defined for all other molecules in a molecular aggregate.

In case of interaction between molecules A and B , OEP object of molecule A interacts directly with wavefunction object of the molecule B . Defining a Solver class that handles such interaction Wavefunction class and OEP class the universal design of OEP-based approaches can be established and developed.

Important: OEP and Wavefunction classes should not be restricted to Hartree-Fock; in general any correlated wavefunction and derived OEP's should be allowed to work with each other.

3.1 OEP Classes

There are many types of OEP's, but the underlying principle is the same and independent of the type of intermolecular interaction. Therefore, the OEP's should be implemented by using a multi-level class design. In turn, this design depends on the way OEP's enter the mathematical expressions, i.e., on the types of matrix elements of the one-electron effective operator \hat{v}^A .

3.1.1 Structure of possible OEP-based expressions and their unification

Structure of OEP-based mathematical expressions is listed below:

| Type | Matrix Element | Comment |
|--------|-------------------|--------------------|
| Type 1 | $(I \hat{v}^A J)$ | $I \in A, J \in B$ |
| Type 2 | $(J \hat{v}^A L)$ | $J, L \in B$ |

In the above table, I , J and K indices correspond to basis functions or molecular orbitals. Basis functions can be primary or auxiliary OEP-specialized density-fitting. Depending on the type of function and matrix element, there are many subtypes of resulting matrix elements that differ in their dimensionality. Examples are given below:

| Matrix Element | DF-based form | ESP-based form |
|---------------------------------|--|--|
| $(\mu \hat{v}^{A[\mu]} \sigma)$ | $\sum_{I \in A} v_{\mu I}^A S_{I\sigma}$ | $\sum_{\alpha \in A} q_{\alpha}^{A[\mu]} V_{\mu\sigma}^{(\alpha)}$ |
| $(i \hat{v}^{A[i]} j)$ | $\sum_{I \in A} v_{ii}^A S_{Ij}$ | $\sum_{\alpha \in A} q_{\alpha}^{A[i]} V_{ij}^{(\alpha)}$ |

| | | |
|-----------------------------------|---|---|
| $\left(j \hat{v}^{A[i]} l\right)$ | $\sum_{\kappa \in A} S_{jl} v_{\kappa}^{A[i]} S_{\kappa l}$ | $\sum_{\alpha \in A} q_{\alpha}^{A[i]} v_{jl}^{(\alpha)}$ |
|-----------------------------------|---|---|

In the formulae above, the OEP-part (stored by OEP instances) and the Solver-part (to be computed by the Solver) are separated. It is apparent that all OEP-parts have the form of 2nd- or 3rd-rank tensors with different class of axes (molecular orbitals, primary/auxiliary basis, atomic space). Therefore, they can be uniquely defined by a unified *tensor object* (storing double precision numbers) and unified *dimension object* storing the information of the axes classes.

In Psi4, a perfect candidate for the above is `psi4::Tensor` class declared in `psi4/libthce/thce.h`. Except from the numeric content its instances also store the information of the dimensions in a form of a vector of `psi4::Dimension` instances.

Another possibility is to use `psi::Matrix` objects, instead of `psi4::Tensor` objects, possibly putting them into a `std::vector` container in case there is more than two axes.

Chapter 4

List of One-Electron Potentials

Here I provide the list of OEP's that have been already derived within the scope of the OEPDev project.

4.1 Electrostatic Energy OEP's

For electrostatic energy calculations, OEP is simply the electrostatic potential due to nuclei and electrons.

3D form:

$$v(\mathbf{r}) = \sum_x \frac{Z_x}{|\mathbf{r} - \mathbf{r}_x|} + \sum_{\mu\nu \in A} P_{\nu\mu} \int d\mathbf{r}' \frac{\phi_\mu^*(\mathbf{r}') \phi_\nu(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

Matrix form:

$$v_{ik} = \sum_{x \in A} Z_x V_{ik}^{(x)} + \sum_{\mu\nu \in A} P_{\nu\mu} (\mu\nu|ik)$$

4.2 Pauli Repulsion OEP's

The following potentials are derived for the evaluation of the Pauli repulsion energy based on Murrell's expressions.

4.2.1 First-order contribution in overlap matrix expansion.

This contribution is simply the electrostatic potential coming from all nuclei and electron density except* from electron density from molecular orbital i that interacts with the generalized overlap density between i of molecule A and j of molecule B .

3D forms:

$$v(\mathbf{r})_{S^{-1}}^{A[i]} = - \sum_{x \in A} \frac{Z_x}{|\mathbf{r} - \mathbf{r}_x|} + \sum_{\mu\nu \in A} \{D_{\nu\mu} - C_{\mu i}^* C_{\nu i}\} \int d\mathbf{r}' \frac{\phi_\mu^*(\mathbf{r}') \phi_\nu(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

Matrix forms:

$$v_{\xi i}(S^{-1}) = \sum_{\kappa \in A} C_{i\kappa} \left\{ - \sum_{x \in A} V_{\kappa \xi}^{(x)} + \sum_{\mu \nu \in A} \{ D_{\nu \mu} - C_{\mu i}^* C_{\nu i} \} (\mu \nu | \xi \kappa) \right\}$$

4.2.2 Second-order contribution in overlap matrix expansion.

To be added here!

4.3 Excitonic Energy Transfer OEP's

The following potentials are derived for the evaluation of the short-range EET couplings based on Fujimoto's TDFI-TI method.

4.3.1 ET contributions.

3D forms:

$$\begin{aligned} v(\mathbf{r})_1^{A[\mu]} &= -C_{\mu L}^* \sum_{x \in A} \frac{Z_x}{|\mathbf{r} - \mathbf{r}_x|} + \sum_{\nu \kappa \in A} \left\{ C_{\mu L}^* D_{\nu \kappa} - \frac{1}{2} C_{\nu L}^* D_{\mu \kappa} \right\} \int d\mathbf{r}' \frac{\phi_{\nu}^*(\mathbf{r}') \phi_{\kappa}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ v(\mathbf{r})_2^{A[\mu]} &= C_{\kappa H} \sum_{\nu \kappa \in A} \left\{ 2C_{\nu L}^* C_{\mu H}^* - C_{\nu H}^* C_{\mu L}^* \right\} \int d\mathbf{r}' \frac{\phi_{\nu}^*(\mathbf{r}') \phi_{\kappa}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\ v(\mathbf{r})_3^{A[\mu]} &= v(\mathbf{r})_1^{A[\mu]} + v(\mathbf{r})_2^{A[\mu]} \end{aligned}$$

Matrix forms:

$$\begin{aligned} v_{\mu \xi}(1) &= -C_{\mu L}^* \sum_{x \in A} V_{\mu \xi}^x + \sum_{\nu \kappa \in A} \left\{ C_{\mu L}^* D_{\nu \kappa} - \frac{1}{2} C_{\nu L}^* D_{\mu \kappa} \right\} (\nu \kappa | \mu \xi) \\ v_{\mu \xi}(2) &= C_{\kappa H} \sum_{\nu \kappa \in A} \left\{ 2C_{\nu L}^* C_{\mu H}^* - C_{\nu H}^* C_{\mu L}^* \right\} (\nu \kappa | \mu \xi) \\ v_{\mu \xi}(3) &= v_{\mu \xi}(1) + v_{\mu \xi}(2) \end{aligned}$$

4.3.2 HT contributions.

Do be derived.

4.3.3 CT contributions.

To be derived.

4.4 Full HF Interaction OEP's

The following potentials are derived for the evaluation of the full Hartree-Fock interaction energy based on the OEPDev equations.

Chapter 5

Density-fitting Specialized for OEP's

To get the ab-initio representation of a OEP, one can use a procedure similar to the typical density fitting or resolution of identity, both of which are nowadays widely used to compute electron-repulsion integrals (ERI's) more efficiently.

5.1 Fitting in Complete Space

An arbitrary one-electron potential of molecule A acting on any state vector associated with molecule A can be expanded in the *auxiliary space* centered on A as

$$v|i) = \sum_{\xi} v|\xi)(\xi|i)$$

under the necessary assumption that the auxiliary basis set is *complete*. In that case, formally one can write the following identity

$$(\eta|v|i) = \sum_{\xi} (\eta|v|\xi)S_{\xi i}$$

The matrix elements of the OEP operator in auxiliary space can be computed in the same way as the matrix elements with any other basis function. In reality, it is almost impossible to reach the completeness of the basis set, however, but it is possible to obtain the **effective** matrix elements of the OEP operator in auxiliary space, rather than compute them as they are in the above equation explicitly. We expand the LHS of the first equation on this page in a series of the auxiliary basis functions scaled by the undetermined expansion coefficients:

$$v|i) = \sum_{\xi} G_{i\xi}|\xi)$$

The expansion coefficients are the effective matrix elements of the OEP operator in auxiliary basis set. Now, multiplying both sides by another auxiliary basis function and subsequently inverting the equation one obtains the expansion coefficients:

$$G_{i\eta} = \sum_{\xi} (i|v|\eta) [S^{-1}]_{\eta\xi}$$

In this way, it is possible to approximately determine the matrix elements of the OEP operator with any other basis function in case the auxiliary basis set is not complete. **In particular**, when the other basis function does not belong to molecule A but to the (changing) environment, it is straightforward to compute the resulting matrix element, which is simply given as

$$(j_{\in B}|v^A|i_{\in A}) = \sum_{\xi} S_{j\xi} G_{i\xi}$$

where j denotes the other (environmental) basis function.

In the above equation, the OEP-part (fragment parameters for molecule A only) and the Solver-part (subject to be computed by solver on the fly) are separated. This then forms a basis for fragment-based approach to solve Quantum Chemistry problems related to the extended molecular aggregates.

5.2 Fitting in Truncated Space

Density fitting scheme from previous section has practical disadvantage of a complete space being usually very large (spanned by large amount of basis set vectors). Any non-complete basis set won't work in the above example. Since most of basis sets used in quantum chemistry do not form a complete set, is beneficial to design a modified scheme. This can be achieved by minimizing the following objective function

$$Z[\{G_{\xi}^{(i)}\}] = \iint d\mathbf{r}_1 d\mathbf{r}_2 \frac{\left[v(\mathbf{r}_1)\phi_i(\mathbf{r}_1) - \sum_{\xi} G_{\xi}^{(i)} \phi_{\xi}(\mathbf{r}_1) \right] \left[v(\mathbf{r}_2)\phi_i(\mathbf{r}_2) - \sum_{\xi} G_{\xi}^{(i)} \phi_{\xi}(\mathbf{r}_2) \right]}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Thus requesting that

$$\frac{\partial Z[\{G_{\xi}^{(i)}\}]}{\partial G_{\mu}^{(i)}} = 0 \text{ for all } \mu$$

we find the coefficients $G_{\xi}^{(i)}$ to be

$$\mathbf{G}^{(i)} = \mathbf{b}^{(i)} \cdot \mathbf{A}^{-1}$$

where

$$b_{\eta}^{(i)} = (\eta || v_i)$$

$$A_{\eta\xi} = (\eta || \xi)$$

The symbol $||$ is to denote the operator r_{12}^{-1} and double integration over \mathbf{r}_1 and \mathbf{r}_2 . Thus, it is clear that in order to use this generalized density fitting scheme one must to compute two-centre electron repulsion integrals (implemented in `oepdev::ERI_1_1`) as well as four-centre asymmetric electron repulsion integrals of the type $(\alpha\beta\gamma||\eta)$ (implemented in `oepdev::ERI_3_1`).

Chapter 6

Implemented Models

6.1 Target Properties

Detailed list of models which is to be implemented in the OEPDev project is given below:

Table 1. Models subject to be implemented and analyzed within oep-dev.

| Pauli energy | Induction energy | EET Coupling |
|------------------------|------------------------|--------------|
| EFP2-Pauli | EFP2-Induced Dipoles | TrCAMM |
| Murrel et al.'s theory | Density Susceptibility | OEP-ET/HT |
| OEP-Murrel et al.'s | | TDFI-TI |
| | | FED |
| Exact (Stone's) | Exact (incl. CT) | Exact (ESD) |

6.2 Target, Benchmark and Competing Models

The target models introduced in the Project shall be tested against the following benchmarks and compared with the following state-of-the-art models:

Table 2. Target models vs benchmarks and competitor models.

| Target Model | Benchmarks | Competing Model |
|------------------------|------------------|----------------------|
| OEP-Murrel et al.'s | Murrel et al.'s | EFP2-Pauli |
| | Exact (Stone's) | |
| OEP-ET/HT + TrCAMM | Exact (ESD) | TDFI-TI |
| | FED | FED |
| | TDFI-TI | |
| Density Susceptibility | Exact (incl. CT) | EFP2-Induced Dipoles |

Chapter 7

Contributing to oep-dev

OepDev is a plugin to Psi4.

Therefore it should follow the programming etiquette of Psi4. Also, oep-dev has additional programming tips to make the code more versatile and easy in further development. Here, I emphasise on most important aspects regarding the **programming rules**.

7.1 Main routine and libraries

Oep-dev has only *one* source file in the plugin base directory, i.e., `main.cc`. This is the main driver routine that handles the functionality of the whole OEP testing platform: specifies options for Psi4 input file and implements test routines based on the options. Other sources are stored in `MODULE/libNAME*` directories where `NAME` is the name of the library with sources and header files, whereas `MODULE` is the directory of the oep-dev module.

Things to remember:

1. **No other sources in base directory.** It is not permitted to place any new source or other files in the plugin base directory (i.e., where `main.cc` resides).
2. **Sources in library directories.** Any additional source code has to be placed in `oepdev/libNAME*` directory (either existing one or a new one; in the latter case remember to add the new `*.cc` files to `CMakeLists.txt` in the plugin base directory).
3. **Miscellanea in special directories.** If you want to add additional documentation, put it in the `doc` directory. If you want to add graphics, put it in the `images` directory.

7.2 Header files in libraries

Header files are handy in obtaining a quick glimpse of the functionality within certain library. Each library directory should contain at least one header file in oep-dev. However, header files can be problematic if not managed properly.

Things to remember:

1. **Header preprocessor variable.** Define the preprocessor variable specifying the existence of include of the particular header file. The format of such is

```
#ifndef MODULE_LIBRARY_HEADER_h
#define MODULE_LIBRARY_HEADER_h
// rest of your code goes here
#endif // MODULE_LIBRARY_HEADER_h
```

Last line is the **end** of the header file. The preprocessor variables represents the directory tree `oepdev/-MODULE/LIBRARY/HEADER.h` structure (where `oepdev` is the base plugin directory). `MODULE` is the

plugin module name (e.g. `oepdev`, the name of the module directory) `LIBRARY` is the name of the library (e.g. `libutil`, should be the same as library directory name) `HEADER` is the name of the header in library directory (e.g. `diis` for `diis.h` header file)

2. **Set module namespace.** To prevent naming clashes with other modules and with `Psi4` it is important to operate in separate namespace (e.g. for a module).

```
namespace MODULE {
// your code goes here
} // EndNameSpace MODULE
```

For instance, all classes and functions in `oepdev` module are implemented within the namespace of the same label. Considering addition of other local namespaces within a module can also be useful in certain cases.

7.3 Environmental variables

Defining the set of intrinsic environmental variables can help in code management and conditional compilation. The `oep-dev` environmental variables are defined in `include/oepdev_files.h` file. Remember also about `psi4` environmental variables defined in `psi4/psifiles.h` header. As a rule, the `oep-dev` environmental variable should have the following format:

```
OEPDEV_XXXX
```

where `XXXX` is the descriptive name of variable.

7.4 Documenting the code

Code has to be documented (at best at a time it is being created). The place for documentation is always in header files. Additional documentation can be also placed in source files. Leaving a chunk of code for a production run without documentation is unacceptable.

Use Doxygen style for documentation all the time. Remember that it supports markdown which can make the documentation even more clear and easy to understand. Additionally you can create a nice `.rst` documentation file for Sphinx program. If you are coding equations, always include formulae in the documentation!

Things to remember:

1. **Descriptions of classes, structures, global functions, etc.** Each programming object should have a description.
2. **Documentation for function arguments and return object.** Usage of functions and class methods should be explained by providing the description of all arguments (use `\param` and `\return` Doxygen keywords).
3. **One-line description of class member variables.** Any class member variable should be preceded by a one-liner documentation (starting from `///`).
4. **Do not be afraid of long names in the code.** Self-documenting code is a blessing!

7.5 Naming conventions

Naming is important because it helps to create more readable and clear self-documented code.

Some loose suggestions:

1. **Do not be afraid of long names in the code, but avoid redundancy.** Examples of good and bad names: good name: `get_density_matrix`; bad name: `get_matrix`. Unless there is only one type of matrix a particular objects can store, `matrix` is not a good name for a getter method. good name: `class Wavefunction`, bad name: `class WFN` good name: `int numberOfErrorVectors`, bad name: `int nvec`, bad name: `the_number_of_error_vectors` good name: `class EFPotential`, probably bad name: `class EffectiveFragmentPotential`. The latter might be understood by some people as a class that inherits from `EffectiveFragment` class. If it is not the case, compromise between abbreviation and long description is OK.
2. **Short names are OK in special situations.** In cases meaning of a particular variable is obvious and it is frequently used in the code locally, it can be named shortly. Examples are: `i` when iterating `no` number of occupied orbitals, `nv` number of virtual orbitals, etc.
3. **Clumped names for variables and dashed names for functions.** Try to distinguish between variable name like `sizeofOEPTypelist` and a method name `get_matrix()` (neither `size_of_OEP_type_list`, nor `getMatrix()`). This is little bit cosmetics, but helps in managing the code when it grows.
4. **Class names start from capital letter.** However, avoid only capital letters in class names, unless it is obvious. Avoid also dashes in class names (they are reserved for global functions and class methods). Examples: good name: `DIISManager`, bad name: `DIIS`. good name: `EETCouplingSolver`, bad name: `EETSolver`, very bad: `EET`.

7.6 Use Object-Oriented Programming

Try to organise your creations in objects having special relationships and data structures. Encapsulation helps in producing self-maintaining code and is much easier to use. Use:

- **factory design** for creating objects
- **container design** for designing data structures
- **polymorphism** when dealing with various flavours of one particular feature in the data structure

Note: In Psi4, factories are frequently implemented as static methods of the base classes, for example `psi::BasisSet::build` static method. It can be followed when building object factories in oep-dev too.

Chapter 8

Advanced Usage

This page is for advanced users.

Make sure you have first read [the introduction](#).

Chapter 9

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Chapter 10

Module Index

10.1 Modules

Here is a list of all modules:

| | |
|---|----|
| The OEPDev solver library | ?? |
| The Generalized One-Electron Potentials library | ?? |
| The Integral Package Library | ?? |
| The Integral Helper Library | ?? |
| The Three-Dimensional Scalar Fields Library | ?? |
| The Multipole Fitting Library | ?? |
| The OEPDev Utilities | ?? |
| The OEPDev Testing Platform Library | ?? |

Chapter 11

Namespace Index

11.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

| | | |
|------------------------|----------------------------------|----|
| oepdev | OEPEv module namespace | ?? |
| psi | Psi4 package namespace | ?? |

Chapter 12

Hierarchical Index

12.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

| | |
|---|----|
| oepdev::AllAOIntegralsIterator | ?? |
| oepdev::AllAOShellCombinationsIterator | ?? |
| CubicScalarGrid | |
| oepdev::CubePointsCollection3D | ?? |
| oepdev::DIISManager | ?? |
| enable_shared_from_this | |
| oepdev::OEPDevSolver | ?? |
| oepdev::ChargeTransferEnergySolver | ?? |
| oepdev::ElectrostaticEnergySolver | ?? |
| oepdev::RepulsionEnergySolver | ?? |
| oepdev::OEPotential | ?? |
| oepdev::ChargeTransferEnergyOEPotential | ?? |
| oepdev::EETCouplingOEPotential | ?? |
| oepdev::ElectrostaticEnergyOEPotential | ?? |
| oepdev::RepulsionEnergyOEPotential | ?? |
| oepdev::ESPSolver | ?? |
| IntegralFactory | |
| oepdev::IntegralFactory | ?? |
| oepdev::Points3DIterator::Point | ?? |
| oepdev::Points3DIterator | ?? |
| oepdev::CubePoints3DIterator | ?? |
| oepdev::RandomPoints3DIterator | ?? |
| oepdev::PointsCollection3D | ?? |
| oepdev::CubePointsCollection3D | ?? |
| oepdev::RandomPointsCollection3D | ?? |
| PotentialInt | |
| oepdev::PotentialInt | ?? |
| oepdev::ScalarField3D | ?? |
| oepdev::ElectrostaticPotential3D | ?? |
| oepdev::OEPotential3D< T > | ?? |
| oepdev::test::Test | ?? |
| TwoBodyAOInt | |
| oepdev::TwoElectronInt | ?? |
| oepdev::ERI_2_2 | ?? |
| oepdev::ERI_3_1 | ?? |
| Wavefunction | |
| oepdev::WavefunctionUnion | ?? |

Chapter 13

Class Index

13.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

| | | |
|---|--|----|
| oepdev::AllAOIntegralsIterator | Loop over all possible ERI within a particular shell | ?? |
| oepdev::AllAOShellCombinationsIterator | Loop over all possible ERI shells | ?? |
| oepdev::ChargeTransferEnergyOEPotential | Generalized One-Electron Potential for Charge-Transfer Interaction Energy | ?? |
| oepdev::ChargeTransferEnergySolver | Compute the Charge-Transfer interaction energy between unperturbed wavefunctions | ?? |
| oepdev::CubePoints3DIterator | Iterator over a collection of points in 3D space. g09 Cube-like order | ?? |
| oepdev::CubePointsCollection3D | G09 cube-like ordered collection of points in 3D space | ?? |
| oepdev::DIISManager | DIIS manager | ?? |
| oepdev::EETCouplingOEPotential | Generalized One-Electron Potential for EET coupling calculations | ?? |
| oepdev::ElectrostaticEnergyOEPotential | Generalized One-Electron Potential for Electrostatic Energy | ?? |
| oepdev::ElectrostaticEnergySolver | Compute the Coulombic interaction energy between unperturbed wavefunctions | ?? |
| oepdev::ElectrostaticPotential3D | Electrostatic potential of a molecule | ?? |
| oepdev::ERI_2_2 | 4-centre ERI of the form $(ab O(2) cd)$ where $O(2) = 1/r_{12}$ | ?? |
| oepdev::ERI_3_1 | 4-centre ERI of the form $(abc O(2) d)$ where $O(2) = 1/r_{12}$ | ?? |
| oepdev::ESPSolver | Charges from Electrostatic Potential (ESP). A solver-type class | ?? |
| oepdev::IntegralFactory | Extended IntegralFactory for computing integrals | ?? |
| oepdev::OEPDevSolver | Solver of properties of molecular aggregates. Abstract base | ?? |
| oepdev::OEPotential | Generalized One-Electron Potential: Abstract base | ?? |
| oepdev::OEPotential3D< T > | Class template for OEP scalar fields | ?? |
| oepdev::Points3DIterator::Point | | ?? |

| | | |
|--|--|----|
| oepdev::Points3DIterator | Iterator over a collection of points in 3D space. Abstract base | ?? |
| oepdev::PointsCollection3D | Collection of points in 3D space. Abstract base | ?? |
| oepdev::PotentialInt | Computes potential integrals | ?? |
| oepdev::RandomPoints3DIterator | Iterator over a collection of points in 3D space. Random collection | ?? |
| oepdev::RandomPointsCollection3D | Collection of random points in 3D space | ?? |
| oepdev::RepulsionEnergyOEPotential | Generalized One-Electron Potential for Pauli Repulsion Energy | ?? |
| oepdev::RepulsionEnergySolver | Compute the Pauli-Repulsion interaction energy between unperturbed wavefunctions | ?? |
| oepdev::ScalarField3D | Scalar field in 3D space. Abstract base | ?? |
| oepdev::test::Test | Manages test routines | ?? |
| oepdev::TwoElectronInt | General Two Electron Integral | ?? |
| oepdev::WavefunctionUnion | Union of two Wavefunction objects | ?? |

Chapter 14

File Index

14.1 File List

Here is a list of all documented files with brief descriptions:

| | |
|--|----|
| main.cc | ?? |
| include/ oepdev_files.h | ?? |
| include/doxygen/ oepdev_manual.h | ?? |
| include/doxygen/ oepdev_modules.h | ?? |
| include/doxygen/ oepdev_namespaces.h | ?? |
| oepdev/libints/ eri.h | ?? |
| oepdev/libints/ recurr.h | ?? |
| oepdev/liboep/ oep.h | ?? |
| oepdev/libpsi/ integral.h | ?? |
| oepdev/libpsi/ potential.h | ?? |
| oepdev/libtest/ test.h | ?? |
| oepdev/libutil/ cphf.h | ?? |
| oepdev/libutil/ diis.h | ?? |
| oepdev/libutil/ esp.h | ?? |
| oepdev/libutil/ integrals_iter.h | ?? |
| oepdev/libutil/ solver.h | ?? |
| oepdev/libutil/ space3d.h | ?? |
| oepdev/libutil/ util.h | ?? |
| oepdev/libutil/ wavefunction_union.h | ?? |

Chapter 15

Module Documentation

15.1 The OEPDev solver library

Classes

- class [oepdev::OEPDevSolver](#)
Solver of properties of molecular aggregates. Abstract base.
- class [oepdev::ElectrostaticEnergySolver](#)
Compute the Coulombic interaction energy between unperturbed wavefunctions.
- class [oepdev::RepulsionEnergySolver](#)
Compute the Pauli-Repulsion interaction energy between unperturbed wavefunctions.
- class [oepdev::ChargeTransferEnergySolver](#)
Compute the Charge-Transfer interaction energy between unperturbed wavefunctions.

15.1.1 Detailed Description

Implementations various solvers for molecular properties as a functions of unperturbed monomeric wavefunctions. This is the place all target OEP-based models are implemented and compared with benchmark models.

15.2 The Generalized One-Electron Potentials library

Classes

- class [oepdev::OEPotential](#)
Generalized One-Electron Potential: Abstract base.
- class [oepdev::ElectrostaticEnergyOEPotential](#)
Generalized One-Electron Potential for Electrostatic Energy.
- class [oepdev::RepulsionEnergyOEPotential](#)
Generalized One-Electron Potential for Pauli Repulsion Energy.
- class [oepdev::ChargeTransferEnergyOEPotential](#)
Generalized One-Electron Potential for Charge-Transfer Interaction Energy.
- class [oepdev::EETCouplingOEPotential](#)
Generalized One-Electron Potential for EET coupling calculations.

15.2.1 Detailed Description

Implements the goal of this project: The Generalized One-Electron Potentials (OEP's). You will find here OEP's for computation of Pauli repulsion energy, charge-transfer energy and others.

15.3 The Integral Package Library

Classes

- class `oepdev::TwoElectronInt`
General Two Electron Integral.
- class `oepdev::ERI_2_2`
4-centre ERI of the form $(ab|O(2)|cd)$ where $O(2) = 1/r^{12}$.
- class `oepdev::ERI_3_1`
4-centre ERI of the form $(abc|O(2)|d)$ where $O(2) = 1/r^{12}$.
- class `oepdev::IntegralFactory`
Extended `IntegralFactory` for computing integrals.
- class `oepdev::PotentialInt`
Computes potential integrals.

Macros

- `#define D1_INDEX(x, i, n) ((81*(x))+(9*(i))+(n))`
Get the index of McMurchie-Davidson-Hermite D1 coefficient stored in the `mdh_buffer_`, that is attributed to the x Cartesian coordinate from angular momentum i of function 1, and the Hermite index n.
- `#define D2_INDEX(x, i, j, n) ((1377*(x))+(153*(i))+(17*(j))+(n))`
Get the index of McMurchie-Davidson-Hermite D2 coefficient stored in the `mdh_buffer_`, that is attributed to the x Cartesian coordinate from angular momenta i, j of function 1 and 2, and the Hermite index n.
- `#define D3_INDEX(x, i, j, k, n) ((18225*(x))+(2025*(i))+(225*(j))+(25*(k))+(n))`
Get the index of McMurchie-Davidson-Hermite D3 coefficient stored in the `mdh_buffer_`, that is attributed to the x Cartesian coordinate from angular momenta i, j and k of function 1, 2 and 3, and the Hermite index n.
- `#define R_INDEX(n, l, m, j) ((14739*(n))+(867*(l))+(51*(m))+(j))`
Get the index of McMurchie-Davidson R coefficient stored in the `mdh_buffer_R_` from angular momenta n, l and m and the Boys index j.

Functions

- double `oepdev::d_N_n1_n2` (int N, int n1, int n2, double PA, double PB, double aP)
Compute McMurchie-Davidson-Hermite (MDH) coefficient for binomial expansion.
- void `oepdev::make_mdh_D1_coeff` (int n1, double aPd, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for monomial expansion.
- void `oepdev::make_mdh_D2_coeff` (int n1, int n2, double aPd, double *PA, double *PB, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion.
- void `oepdev::make_mdh_D3_coeff` (int n1, int n2, int n3, double aPd, double *PA, double *PB, double *PC, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for trinomial expansion.
- void `oepdev::make_mdh_D2_coeff_explicit_recursion` (int n1, int n2, double aP, double *PA, double *PB, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion by explicit recursion. This function makes the same changes to buffers as `oepdev::make_mdh_D2_coeff`, but implements it through explicit recursion by calls to `oepdev::d_N_n1_n2`. Therefore, it is slightly slower. Here for debugging purposes.
- void `oepdev::make_mdh_R_coeff` (int N, int L, int M, double alpha, double a, double b, double c, double *F, double *buffer)
Compute the McMurchie-Davidson R coefficients.

15.3.1 Detailed Description

Implementations of various one- and two-body integrals via McMurchie-Davidson recurrence scheme. Here, we define the primitive Gaussian type functions (GTO's)

$$\begin{aligned}\phi_i(\mathbf{r}) &\equiv x_A^{n_1} y_A^{l_1} z_A^{m_1} e^{-\alpha_1 r_A^2} \\ \phi_j(\mathbf{r}) &\equiv x_B^{n_2} y_B^{l_2} z_B^{m_2} e^{-\alpha_2 r_B^2} \\ \phi_k(\mathbf{r}) &\equiv x_C^{n_3} y_C^{l_3} z_C^{m_3} e^{-\alpha_3 r_C^2}\end{aligned}$$

in which $\mathbf{r}_A \equiv \mathbf{r} - \mathbf{A}$ and so on. \mathbf{A} is the centre of the GTO, α_1 its exponent, whereas n_1, l_1, m_1 the Cartesian angular momenta, with the total angular momentum $\theta_1 = n_1 + l_1 + m_1$.

In OEPDev implementations, the following definition shall be in use:

$$\begin{aligned}\mathbf{P} &\equiv \frac{\alpha_1 \mathbf{A} + \alpha_2 \mathbf{B}}{\alpha_1 + \alpha_2} \\ \mathbf{Q} &\equiv \frac{\alpha_3 \mathbf{C} + \alpha_4 \mathbf{D}}{\alpha_3 + \alpha_4} \\ \mathbf{R} &\equiv \frac{\alpha_1 \mathbf{A} + \alpha_2 \mathbf{B} + \alpha_3 \mathbf{C}}{\alpha_1 + \alpha_2 + \alpha_3} \\ \alpha_P &\equiv \alpha_1 + \alpha_2 \\ \alpha_Q &\equiv \alpha_3 + \alpha_4 \\ \alpha_R &\equiv \alpha_1 + \alpha_2 + \alpha_3\end{aligned}$$

The unnormalized products of primitive GTO's are denoted here as

$$\begin{aligned}[ij] &\equiv \phi_i(\mathbf{r}) \phi_j(\mathbf{r}) \\ [ijk] &\equiv \phi_i(\mathbf{r}) \phi_j(\mathbf{r}) \phi_k(\mathbf{r})\end{aligned}$$

15.3.2 Hermite Operators

It is convenient to define

$$\Lambda_j(x_P; \alpha_P) \equiv \left(\frac{\partial}{\partial P_x} \right)^j = \alpha_P^{j/2} H_j(\sqrt{\alpha_P} x_P)$$

where $H_j(x)$ is the Hermite polynomial of order j evaluated at x . Introduction of the above Hermite operator can be used by invoking the recurrence relationship due to Hermite polynomial properties:

$$x_A \Lambda_j(x_P; \alpha_P) = j \Lambda_{j-1} + |\mathbf{P} - \mathbf{A}|_x \Lambda_j + \frac{1}{2\alpha_P} \Lambda_{j+1}$$

This can be directly used to derive very useful McMurchie-Davidson-Hermite coefficients as expansion coefficients of the polynomial expansions.

15.3.2.1 Polynomial Expansions as Hermite Series

By using the previous relation, it is possible to express the following expansions in Hermite series:

$$\begin{aligned}x_A^{n_1} &= \sum_{N=0}^{n_1} d_N^{n_1} \Lambda_N(x_A; \alpha_A) \\ x_A^{n_1} x_B^{n_2} &= \sum_{N=0}^{n_1+n_2} d_N^{n_1 n_2} \Lambda_N(x_P; \alpha_P) \\ x_A^{n_1} x_B^{n_2} x_C^{n_3} &= \sum_{N=0}^{n_1+n_2+n_3} d_N^{n_1 n_2 n_3} \Lambda_N(x_R; \alpha_R)\end{aligned}$$

The recurrence relationships can be easily found and they read

$$d_N^{n_1+1} = \frac{1}{2\alpha_A} d_{N-1}^{n_1} + (N+1) d_{N+1}^{n_1}$$

as well as

$$d_N^{n_1+1, n_2} = \frac{1}{2\alpha_P} d_{N-1}^{n_1 n_2} + |\mathbf{P} - \mathbf{A}|_x d_N^{n_1 n_2} + (N+1) d_{N+1}^{n_1 n_2}$$

$$d_N^{n_1, n_2+1} = \frac{1}{2\alpha_P} d_{N-1}^{n_1 n_2} + |\mathbf{P} - \mathbf{B}|_x d_N^{n_1 n_2} + (N+1) d_{N+1}^{n_1 n_2}$$

and

$$d_N^{n_1+1, n_2, n_3} = \frac{1}{2\alpha_R} d_{N-1}^{n_1 n_2 n_3} + |\mathbf{R} - \mathbf{A}|_x d_N^{n_1 n_2 n_3} + (N+1) d_{N+1}^{n_1 n_2 n_3}$$

$$d_N^{n_1, n_2+1, n_3} = \frac{1}{2\alpha_R} d_{N-1}^{n_1 n_2 n_3} + |\mathbf{R} - \mathbf{B}|_x d_N^{n_1 n_2 n_3} + (N+1) d_{N+1}^{n_1 n_2 n_3}$$

$$d_N^{n_1, n_2, n_3+1} = \frac{1}{2\alpha_R} d_{N-1}^{n_1 n_2 n_3} + |\mathbf{R} - \mathbf{C}|_x d_N^{n_1 n_2 n_3} + (N+1) d_{N+1}^{n_1 n_2 n_3}$$

respectively. The first elements are given by

$$d_0^0 = 1$$

$$d_0^{00} = 1$$

$$d_0^{000} = 1$$

By using the above formalisms, it is straightforward to express the doublet of primitive GTO's as

$$[ij] = E_{ij} \sum_{N=0}^{n_1+n_2} \sum_{L=0}^{l_1+l_2} \sum_{M=0}^{m_1+m_2} d_N^{n_1 n_2} d_L^{l_1 l_2} d_M^{m_1 m_2} \Lambda_N(x_P) \Lambda_L(y_P) \Lambda_M(z_P) e^{-\alpha_P r_P^2}$$

Analogously, the triplet of primitive GTO's is given by

$$[ijk] = E_{ijk} \sum_{N=0}^{n_1+n_2+n_3} \sum_{L=0}^{l_1+l_2+l_3} \sum_{M=0}^{m_1+m_2+m_3} d_N^{n_1 n_2 n_3} d_L^{l_1 l_2 l_3} d_M^{m_1 m_2 m_3} \Lambda_N(x_R) \Lambda_L(y_R) \Lambda_M(z_R) e^{-\alpha_R r_R^2}$$

The multiplicative constants are given by

$$E_{ij}(\alpha_1, \alpha_2) = \exp \left[-\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} |\mathbf{A} - \mathbf{B}|^2 \right]$$

$$E_{ijk}(\alpha_1, \alpha_2, \alpha_3) = \exp \left[-\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} |\mathbf{A} - \mathbf{B}|^2 \right] \exp \left[-\frac{(\alpha_1 + \alpha_2) \alpha_3}{\alpha_1 + \alpha_2 + \alpha_3} |\mathbf{P} - \mathbf{C}|^2 \right]$$

15.3.3 One-Body Integrals over Hermite Functions

The fundamental Hermite integrals that appear during computations of any kind of one-body integrals over GTO's are as follows

$$[NLM|\Theta(1)] \equiv \int d\mathbf{r}_1 \Theta(\mathbf{r}_1) \Lambda_N(x_{1P}; \alpha_P) \Lambda_L(y_{1P}; \alpha_P) \Lambda_M(z_{1P}; \alpha_P) e^{-\alpha_P r_{1P}^2}$$

It immediately follows that the overlap, dipole, quadrupole and potential integrals are given as

$$[NLM|1] = \delta_{N0} \delta_{L0} \delta_{M0} \left(\frac{\pi}{\alpha_P} \right)^{3/2}$$

$$[NLM|x_C] = [\delta_{N1} + |\mathbf{P}\mathbf{C}|_x \delta_{N0}] \delta_{L0} \delta_{M0} \left(\frac{\pi}{\alpha_P} \right)^{3/2}$$

$$[NLM|x_C^2] = \left[2\delta_{N2} + 2|\mathbf{P}\mathbf{C}|_x \delta_{N1} + \left(|\mathbf{P}\mathbf{C}|_x^2 + \frac{1}{2\alpha_P} \right) \delta_{N0} \right] \delta_{L0} \delta_{M0} \left(\frac{\pi}{\alpha_P} \right)^{3/2}$$

$$[NLM|x_C y_C] = (\delta_{N1} + |\mathbf{P}\mathbf{C}|_x \delta_{N0}) (\delta_{L1} + |\mathbf{P}\mathbf{C}|_y \delta_{L0}) \delta_{M0} \left(\frac{\pi}{\alpha_P} \right)^{3/2}$$

$$[NLM|r_C^{-1}] = \frac{2\pi}{\alpha_P} R_{NLM}$$

The coefficients R_{NLM} are discussed in separate section below.

15.3.4 Two-Body Integrals over Hermite Functions

The fundamental Hermite integrals that appear during computations of any kind of two-electron integrals over GTO's are as follows

$$[N_1 L_1 M_1 | N_2 L_2 M_2] \equiv \iint d\mathbf{r}_1 d\mathbf{r}_2 \Lambda_{N_1}(x_{1P}; \alpha_P) \Lambda_{L_1}(y_{1P}; \alpha_P) \Lambda_{M_1}(z_{1P}; \alpha_P) \Lambda_{N_2}(x_{2Q}; \alpha_Q) \Lambda_{L_2}(y_{2Q}; \alpha_Q) \Lambda_{M_2}(z_{2Q}; \alpha_Q) e^{-\alpha_P r_{1P}^2 - \alpha_Q r_{2Q}^2}$$

The above formula dramatically reduces to the following

$$[N_1 L_1 M_1 | N_2 L_2 M_2] = \lambda (-)^{N_2+L_2+M_2} R_{N_1+N_2, L_1+L_2, M_1+M_2}$$

with

$$\lambda \equiv \frac{2\pi^{5/2}}{\alpha_P \alpha_Q \sqrt{\alpha_P + \alpha_Q}}$$

To compute the $R_{N_1+N_2, L_1+L_2, M_1+M_2}$ coefficients, the parameter T is given by

$$T = \frac{\alpha_P \alpha_Q}{\alpha_P + \alpha_Q} |\mathbf{P} - \mathbf{Q}|^2$$

15.3.5 The R(N,L,M) Coefficients

The R coefficients are defined as

$$R_{NLM} \equiv \left(\frac{\partial}{\partial a} \right)^N \left(\frac{\partial}{\partial b} \right)^L \left(\frac{\partial}{\partial c} \right)^M \int_0^1 e^{-Tu^2} du$$

with

$$T \equiv \alpha (a^2 + b^2 + c^2)$$

By extending the above definition to more general

$$R_{NLMj} \equiv (-\sqrt{\alpha})^{N+L+M} (-2\alpha)^j \int_0^1 u^{N+L+M+2j} H_N(au\sqrt{\alpha}) H_L(bu\sqrt{\alpha}) H_M(cu\sqrt{\alpha}) e^{-Tu^2} du$$

one can see that

$$R_{000j} = (-2\alpha)^j F_j(T)$$

The Boys function is here given by

$$F_j(T) \equiv \int_0^1 u^{2j} e^{-Tu^2} du$$

and its efficient implementation can be discussed elsewhere. In Psi4, `psi::Taylor_Fjt` class is used for this purpose.

Now, it is possible to show that the following recursion relationships are true:

$$R_{0,0,M+1,j} = cR_{0,0,M,j+1} + MR_{0,0,M-1,j+1}$$

$$R_{0,L+1,M,j} = bR_{0,L,M,j+1} + LR_{0,L-1,M,j+1}$$

$$R_{N+1,L,M,j} = aR_{N,L,M,j+1} + NR_{N-1,L,M,j+1}$$

This scheme is implemented in OEPDev.

15.3.6 Function Documentation

15.3.6.1 double oepdev::d_N_n1_n2 (int N, int n1, int n2, double PA, double PB, double aP)

Compute McMurchie-Davidson-Hermite (MDH) coefficient for binomial expansion.

Parameters

| | |
|-----------|--|
| <i>N</i> | - increment in the summation of MDH series |
| <i>n1</i> | - angular momentum of first function |
| <i>n2</i> | - angular momentum of second function |
| <i>PA</i> | - cartesian component of P-A distance |
| <i>PB</i> | - cartesian component of P-B distance |
| <i>aP</i> | - free parameter of MDH expansion |

Returns

the McMurchie-Davidson-Hermite coefficient

15.3.6.2 void oepdev::make_mdh_D1_coeff (int *n1*, double *aPd*, double * *buffer*)

Compute the McMurchie-Davidson-Hermite coefficients for monomial expansion.

Parameters

| | |
|---------------|---|
| <i>n1</i> | - angular momentum of first function |
| <i>aPd</i> | - parameter equal to 0.500/ <i>Pa</i> where <i>Pa</i> is exponent |
| <i>buffer</i> | - the McMurchie-Davidson-Hermite 3-dimensional array (raveled to vector): <ul style="list-style-type: none"> • axis 0: dimension 3 (x, y or z Cartesian component) • axis 1: dimension <i>n1</i>+1 (0 to <i>n1</i>) • axis 2: dimension <i>n1</i>+1 (0 to <i>n1</i>) |

See Also

[D1_INDEX](#)

15.3.6.3 void oepdev::make_mdh_D2_coeff (int *n1*, int *n2*, double *aPd*, double * *PA*, double * *PB*, double * *buffer*)

Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion.

Parameters

| | |
|---------------|---|
| <i>n1</i> | - angular momentum of first function |
| <i>n2</i> | - angular momentum of second function |
| <i>aPd</i> | - parameter equal to 0.500/ <i>Pa</i> where <i>Pa</i> is exponent |
| <i>PA</i> | - cartesian components of P-A distance |
| <i>PB</i> | - cartesian components of P-B distance |
| <i>buffer</i> | - the McMurchie-Davidson-Hermite 4-dimensional array (raveled to vector): <ul style="list-style-type: none"> • axis 0: dimension 3 (x, y or z Cartesian component) • axis 1: dimension <i>n1</i>+1 (0 to <i>n1</i>) • axis 2: dimension <i>n2</i>+1 (0 to <i>n2</i>) • axis 3: dimension <i>n1</i>+<i>n2</i>+1 (0 to <i>n1</i>+<i>n2</i>) |

See Also

[D2_INDEX](#)

15.3.6.4 `void oepdev::make_mdh_D2_coeff_explicit_recursion (int n1, int n2, double aP, double * PA, double * PB, double * buffer)`

Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion by explicit recursion. This function makes the same changes to buffers as [oepdev::make_mdh_D2_coeff](#), but implements it through explicit recursion by calls to [oepdev::d_N_n1_n2](#). Therefore, it is slightly slower. Here for debugging purposes.

Parameters

| | |
|---------------|---|
| <i>n1</i> | - angular momentum of first function |
| <i>n2</i> | - angular momentum of second function |
| <i>aPd</i> | - parameter equal to 0.500/ <i>Pa</i> where <i>Pa</i> is exponent |
| <i>PA</i> | - cartesian components of P-A distance |
| <i>PB</i> | - cartesian components of P-B distance |
| <i>buffer</i> | - the McMurchie-Davidson-Hermite 4-dimensional array (raveled to vector): <ul style="list-style-type: none"> • axis 0: dimension 3 (x, y or z Cartesian component) • axis 1: dimension <i>n1</i>+1 (0 to <i>n1</i>) • axis 2: dimension <i>n2</i>+1 (0 to <i>n2</i>) • axis 3: dimension <i>n1</i>+<i>n2</i>+1 (0 to <i>n1</i>+<i>n2</i>) |

See Also

[D2_INDEX](#)

15.3.6.5 `void oepdev::make_mdh_D3_coeff (int n1, int n2, int n3, double aPd, double * PA, double * PB, double * PC, double * buffer)`

Compute the McMurchie-Davidson-Hermite coefficients for trinomial expansion.

Parameters

| | |
|---------------|---|
| <i>n1</i> | - angular momentum of first function |
| <i>n2</i> | - angular momentum of second function |
| <i>n3</i> | - angular momentum of third function |
| <i>aPd</i> | - parameter equal to 0.500/ <i>Pa</i> where <i>Pa</i> is exponent |
| <i>PA</i> | - cartesian components of P-A distance |
| <i>PB</i> | - cartesian components of P-B distance |
| <i>PC</i> | - cartesian components of P-C distance |
| <i>buffer</i> | - the McMurchie-Davidson-Hermite 5-dimensional array (raveled to vector): <ul style="list-style-type: none"> • axis 0: dimension 3 (x, y or z Cartesian component) • axis 1: dimension <i>n1</i>+1 (0 to <i>n1</i>) • axis 2: dimension <i>n2</i>+1 (0 to <i>n2</i>) • axis 3: dimension <i>n3</i>+1 (0 to <i>n3</i>) • axis 4: dimension <i>n1</i>+<i>n2</i>+<i>n3</i>+1 (0 to <i>n1</i>+<i>n2</i>+<i>n3</i>) |

See Also

[D3_INDEX](#)


```
15.3.6.6 void oepdev::make_mdh_R_coeff ( int N, int L, int M, double alpha, double a, double b, double c, double * F,  
double * buffer )
```

Compute the McMurchie-Davidson R coefficients.

Parameters

| | |
|----------|--|
| N | - increment in the summation of MDH series along x direction |
| L | - increment in the summation of MDH series along y direction |
| M | - increment in the summation of MDH series along z direction |
| α | - alpha parameter of R coefficient |
| a | - x component of PQ vector of R coefficient |
| b | - y component of PQ vector of R coefficient |
| c | - z component of PQ vector of R coefficient |
| F | - array of Boys function values for given alpha and PQ |
| $buffer$ | - the McMurchie-Davidson 4-dimensional array (raveled to vector): <ul style="list-style-type: none"> • axis 0: dimension $N+1$ • axis 1: dimension $L+1$ • axis 2: dimension $M+1$ • axis 3: dimension $N+L+M+1$ (j-th element) |

15.4 The Integral Helper Library

Classes

- class [oepdev::AllAOShellCombinationsIterator](#)
Loop over all possible ERI shells.
- class [oepdev::AllAOIntegralsIterator](#)
Loop over all possible ERI within a particular shell.

15.4.1 Detailed Description

You will find here various iterators to go through shells while computing ERI, or iterators over ERI itself.

15.5 The Three-Dimensional Scalar Fields Library

Classes

- class [oepdev::Points3DIterator](#)
Iterator over a collection of points in 3D space. Abstract base.
- class [oepdev::CubePoints3DIterator](#)
Iterator over a collection of points in 3D space. g09 Cube-like order.
- class [oepdev::RandomPoints3DIterator](#)
Iterator over a collection of points in 3D space. Random collection.
- class [oepdev::PointsCollection3D](#)
Collection of points in 3D space. Abstract base.
- class [oepdev::RandomPointsCollection3D](#)
Collection of random points in 3D space.
- class [oepdev::CubePointsCollection3D](#)
G09 cube-like ordered collection of points in 3D space.
- class [oepdev::ScalarField3D](#)
Scalar field in 3D space. Abstract base.
- class [oepdev::ElectrostaticPotential3D](#)
Electrostatic potential of a molecule.
- class [oepdev::OEPotential3D< T >](#)
Class template for OEP scalar fields.

Functions

- [oepdev::OEPotential3D< T >::OEPotential3D](#) (const int &np, const double &padding, std::shared_ptr< T > oep, const std::string &oepType)
Construct random spherical collection of scalar field of type T.
- [oepdev::OEPotential3D< T >::OEPotential3D](#) (const int &nx, const int &ny, const int &nz, const double &px, const double &py, const double &pz, std::shared_ptr< T > oep, const std::string &oepType, psi::Options &options)
Construct ordered 3D collection of scalar field of type T.
- virtual [oepdev::OEPotential3D< T >::~~OEPotential3D](#) ()
Destructor.
- virtual void [oepdev::OEPotential3D< T >::print](#) () const
Print information of the object to Psi4 output.
- virtual double [oepdev::OEPotential3D< T >::compute_xyz](#) (const double &x, const double &y, const double &z)
Compute a value of scalar field at point (x, y, z)

15.5.1 Detailed Description

Handles all sorts of scalar distributions in 3D Euclidean space, such as potentials defined at particular collection of points. In this Module, you will also find handling both random and ordered points collections in a form of a G09 cube, as well as handling G09 Cube files.

15.5.2 Function Documentation

15.5.2.1 `template<class T > oepdev::OEPotential3D< T >::OEPotential3D (const int & np, const double & padding,
std::shared_ptr< T > oep, const std::string & oepType)`

Construct random spherical collection of scalar field of type T.

The points are drawn according to uniform distribution in 3D space.

Parameters

| | |
|----------------|-----------------------------------|
| <i>np</i> | - number of points to draw |
| <i>padding</i> | - spherical padding distance (au) |
| <i>oep</i> | - OEP object of type T |
| <i>oepType</i> | - type of OEP |

15.5.2.2 `template<class T > oepdev::OEPotential3D< T >::OEPotential3D (const int & nx, const int & ny, const int & nz, const double & px, const double & py, const double & pz, std::shared_ptr< T > oep, const std::string & oepType, psi::Options & options)`

Construct ordered 3D collection of scalar field of type T.

The points are generated according to Gaussian cube file format.

Parameters

| | |
|----------------|--------------------------------------|
| <i>nx</i> | - number of points along x direction |
| <i>ny</i> | - number of points along y direction |
| <i>nz</i> | - number of points along z direction |
| <i>px</i> | - padding distance along x direction |
| <i>py</i> | - padding distance along y direction |
| <i>pz</i> | - padding distance along z direction |
| <i>oep</i> | - OEP object of type T |
| <i>oepType</i> | - type of OEP |
| <i>options</i> | - Psi4 options object |

15.6 The Multipole Fitting Library

Classes

- class [oepdev::ESPSolver](#)
Charges from Electrostatic Potential (ESP). A solver-type class.

Typedefs

- using **oepdev::SharedScalarField3D** = std::shared_ptr< ScalarField3D >

15.6.1 Detailed Description

Implements methods to fit the generalized multipole moments of a generalized density distribution based on the input generalized potential scalar field. Among others, you will find here the electrostatic potential (ESP) fitting method.

15.7 The OEPDev Utilities

Classes

- class `oepdev::DIISManager`
DIIS manager.
- class `oepdev::WavefunctionUnion`
Union of two Wavefunction objects.

Macros

- `#define OEPDEV_USE_PSI4_DIIS_MANAGER 0`
Use DIIS from Psi4 (1) or OEPDev (0)?
- `#define OEPDEV_MAX_AM 8`
L_max.
- `#define OEPDEV_N_MAX_AM 17`
2L_max+1
- `#define OEPDEV_CRIT_ERI 1e-9`
*ERI criterion for E12, E34, E123 and lambda*EXY coefficients.*
- `#define OEPDEV_SIZE_BUFFER_R 250563`
*Size of R buffer (OEPDEV_N_MAX_AM*OEPDEV_N_MAX_AM*OEPDEV_N_MAX_AM*OEPDEV_N_MAX_AM*3)*
- `#define OEPDEV_SIZE_BUFFER_D2 3264`
Size of D2 buffer (3(OEPDEV_MAX_AM+1)*(OEPDEV_MAX_AM+1)*OEPDEV_N_MAX_AM)*

Functions

- void `oepdev::preamble` (void)
Print preamble for module OEPDEV.
- `std::shared_ptr< SuperFunctional > oepdev::create_superfunctional` (std::string name, Options &options)
Set up DFT functional.
- `std::shared_ptr< Molecule > oepdev::extract_monomer` (std::shared_ptr< const Molecule > molecule_dimer, int id)
Extract molecule from dimer.
- `std::shared_ptr< Wavefunction > oepdev::solve_scf` (std::shared_ptr< Molecule > molecule, std::shared_ptr< BasisSet > primary, std::shared_ptr< SuperFunctional > functional, Options &options, std::shared_ptr< PSIO > psio)
Solve RHF-SCF equations for a given molecule in a given basis set.

15.7.1 Detailed Description

Contains utility functions such as printing OEPDev preamble to the output file, class for wavefunction union etc.

15.7.2 Function Documentation

15.7.2.1 `std::shared_ptr< SuperFunctional > oepdev::create_superfunctional (std::string name, Options &options)`

Set up DFT functional.

Now it accepts only pure HF functional.

Parameters

| | |
|----------------|---|
| <i>name</i> | name of the functional ("HF" is now only available) |
| <i>options</i> | psi::Options object |

Returns

psi::SharedSuperFunctional object with functional.

15.7.2.2 `std::shared_ptr< Molecule > oepdev::extract_monomer (std::shared_ptr< const Molecule > molecule_dimer, int id)`

Extract molecule from dimer.

Parameters

| | |
|-----------------------|---------------------------------------|
| <i>molecule_dimer</i> | psi::SharedMolecule object with dimer |
| <i>id</i> | index of a molecule (starts from 1) |

Returns

psi::SharedMolecule object with indicated monomer

15.7.2.3 `std::shared_ptr< Wavefunction > oepdev::solve_scf (std::shared_ptr< Molecule > molecule, std::shared_ptr< BasisSet > primary, std::shared_ptr< SuperFunctional > functional, Options & options, std::shared_ptr< PSIO > psio)`

Solve RHF-SCF equations for a given molecule in a given basis set.

Parameters

| | |
|-------------------|--|
| <i>molecule</i> | psi::SharedMolecule object with molecule |
| <i>primary</i> | shared primary basis set |
| <i>functional</i> | DFT functional |
| <i>options</i> | psi::Options object |
| <i>psio</i> | psi::PSIO object |

Returns

psi::SharedWavefunction SCF wavefunction of the molecule

15.8 The OEPDev Testing Platform Library

Classes

- class `oepdev::test::Test`
Manages test routines.

15.8.1 Detailed Description

Testing platform at C++ level of code. You can add more tests here when developing new functionalities.

Chapter 16

Namespace Documentation

16.1 oepdev Namespace Reference

OEPDev module namespace.

Classes

- class [TwoElectronInt](#)
General Two Electron Integral.
- class [ERI_2_2](#)
4-centre ERI of the form $(ab|O(2)|cd)$ where $O(2) = 1/r_{12}$.
- class [ERI_3_1](#)
4-centre ERI of the form $(abc|O(2)|d)$ where $O(2) = 1/r_{12}$.
- class [OEPotential](#)
Generalized One-Electron Potential: Abstract base.
- class [ElectrostaticEnergyOEPotential](#)
Generalized One-Electron Potential for Electrostatic Energy.
- class [RepulsionEnergyOEPotential](#)
Generalized One-Electron Potential for Pauli Repulsion Energy.
- class [ChargeTransferEnergyOEPotential](#)
Generalized One-Electron Potential for Charge-Transfer Interaction Energy.
- class [EETCouplingOEPotential](#)
Generalized One-Electron Potential for EET coupling calculations.
- class [IntegralFactory](#)
Extended [IntegralFactory](#) for computing integrals.
- class [PotentialInt](#)
Computes potential integrals.
- class [DIISManager](#)
DIIS manager.
- class [ESPSolver](#)
Charges from Electrostatic Potential (ESP). A solver-type class.
- class [AllAOShellCombinationsIterator](#)
Loop over all possible ERI shells.
- class [AllAOIntegralsIterator](#)
Loop over all possible ERI within a particular shell.
- class [OEPDevSolver](#)
Solver of properties of molecular aggregates. Abstract base.

- class [ElectrostaticEnergySolver](#)
Compute the Coulombic interaction energy between unperturbed wavefunctions.
- class [RepulsionEnergySolver](#)
Compute the Pauli-Repulsion interaction energy between unperturbed wavefunctions.
- class [ChargeTransferEnergySolver](#)
Compute the Charge-Transfer interaction energy between unperturbed wavefunctions.
- class [Points3DIterator](#)
Iterator over a collection of points in 3D space. Abstract base.
- class [CubePoints3DIterator](#)
Iterator over a collection of points in 3D space. g09 Cube-like order.
- class [RandomPoints3DIterator](#)
Iterator over a collection of points in 3D space. Random collection.
- class [PointsCollection3D](#)
Collection of points in 3D space. Abstract base.
- class [RandomPointsCollection3D](#)
Collection of random points in 3D space.
- class [CubePointsCollection3D](#)
G09 cube-like ordered collection of points in 3D space.
- class [ScalarField3D](#)
Scalar field in 3D space. Abstract base.
- class [ElectrostaticPotential3D](#)
Electrostatic potential of a molecule.
- class [OEPotential3D](#)
Class template for OEP scalar fields.
- class [WavefunctionUnion](#)
Union of two Wavefunction objects.

Typedefs

- using **SharedWavefunction** = std::shared_ptr< Wavefunction >
- using **SharedBasisSet** = std::shared_ptr< BasisSet >
- using **SharedTensor** = std::shared_ptr< Tensor >
- using **SharedMatrix** = std::shared_ptr< Matrix >
- using **SharedVector** = std::shared_ptr< Vector >
- using **SharedScalarField3D** = std::shared_ptr< [ScalarField3D](#) >
- using **SharedIntegralFactory** = std::shared_ptr< [IntegralFactory](#) >
- using **SharedTwoBodyAOInt** = std::shared_ptr< TwoBodyAOInt >
- using **SharedWavefunctionUnion** = std::shared_ptr< [WavefunctionUnion](#) >
- using **SharedOEPotential** = std::shared_ptr< [OEPotential](#) >
- using **SharedMolecule** = std::shared_ptr< Molecule >
- using **SharedSuperFunctional** = std::shared_ptr< SuperFunctional >
- using **SharedMOSpace** = std::shared_ptr< MOSpace >
- using **SharedMOSpaceVector** = std::vector< std::shared_ptr< MOSpace >>
- using **SharedIntegralTransform** = std::shared_ptr< IntegralTransform >
- using **SharedLocalizer** = std::shared_ptr< Localizer >

Functions

- **n_max_am_** (2 *max_am_+1)
- double **d_N_n1_n2** (int N, int n1, int n2, double PA, double PB, double aP)
Compute McMurchie-Davidson-Hermite (MDH) coefficient for binomial expansion.
- void **make_mdh_D2_coeff_explicit_recursion** (int n1, int n2, double aP, double *PA, double *PB, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion by explicit recursion. This function makes the same changes to buffers as `oepdev::make_mdh_D2_coeff`, but implements it through explicit recursion by calls to `oepdev::d_N_n1_n2`. Therefore, it is slightly slower. Here for debugging purposes.
- void **make_mdh_D1_coeff** (int n1, double aPd, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for monomial expansion.
- void **make_mdh_D2_coeff** (int n1, int n2, double aPd, double *PA, double *PB, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion.
- void **make_mdh_D3_coeff** (int n1, int n2, int n3, double aPd, double *PA, double *PB, double *PC, double *buffer)
Compute the McMurchie-Davidson-Hermite coefficients for trinomial expansion.
- void **make_mdh_R_coeff** (int N, int L, int M, double alpha, double a, double b, double c, double *F, double *buffer)
Compute the McMurchie-Davidson R coefficients.
- void **preamble** (void)
Print preamble for module OEPDEV.
- std::shared_ptr< SuperFunctional > **create_superfunctional** (std::string name, Options &options)
Set up DFT functional.
- std::shared_ptr< Molecule > **extract_monomer** (std::shared_ptr< const Molecule > molecule_dimer, int id)
Extract molecule from dimer.
- std::shared_ptr< Wavefunction > **solve_scf** (std::shared_ptr< Molecule > molecule, std::shared_ptr< BasisSet > primary, std::shared_ptr< SuperFunctional > functional, Options &options, std::shared_ptr< PSIO > psio)
Solve RHF-SCF equations for a given molecule in a given basis set.

16.1.1 Detailed Description

OEPDev module namespace. Contains:

16.2 psi Namespace Reference

Psi4 package namespace.

Typedefs

- using **SharedVetor** = std::shared_ptr< Vector >
- using **SharedBasisSet** = std::shared_ptr< BasisSet >
- using **SharedMolecule** = std::shared_ptr< Molecule >
- using **SharedMatrix** = std::shared_ptr< Matrix >
- using **SharedWavefunction** = std::shared_ptr< Wavefunction >

Functions

- int [read_options](#) (std::string name, Options &options)
Options for the OEPDev plugin.
- SharedWavefunction [oepdev](#) (SharedWavefunction ref_wfn, Options &options)
Main routine of the OEPDev plugin.

16.2.1 Detailed Description

Psi4 package namespace. Contains all Psi4 functionalities.

16.2.2 Function Documentation

16.2.2.1 SharedWavefunction psi::oepdev (SharedWavefunction ref_wfn, Options & options)

Main routine of the OEPDev plugin.

Created with intention to test various models of the interaction energy between two molecules, described by the Hartree-Fock-Roothaan-Hall theory or the configuration interaction with singles theory.

In particular, the plugin tests the models of:

1. the Pauli repulsion and CT interaction energy (Project II)
2. the Induction interaction energy (Project III)
3. the excitation energy transfer couplings (Project I)

against benchmarks (exact or reference solutions). The list of implemented models can be found in [Implemented Models](#) .

Parameters

| | |
|----------------|--------------------------------|
| <i>ref_wfn</i> | shared wavefunction of a dimer |
| <i>options</i> | psi::Options object |

Returns

psi::SharedWavefunction (either ref_wfn or wavefunction union)

16.2.2.2 int psi::read_options (std::string name, Options & options)

Options for the OEPDev plugin.

Parameters

| | |
|----------------|-------------------------|
| <i>name</i> | name of driver function |
| <i>options</i> | psi::Options object |

Returns

true

Chapter 17

Class Documentation

17.1 oepdev::AllAOIntegralsIterator Class Reference

Loop over all possible ERI within a particular shell.

```
#include <integrals_iter.h>
```

Public Member Functions

- [AllAOIntegralsIterator](#) (const [AllAOShellCombinationsIterator](#) &shellIter)
Construct by shell iterator (const object)
- [AllAOIntegralsIterator](#) (std::shared_ptr< [AllAOShellCombinationsIterator](#) > shellIter)
Construct by shell iterator (pointed by shared pointer)
- void [first](#) ()
First iteration.
- void [next](#) ()
Next iteration.
- bool [is_done](#) ()
Check status of iterations.
- int [i](#) () const
Grab the current integral i index.
- int [j](#) () const
Grab the current integral j index.
- int [k](#) () const
Grab the current integral k index.
- int [l](#) () const
Grab the current integral l index.
- int [index](#) () const

17.1.1 Detailed Description

Loop over all possible ERI within a particular shell.

Constructed by providing a const reference or shared pointer to an [AllAOShellCombinationsIterator](#) object.

Suggested usage:

See Also

[AllAOShellCombinationsIterator](#)

Examples:

[example_integrals_iter.cc](#).

17.1.2 Constructor & Destructor Documentation

17.1.2.1 `oepdev::AllAOShellCombinationsIterator::AllAOShellCombinationsIterator (const AllAOShellCombinationsIterator & shellIter)`

Construct by shell iterator (const object)

Parameters

| | |
|------------------|-------------------------|
| <i>shellIter</i> | - shell iterator object |
|------------------|-------------------------|

17.1.2.2 `oepdev::AllAOShellCombinationsIterator::AllAOShellCombinationsIterator (std::shared_ptr< AllAOShellCombinationsIterator > shellIter)`

Construct by shell iterator (pointed by shared pointer)

Parameters

| | |
|------------------|-------------------------|
| <i>shellIter</i> | - shell iterator object |
|------------------|-------------------------|

17.1.3 Member Function Documentation

17.1.3.1 `int oepdev::AllAOShellCombinationsIterator::index () const` `[inline]`

Grab the current index of integral value stored in the buffer

Examples:

[example_integrals_iter.cc](#).

The documentation for this class was generated from the following files:

- [oepdev/libutil/integrals_iter.h](#)
- [oepdev/libutil/integrals_iter.cc](#)

17.2 oepdev::AllAOShellCombinationsIterator Class Reference

Loop over all possible ERI shells.

```
#include <integrals_iter.h>
```

Public Member Functions

- [AllAOShellCombinationsIterator](#) (SharedBasisSet [bs_1](#), SharedBasisSet [bs_2](#), SharedBasisSet [bs_3](#), SharedBasisSet [bs_4](#))
Construct by providing basis sets for each axis. The basis sets must be defined for the same molecule.
- [AllAOShellCombinationsIterator](#) (SharedIntegralFactory integrals)
Construct by providing integral factory.

- **AllAOShellCombinationsIterator** (psi::IntegralFactory integrals)
- void **first** ()
First iteration.
- void **next** ()
Next iteration.
- bool **is_done** ()
Check status of iterations.
- int **P** () const
Grab the current shell P index.
- int **Q** () const
Grab the current shell Q index.
- int **R** () const
Grab the current shell R index.
- int **S** () const
Grab the current shell S index.
- SharedBasisSet **bs_1** () const
Grab the basis set of axis 1.
- SharedBasisSet **bs_2** () const
Grab the basis set of axis 2.
- SharedBasisSet **bs_3** () const
Grab the basis set of axis 3.
- SharedBasisSet **bs_4** () const
Grab the basis set of axis 4.
- void **compute_shell** (SharedTwoBodyAOInt tei) const
Compute ERI's for the current shell. The eris are stored in the buffer of the argument object.

17.2.1 Detailed Description

Loop over all possible ERI shells.

Constructed by providing shared pointer to [IntegralFactory](#) object or shared pointers to four basis set spaces.

Suggested usage:

```
SharedIntegralFactory ints = std::make_shared<IntegralFactory>(bs1, bs2, bs3, bs4);
SharedTwoBodyAOInt tei(ints->eri());
AllAOShellCombinationsIterator shellIter(ints);
const double * buffer = tei->buffer();
for (shellIter.first(); shellIter.is_done()==false; shellIter.next())
{
    shellIter.compute_shell(tei);
    AllAOIntegralsIterator intsIter(shellIter);
    for (intsIter.first(); intsIter.is_done()==false; intsIter.next())
    {
        // Grab (ij|kl) integrals and indices here
        int i = intsIter.i();
        int j = intsIter.j();
        int k = intsIter.k();
        int l = intsIter.l();
        double integral = buffer[intsIter.index()];
    }
}
```

Examples:

[example_integrals_iter.cc](#).

17.2.2 Constructor & Destructor Documentation

17.2.2.1 `oepdev::AllAOShellCombinationsIterator::AllAOShellCombinationsIterator (SharedBasisSet bs_1, SharedBasisSet bs_2, SharedBasisSet bs_3, SharedBasisSet bs_4)`

Construct by providing basis sets for each axis. The basis sets must be defined for the same molecule.

Parameters

| | |
|-------------|-----------------------|
| <i>bs_1</i> | - basis set of axis 1 |
| <i>bs_2</i> | - basis set of axis 2 |
| <i>bs_3</i> | - basis set of axis 3 |
| <i>bs_4</i> | - basis set of axis 4 |

17.2.2.2 oepdev::AllAOShellCombinationsIterator::AllAOShellCombinationsIterator (SharedIntegralFactory *integrals*)

Construct by providing integral factory.

Parameters

| | |
|------------------|---------------------------|
| <i>integrals</i> | - integral factory object |
|------------------|---------------------------|

17.2.3 Member Function Documentation

17.2.3.1 void oepdev::AllAOShellCombinationsIterator::compute_shell (SharedTwoBodyAOInt *tei*) const

Compute ERI's for the current shell. The eris are stored in the buffer of the argument object.

Parameters

| | |
|------------|----------------------------|
| <i>tei</i> | - two electron AO integral |
|------------|----------------------------|

Examples:

[example_integrals_iter.cc](#).

The documentation for this class was generated from the following files:

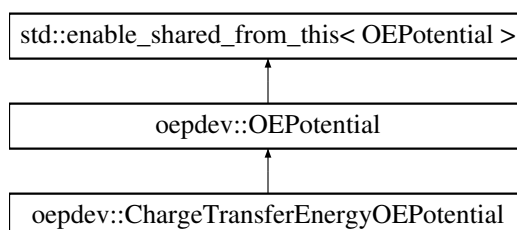
- oepdev/libutil/[integrals_iter.h](#)
- oepdev/libutil/[integrals_iter.cc](#)

17.3 oepdev::ChargeTransferEnergyOEPotential Class Reference

Generalized One-Electron Potential for Charge-Transfer Interaction Energy.

```
#include <oep.h>
```

Inheritance diagram for oepdev::ChargeTransferEnergyOEPotential:



Public Member Functions

- **ChargeTransferEnergyOEPotential** (SharedWavefunction [wfn](#), SharedBasisSet auxiliary, Options &options)
- **ChargeTransferEnergyOEPotential** (SharedWavefunction [wfn](#), Options &options)
- virtual void **compute** (const std::string &oepType) override

- virtual void [compute_3D](#) (const std::string &oepType, const double &x, const double &y, const double &z, double &v) override
- virtual void **print_header** () const override

Additional Inherited Members

17.3.1 Detailed Description

Generalized One-Electron Potential for Charge-Transfer Interaction Energy.

Contains the following OEP types:

- `Otto-Ladik.V1` - DF-based term
- `Otto-Ladik.V2` - ESP-based term
- `Otto-Ladik.V3` - ESP-based term

17.3.2 Member Function Documentation

17.3.2.1 void `ChargeTransferEnergyOEPotential::compute_3D` (const std::string & *oepType*, const double & *x*, const double & *y*, const double & *z*, double & *v*) `[override]`, `[virtual]`

Compute value of potential in point x, y, z and save at v

Implements [oepdev::OEPotential](#).

The documentation for this class was generated from the following files:

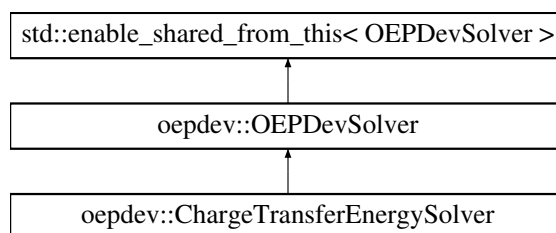
- `oepdev/liboep/oep.h`
- `oepdev/liboep/oep.cc`

17.4 oepdev::ChargeTransferEnergySolver Class Reference

Compute the Charge-Transfer interaction energy between unperturbed wavefunctions.

```
#include <solver.h>
```

Inheritance diagram for `oepdev::ChargeTransferEnergySolver`:



Public Member Functions

- **ChargeTransferEnergySolver** (SharedWavefunctionUnion wfn_union)
- virtual double [compute_oep_based](#) (const std::string &method="DEFAULT")
Compute property by using OEP's.
- virtual double [compute_benchmark](#) (const std::string &method="DEFAULT")
Compute property by using benchmark method.

Additional Inherited Members

17.4.1 Detailed Description

Compute the Charge-Transfer interaction energy between unperturbed wavefunctions.

The implemented methods are shown below

| Keyword | Method Description |
|--------------------------|--|
| Benchmark Methods | |
| OTTO_LADIK | *Default*. CT energy at HF level from Otto and Ladik (1975). |
| EFP2 | CT energy at HF level from EFP2 model. |
| OEP-Based Methods | |
| OTTO_LADIK | *Default*. OEP-based Otto-Ladik expressions. |

Table 17.1: Methods available in the Solver

In order to construct this solver, **always** use the `OEPDevSolver::build` static factory method.

Below the detailed description of the implemented equations is given for each of the above provided methods. In the formulae across, it is assumed that the orbitals are real. The Coulomb notation for electron repulsion integrals (ERI's) is adopted; i.e.,

$$(ac|bd) = \iint d\mathbf{r}_1 d\mathbf{r}_2 \phi_a(\mathbf{r}_1) \phi_c(\mathbf{r}_1) \frac{1}{r_{12}} \phi_b(\mathbf{r}_2) \phi_d(\mathbf{r}_2)$$

Greek subscripts denote basis set orbitals whereas Italic subscripts denote the occupied molecular orbitals.

The CT energy between molecules *A* and *B* is given by

$$E^{\text{CT}} = E^{A^+B^-} + E^{A^-B^+}$$

Benchmark Methods

CT energy at HF level by Otto and Ladik (1975).

For a closed-shell system, CT energy equation of Otto and Ladik becomes

$$E^{A^+B^-} \approx 2 \sum_{i \in A}^{\text{Occ}_A} \sum_{n \in B}^{\text{Vir}_B} \frac{V_{in}^2}{\epsilon_i - \epsilon_n}$$

where

$$V_{in} = V_{in}^B + 2 \sum_{j \in B}^{\text{Occ}_B} (in|jj) - \sum_{k \in A}^{\text{Occ}_A} S_{kn} \left\{ V_{ik}^B + 2 \sum_{j \in B}^{\text{Occ}_B} (ik|jj) \right\} \\ - \sum_{j \in B}^{\text{Occ}_B} \left[S_{ij} \left\{ V_{nj}^A + 2 \sum_{k \in A}^{\text{Occ}_A} (1 - \delta_{ik})(nj|kk) \right\} - (nj|ij) \right] + \sum_{k \in A}^{\text{Occ}_A} \sum_{j \in B}^{\text{Occ}_B} S_{kj} (1 - \delta_{ik})(ik|nj)$$

and analogously the twin term.

CT energy at HF level by EFP2.

In EFP2 method, CT energy is given as

$$E^{A+B-} \approx 2 \sum_{i \in A} \sum_{n \in B}^{\text{Occ}_A \text{Vir}_B} \frac{V_{in}^2}{F_{ii} - T_{nn}}$$

where

$$V_{in}^2 = \frac{V_{in}^B - \sum_{m \in A}^{\text{All}_A} V_{im} S_{mn}^B}{1 - \sum_{m \in A}^{\text{All}_A} S_{mn}^2} \left\{ V_{in}^B - \sum_{m \in A}^{\text{All}_A} V_{im}^B S_{mn} + \sum_{j \in B}^{\text{Occ}_B} S_{ij} \left(T_{nj} - \sum_{m \in A}^{\text{All}_A} S_{nm} T_{mj} \right) \right\}$$

and analogously the twin term.

OEP-Based Methods

OEP-Based Otto-Ladik's theory

After introducing OEP's, the original Otto-Ladik's theory is reformulated *without* approximation as

$$E^{A+B-} \approx 2 \sum_{i \in A} \sum_{n \in B}^{\text{Occ}_A \text{Vir}_B} \frac{\left(V_{in}^{\text{DF}} + V_{in}^{\text{ESP,A}} + V_{in}^{\text{ESP,B}} \right)^2}{\epsilon_i - \epsilon_n}$$

where

$$\begin{aligned} V_{in}^{\text{DF}} &= \sum_{\eta \in B}^{\text{Aux}_B} S_{i\eta} G_{\eta n}^B \\ V_{in}^{\text{ESP,A}} &= \sum_{k \in A}^{\text{Occ}_A} \sum_{j \in B}^{\text{Occ}_B} S_{kj} \sum_{x \in A} V_{nj}^{(x)} q_{ik}^{(x)} \\ V_{in}^{\text{ESP,B}} &= - \sum_{k \in A}^{\text{Occ}_A} S_{kn} V_{ik}^B \end{aligned}$$

The OEP matrix for density fitted part is given by

$$G_{\eta n}^B = \sum_{\eta' \in B}^{\text{Aux}_B} [S^{-1}]_{\eta\eta'} \left\{ V_{\eta'n}^B + \sum_{j \in B}^{\text{Occ}_B} [2(\eta'n|jj) - (\eta'j|nj)] \right\}$$

The OEP ESP-A charges are fit to reproduce the OEP potential

$$v_{ik}^A(\mathbf{r}) \equiv (1 - \delta_{ik}) \int \frac{\phi_i(\mathbf{r}') \phi_k(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - \delta_{ik} \left(\sum_{x \in A} \frac{-Z_x}{|\mathbf{r} - \mathbf{r}_x|} + 2 \sum_{k \in A}^{\text{Occ}_A} \int \frac{\phi_k(\mathbf{r}') \phi_k(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - 2 \int \frac{\phi_i(\mathbf{r}') \phi_i(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \right)$$

so that

$$v_{ik}^A(\mathbf{r}) \cong \sum_{x \in A} \frac{q_{ik}^{(x)}}{|\mathbf{r} - \mathbf{r}_x|}$$

The OEP ESP-B charges are fit to reproduce the electrostatic potential of molecule *B* (they are standard ESP charges).

17.4.2 Member Function Documentation

17.4.2.1 `double ChargeTransferEnergySolver::compute_benchmark (const std::string & method = "DEFAULT")`
`[virtual]`

Compute property by using benchmark method.

Each solver object has one `DEFAULT` benchmark method

Parameters

| | |
|---------------|--------------------|
| <i>method</i> | - benchmark method |
|---------------|--------------------|

Implements [oepdev::OEPDevSolver](#).

```
17.4.2.2 double ChargeTransferEnergySolver::compute_oep_based ( const std::string & method = "DEFAULT" )
           [virtual]
```

Compute property by using OEP's.

Each solver object has one `DEFAULT` OEP-based method.

Parameters

| | |
|---------------|------------------------|
| <i>method</i> | - flavour of OEP model |
|---------------|------------------------|

Implements [oepdev::OEPDevSolver](#).

The documentation for this class was generated from the following files:

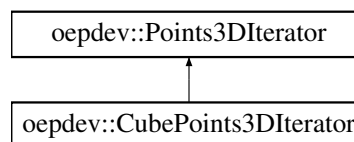
- [oepdev/libutil/solver.h](#)
- [oepdev/libutil/solver.cc](#)

17.5 oepdev::CubePoints3DIterator Class Reference

Iterator over a collection of points in 3D space. g09 Cube-like order.

```
#include <space3d.h>
```

Inheritance diagram for `oepdev::CubePoints3DIterator`:



Public Member Functions

- **CubePoints3DIterator** (const int &nx, const int &ny, const int &nz, const double &dx, const double &dy, const double &dz, const double &ox, const double &oy, const double &oz)
- virtual void [first](#) ()
Initialize first iteration.
- virtual void [next](#) ()
Step to next iteration.

Protected Attributes

- const int **nx_**
- const int **ny_**
- const int **nz_**
- const double **dx_**
- const double **dy_**
- const double **dz_**
- const double **ox_**

- const double **oy_**
- const double **oz_**
- int **ii_**
- int **jj_**
- int **kk_**

Additional Inherited Members

17.5.1 Detailed Description

Iterator over a collection of points in 3D space. g09 Cube-like order.

Note: Always create instances by using static factory method from [Points3DIterator](#). Do not use constructor of this class.

The documentation for this class was generated from the following files:

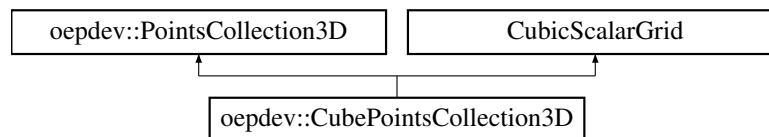
- oepdev/libutil/space3d.h
- oepdev/libutil/space3d.cc

17.6 oepdev::CubePointsCollection3D Class Reference

G09 cube-like ordered collection of points in 3D space.

```
#include <space3d.h>
```

Inheritance diagram for oepdev::CubePointsCollection3D:



Public Member Functions

- **CubePointsCollection3D** ([Collection](#) collectionType, const int &nx, const int &ny, const int &nz, const double &px, const double &py, const double &pz, psi::SharedBasisSet bs, psi::Options &options)
- virtual void [print](#) () const
Print the information to Psi4 output file.
- virtual void **write_cube_file** (psi::SharedMatrix v, const std::string &name)

Additional Inherited Members

17.6.1 Detailed Description

G09 cube-like ordered collection of points in 3D space.

Note: Do not use constructors of this class explicitly. Instead, use static factory methods of the superclass to create instances.

The documentation for this class was generated from the following files:

- oepdev/libutil/space3d.h
- oepdev/libutil/space3d.cc

17.7 oepdev::DIISManager Class Reference

DIIS manager.

```
#include <diis.h>
```

Public Member Functions

- [DIISManager](#) (int dim, int na, int nb)
 - [~DIISManager](#) ()
- Destructor.*
- void [put](#) (const std::shared_ptr< const Matrix > &error, const std::shared_ptr< const Matrix > &vector)
 - void [compute](#) (void)
 - void [update](#) (std::shared_ptr< Matrix > &other)

17.7.1 Detailed Description

DIIS manager.

Instance can interact directly with the process of solving vector quantities in iterative manner. One needs to pass the dimensions of solution vector as well as the DIIS subspace size. The iterative procedure requires providing the current vector and also an estimate of the error vector. The updated DIIS vector can be copied to an old vector through the Instance.

17.7.2 Constructor & Destructor Documentation

17.7.2.1 oepdev::DIISManager::DIISManager (int *dim*, int *na*, int *nb*)

Constructor.

Parameters

| | |
|------------|----------------------------|
| <i>dim</i> | Size of DIIS subspace |
| <i>na</i> | Number of solution rows |
| <i>nb</i> | Number of solution columns |

17.7.3 Member Function Documentation

17.7.3.1 void oepdev::DIISManager::compute (void)

Perform DIIS interpolation.

17.7.3.2 void oepdev::DIISManager::put (const std::shared_ptr< const Matrix > & *error*, const std::shared_ptr< const Matrix > & *vector*)

Put the current solution to the DIIS manager.

Parameters

| | |
|---------------|--|
| <i>error</i> | Shared matrix with current solution error |
| <i>vector</i> | Shared matrix with current solution vector |

17.7.3.3 void oepdev::DIISManager::update (std::shared_ptr< Matrix > & other)

Update solution vector. Pass the Shared pointer to current solution. Then it will be overridden by the updated DIIS solution.

The documentation for this class was generated from the following files:

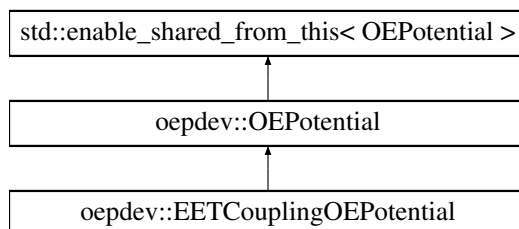
- oepdev/libutil/diis.h
- oepdev/libutil/diis.cc

17.8 oepdev::EETCouplingOEPotential Class Reference

Generalized One-Electron Potential for EET coupling calculations.

```
#include <oep.h>
```

Inheritance diagram for oepdev::EETCouplingOEPotential:



Public Member Functions

- **EETCouplingOEPotential** (SharedWavefunction [wfn](#), SharedBasisSet auxiliary, Options &options)
- **EETCouplingOEPotential** (SharedWavefunction [wfn](#), Options &options)
- virtual void **compute** (const std::string &oepType) override
- virtual void **compute_3D** (const std::string &oepType, const double &x, const double &y, const double &z, double &v) override
- virtual void **print_header** () const override

Additional Inherited Members

17.8.1 Detailed Description

Generalized One-Electron Potential for EET coupling calculations.

Contains the following OEP types:

- Fujimoto.ET1
- Fujimoto.ET2
- Fujimoto.HT1
- Fujimoto.HT1
- Fujimoto.HT2
- Fujimoto.CT1
- Fujimoto.CT2

17.8.2 Member Function Documentation

17.8.2.1 `void EETCouplingOEPotential::compute_3D (const std::string & oepType, const double & x, const double & y, const double & z, double & v) [override], [virtual]`

Compute value of potential in point x, y, z and save at v

Implements [oepdev::OEPotential](#).

The documentation for this class was generated from the following files:

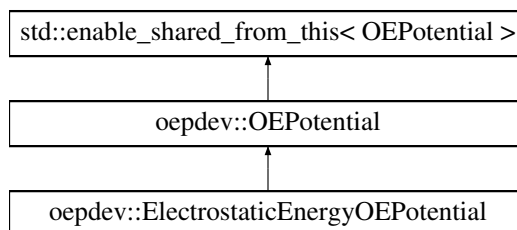
- [oepdev/liboep/oep.h](#)
- [oepdev/liboep/oep.cc](#)

17.9 oepdev::ElectrostaticEnergyOEPotential Class Reference

Generalized One-Electron Potential for Electrostatic Energy.

```
#include <oep.h>
```

Inheritance diagram for oepdev::ElectrostaticEnergyOEPotential:



Public Member Functions

- [ElectrostaticEnergyOEPotential](#) (SharedWavefunction [wfn](#), Options &options)
Only ESP-based potential is worth implementing.
- virtual void **compute** (const std::string &oepType) override
- virtual void **compute_3D** (const std::string &oepType, const double &x, const double &y, const double &z, double &v) override
- virtual void **print_header** () const override

Additional Inherited Members

17.9.1 Detailed Description

Generalized One-Electron Potential for Electrostatic Energy.

Contains the following OEP types:

- v

17.9.2 Member Function Documentation

17.9.2.1 `void ElectrostaticEnergyOEPotential::compute_3D (const std::string & oepType, const double & x, const double & y, const double & z, double & v) [override], [virtual]`

Compute value of potential in point x, y, z and save at v

Implements [oepdev::OEPotential](#).

The documentation for this class was generated from the following files:

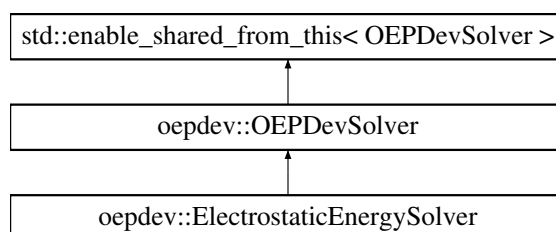
- [oepdev/liboep/oep.h](#)
- [oepdev/liboep/oep.cc](#)

17.10 oepdev::ElectrostaticEnergySolver Class Reference

Compute the Coulombic interaction energy between unperturbed wavefunctions.

```
#include <solver.h>
```

Inheritance diagram for oepdev::ElectrostaticEnergySolver:



Public Member Functions

- **ElectrostaticEnergySolver** (SharedWavefunctionUnion wfn_union)
- virtual double [compute_oep_based](#) (const std::string &method="DEFAULT")
Compute property by using OEP's.
- virtual double [compute_benchmark](#) (const std::string &method="DEFAULT")
Compute property by using benchmark method.

Additional Inherited Members

17.10.1 Detailed Description

Compute the Coulombic interaction energy between unperturbed wavefunctions.

The implemented methods are shown in below

Below the detailed description of the above methods is given.

Benchmark Methods

Exact Coulombic energy from atomic orbital expansions.

The Coulombic interaction energy is given by

$$E^{\text{Coul}} = E^{\text{Nuc-Nuc}} + E^{\text{Nuc-El}} + E^{\text{El-El}}$$

where the nuclear-nuclear repulsion energy is

$$E^{\text{Nuc-Nuc}} = \sum_{x \in A} \sum_{y \in B} \frac{Z_x Z_y}{|\mathbf{r}_x - \mathbf{r}_y|}$$

| Keyword | Method Description |
|--------------------------|--|
| Benchmark Methods | |
| AO_EXPANDED | *Default*. Exact Coulombic energy from atomic orbital expansions. |
| MO_EXPANDED | Exact Coulombic energy from molecular orbital expansions |
| OEP-Based Methods | |
| ESP_SYMMETRIZED | *Default*. Coulombic energy from ESP charges interacting with nuclei and electronic density. Symmetrized with respect to monomers. |

Table 17.2: Methods available in the Solver

the nuclear-electronic attraction energy is

$$E^{\text{Nuc-EI}} = \sum_{x \in A} \sum_{\lambda \sigma \in B} Z_x V_{\lambda \sigma}^{(x)} \left(D_{\lambda \sigma}^{(\alpha)} + D_{\lambda \sigma}^{(\beta)} \right) + \sum_{y \in B} \sum_{\mu \nu \in A} Z_y V_{\mu \nu}^{(y)} \left(D_{\mu \nu}^{(\alpha)} + D_{\mu \nu}^{(\beta)} \right)$$

and the electron-electron repulsion energy is

$$E^{\text{EI-EI}} = \sum_{\mu \nu \in A} \sum_{\lambda \sigma \in B} \left\{ D_{\mu \nu}^{(\alpha)} + D_{\mu \nu}^{(\beta)} \right\} \left\{ D_{\lambda \sigma}^{(\alpha)} + D_{\lambda \sigma}^{(\beta)} \right\} (\mu \nu | \lambda \sigma)$$

In the above equations,

$$V_{\lambda \sigma}^{(x)} \equiv \int \frac{\varphi_{\lambda}^*(\mathbf{r}) \varphi_{\sigma}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}_x|} d\mathbf{r}$$

Exact Coulombic energy from molecular orbital expansion.

This approach is fully equivalent to the atomic orbital expansion shown above. For the closed shell case, the Coulombic interaction energy is given by

$$E^{\text{Coul}} = E^{\text{Nuc-Nuc}} + E^{\text{Nuc-EI}} + E^{\text{EI-EI}}$$

where the nuclear-nuclear repulsion energy is

$$E^{\text{Nuc-Nuc}} = \sum_{x \in A} \sum_{y \in B} \frac{Z_x Z_y}{|\mathbf{r}_x - \mathbf{r}_y|}$$

the nuclear-electronic attraction energy is

$$E^{\text{Nuc-EI}} = 2 \sum_{i \in A} \sum_{y \in B} V_{ii}^{(y)} + 2 \sum_{j \in B} \sum_{x \in A} V_{jj}^{(x)}$$

and the electron-electron repulsion energy is

$$E^{\text{EI-EI}} = 4 \sum_{i \in A} \sum_{j \in B} (ii | jj)$$

OEP-Based Methods

Coulombic energy from ESP charges interacting with nuclei and electronic density.

In this approach, nuclear and electronic density of either species is approximated by ESP charges. In order to achieve symmetric expression, the interaction is computed twice (ESP of A interacting with density matrix and

nuclear charges of B and vice versa) and then divided by 2. Thus,

$$E^{\text{Coul}} \approx \frac{1}{2} \left[\sum_{x \in A} \sum_{y \in B} \frac{Z_x q_y}{|\mathbf{r}_x - \mathbf{r}_y|} + \sum_{y \in B} \sum_{\mu \nu \in A} q_y V_{\mu \nu}^{(y)} \left(D_{\mu \nu}^{(\alpha)} + D_{\mu \nu}^{(\beta)} \right) + \sum_{y \in B} \sum_{x \in A} \frac{q_x Z_y}{|\mathbf{r}_x - \mathbf{r}_y|} + \sum_{x \in A} \sum_{\lambda \sigma \in B} Z_x V_{\lambda \sigma}^{(x)} \left(D_{\lambda \sigma}^{(\alpha)} + D_{\lambda \sigma}^{(\beta)} \right) \right]$$

If the basis set is large and the number of ESP centres $q_{x(y)}$ is sufficient, the sum of first two contributions equals the sum of the latter two contributions.

Notes:

- This solver also computes and prints the ESP-ESP point charge interaction energy,

$$E^{\text{Coul,ESP}} \approx \sum_{x \in A} \sum_{y \in B} \frac{q_x q_y}{|\mathbf{r}_x - \mathbf{r}_y|}$$

for reference purposes.

- In order to construct this solver, **always** use the `OEPDevSolver::build` static factory method.

17.10.2 Member Function Documentation

17.10.2.1 `double ElectrostaticEnergySolver::compute_benchmark (const std::string & method = "DEFAULT")`
[virtual]

Compute property by using benchmark method.

Each solver object has one `DEFAULT` benchmark method

Parameters

| | |
|---------------|--------------------|
| <i>method</i> | - benchmark method |
|---------------|--------------------|

Implements [oepdev::OEPDevSolver](#).

17.10.2.2 `double ElectrostaticEnergySolver::compute_oep_based (const std::string & method = "DEFAULT")`
[virtual]

Compute property by using OEP's.

Each solver object has one `DEFAULT` OEP-based method.

Parameters

| | |
|---------------|------------------------|
| <i>method</i> | - flavour of OEP model |
|---------------|------------------------|

Implements [oepdev::OEPDevSolver](#).

The documentation for this class was generated from the following files:

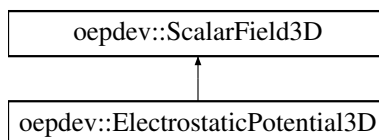
- [oepdev/libutil/solver.h](#)
- [oepdev/libutil/solver.cc](#)

17.11 oepdev::ElectrostaticPotential3D Class Reference

Electrostatic potential of a molecule.

```
#include <space3d.h>
```

Inheritance diagram for `oepdev::ElectrostaticPotential3D`:



Public Member Functions

- **ElectrostaticPotential3D** (const int &np, const double &padding, psi::SharedWavefunction [wfn](#), psi::Options &options)
- **ElectrostaticPotential3D** (const int &nx, const int &ny, const int &nz, const double &px, const double &py, const double &pz, psi::SharedWavefunction [wfn](#), psi::Options &options)
- virtual double [compute_xyz](#) (const double &x, const double &y, const double &z)
Compute a value of scalar field at point (x, y, z)
- virtual void [print](#) () const
Print information of the object to Psi4 output.

Additional Inherited Members

17.11.1 Detailed Description

Electrostatic potential of a molecule.

Computes the electrostatic potential of a molecule directly from the wavefunction. The electrostatic potential $v(\mathbf{r})$ at point \mathbf{r} is computed from the following formula:

$$v(\mathbf{r}) = v_{\text{nuc}}(\mathbf{r}) + v_{\text{el}}(\mathbf{r})$$

where the nuclear and electronic contributions are defined accordingly as

$$v_{\text{nuc}}(\mathbf{r}) = \sum_x \frac{Z_x}{|\mathbf{r} - \mathbf{r}_x|}$$

$$v_{\text{el}}(\mathbf{r}) = \sum_{\mu\nu} \left\{ D_{\mu\nu}^{(\alpha)} + D_{\mu\nu}^{(\beta)} \right\} V_{\nu\mu}(\mathbf{r})$$

In the above equations, Z_x denotes the charge of x th nucleus, $D_{\mu\nu}^{(\omega)}$ is the one-particle (relaxed) density matrix element in AO basis associated with the ω electron spin, and $V_{\nu\mu}(\mathbf{r})$ is the potential one-electron integral defined by

$$V_{\nu\mu}(\mathbf{r}) \equiv \int d\mathbf{r}' \phi_{\nu}^*(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \phi_{\mu}(\mathbf{r}')$$

The documentation for this class was generated from the following files:

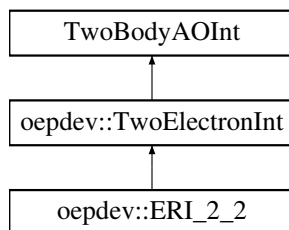
- oepdev/libutil/space3d.h
- oepdev/libutil/space3d.cc

17.12 oepdev::ERI_2_2 Class Reference

4-centre ERI of the form (ab|O(2)|cd) where O(2) = 1/r¹².

```
#include <eri.h>
```

Inheritance diagram for oepdev::ERI_2_2:



Public Member Functions

- [ERI_2_2](#) (const [IntegralFactory](#) *integral, int deriv=0, bool use_shell_pairs=false)
Constructor. Use [oepdev::IntegralFactory](#) to generate this object.
- [~ERI_2_2](#) ()
Destructor.

Protected Member Functions

- `size_t` [compute_quartet](#) (int, int, int, int)
Compute ERI's between 4 shells.

Protected Attributes

- double * [mdh_buffer_12_](#)
Buffer for McMurchie-Davidson-Hermite coefficients for binomial expansion (shells 1 and 2)
- double * [mdh_buffer_34_](#)
Buffer for McMurchie-Davidson-Hermite coefficients for binomial expansion (shells 3 and 4)

17.12.1 Detailed Description

4-centre ERI of the form $(ab|O(2)|cd)$ where $O(2) = 1/r_{12}$.

ERI's are computed for a shell quartet (PQ|RS) and stored in the `target_full_` buffer, accessible through `buffer()` method:

For each $(n_1, l_1, m_1) \in P$:
 For each $(n_2, l_2, m_2) \in Q$:
 For each $(n_3, l_3, m_3) \in R$:
 For each $(n_4, l_4, m_4) \in S$:
 $ERI = (AB|CD)[\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}]$

For detailed description of the McMurchie-Davidson scheme, refer to [The Integral Package Library](#).

17.12.2 Implementation

A set of ERI's in a shell is decontracted as

$$(AB|CD)[\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}] = \sum_{ijkl} c_i(\alpha_1) c_j(\alpha_2) c_k(\alpha_3) c_l(\alpha_4) (ij|kl)[\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}]$$

where the primitive ERI is given by

$$(ij|kl)[\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}] = E_{ij}(\alpha_1, \alpha_2) E_{kl}(\alpha_3, \alpha_4) \\ \times \sum_{N_1=0}^{n_1+n_2} \sum_{L_1=0}^{l_1+l_2} \sum_{M_1=0}^{m_1+m_2} \sum_{N_2=0}^{n_3+n_4} \sum_{L_2=0}^{l_3+l_4} \sum_{M_2=0}^{m_3+m_4} d_{N_1}^{n_1 n_2} d_{L_1}^{l_1 l_2} d_{M_1}^{m_1 m_2} d_{N_2}^{n_3 n_4} d_{L_2}^{l_3 l_4} d_{M_2}^{m_3 m_4} [N_1 L_1 M_1 | N_2 L_2 M_2]$$

In the above equation, the multiplicative constants are given as

$$E_{ij}(\alpha_1, \alpha_2) = \exp \left[-\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} |\mathbf{A} - \mathbf{B}|^2 \right] \\ E_{kl}(\alpha_3, \alpha_4) = \exp \left[-\frac{\alpha_3 \alpha_4}{\alpha_3 + \alpha_4} |\mathbf{C} - \mathbf{D}|^2 \right]$$

The documentation for this class was generated from the following files:

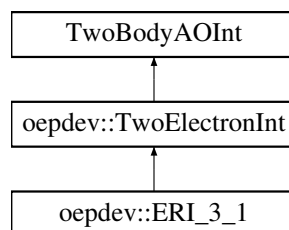
- oepdev/libints/eri.h
- oepdev/libints/eri.cc

17.13 oepdev::ERI_3_1 Class Reference

4-centre ERI of the form (abc|O(2)|d) where O(2) = 1/r¹².

```
#include <eri.h>
```

Inheritance diagram for oepdev::ERI_3_1:



Public Member Functions

- [ERI_3_1](#) (const [IntegralFactory](#) *integral, int deriv=0, bool use_shell_pairs=false)
Constructor. Use [oepdev::IntegralFactory](#) to generate this object.
- [~ERI_3_1](#) ()
Destructor.

Protected Member Functions

- `size_t` [compute_quartet](#) (int, int, int, int)
Compute ERI's between 4 shells.

Protected Attributes

- `double *` [mdh_buffer_123_](#)
Buffer for McMurchie-Davidson-Hermite coefficients for trinomial expansion (shells 1, 2 and 3)
- `double *` [mdh_buffer_4_](#)
Buffer for McMurchie-Davidson-Hermite coefficients for monomial expansion (shell 4)

17.13.1 Detailed Description

4-centre ERI of the form $(abc|O(2)|d)$ where $O(2) = 1/r12$.

ERI's are computed for a shell quartet $(PQR|S)$ and stored in the `target_full_` buffer, accessible through `buffer()` method:

For each $(n_1, l_1, m_1) \in P$:
 For each $(n_2, l_2, m_2) \in Q$:
 For each $(n_3, l_3, m_3) \in R$:
 For each $(n_4, l_4, m_4) \in S$:
 ERI = $(ABC|D)[\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}]$

For detailed description of the McMurchie-Davidson scheme, refer to [The Integral Package Library](#).

17.13.2 Implementation

A set of ERI's in a shell is decontracted as

$$(ABC|D)[\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}] = \sum_{ijkl} c_i(\alpha_1) c_j(\alpha_2) c_k(\alpha_3) c_l(\alpha_4) (ijk|l) [\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}]$$

where the primitive ERI is given by

$$(ijk|l) [\{\alpha\}, \mathbf{n}, \mathbf{l}, \mathbf{m}] = E_{ijk}(\alpha_1, \alpha_2, \alpha_3) \times \sum_{N_1=0}^{n_1+n_2+n_3} \sum_{L_1=0}^{l_1+l_2+l_3} \sum_{M_1=0}^{m_1+m_2+m_3} \sum_{N_2=0}^{n_4} \sum_{L_2=0}^{l_4} \sum_{M_2=0}^{m_4} d_{N_1}^{n_1 n_2 n_3} d_{L_1}^{l_1 l_2 l_3} d_{M_1}^{m_1 m_2 m_3} d_{N_2}^{n_4} d_{L_2}^{l_4} d_{M_2}^{m_4} [N_1 L_1 M_1 | N_2 L_2 M_2]$$

In the above equation, the multiplicative constants are given as

$$E_{ijk}(\alpha_1, \alpha_2, \alpha_3) = \exp \left[-\frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} |\mathbf{A} - \mathbf{B}|^2 \right] \exp \left[-\frac{(\alpha_1 + \alpha_2) \alpha_3}{\alpha_1 + \alpha_2 + \alpha_3} |\mathbf{P} - \mathbf{C}|^2 \right]$$

The documentation for this class was generated from the following files:

- [oepdev/libints/eri.h](#)
- [oepdev/libints/eri.cc](#)

17.14 oepdev::ESPSolver Class Reference

Charges from Electrostatic Potential (ESP). A solver-type class.

```
#include <esp.h>
```

Public Member Functions

- [ESPSolver](#) (SharedScalarField3D field)
Construct from scalar field.
- [ESPSolver](#) (SharedScalarField3D field, psi::SharedMatrix [centres](#))
Construct from scalar field.
- virtual [~ESPSolver](#) ()
Destructor.
- virtual psi::SharedVector [charges](#) () const
Get the (fit) charges.
- virtual psi::SharedMatrix [centres](#) () const
Get the charge distribution centres.
- virtual void [compute](#) ()
Perform fitting of effective charges.

Protected Attributes

- const int `nCentres_`
Number of fit centres.
- SharedScalarField3D `field_`
Scalar field.
- psi::SharedVector `charges_`
Charges to be fit.
- psi::SharedMatrix `centres_`
Centres, at which fit charges will reside.

17.14.1 Detailed Description

Charges from Electrostatic Potential (ESP). A solver-type class.

Solves the least-squares problem to fit the generalized charges q_m , that reproduce the reference generalized potential $v^{\text{ref}}(\mathbf{r})$ supplied by the `ScalarField3D` object:

$$\int d\mathbf{r}' \left[v^{\text{ref}}(\mathbf{r}') - \sum_m \frac{q_m}{|\mathbf{r}' - \mathbf{r}_m|} \right]^2 \rightarrow \text{minimize}$$

The charges are subject to the following constraint:

$$\sum_m q_m = 0$$

Method description.

M generalized charges is found by solving the matrix equation

$$\begin{pmatrix} \mathbf{A} & 0 \\ 0 & 1 \end{pmatrix}^{-1} \cdot \begin{pmatrix} \mathbf{b} \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{q} \\ \lambda \end{pmatrix}$$

where the \mathbf{A} matrix of dimension $M \times M$ and \mathbf{b} vector of length M are given as

$$A_{mn} = \sum_i \frac{1}{r_{im} r_{in}}$$

$$b_m = \sum_i \frac{v^{\text{ref}}(\mathbf{r}_m)}{r_{im}}$$

In the above equation, summations run over all sample points, at which reference potential is known.

17.14.2 Constructor & Destructor Documentation

17.14.2.1 oepdev::ESPSolver::ESPSolver (SharedScalarField3D *field*)

Construct from scalar field.

Assume that the centres are on atoms associated with the scalar field.

Parameters

| | |
|--------------|------------------------------|
| <i>field</i> | - oepdev scalar field object |
|--------------|------------------------------|

17.14.2.2 oepdev::ESPSolver::ESPSolver (SharedScalarField3D *field*, psi::SharedMatrix *centres*)

Construct from scalar field.

Solve ESP equations for a custom set of charge distribution centres.

Parameters

| | |
|----------------|--|
| <i>field</i> | - oepdev scalar field object |
| <i>centres</i> | - matrix with coordinates of charge distribution centres |

The documentation for this class was generated from the following files:

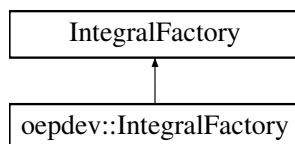
- oepdev/libutil/[esp.h](#)
- oepdev/libutil/[esp.cc](#)

17.15 oepdev::IntegralFactory Class Reference

Extended [IntegralFactory](#) for computing integrals.

```
#include <integral.h>
```

Inheritance diagram for oepdev::IntegralFactory:



Public Member Functions

- [IntegralFactory](#) (std::shared_ptr< psi::BasisSet > bs1, std::shared_ptr< psi::BasisSet > bs2, std::shared_ptr< psi::BasisSet > bs3, std::shared_ptr< psi::BasisSet > bs4)
Initialize integral factory given a BasisSet for each center. Becomes (bs1 bs2 | bs3 bs4).
- [IntegralFactory](#) (std::shared_ptr< psi::BasisSet > bs1, std::shared_ptr< psi::BasisSet > bs2)
Initialize integral factory given a BasisSet for two centres. Becomes (bs1 bs2 | bs1 bs2).
- [IntegralFactory](#) (std::shared_ptr< psi::BasisSet > bs1)
Initialize integral factory given a BasisSet for two centres. Becomes (bs1 bs1 | bs1 bs1).
- virtual [~IntegralFactory](#) ()
Destructor.
- virtual psi::TwoBodyAOInt * [eri_1_1](#) (int deriv=0, bool use_shell_pairs=false)
Returns an ERI_1_1 integral object.
- virtual psi::TwoBodyAOInt * [eri_2_1](#) (int deriv=0, bool use_shell_pairs=false)
Returns an ERI_2_1 integral object.
- virtual psi::TwoBodyAOInt * [eri_2_2](#) (int deriv=0, bool use_shell_pairs=false)
Returns an ERI_2_2 integral object.
- virtual psi::TwoBodyAOInt * [eri_3_1](#) (int deriv=0, bool use_shell_pairs=false)
Returns an ERI_3_1 integral object.

17.15.1 Detailed Description

Extended [IntegralFactory](#) for computing integrals.

In addition to integrals available in Psi4, [oepdev::IntegralFactory](#) enables to compute also:

- OEI's:
 - none at that moment
- ERI's:

- integrals of type (a|b) - `oepdev::ERI_1_1`
- integrals of type (ab|c) - `oepdev::ERI_2_1`
- integrals of type (abc|d) - `oepdev::ERI_3_1`
- integrals of type (ab|cd) - `oepdev::ERI_2_2` (also in Psi4 as `psi::ERI`)

The documentation for this class was generated from the following files:

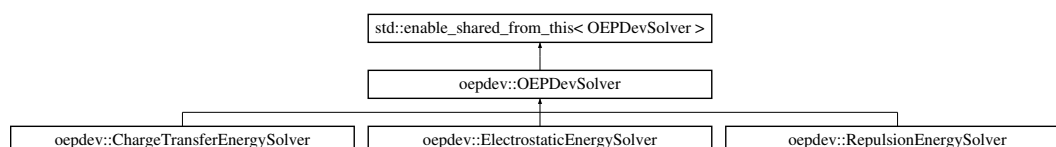
- `oepdev/libpsi/integral.h`
- `oepdev/libpsi/integral.cc`

17.16 oepdev::OEPDevSolver Class Reference

Solver of properties of molecular aggregates. Abstract base.

```
#include <solver.h>
```

Inheritance diagram for `oepdev::OEPDevSolver`:



Public Member Functions

- `OEPDevSolver` (SharedWavefunctionUnion wfn_union)
Take wavefunction union and initialize the Solver.
- virtual `~OEPDevSolver` ()
Destructor.
- virtual double `compute_oe_based` (const std::string &method="DEFAULT")=0
Compute property by using OEP's.
- virtual double `compute_benchmark` (const std::string &method="DEFAULT")=0
Compute property by using benchmark method.

Static Public Member Functions

- static std::shared_ptr
 < `OEPDevSolver` > `build` (const std::string &target, SharedWavefunctionUnion wfn_union)
Build a solver of a particular property for given molecular cluster.

Protected Attributes

- SharedWavefunctionUnion `wfn_union_`
Wavefunction union.
- std::vector< std::string > `methods_oeBased_`
Names of all OEP-based methods implemented for a solver.
- std::vector< std::string > `methods_benchmark_`
Names of all benchmark methods implemented for a solver.

17.16.1 Detailed Description

Solver of properties of molecular aggregates. Abstract base.

Uses only a wavefunction union object to initialize. Available solvers:

- ELECTROSTATIC ENERGY
- REPULSION ENERGY
- CHARGE TRANSFER ENERGY

17.16.2 Constructor & Destructor Documentation

17.16.2.1 OEPDevSolver::OEPDevSolver (SharedWavefunctionUnion *wfn_union*)

Take wavefunction union and initialize the Solver.

Parameters

| | |
|------------------|--|
| <i>wfn_union</i> | - wavefunction union of isolated molecular wavefunctions |
|------------------|--|

17.16.3 Member Function Documentation

17.16.3.1 std::shared_ptr< OEPDevSolver > OEPDevSolver::build (const std::string & *target*, SharedWavefunctionUnion *wfn_union*) [static]

Build a solver of a particular property for given molecular cluster.

Parameters

| | |
|------------------|--|
| <i>target</i> | - target property |
| <i>wfn_union</i> | - wavefunction union of isolated molecular wavefunctions |

Implemented target properties:

- ELECTROSTATIC_ENERGY - Coulombic interaction energy between unperturbed wavefunctions.
- REPULSION_ENERGY - Pauli repulsion interaction energy between unperturbed wavefunctions.

See Also

[ElectrostaticEnergySolver](#)

17.16.3.2 double OEPDevSolver::compute_benchmark (const std::string & *method* = "DEFAULT") [pure virtual]

Compute property by using benchmark method.

Each solver object has one DEFAULT benchmark method

Parameters

| | |
|---------------|--------------------|
| <i>method</i> | - benchmark method |
|---------------|--------------------|

Implemented in [oepdev::ChargeTransferEnergySolver](#), [oepdev::RepulsionEnergySolver](#), and [oepdev::ElectrostaticEnergySolver](#).

17.16.3.3 `double OEPDevSolver::compute_oep_based (const std::string & method = "DEFAULT") [pure virtual]`

Compute property by using OEP's.

Each solver object has one `DEFAULT` OEP-based method.

Parameters

| | |
|---------------|------------------------|
| <i>method</i> | - flavour of OEP model |
|---------------|------------------------|

Implemented in [oepdev::ChargeTransferEnergySolver](#), [oepdev::RepulsionEnergySolver](#), and [oepdev::ElectrostaticEnergySolver](#).

The documentation for this class was generated from the following files:

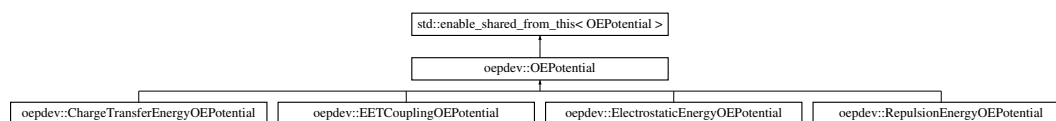
- [oepdev/libutil/solver.h](#)
- [oepdev/libutil/solver.cc](#)

17.17 oepdev::OEPotential Class Reference

Generalized One-Electron Potential: Abstract base.

```
#include <oep.h>
```

Inheritance diagram for `oepdev::OEPotential`:



Public Member Functions

- [OEPotential](#) (SharedWavefunction [wfn](#), Options &options)
ESP-based OEP object.
- [OEPotential](#) (SharedWavefunction [wfn](#), SharedBasisSet auxiliary, Options &options)
DF-based OEP object.
- virtual [~OEPotential](#) ()
Destructor.
- virtual void [rotate](#) (const Matrix &rotmat)
Rotate.
- virtual void [translate](#) (const Vector &trans)
Translate.
- virtual void [superimpose](#) (const Matrix &refGeometry, const std::vector< int > &supList, const std::vector< int > &reordList)
Superimpose.
- std::string [name](#) () const
Retrieve name of this OEP.
- SharedMatrix [matrix](#) (const std::string &oepType) const
Retrieve matrix potential.
- SharedWavefunction [wfn](#) () const
Retrieve wavefunction object.
- void [set_name](#) (const std::string &name)
- virtual void [print_header](#) () const =0

- virtual void **compute** (const std::string &oeptype)=0
- virtual void **compute** (void)
- virtual void **write_cube** (const std::string &oeptype, const std::string &fileName)
- virtual void **compute_3D** (const std::string &oeptype, const double &x, const double &y, const double &z, double &v)=0

Static Public Member Functions

- static std::shared_ptr
< [OEPotential](#) > **build** (const std::string &category, SharedWavefunction [wfn](#), Options &options)
Build ESP-based OEP object.
- static std::shared_ptr
< [OEPotential](#) > **build** (const std::string &category, SharedWavefunction [wfn](#), SharedBasisSet auxiliary, Options &options)
Build DF-based OEP object.

Public Attributes

- const bool [is_density_fitted](#)
Is this OEP density-fitted?
- const bool [is_esp_based](#)
Is this OEP ESP-based?

Protected Attributes

- Options [options_](#)
Psi4 options.
- SharedWavefunction [wfn_](#)
Wavefunction.
- SharedBasisSet [primary_](#)
Primary Basis set.
- SharedBasisSet [auxiliary_](#)
Auxiliary Basis set.
- std::string [name_](#)
Name of this OEP.
- std::vector< std::string > [oeptypes_](#)
Types of OEP's within the scope of this object.
- std::map< std::string, SharedMatrix > [oepmatrices_](#)
OEP's matrix forms for each OEP type.
- std::shared_ptr
< psi::IntegralFactory > [intsfactory_](#)
Integral factory.
- std::shared_ptr< psi::Matrix > [potmat_](#)
Matrix of potential one-electron integrals.
- std::shared_ptr
< psi::OneBodyAOInt > [OEInt_](#)
One-electron integral shared pointer.
- std::shared_ptr< [PotentialInt](#) > [potInt_](#)
One-electron potential shared pointer.

17.17.1 Detailed Description

Generalized One-Electron Potential: Abstract base.

Manages OEP's in matrix and 3D forms. Available OEP categories:

- ELECTROSTATIC ENERGY
- REPULSION ENERGY
- CHARGE TRANSFER ENERGY
- EET COUPLING CONSTANT

17.17.2 Constructor & Destructor Documentation

17.17.2.1 OEPotential::OEPotential (SharedWavefunction *wfn*, Options & *options*)

ESP-based OEP object.

Parameters

| | |
|----------------|----------------|
| <i>wfn</i> | - wavefunction |
| <i>options</i> | - Psi4 options |

17.17.2.2 OEPotential::OEPotential (SharedWavefunction *wfn*, SharedBasisSet *auxiliary*, Options & *options*)

DF-based OEP object.

Parameters

| | |
|------------------|--|
| <i>wfn</i> | - wavefunction |
| <i>auxiliary</i> | - basis set for density fitting of OEP's |
| <i>options</i> | - Psi4 options |

17.17.3 Member Function Documentation

17.17.3.1 std::shared_ptr< OEPotential > OEPotential::build (const std::string & *category*, SharedWavefunction *wfn*, Options & *options*) [static]

Build ESP-based OEP object.

Parameters

| | |
|----------------|----------------|
| <i>type</i> | - OEP category |
| <i>wfn</i> | - wavefunction |
| <i>options</i> | - Psi4 options |

17.17.3.2 std::shared_ptr< OEPotential > OEPotential::build (const std::string & *category*, SharedWavefunction *wfn*, SharedBasisSet *auxiliary*, Options & *options*) [static]

Build DF-based OEP object.

Parameters

| | |
|------------------|--|
| <i>type</i> | - OEP category |
| <i>wfn</i> | - wavefunction |
| <i>auxiliary</i> | - basis set for density fitting of OEP's |
| <i>options</i> | - Psi4 options |

17.17.3.3 `void OEPotential::compute_3D (const std::string & oepType, const double & x, const double & y, const double & z, double & v)` `[pure virtual]`

Compute value of potential in point x, y, z and save at v

Implemented in [oepdev::EETCouplingOEPotential](#), [oepdev::ChargeTransferEnergyOEPotential](#), [oepdev::RepulsionEnergyOEPotential](#), and [oepdev::ElectrostaticEnergyOEPotential](#).

17.17.3.4 `void OEPotential::write_cube (const std::string & oepType, const std::string & fileName)` `[virtual]`

Write potential to a cube file

The documentation for this class was generated from the following files:

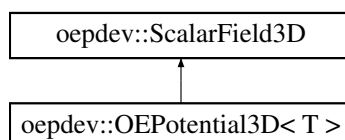
- [oepdev/liboep/oep.h](#)
- [oepdev/liboep/oep.cc](#)

17.18 oepdev::OEPotential3D< T > Class Template Reference

Class template for OEP scalar fields.

```
#include <space3d.h>
```

Inheritance diagram for `oepdev::OEPotential3D< T >`:



Public Member Functions

- [OEPotential3D](#) (const int &np, const double &padding, std::shared_ptr< T > oep, const std::string &oepType)
Construct random spherical collection of scalar field of type T.
- [OEPotential3D](#) (const int &nx, const int &ny, const int &nz, const double &px, const double &py, const double &pz, std::shared_ptr< T > oep, const std::string &oepType, psi::Options &options)
Construct ordered 3D collection of scalar field of type T.
- virtual [~OEPotential3D](#) ()
Destructor.
- virtual double [compute_xyz](#) (const double &x, const double &y, const double &z)
Compute a value of scalar field at point (x, y, z)
- virtual void [print](#) () const
Print information of the object to Psi4 output.

Protected Attributes

- `std::shared_ptr< T > oep_`
Shared pointer to the instance of class T
- `std::string oepType_`
Descriptor of the scalar field type stored in instance of T

Additional Inherited Members

17.18.1 Detailed Description

`template<class T>class oepdev::OEPotential3D< T >`

Class template for OEP scalar fields.

Used for special type of classes T that contain following public member functions:

```
class T : public std::enable_shared_from_this<T> {
public:
    void compute_3D(const std::string& descriptor,
                  const double& x, const double& y, const double& z,
                  double& v);

    shared_ptr<psi::Wavefunction> wfn() const {return wfn_;}
};
```

with the `descriptor` of a certain scalar field type, `x`, `y`, `z` the points in 3D space in which the scalar field has to be computed and stored at `v`. Instances of T should store shared pointer to wavefunction object. List of classes T that are compatible with this class template and are currently implemented in oepdev is given below:

- `oepdev::OEPotential` abstract base (do not use derived classes as T)

Template parameters:

Template Parameters

| | |
|----------------|---|
| <code>T</code> | the compatible class (e.g. <code>oepdev::OEPotential</code>) |
|----------------|---|

The documentation for this class was generated from the following file:

- `oepdev/libutil/space3d.h`

17.19 oepdev::Points3DIterator::Point Struct Reference

Public Attributes

- double `x`
- double `y`
- double `z`
- int `index`

The documentation for this struct was generated from the following file:

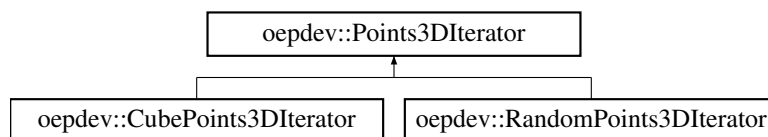
- `oepdev/libutil/space3d.h`

17.20 oepdev::Points3DIterator Class Reference

Iterator over a collection of points in 3D space. Abstract base.

```
#include <space3d.h>
```

Inheritance diagram for oepdev::Points3DIterator:



Classes

- struct [Point](#)

Public Member Functions

- [Points3DIterator](#) (const int &np)
Plain constructor. Initializes the abstract features.
- virtual [~Points3DIterator](#) ()
Destructor.
- virtual bool [is_done](#) ()
Check if iteration is finished.
- virtual void [first](#) ()=0
Initialize first iteration.
- virtual void [next](#) ()=0
Step to next iteration.
- virtual double [x](#) () const
- virtual double [y](#) () const
- virtual double [z](#) () const
- virtual int [index](#) () const

Static Public Member Functions

- static shared_ptr
< [Points3DIterator](#) > [build](#) (const int &nx, const int &ny, const int &nz, const double &dx, const double &dy, const double &dz, const double &ox, const double &oy, const double &oz)
Build G09 Cube collection iterator.
- static shared_ptr
< [Points3DIterator](#) > [build](#) (const int &np, const double &radius, const double &cx, const double &cy, const double &cz)
Build random collection iterator.
- static shared_ptr
< [Points3DIterator](#) > [build](#) (const int &np, const double &pad, psi::SharedMolecule mol)
Build random collection iterator.

Protected Attributes

- const int `np_`
Number of points.
- bool `done_`
Status of the iterator.
- int `index_`
Current index.
- `Point` `current_`

17.20.1 Detailed Description

Iterator over a collection of points in 3D space. Abstract base.

Points3DIterators are constructed either as iterators over:

- a random collections or
- an ordered (g09 cube-like) collections. **Note:** Always create instances by using static factory methods.

17.20.2 Constructor & Destructor Documentation

17.20.2.1 oepdev::Points3DIterator::Points3DIterator (const int & np)

Plain constructor. Initializes the abstract features.

Parameters

| | |
|-----------------|---|
| <code>np</code> | - number of points this iterator is constructed for |
|-----------------|---|

17.20.3 Member Function Documentation

17.20.3.1 `std::shared_ptr< Points3DIterator > oepdev::Points3DIterator::build (const int & nx, const int & ny, const int & nz, const double & dx, const double & dy, const double & dz, const double & ox, const double & oy, const double & oz) [static]`

Build G09 Cube collection iterator.

The points are generated according to Gaussian cube file format.

Parameters

| | |
|-----------------|--------------------------------------|
| <code>nx</code> | - number of points along x direction |
| <code>ny</code> | - number of points along y direction |
| <code>nz</code> | - number of points along z direction |
| <code>dx</code> | - spacing distance along x direction |
| <code>dy</code> | - spacing distance along y direction |
| <code>dz</code> | - spacing distance along y direction |
| <code>ox</code> | - coordinate x of cube origin |
| <code>oy</code> | - coordinate y of cube origin |
| <code>oz</code> | - coordinate z of cube origin |

17.20.3.2 `std::shared_ptr< Points3DIterator > oepdev::Points3DIterator::build (const int & np, const double & radius, const double & cx, const double & cy, const double & cz) [static]`

Build random collection iterator.

The points are drawn according to uniform distribution in 3D space.

Parameters

| | |
|---------------|---|
| <i>np</i> | - number of points to draw |
| <i>radius</i> | - sphere radius inside which points are to be drawn |
| <i>cx</i> | - coordinate x of sphere's centre |
| <i>cy</i> | - coordinate y of sphere's centre |
| <i>cz</i> | - coordinate z of sphere's centre |

17.20.3.3 `shared_ptr< Points3DIterator > oepdev::Points3DIterator::build (const int & np, const double & pad, psi::SharedMolecule mol) [static]`

Build random collection iterator.

The points are drawn according to uniform distribution in 3D space enclosing a molecule given. All drawn points lie outside the van der Waals volume.

Parameters

| | |
|------------|---|
| <i>np</i> | - number of points to draw |
| <i>pad</i> | - radius padding of a minimal sphere enclosing the molecule |
| <i>mol</i> | - Psi4 molecule object |

The documentation for this class was generated from the following files:

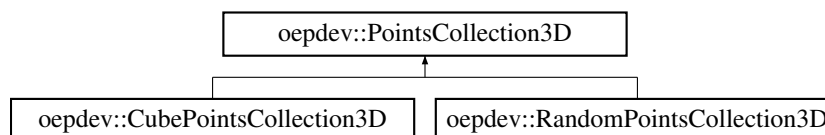
- oepdev/libutil/space3d.h
- oepdev/libutil/space3d.cc

17.21 oepdev::PointsCollection3D Class Reference

Collection of points in 3D space. Abstract base.

```
#include <space3d.h>
```

Inheritance diagram for oepdev::PointsCollection3D:



Public Types

- enum `Collection` { `Random`, `Cube` }
- Public descriptor of collection type.*

Public Member Functions

- `PointsCollection3D (Collection collectionType, int &np)`
Initialize abstract features.
- `PointsCollection3D (Collection collectionType, const int &np)`
- `virtual ~PointsCollection3D ()`
Destructor.
- `virtual int npoints () const`
Get the number of points.

- virtual shared_ptr
< Points3DIterator > points_iterator () const
Get the iterator over this collection of points.
- virtual Collection get_type () const
Get the collection type.
- virtual void print () const =0
Print the information to Psi4 output file.

Static Public Member Functions

- static shared_ptr
< PointsCollection3D > build (const int &npoints, const double &radius, const double &cx=0.0, const double &cy=0.0, const double &cz=0.0)
Build random collection of points.
- static shared_ptr
< PointsCollection3D > build (const int &npoints, const double &padding, psi::SharedMolecule mol)
Build random collection of points.
- static shared_ptr
< PointsCollection3D > build (const int &nx, const int &ny, const int &nz, const double &px, const double &py, const double &pz, psi::SharedBasisSet bs, psi::Options &options)
Build G09 Cube collection of points.

Protected Attributes

- const int np_
Number of points.
- Collection collectionType_
Collection type.
- shared_ptr< Points3DIterator > pointsIterator_
iterator over points collection

17.21.1 Detailed Description

Collection of points in 3D space. Abstract base.

Create random or ordered (g09 cube-like) collections of points in 3D space.

Note: Always create instances by using static factory methods.

17.21.2 Constructor & Destructor Documentation

17.21.2.1 oepdev::PointsCollection3D::PointsCollection3D (Collection collectionType, int & np)

Initialize abstract features.

Parameters

| | |
|-----------|----------------------------------|
| <i>np</i> | - number of points to be created |
|-----------|----------------------------------|

17.21.3 Member Function Documentation

17.21.3.1 `std::shared_ptr< PointsCollection3D > oepdev::PointsCollection3D::build (const int & npoints, const double & radius, const double & cx = 0.0, const double & cy = 0.0, const double & cz = 0.0) [static]`

Build random collection of points.

Points uniformly span a sphere.

Parameters

| | |
|----------------|---|
| <i>npoints</i> | - number of points to draw |
| <i>radius</i> | - sphere radius inside which points are to be drawn |
| <i>cx</i> | - coordinate x of sphere's centre |
| <i>cy</i> | - coordinate y of sphere's centre |
| <i>cz</i> | - coordinate z of sphere's centre |

17.21.3.2 `std::shared_ptr< PointsCollection3D > oepdev::PointsCollection3D::build (const int & npoints, const double & padding, psi::SharedMolecule mol) [static]`

Build random collection of points.

Points uniformly span space inside a sphere enclosing a molecule. excluding the van der Waals volume.

Parameters

| | |
|----------------|---|
| <i>np</i> | - number of points to draw |
| <i>padding</i> | - radius padding of a minimal sphere enclosing the molecule |
| <i>mol</i> | - Psi4 molecule object |

17.21.3.3 `std::shared_ptr< PointsCollection3D > oepdev::PointsCollection3D::build (const int & nx, const int & ny, const int & nz, const double & px, const double & py, const double & pz, psi::SharedBasisSet bs, psi::Options & options) [static]`

Build G09 Cube collection of points.

The points span a parallelepiped according to Gaussian cube file format.

Parameters

| | |
|----------------|--------------------------------------|
| <i>nx</i> | - number of points along x direction |
| <i>ny</i> | - number of points along y direction |
| <i>nz</i> | - number of points along z direction |
| <i>px</i> | - padding distance along x direction |
| <i>py</i> | - padding distance along y direction |
| <i>pz</i> | - padding distance along z direction |
| <i>bs</i> | - Psi4 basis set object |
| <i>options</i> | - Psi4 options object |

The documentation for this class was generated from the following files:

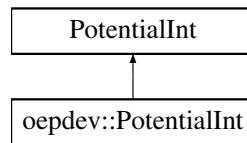
- oepdev/libutil/space3d.h
- oepdev/libutil/space3d.cc

17.22 oepdev::PotentialInt Class Reference

Computes potential integrals.

```
#include <potential.h>
```

Inheritance diagram for oepdev::PotentialInt:



Public Member Functions

- [PotentialInt](#) (std::vector< psi::SphericalTransform > &st, std::shared_ptr< psi::BasisSet > bs1, std::shared_ptr< psi::BasisSet > bs2, int deriv=0)
Constructor. Initialize identically like in psi::Potentillnt.
- [PotentialInt](#) (std::vector< psi::SphericalTransform > &st, std::shared_ptr< psi::BasisSet > bs1, std::shared_ptr< psi::BasisSet > bs2, std::shared_ptr< psi::Matrix > Qxyz, int deriv=0)
Constructor. Takes an arbitrary collection of charges.
- [PotentialInt](#) (std::vector< psi::SphericalTransform > &, std::shared_ptr< psi::BasisSet >, std::shared_ptr< psi::BasisSet >, const double &x, const double &y, const double &z, const double &q=1.0, int deriv=0)
Constructor. Computes potential for one point x, y, z for a test particle of charge q.
- void [set_charge_field](#) (const double &x, const double &y, const double &z, const double &q=1.0)
Mutator. Set the charge field to be a x, y, z point of charge q.

17.22.1 Detailed Description

Computes potential integrals.

17.22.2 Constructor & Destructor Documentation

17.22.2.1 `oepdev::PotentialInt::PotentialInt (std::vector< psi::SphericalTransform > & st, std::shared_ptr< psi::BasisSet > bs1, std::shared_ptr< psi::BasisSet > bs2, int deriv = 0)`

Constructor. Initialize identically like in psi::Potentillnt.

Parameters

| | |
|--------------|------------------------------|
| <i>st</i> | - Spherical transform object |
| <i>bs1</i> | - basis set for first space |
| <i>bs2</i> | - basis set for second space |
| <i>deriv</i> | - derivative level |

17.22.2.2 `oepdev::PotentialInt::PotentialInt (std::vector< psi::SphericalTransform > & st, std::shared_ptr< psi::BasisSet > bs1, std::shared_ptr< psi::BasisSet > bs2, std::shared_ptr< psi::Matrix > Qxyz, int deriv = 0)`

Constructor. Takes an arbitrary collection of charges.

Parameters

| | |
|-----------|------------------------------|
| <i>st</i> | - Spherical transform object |
|-----------|------------------------------|

| | |
|--------------|---|
| <i>bs1</i> | - basis set for first space |
| <i>bs2</i> | - basis set for second space |
| <i>Qxyz</i> | - matrix with charges and their positions |
| <i>deriv</i> | - derivative level |

17.22.2.3 oepdev::PotentialInt::PotentialInt (std::vector< psi::SphericalTransform > & *st*, std::shared_ptr< psi::BasisSet > *bs1*, std::shared_ptr< psi::BasisSet > *bs2*, const double & *x*, const double & *y*, const double & *z*, const double & *q* = 1.0, int *deriv* = 0)

Constructor. Computes potential for one point x, y, z for a test particle of charge q.

Parameters

| | |
|--------------|------------------------------|
| <i>st</i> | - Spherical transform object |
| <i>bs1</i> | - basis set for first space |
| <i>bs2</i> | - basis set for second space |
| <i>x</i> | - x coordinate of q |
| <i>y</i> | - y coordinate of q |
| <i>z</i> | - z coordinate of q |
| <i>q</i> | - value of the probe charge |
| <i>deriv</i> | - derivative level |

17.22.3 Member Function Documentation

17.22.3.1 void oepdev::PotentialInt::set_charge_field (const double & *x*, const double & *y*, const double & *z*, const double & *q* = 1.0)

Mutator. Set the charge field to be a x, y, z point of charge q.

Parameters

| | |
|----------|-----------------------------|
| <i>x</i> | - x coordinate of q |
| <i>y</i> | - y coordinate of q |
| <i>z</i> | - z coordinate of q |
| <i>q</i> | - value of the probe charge |

The documentation for this class was generated from the following files:

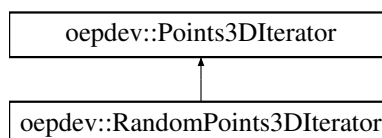
- oepdev/libpsi/potential.h
- oepdev/libpsi/potential.cc

17.23 oepdev::RandomPoints3DIterator Class Reference

Iterator over a collection of points in 3D space. Random collection.

```
#include <space3d.h>
```

Inheritance diagram for oepdev::RandomPoints3DIterator:



Public Member Functions

- **RandomPoints3DIterator** (const int &np, const double &radius, const double &cx, const double &cy, const double &cz)
- **RandomPoints3DIterator** (const int &np, const double &pad, psi::SharedMolecule mol)
- virtual void **first** ()
Initialize first iteration.
- virtual void **next** ()
Step to next iteration.

Protected Member Functions

- virtual double **random_double** ()
- virtual void **draw_random_point** ()
- virtual bool **is_in_vdWsphere** (double x, double y, double z) const

Protected Attributes

- double **cx_**
- double **cy_**
- double **cz_**
- double **radius_**
- double **r_**
- double **phi_**
- double **theta_**
- double **x_**
- double **y_**
- double **z_**
- psi::SharedMatrix **excludeSpheres_**
- std::map< std::string, double > **vdwRadius_**
- std::default_random_engine **randomNumberGenerator_**
- std::uniform_real_distribution
< double > **randomDistribution_**

Additional Inherited Members

17.23.1 Detailed Description

Iterator over a collection of points in 3D space. Random collection.

Note: Always create instances by using static factory method from [Points3DIterator](#). Do not use constructors of this class.

The documentation for this class was generated from the following files:

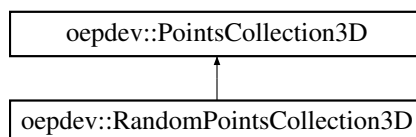
- oepdev/libutil/space3d.h
- oepdev/libutil/space3d.cc

17.24 oepdev::RandomPointsCollection3D Class Reference

Collection of random points in 3D space.

```
#include <space3d.h>
```

Inheritance diagram for oepdev::RandomPointsCollection3D:



Public Member Functions

- **RandomPointsCollection3D** ([Collection](#) collectionType, const int &npoints, const double &radius, const double &cx, const double &cy, const double &cz)
- **RandomPointsCollection3D** ([Collection](#) collectionType, const int &npoints, const double &padding, psi::SharedMolecule mol)
- virtual void [print](#) () const

Print the information to Psi4 output file.

Additional Inherited Members

17.24.1 Detailed Description

Collection of random points in 3D space.

Note: Do not use constructors of this class explicitly. Instead, use static factory methods of the superclass to create instances.

The documentation for this class was generated from the following files:

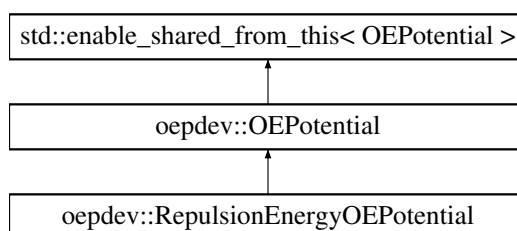
- oepdev/libutil/space3d.h
- oepdev/libutil/space3d.cc

17.25 oepdev::RepulsionEnergyOEPotential Class Reference

Generalized One-Electron Potential for Pauli Repulsion Energy.

```
#include <oep.h>
```

Inheritance diagram for oepdev::RepulsionEnergyOEPotential:



Public Member Functions

- **RepulsionEnergyOEPotential** (SharedWavefunction [wfn](#), SharedBasisSet auxiliary, Options &options)
- **RepulsionEnergyOEPotential** (SharedWavefunction [wfn](#), Options &options)
- virtual void **compute** (const std::string &oepType) override
- virtual void **compute_3D** (const std::string &oepType, const double &x, const double &y, const double &z, double &v) override
- virtual void **print_header** () const override

Additional Inherited Members

17.25.1 Detailed Description

Generalized One-Electron Potential for Pauli Repulsion Energy.

Contains the following OEP types:

- Murrell-etal.S1
- Otto-Ladik.S2

17.25.2 Member Function Documentation

17.25.2.1 void RepulsionEnergyOEPotential::compute_3D (const std::string & oepType, const double & x, const double & y, const double & z, double & v) [override],[virtual]

Compute value of potential in point x, y, z and save at v

Implements [oepdev::OEPotential](#).

The documentation for this class was generated from the following files:

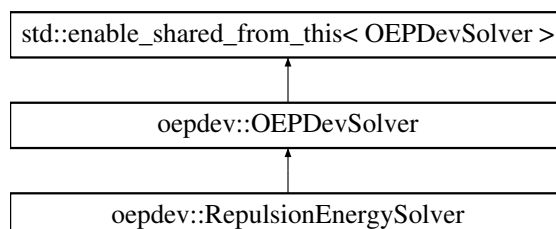
- [oepdev/liboep/oep.h](#)
- [oepdev/liboep/oep.cc](#)

17.26 oepdev::RepulsionEnergySolver Class Reference

Compute the Pauli-Repulsion interaction energy between unperturbed wavefunctions.

```
#include <solver.h>
```

Inheritance diagram for oepdev::RepulsionEnergySolver:



Public Member Functions

- **RepulsionEnergySolver** (SharedWavefunctionUnion wfn_union)
- virtual double **compute_oep_based** (const std::string &method="DEFAULT")

Compute property by using OEP's.

- virtual double `compute_benchmark` (const std::string &method="DEFAULT")

Compute property by using benchmark method.

Additional Inherited Members

17.26.1 Detailed Description

Compute the Pauli-Repulsion interaction energy between unperturbed wavefunctions.

The implemented methods are shown below *Note*:

| Keyword | Method Description |
|--------------------------|--|
| Benchmark Methods | |
| HAYES_STONE | *Default*. Pauli Repulsion energy at HF level from Hayes and Stone (1984). |
| DENSITY_BASED | Pauli Repulsion energy at HF level from Mandado and Hermida-Ramon (2012). |
| MURRELL_ETAL | Approximate Pauli Repulsion energy at HF level from Murrell et al (1967). |
| OTTO_LADIK | Approximate Pauli Repulsion energy at HF level from Otto and Ladik (1975). |
| EFP2 | Approximate Pauli Repulsion energy at HF level from EFP2 model. |
| OEP-Based Methods | |
| MURRELL_ETAL_MIX | *Default*. OEP-Murrell et al's: S1 term via DF-OEP, S2 term via ESP-OEP. |
| MURRELL_ETAL_ESP | OEP-Murrell et al's: S1 and S2 via ESP-OEP |

Table 17.3: Methods available in the Solver

- This solver also computes and prints the exchange energy at HF level (formulae are given below) for reference purposes.
- In order to construct this solver, **always** use the `OEPDevSolver::build` static factory method.

Below the detailed description of the implemented equations is given for each of the above provided methods. In the formulae across, it is assumed that the orbitals are real. The Coulomb notation for electron repulsion integrals (ERI's) is adopted; i.e,

$$(ac|bd) = \iint d\mathbf{r}_1 d\mathbf{r}_2 \phi_a(\mathbf{r}_1) \phi_c(\mathbf{r}_1) \frac{1}{r_{12}} \phi_b(\mathbf{r}_2) \phi_d(\mathbf{r}_2)$$

Greek subscripts denote basis set orbitals whereas Italic subscripts denote the occupied molecular orbitals.

Benchmark Methods

Pauli Repulsion energy at HF level by Hayes and Stone (1984).

For a closed-shell system, equation of Hayes and Stone (1984) becomes

$$E^{\text{Rep}} = 2 \sum_{kl} (V_{kl}^A + V_{kl}^B + T_{kl}) \left[[\mathbf{S}^{-1}]_{lk} - \delta_{lk} \right] + \sum_{klmn} (kl|mn) \left\{ 2[\mathbf{S}^{-1}]_{kl} [\mathbf{S}^{-1}]_{mn} - [\mathbf{S}^{-1}]_{kn} [\mathbf{S}^{-1}]_{lm} - 2\delta_{kl} \delta_{mn} + \delta_{kn} \delta_{lm} \right\}$$

where \mathbf{S} is the overlap matrix between the doubly-occupied orbitals. The exact, pure exchange energy is for a closed shell case given as

$$E^{\text{Ex,pure}} = -2 \sum_{a \in A} \sum_{b \in B} (ab|ba)$$

Similarity transformation of molecular orbitals does not affect the resulting energies. The overall exchange-repulsion interaction energy is then (always net repulsive)

$$E^{\text{Ex-Rep}} = E^{\text{Ex,pure}} + E^{\text{Rep}}$$

Repulsion energy of Mandado and Hermida-Ramon (2011)

At the Hartree-Fock level, the exchange-repulsion energy from the density-based scheme of Mandado and Hermida-Ramon (2011) is fully equivalent to the method by Hayes and Stone (1984). However, density-based method enables to compute exchange-repulsion energy at any level of theory. It is derived based on the Pauli deformation density matrix,

$$\Delta \mathbf{D}^{\text{Pauli}} \equiv \mathbf{D}^{oo} - \mathbf{D}$$

where \mathbf{D}^{oo} and \mathbf{D} are the density matrix formed from mutually orthogonal sets of molecular orbitals within the entire aggregate (formed by symmetric orthogonalization of MO's) and the density matrix of the unperturbed system (that can be understood as a Hadamard sum $\mathbf{D} \equiv \mathbf{D}^A \oplus \mathbf{D}^B$).

At HF level, the Pauli deformation density matrix is given by

$$\Delta \mathbf{D}^{\text{Pauli}} = \mathbf{C} [\mathbf{S}^{-1} - \mathbf{1}] \mathbf{C}^\dagger$$

whereas the density matrix constructed from mutually orthogonal orbitals is

$$\mathbf{D}^{oo} = \mathbf{C} \mathbf{S}^{-1} \mathbf{C}^\dagger$$

In the above equations, \mathbf{S} is the overlap matrix between doubly occupied molecular orbitals of the entire aggregate.

Here, the expressions for the exchange-repulsion energy at any level of theory are shown for the case of open-shell system. The net repulsive energy is given as

$$E^{\text{Ex-Rep}} = E^{\text{Rep,1}} + E^{\text{Rep,2}} + E^{\text{Ex}}$$

where the one- and two-electron part of the repulsion energy is

$$E^{\text{Rep,1}} = E^{\text{Rep,Kin}} + E^{\text{Rep,Nuc}}$$

$$E^{\text{Rep,2}} = E^{\text{Rep,el-}\Delta} + E^{\text{Rep,}\Delta-\Delta}$$

The kinetic and nuclear contributions are

$$E^{\text{Rep,Kin}} = 2 \sum_{\alpha\beta \in A,B} \Delta D_{\alpha\beta}^{\text{Pauli}} T_{\alpha\beta}$$

$$E^{\text{Rep,Nuc}} = 2 \sum_{\alpha\beta \in A,B} \Delta D_{\alpha\beta}^{\text{Pauli}} \sum_{z \in A,B} V_{\alpha\beta}^{(z)}$$

whereas the electron-deformation and deformation-deformation interaction contributions are

$$E^{\text{Rep,el-}\Delta} = 4 \sum_{\alpha\beta\gamma\delta \in A,B} \Delta D_{\alpha\beta}^{\text{Pauli}} D_{\gamma\delta} (\alpha\beta|\gamma\delta)$$

$$E^{\text{Rep,}\Delta-\Delta} = 2 \sum_{\alpha\beta\gamma\delta \in A,B} \Delta D_{\alpha\beta}^{\text{Pauli}} \Delta D_{\gamma\delta}^{\text{Pauli}} (\alpha\beta|\gamma\delta)$$

The associated exchange energy is given by

$$E^{\text{Ex}} = - \sum_{\alpha\beta\gamma\delta \in A,B} \left[D_{\alpha\delta}^{oo} D_{\beta\gamma}^{oo} - D_{\alpha\delta}^A D_{\beta\gamma}^A - D_{\alpha\delta}^B D_{\beta\gamma}^B \right] (\alpha\beta|\gamma\delta)$$

It is important to emphasise that, although, at HF level, the particular 'repulsive' and 'exchange' energies computed by using either Hayes and Stone or Mandado and Hermida-Ramon methods are not equal to each other, they sum up to exactly the same exchange-repulsion energy, $E^{\text{Ex-Rep}}$. Therefore, these methods at HF level are fully equivalent but the nature of partitioning of repulsive and exchange parts is different. It is also noted that the orbital localization does *not* affect the resulting energies, as opposed to the few approximate methods described below (Otto-Ladik and EFP2 methods).

Approximate Pauli Repulsion energy at HF level from Murrell et al.

By expanding the overlap matrix in a Taylor series one can show that the Pauli repulsion energy is approximately given as

$$E^{\text{Rep}} = E^{\text{Rep}}(\mathcal{O}(S)) + E^{\text{Rep}}(\mathcal{O}(S^2))$$

where the first-order term is

$$E^{\text{Rep}}(\mathcal{O}(S)) = -2 \sum_{a \in A} \sum_{b \in B} S_{ab} \left\{ V_{ab}^A + \sum_{c \in A} [2(ab|cc) - (ac|bc)] + V_{ab}^B + \sum_{d \in B} [2(ab|dd) - (ad|bd)] \right\}$$

whereas the second-order term is

$$E^{\text{Rep}}(\mathcal{O}(S^2)) = 2 \sum_{a \in A} \sum_{b \in B} S_{ab} \left\{ \sum_{c \in A} S_{bc} \left[V_{ac}^B + 2 \sum_{d \in B} (ac|dd) \right] + \sum_{d \in B} S_{ad} \left[V_{bd}^A + 2 \sum_{x \in A} (bd|cc) \right] - \sum_{c \in A} \sum_{d \in B} S_{cd} (ac|bd) \right\}$$

Thus derived repulsion energy is invariant with respect to transformation of molecular orbitals, similarly as Hayes--Stone's method and density-based method. By using OEP technique, the above theory can be exactly re-cast *without* any further approximations.

Approximate Pauli Repulsion energy at HF level from Otto and Ladik (1975).

The Pauli repulsion energy is approximately given as

$$E^{\text{Rep}} = E^{\text{Rep}}(\mathcal{O}(S)) + E^{\text{Rep}}(\mathcal{O}(S^2))$$

where the first-order term is

$$E^{\text{Rep}}(\mathcal{O}(S)) = -2 \sum_{a \in A} \sum_{b \in B} S_{ab} \left\{ V_{ab}^A + 2 \sum_{c \in A} (ab|cc) - (ab|aa) + V_{ab}^B + 2 \sum_{d \in B} (ab|dd) - (ab|bb) \right\}$$

whereas the second-order term is

$$E^{\text{Rep}}(\mathcal{O}(S^2)) = 2 \sum_{a \in A} \sum_{b \in B} S_{ab}^2 \left\{ V_{aa}^B + V_{bb}^A + 2 \sum_{c \in A} (cc|bb) + 2 \sum_{d \in B} (aa|dd) - (aa|bb) \right\}$$

Thus derived repulsion energy is *not* invariant with respect to transformation of molecular orbitals, in contrast to Hayes-Stone's method and density-based method. It was shown that good results are obtained when using localized molecular orbitals, whereas using canonical molecular orbitals brings poor results. By using OEP technique, the above theory can be exactly re-cast *without* any further approximations.

Approximate Pauli Repulsion energy at HF level from Jensen and Gordon (1996).

The Pauli repulsion energy used within the EFP2 approach is approximately given as

$$E^{\text{Rep}} = E^{\text{Rep}}(\mathcal{O}(S)) + E^{\text{Rep}}(\mathcal{O}(S^2))$$

where the first-order term is

$$E^{\text{Rep}}(\mathcal{O}(S)) = -2 \sum_{a \in A} \sum_{b \in B} S_{ab} \left\{ \sum_{c \in A} F_{ac}^A S_{cb} + \sum_{d \in B} F_{bd}^B S_{da} - 2T_{ab} \right\}$$

whereas the second-order term is

$$E^{\text{Rep}}(\mathcal{O}(S^2)) = 2 \sum_{a \in A} \sum_{b \in B} S_{ab}^2 \left\{ \sum_{x \in A} \frac{-Z_x}{R_{xb}} + \sum_{y \in B} \frac{-Z_y}{R_{ya}} + \sum_{c \in A} \frac{2}{R_{bc}} + \sum_{d \in B} \frac{2}{R_{ad}} - \frac{1}{R_{ab}} \right\}$$

Thus derived repulsion energy is *not* invariant with respect to transformation of molecular orbitals, in contrast to Hayes-Stone's method and density-based method. It was shown that good results are obtained when using localized molecular orbitals, whereas using canonical molecular orbitals brings poor results.

In EFP2, exchange energy is approximated by spherical Gaussian approximation (SGO). The result of this is the following formula for the exchange energy:

$$E^{\text{Ex}} \approx -4 \sum_{a \in A} \sum_{b \in B} \sqrt{\frac{-2 \ln |S_{ab}|}{\pi}} \frac{S_{ab}^2}{R_{ab}}$$

In all the above formulas, R_{ij} are distances between position vectors of i -th and j -th point. The LMO centroids are defined by

$$\mathbf{r}_a = (a|\mathbf{r}|a)$$

where a denotes the occupied molecular orbital.

OEP-Based Methods

The Murrell et al's theory of Pauli repulsion for S-1 term and the Otto-Ladik's theory for S-2 term is here re-cast by introducing OEP's. The S-1 term is expressed via DF-OEP, whereas the S-2 term via ESP-OEP.

S-1 term (Murrell et al.)

The OEP reduction without any approximations leads to the following formula

$$E^{\text{Rep}}(\mathcal{O}(S^1)) = -2 \sum_{a \in A} \sum_{b \in B} S_{ab} \left\{ \sum_{\xi \in A} S_{b\xi} G_{\xi a}^A + \sum_{\eta \in B} S_{a\eta} G_{\eta b}^B \right\}$$

where the OEP matrices are given as

$$G_{\xi a}^A = \sum_{\xi' \in A} [\mathbf{S}^{-1}]_{\xi \xi'} \sum_{\alpha \in A} \left\{ C_{\alpha a} V_{\alpha \xi'}^A + \sum_{\mu \nu \in A} [2C_{\alpha a} D_{\mu \nu} - C_{\nu a} D_{\alpha \mu}] (\alpha \xi' | \mu \nu) \right\}$$

and analogously for molecule B . Here, the nuclear attraction integrals are denoted by $V_{\alpha \xi'}^A$.

S-2 term (Otto-Ladik)

After the OEP reduction, this contribution under Otto-Ladik approximation has the following form:

$$E^{\text{Rep}}(\mathcal{O}(S^2)) = 2 \sum_{a \in A} \sum_{b \in B} S_{ab}^2 \left\{ \sum_{x \in A} q_{xa} V_{bb}^{(x)} + \sum_{y \in B} q_{yb} V_{aa}^{(y)} \right\}$$

where the ESP charges associated with each occupied molecular orbital reproduce the *effective potential* of molecule in question, i.e.,

$$\sum_{x \in A} \frac{q_{xa}}{|\mathbf{r} - \mathbf{r}_x|} \cong v_a^A(\mathbf{r})$$

where the potential is given by

$$v_a^A(\mathbf{r}) = \sum_{x \in A} \frac{-Z_x}{|\mathbf{r} - \mathbf{r}_x|} + 2 \sum_{c \in A} \int \frac{\phi_c(\mathbf{r}') \phi_c(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - \frac{1}{2} \int \frac{\phi_a(\mathbf{r}') \phi_a(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'$$

17.26.2 Member Function Documentation

17.26.2.1 `double RepulsionEnergySolver::compute_benchmark (const std::string & method = "DEFAULT")`
`[virtual]`

Compute property by using benchmark method.

Each solver object has one `DEFAULT` benchmark method

Parameters

| | |
|---------------|--------------------|
| <i>method</i> | - benchmark method |
|---------------|--------------------|

Implements [oepdev::OEPDevSolver](#).

17.26.2.2 `double RepulsionEnergySolver::compute_oep_based (const std::string & method = "DEFAULT")`
`[virtual]`

Compute property by using OEP's.

Each solver object has one `DEFAULT` OEP-based method.

Parameters

| | |
|---------------|------------------------|
| <i>method</i> | - flavour of OEP model |
|---------------|------------------------|

Implements [oepdev::OEPDevSolver](#).

The documentation for this class was generated from the following files:

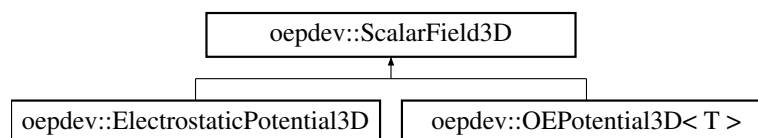
- [oepdev/libutil/solver.h](#)
- [oepdev/libutil/solver.cc](#)

17.27 oepdev::ScalarField3D Class Reference

Scalar field in 3D space. Abstract base.

```
#include <space3d.h>
```

Inheritance diagram for `oepdev::ScalarField3D`:



Public Member Functions

- [ScalarField3D](#) (const int &np, const double &pad, psi::SharedWavefunction [wfn](#), psi::Options &options)
Construct potential on random grid by providing wavefunction.
- [ScalarField3D](#) (const int &nx, const int &ny, const int &nz, const double &px, const double &py, const double &pz, std::shared_ptr< psi::Wavefunction > [wfn](#), psi::Options &options)
Construct potential on cube grid by providing wavefunction.
- virtual [~ScalarField3D](#) ()
Destructor.
- virtual int [npoints](#) () const
Get the number of points at which the scalar field is defined.
- virtual std::shared_ptr< [PointsCollection3D](#) > [points_collection](#) () const
Get the collection of points.
- virtual std::shared_ptr< psi::Matrix > [data](#) () const
Get the data matrix in a form { [x, y, z, f(x, y, z)] }.

- virtual std::shared_ptr< psi::Wavefunction > **wfn** () const
Get the wavefunction.
- virtual bool **is_computed** () const
Get the information if data is already computed or not.
- virtual void **compute** ()
Compute the scalar field in each point from the point collection.
- virtual double **compute_xyz** (const double &x, const double &y, const double &z)=0
Compute a value of scalar field at point (x, y, z)
- virtual void **write_cube_file** (const std::string &name)
Write the cube file (only for Cube collections, otherwise does nothing)
- virtual void **print** () const =0
Print information of the object to Psi4 output.

Static Public Member Functions

- static shared_ptr< **ScalarField3D** > **build** (const std::string &type, const int &np, const double &pad, psi::SharedWavefunction **wfn**, psi::Options &options)
Build scalar field of random points.
- static shared_ptr< **ScalarField3D** > **build** (const std::string &type, const int &nx, const int &ny, const int &nz, const double &px, const double &py, const double &pz, psi::SharedWavefunction **wfn**, psi::Options &options)
Build scalar field of points on a g09-cube grid.

Protected Attributes

- std::shared_ptr< **PointsCollection3D** > **pointsCollection_**
Collection of points at which the scalar field is to be computed.
- std::shared_ptr< psi::Matrix > **data_**
The data matrix in a form { [x, y, z, f(x, y, z)] }.
- std::shared_ptr< psi::Wavefunction > **wfn_**
Wavefunction.
- psi::Matrix **geom_**
Geometry of a molecule.
- std::shared_ptr< psi::IntegralFactory > **fact_**
Integral factory.
- std::shared_ptr< psi::Matrix > **pot_**
Matrix of potential one-electron integrals.
- std::shared_ptr< psi::OneBodyAOInt > **oneInt_**
One-electron integral shared pointer.
- std::shared_ptr< **PotentialInt** > **potInt_**
One-electron potential shared pointer.
- std::shared_ptr< psi::BasisSet > **primary_**
Basis set.
- int **nbf_**
Number of basis functions.
- bool **isComputed_**
Has data already computed?

17.27.1 Detailed Description

Scalar field in 3D space. Abstract base.

Create scalar field defined at points distributed randomly or as an ordered g09 cube-like collection. Currently implemented scalar fields are:

- Electrostatic potential - computes electrostatic potential (requires wavefunction)
- Template of generic classes - compute custom scalar fields (requires generic object that is able to compute the field in 3D space)

Note: Always create instances by using static factory methods `build`. The following types of scalar field are currently implemented:

- `ELECTROSTATIC POTENTIAL`

17.27.2 Member Function Documentation

17.27.2.1 `std::shared_ptr< ScalarField3D > oepdev::ScalarField3D::build (const std::string & type, const int & np, const double & pad, psi::SharedWavefunction wfn, psi::Options & options) [static]`

Build scalar field of random points.

Parameters

| | |
|----------------|---|
| <i>type</i> | - type of scalar field |
| <i>np</i> | - number of points |
| <i>pad</i> | - radius padding of a minimal sphere enclosing the molecule |
| <i>wfn</i> | - Psi4 Wavefunction containing the molecule |
| <i>options</i> | - Psi4 options |

17.27.2.2 `std::shared_ptr< ScalarField3D > oepdev::ScalarField3D::build (const std::string & type, const int & nx, const int & ny, const int & nz, const double & px, const double & py, const double & pz, psi::SharedWavefunction wfn, psi::Options & options) [static]`

Build scalar field of points on a g09-cube grid.

Parameters

| | |
|----------------|---|
| <i>type</i> | - type of scalar field |
| <i>nx</i> | - number of points along x direction |
| <i>ny</i> | - number of points along y direction |
| <i>nz</i> | - number of points along z direction |
| <i>px</i> | - padding distance along x direction |
| <i>py</i> | - padding distance along y direction |
| <i>pz</i> | - padding distance along z direction |
| <i>wfn</i> | - Psi4 Wavefunction containing the molecule |
| <i>options</i> | - Psi4 options |

The documentation for this class was generated from the following files:

- `oepdev/libutil/space3d.h`
- `oepdev/libutil/space3d.cc`

17.28 oepdev::test::Test Class Reference

Manages test routines.

```
#include <test.h>
```

Public Member Functions

- [Test](#) (std::shared_ptr< psi::Wavefunction > wfn, psi::Options &options)
Construct the tester.
- [~Test](#) ()
Destructor.
- double [run](#) (void)
Perform the test.

Protected Member Functions

- double [test_eri_2_2](#) (void)
Test the oepdev::ERI_2_2 class against psi::ERI.
- double [test_eri_1_1](#) (void)
Test the oepdev::ERI_1_1 class against psi::ERI.

Protected Attributes

- std::shared_ptr
 < psi::Wavefunction > [wfn_](#)
Wavefunction object.
- psi::Options [options_](#)
Psi4 Options.

17.28.1 Detailed Description

Manages test routines.

The documentation for this class was generated from the following files:

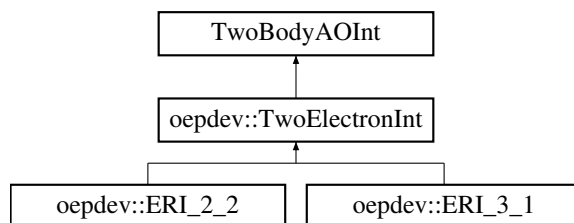
- oepdev/libtest/[test.h](#)
- oepdev/libtest/test.cc

17.29 oepdev::TwoElectronInt Class Reference

General Two Electron Integral.

```
#include <eri.h>
```

Inheritance diagram for oepdev::TwoElectronInt:



Public Member Functions

- **TwoElectronInt** (const [IntegralFactory](#) *integral, int deriv, bool use_shell_pairs)
- virtual size_t [compute_shell](#) (int, int)
Compute ERI's between 2 shells. Result is stored in buffer.
- virtual size_t [compute_shell](#) (int, int, int)
Compute ERI's between 3 shells. Result is stored in buffer.
- virtual size_t [compute_shell](#) (int, int, int, int)
Compute ERI's between 4 shells. Result is stored in buffer.
- virtual size_t [compute_shell](#) (const psi::AOShellCombinationsIterator &)
- virtual size_t [compute_shell_deriv1](#) (int, int)
Compute first derivatives of ERI's between 2 shells.
- virtual size_t [compute_shell_deriv2](#) (int, int)
Compute second derivatives of ERI's between 2 shells.
- virtual size_t [compute_shell_deriv1](#) (int, int, int)
Compute first derivatives of ERI's between 3 shells.
- virtual size_t [compute_shell_deriv2](#) (int, int, int)
Compute second derivatives of ERI's between 3 shells.
- virtual size_t [compute_shell_deriv1](#) (int, int, int, int)
Compute first derivatives of ERI's between 4 shells.
- virtual size_t [compute_shell_deriv2](#) (int, int, int, int)
Compute second derivatives of ERI's between 4 shells.

Protected Member Functions

- int [get_cart_am](#) (int am, int n, int x)
Get the angular momentum per Cartesian component.
- double [get_R](#) (int N, int L, int M)
Get the (N,L,M)th McMurchie-Davidson coefficient.
- virtual size_t [compute_quartet](#) (int, int, int, int)
Computes the ERI's between four shells.
- virtual size_t [compute_triplet](#) (int, int, int)
Computes the ERI's between three shells.
- virtual size_t [compute_doublet](#) (int, int)
Computes the ERI's between three shells.

Protected Attributes

- const int [max_am_](#)
Maximum angular momentum.
- const int [n_max_am_](#)
Maximum number of angular momentum functions.

- `psi::Fjt * fjt_`
Computes the fundamental: Boys function value at T for degree v.
- `bool use_shell_pairs_`
Should we use shell pair information?
- `const double cartMap_ [60]`
Map of Cartesian components per each am.
- `const double df_ [8]`
Double factorial array.
- `double * mdh_buffer_R_`
Buffer for the McMurchie-Davidson-Hermite R coefficients.

17.29.1 Detailed Description

General Two Electron Integral.

The integral can be defined for any number of Gaussian centres, thus it is not limited to 2-by-2 four-centre ERI.

17.29.2 Member Function Documentation

17.29.2.1 `size_t oepdev::TwoElectronInt::compute_shell (const psi::AOShellCombinationsIterator & shellIter)`
[virtual]

Compute ERIs between 4 shells. Result is stored in buffer. Only for use with [ERI_2_2](#) and the same basis sets, otherwise shell pairs won't be compatible.

The documentation for this class was generated from the following files:

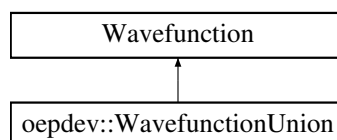
- `oepdev/libints/eri.h`
- `oepdev/libints/eri.cc`

17.30 oepdev::WavefunctionUnion Class Reference

Union of two Wavefunction objects.

```
#include <wavefunction_union.h>
```

Inheritance diagram for `oepdev::WavefunctionUnion`:



Public Member Functions

- [WavefunctionUnion](#) (SharedWavefunction ref_wfn, Options &options)
Constructor.
- `virtual ~WavefunctionUnion ()`
Destructor.
- `virtual double compute_energy ()`
Compute Energy (now blank)
- `virtual double nuclear_repulsion_interaction_energy ()`

- Compute Nuclear Repulsion Energy between unions.*

 - void [localize_orbitals](#) ()

Localize Molecular Orbitals.
- void [transform_integrals](#) ()

Transform Integrals (2- and 4-index transformations)
- int [l_nmo](#) (int n) const

*Get number of molecular orbitals of the *n*th fragment.*
- int [l_nso](#) (int n) const

*Get number of symmetry orbitals of the *n*th fragment.*
- int [l_ndocc](#) (int n) const

*Get number of doubly occupied orbitals of the *n*th fragment.*
- int [l_nvir](#) (int n) const

*Get number of virtual orbitals of the *n*th fragment.*
- int [l_nalpha](#) (int n) const

*Get the number of the alpha electrons of the *n*th fragment.*
- int [l_nbeta](#) (int n) const

*Get the number of the beta electrons of the *n*th fragment.*
- int [l_nbf](#) (int n) const

*Get number of basis functions of the *n*th fragment.*
- int [l_noffs_ao](#) (int n) const

*Get the basis set offset of the *n*th fragment.*
- double [l_energy](#) (int n) const

*Get the reference energy of the *n*th fragment.*
- SharedMolecule [l_molecule](#) (int n) const

*Get the molecule object of the *n*th fragment.*
- SharedBasisSet [l_primary](#) (int n) const

*Get the primary basis set object of the *n*th fragment.*
- SharedBasisSet [l_auxiliary](#) (int n) const

*Get the auxiliary basis set object of the *n*th fragment.*
- SharedWavefunction [l_wfn](#) (int n) const

*Get the wavefunction object of the *n*th fragment.*
- SharedMOSpace [l_mospace](#) (int n, const std::string &label) const

*Get the MO space named `label` (either `OCC` or `VIR`) of the *n*th fragment.*
- SharedLocalizer [l_localizer](#) (int n) const

*Get the orbital localizer object of the *n*th fragment.*
- SharedIntegralTransform [integrals](#) (void) const

Get the integral transform object of the entire union.
- bool [has_localized_orbitals](#) (void) const

If union got its molecular orbital localized or not.
- SharedBasisSet [primary](#) (void) const

Get the primary basis set for the entire union.
- SharedMOSpace [mospace](#) (const std::string &label) const

Get the MO space named `label` (either `OCC` or `VIR`)
- SharedMatrix [Ca_subset](#) (const std::string &basis="SO", const std::string &subset="ALL")
- SharedMatrix [Cb_subset](#) (const std::string &basis="SO", const std::string &subset="ALL")
- SharedMatrix [C_subset_helper](#) (SharedMatrix C, const Dimension &noccpi, SharedVector epsilon, const std::string &basis, const std::string &subset)

Helpers for `Ca_` and `Cb_` matrix transformers.
- SharedVector [epsilon_subset_helper](#) (SharedVector epsilon, const Dimension &noccpi, const std::string &basis, const std::string &subset)

Helper for epsilon transformer.

- void [print_header](#) (void)
Print information about this wavefunction union.
- void [print_mo_integrals](#) (void)
Print the MO integrals.

Protected Attributes

- int [nIsolatedMolecules_](#)
Number of isolated molecules.
- SharedWavefunction [dimer_wavefunction_](#)
The wavefunction for a dimer (electrons relaxed in the field of monomers)
- SharedIntegralTransform [integrals_](#)
Integral transform object (2- and 4-index transformations)
- bool [hasLocalizedOrbitals_](#)
whether orbitals of the union were localized (or not)
- std::map< const std::string, SharedMOSpace > [mospacesUnion_](#)
Dictionary of MO spaces for the entire union (OCC and VIR)
- std::vector< SharedMolecule > [l_molecule_](#)
List of molecules.
- std::vector< SharedBasisSet > [l_primary_](#)
List of primary basis functions per molecule.
- std::vector< SharedBasisSet > [l_auxiliary_](#)
List of auxiliary basis functions per molecule.
- std::vector< SharedWavefunction > [l_wfn_](#)
List of original isolated wavefunctions (electrons unrelaxed)
- std::vector< std::string > [l_name_](#)
List of names of isolated wavefunctions.
- std::vector< int > [l_nbf_](#)
List of basis function numbers per molecule.
- std::vector< int > [l_nmo_](#)
List of numbers of molecular orbitals (MO's) per molecule.
- std::vector< int > [l_nso_](#)
List of numbers of SO's per molecule.
- std::vector< int > [l_ndocc_](#)
List of numbers of doubly occupied orbitals per molecule.
- std::vector< int > [l_nvir_](#)
List of numbers of virtual orbitals per molecule.
- std::vector< int > [l_noffs_ao_](#)
List of basis set offsets per molecule.
- std::vector< double > [l_energy_](#)
List of energies of isolated wavefunctions.
- std::vector< double > [l_efzc_](#)
List of frozen-core energies per isolated wavefunction.
- std::vector< bool > [l_density_fitted_](#)
List of information per wfn whether it was obtained using DF or not.
- std::vector< int > [l_nalpha_](#)
List of numbers of alpha electrons per isolated wavefunction.
- std::vector< int > [l_nbeta_](#)
List of numbers of beta electrons per isolated wavefunction.

- `std::vector< int > l_nfrzc_`
List of numbers of frozen-core orbitals per isolated molecule.
- `std::vector< SharedLocalizer > l_localizer_`
List of orbital localizers.
- `std::vector< std::map< const std::string, SharedMOSpace > > l_mospace_`
List of dictionaries of MO spaces.

17.30.1 Detailed Description

Union of two Wavefunction objects.

The [WavefunctionUnion](#) is the union of two unperturbed Wavefunctions.

Notes:

1. Works only for C1 symmetry! Therefore `this->nirrep() = 1`.
2. Does not set `reference_wavefunction_`
3. Sets `oeprop_` for the union of uncoupled molecules
4. Performs Hadamard sums on `H_`, `Fa_`, `Da_`, `Ca_` and `S_` based on uncoupled wavefunctions.
5. Since it is based on shallow copy of the original Wavefunction, it **changes** contents of this wavefunction. Reallocate and copy if you want to keep the original wavefunction.

Warnings:

1. Gradients, Hessians and frequencies are not touched, hence they are **wrong**!
2. Lagrangian (if present) is not touched, hence its **wrong**!
3. Ca/Cb and epsilon subsets were reimplemented from `psi::Wavefunction` to remove sorting of orbitals. However, the corresponding member functions are not virtual in `psi::Wavefunction`. This could bring problems when upcasting.

The following variables are *shallow* copies of variables inside the Wavefunction object, that is created for the *whole* molecule cluster:

- `basissets_` (DF/RI/F12/etc basis sets)
- `basisset_` (ORBITAL basis set)
- `sobasisset_` (Primary basis set for SO integrals)
- `AO2SO_` (AO2SO conversion matrix (AO in rows, SO in cols))
- `molecule_` (Molecule that this wavefunction is run on)
- `options_` (Options object)
- `psio_` (PSI file access variables)
- `integral_` (Integral factory)
- `factory_` (Matrix factory for creating standard sized matrices)
- `memory_` (How much memory you have access to)
- `nalpha_, nbeta_` (Total alpha and beta electrons)
- `nfrzc_` (Total frozen core orbitals)

- `doccpi_` (Number of doubly occupied per irrep)
- `soccpi_` (Number of singly occupied per irrep)
- `frzcpi_` (Number of frozen core per irrep)
- `frzvpi_` (Number of frozen virtuals per irrep)
- `nalphapi_` (Number of alpha electrons per irrep)
- `nbetapi_` (Number of beta electrons per irrep)
- `nsopi_` (Number of so per irrep)
- `nmopi_` (Number of mo per irrep)
- `nso_` (Total number of SOs)
- `nmo_` (Total number of MOs)
- `nirrep_` (Number of irreps; must be equal to 1 due to symmetry reasons)
- `same_a_b_dens_` and `same_a_b_orbs_` The rest is altered so that the Wavefunction parameters reflect a cluster of non-interacting (uncoupled, isolated, unrelaxed) molecular electron densities.

17.30.2 Constructor & Destructor Documentation

17.30.2.1 `oepdev::WavefunctionUnion::WavefunctionUnion (SharedWavefunction ref_wfn, Options & options)`

Constructor.

Provide wavefunction with molecule containing at least 2 fragments.

Parameters

| | |
|----------------|--------------------------|
| <i>ref_wfn</i> | - reference wavefunction |
| <i>options</i> | - Psi4 options |

17.30.3 Member Function Documentation

17.30.3.1 `SharedMatrix oepdev::WavefunctionUnion::Ca_subset (const std::string & basis = "SO", const std::string & subset = "ALL")`

Return a subset of the Ca matrix in a desired basis

Parameters

| | |
|---------------|--|
| <i>basis</i> | the symmetry basis to use AO, SO |
| <i>subset</i> | the subset of orbitals to return ALL, ACTIVE, FROZEN, OCC, VIR, FROZEN_OCC, ACTIVE_OCC, ACTIVE_VIR, FROZEN_VIR |

Returns

the matrix in Pitzer order in the desired basis

17.30.3.2 `SharedMatrix oepdev::WavefunctionUnion::Cb_subset (const std::string & basis = "SO", const std::string & subset = "ALL")`

Return a subset of the Cb matrix in a desired basis

Parameters

| | |
|---------------|--|
| <i>basis</i> | the symmetry basis to use AO, SO |
| <i>subset</i> | the subset of orbitals to return ALL, ACTIVE, FROZEN, OCC, VIR, FROZEN_OCC, ACTIVE_OCC, ACTIVE_VIR, FROZEN_VIR |

Returns

the matrix in Pitzer order in the desired basis

The documentation for this class was generated from the following files:

- oepdev/libutil/[wavefunction_union.h](#)
- oepdev/libutil/wavefunction_union.cc

Chapter 18

File Documentation

18.1 include/oepdev_files.h File Reference

Macros

- `#define OEPDEV_USE_PSI4_DIIS_MANAGER 0`
Use DIIS from Psi4 (1) or OEPDev (0)?
- `#define OEPDEV_MAX_AM 8`
L_max.
- `#define OEPDEV_N_MAX_AM 17`
2L_max+1
- `#define OEPDEV_CRIT_ERI 1e-9`
*ERI criterion for E12, E34, E123 and lambda*EXY coefficients.*
- `#define OEPDEV_SIZE_BUFFER_R 250563`
*Size of R buffer (OEPDEV_N_MAX_AM*OEPDEV_N_MAX_AM*OEPDEV_N_MAX_AM*OEPDEV_N_MAX_AM*3)*
- `#define OEPDEV_SIZE_BUFFER_D2 3264`
Size of D2 buffer (3(OEPDEV_MAX_AM+1)*(OEPDEV_MAX_AM+1)*OEPDEV_N_MAX_AM)*

18.2 main.cc File Reference

```
#include <cstdlib>
#include <cstdio>
#include <string>
#include "psi4/psi4-dec.h"
#include "psi4/psifiles.h"
#include "psi4/libdpd/dpd.h"
#include "include/oepdev_files.h"
#include "psi4/libparallel/parallel.h"
#include "psi4/liboptions/liboptions.h"
#include "psi4/libpsio/psio.h"
#include "psi4/libpsio/psio.hpp"
#include "psi4/libmints/molecule.h"
#include "psi4/libmints/wavefunction.h"
#include "psi4/libmints/basisset.h"
#include "psi4/libfunctional/superfunctional.h"
#include "oepdev/libutil/util.h"
#include "oepdev/libutil/cphf.h"
```

Namespaces

- [psi](#)

Psi4 package namespace.

Typedefs

- using **SharedMolecule** = std::shared_ptr< Molecule >
- using **SharedSuperFunctional** = std::shared_ptr< SuperFunctional >
- using **SharedWavefunction** = std::shared_ptr< Wavefunction >
- using **SharedVector** = std::shared_ptr< Vector >
- using **SharedMatrix** = std::shared_ptr< Matrix >
- using **SharedBasisSet** = std::shared_ptr< BasisSet >
- using **SharedUnion** = std::shared_ptr< [oepdev::WavefunctionUnion](#) >
- using **SharedPSIO** = std::shared_ptr< PSIO >
- using **SharedCPHF** = std::shared_ptr< [oepdev::CPHF](#) >
- using **SharedMOSpace** = std::shared_ptr< MOSpace >
- using **SharedIntegralTransform** = std::shared_ptr< IntegralTransform >
- using **SharedIntegralFactory** = std::shared_ptr< IntegralFactory >
- using **SharedTwoBodyAOInt** = std::shared_ptr< TwoBodyAOInt >
- using **SharedMOSpaceVector** = std::vector< std::shared_ptr< MOSpace >>
- using **intVector** = std::vector< int >
- using **SharedLocalizer** = std::shared_ptr< Localizer >
- using **SharedOEPotential** = std::shared_ptr< [oepdev::OEPotential](#) >
- using **SharedField3D** = std::shared_ptr< [oepdev::ScalarField3D](#) >

Functions

- int [psi::read_options](#) (std::string name, Options &options)
Options for the OEPDev plugin.
- SharedWavefunction [psi::oepdev](#) (SharedWavefunction ref_wfn, Options &options)
Main routine of the OEPDev plugin.

18.3 oepdev/libints/eri.h File Reference

```
#include "psi4/libpsi4util/exception.h"
#include "psi4/libmints/integral.h"
#include "psi4/libmints/basisset.h"
#include "psi4/libmints/fjt.h"
#include "../libpsi/integral.h"
#include "recurr.h"
```

Classes

- class [oepdev::TwoElectronInt](#)
General Two Electron Integral.
- class [oepdev::ERI_2_2](#)
4-centre ERI of the form $(ab|O(2)|cd)$ where $O(2) = 1/r12$.
- class [oepdev::ERI_3_1](#)
4-centre ERI of the form $(abc|O(2)|d)$ where $O(2) = 1/r12$.

Namespaces

- [oepdev](#)

OEPEv module namespace.

18.4 oepdev/libints/recur.h File Reference

Namespaces

- [oepdev](#)

OEPEv module namespace.

Macros

- `#define D1_INDEX(x, i, n) ((81*(x))+(9*(i))+(n))`

Get the index of McMurchie-Davidson-Hermite D1 coefficient stored in the `mdh_buffer_`, that is attributed to the x Cartesian coordinate from angular momentum i of function 1, and the Hermite index n .

- `#define D2_INDEX(x, i, j, n) ((1377*(x))+(153*(i))+(17*(j))+(n))`

Get the index of McMurchie-Davidson-Hermite D2 coefficient stored in the `mdh_buffer_`, that is attributed to the x Cartesian coordinate from angular momenta i, j of function 1 and 2, and the Hermite index n .

- `#define D3_INDEX(x, i, j, k, n) ((18225*(x))+(2025*(i))+(225*(j))+(25*(k))+(n))`

Get the index of McMurchie-Davidson-Hermite D3 coefficient stored in the `mdh_buffer_`, that is attributed to the x Cartesian coordinate from angular momenta i, j and k of function 1, 2 and 3, and the Hermite index n .

- `#define R_INDEX(n, l, m, j) ((14739*(n))+(867*(l))+(51*(m))+(j))`

Get the index of McMurchie-Davidson R coefficient stored in the `mdh_buffer_R_` from angular momenta n, l and m and the Boys index j .

Functions

- `double oepdev::d_N_n1_n2 (int N, int n1, int n2, double PA, double PB, double aP)`

Compute McMurchie-Davidson-Hermite (MDH) coefficient for binomial expansion.

- `void oepdev::make_mdh_D1_coeff (int n1, double aPd, double *buffer)`

Compute the McMurchie-Davidson-Hermite coefficients for monomial expansion.

- `void oepdev::make_mdh_D2_coeff (int n1, int n2, double aPd, double *PA, double *PB, double *buffer)`

Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion.

- `void oepdev::make_mdh_D3_coeff (int n1, int n2, int n3, double aPd, double *PA, double *PB, double *PC, double *buffer)`

Compute the McMurchie-Davidson-Hermite coefficients for trinomial expansion.

- `void oepdev::make_mdh_D2_coeff_explicit_recursion (int n1, int n2, double aP, double *PA, double *PB, double *buffer)`

Compute the McMurchie-Davidson-Hermite coefficients for binomial expansion by explicit recursion. This function makes the same changes to buffers as `oepdev::make_mdh_D2_coeff`, but implements it through explicit recursion by calls to `oepdev::d_N_n1_n2`. Therefore, it is slightly slower. Here for debugging purposes.

- `void oepdev::make_mdh_R_coeff (int N, int L, int M, double alpha, double a, double b, double c, double *F, double *buffer)`

Compute the McMurchie-Davidson R coefficients.

18.5 oepdev/liboep/oep.h File Reference

```
#include <cstdio>
#include <string>
#include <vector>
#include <map>
#include "psi4/libparallel/parallel.h"
#include "psi4/liboptions/liboptions.h"
#include "psi4/libmints/wavefunction.h"
#include "psi4/libmints/basisset.h"
#include "psi4/libmints/matrix.h"
#include "psi4/libmints/vector.h"
#include "psi4/libthce/thce.h"
#include "psi4/libcubeprop/csg.h"
#include "../libutil/space3d.h"
```

Classes

- class [oepdev::OEPotential](#)
Generalized One-Electron Potential: Abstract base.
- class [oepdev::ElectrostaticEnergyOEPotential](#)
Generalized One-Electron Potential for Electrostatic Energy.
- class [oepdev::RepulsionEnergyOEPotential](#)
Generalized One-Electron Potential for Pauli Repulsion Energy.
- class [oepdev::ChargeTransferEnergyOEPotential](#)
Generalized One-Electron Potential for Charge-Transfer Interaction Energy.
- class [oepdev::EETCouplingOEPotential](#)
Generalized One-Electron Potential for EET coupling calculations.

Namespaces

- [oepdev](#)
OEPEv module namespace.

Typedefs

- using [oepdev::SharedWavefunction](#) = std::shared_ptr< Wavefunction >
- using [oepdev::SharedBasisSet](#) = std::shared_ptr< BasisSet >
- using [oepdev::SharedTensor](#) = std::shared_ptr< Tensor >
- using [oepdev::SharedMatrix](#) = std::shared_ptr< Matrix >
- using [oepdev::SharedVector](#) = std::shared_ptr< Vector >

18.6 oepdev/libpsi/integral.h File Reference

```
#include "psi4/libmints/integral.h"
#include "psi4/libmints/basisset.h"
```

Classes

- class [oepdev::IntegralFactory](#)
Extended [IntegralFactory](#) for computing integrals.

Namespaces

- [oepdev](#)
OEPPDev module namespace.

18.7 oepdev/libpsi/potential.h File Reference

```
#include <vector>
#include "psi4/psi4-dec.h"
#include "psi4/libparallel/parallel.h"
#include "psi4/liboptions/liboptions.h"
#include "psi4/libpsio/psio.h"
#include "psi4/libmints/typedefs.h"
#include "psi4/libmints/onebody.h"
#include "psi4/libmints/potential.h"
#include "psi4/libmints/sointegral_onebody.h"
#include "psi4/libmints/osrecur.h"
```

Classes

- class [oepdev::PotentialInt](#)
Computes potential integrals.

Namespaces

- [oepdev](#)
OEPPDev module namespace.

18.8 oepdev/libtest/test.h File Reference

```
#include <vector>
#include "psi4/psi4-dec.h"
#include "psi4/libparallel/parallel.h"
#include "psi4/liboptions/liboptions.h"
#include "psi4/libpsio/psio.h"
#include "psi4/libmints/integral.h"
#include "psi4/libmints/wavefunction.h"
#include "psi4/libmints/basisset.h"
#include "psi4/libqt/qt.h"
#include "../libpsi/integral.h"
#include "../libutil/integrals_iter.h"
```

Classes

- class [oepdev::test::Test](#)
Manages test routines.

Namespaces

- [oepdev](#)
OEPEv module namespace.

18.9 oepdev/libutil/diis.h File Reference

```
#include <stdio>
#include <string>
#include <vector>
#include "psi4/libparallel/parallel.h"
#include "psi4/libciomr/libciomr.h"
#include "psi4/libmints/vector.h"
#include "psi4/libmints/matrix.h"
#include "psi4/libqt/qt.h"
```

Classes

- class [oepdev::DIISManager](#)
DIIS manager.

Namespaces

- [oepdev](#)
OEPEv module namespace.

18.10 oepdev/libutil/esp.h File Reference

```
#include "psi4/libmints/vector.h"
#include "space3d.h"
```

Classes

- class [oepdev::ESPSolver](#)
Charges from Electrostatic Potential (ESP). A solver-type class.

Namespaces

- [psi](#)
Psi4 package namespace.
- [oepdev](#)
OEPEv module namespace.

Typedefs

- using **psi::SharedVetor** = std::shared_ptr< Vector >
- using **oepdev::SharedScalarField3D** = std::shared_ptr< ScalarField3D >

18.11 oepdev/libutil/integrals_iter.h File Reference

```
#include <cstdio>
#include "psi4/libparallel/parallel.h"
#include "psi4/libmints/basisset.h"
#include "psi4/libmints/integral.h"
```

Classes

- class [oepdev::AllAOShellCombinationsIterator](#)
Loop over all possible ERI shells.
- class [oepdev::AllAOIntegralsIterator](#)
Loop over all possible ERI within a particular shell.

Namespaces

- [oepdev](#)
OEPEv module namespace.

Typedefs

- using **oepdev::SharedIntegralFactory** = std::shared_ptr< IntegralFactory >
- using **oepdev::SharedTwoBodyAOInt** = std::shared_ptr< TwoBodyAOInt >

18.12 oepdev/libutil/solver.h File Reference

```
#include <cstdio>
#include <string>
#include <map>
#include "psi4/psi4-dec.h"
#include "psi4/libparallel/parallel.h"
#include "psi4/liboptions/liboptions.h"
#include "psi4/libpsio/psio.h"
#include "psi4/libmints/potential.h"
#include "psi4/libmints/integral.h"
#include "wavefunction_union.h"
#include "integrals_iter.h"
#include "../liboep/oep.h"
```

Classes

- class [oepdev::OEPEvSolver](#)
Solver of properties of molecular aggregates. Abstract base.

- class [oepdev::ElectrostaticEnergySolver](#)

Compute the Coulombic interaction energy between unperturbed wavefunctions.

- class [oepdev::RepulsionEnergySolver](#)

Compute the Pauli-Repulsion interaction energy between unperturbed wavefunctions.

- class [oepdev::ChargeTransferEnergySolver](#)

Compute the Charge-Transfer interaction energy between unperturbed wavefunctions.

Namespaces

- [oepdev](#)

OEPEDev module namespace.

Typedefs

- using **oepdev::SharedWavefunctionUnion** = std::shared_ptr< WavefunctionUnion >
- using **oepdev::SharedOEPotential** = std::shared_ptr< OEPotential >

18.13 oepdev/libutil/util.h File Reference

```
#include <cstdio>
#include <string>
#include <map>
#include "psi4/psi4-dec.h"
#include "psi4/libparallel/parallel.h"
#include "psi4/liboptions/liboptions.h"
#include "psi4/libpsio/psio.h"
#include "psi4/libciomr/libciomr.h"
#include "psi4/libpsio/psio.hpp"
#include "psi4/libiwl/iwl.h"
#include "psi4/libqt/qt.h"
#include "psi4/libmints/molecule.h"
#include "psi4/libmints/writer.h"
#include "psi4/libmints/writer_file_prefix.h"
#include "psi4/libmints/wavefunction.h"
#include "psi4/libmints/basisset.h"
#include "psi4/libmints/vector.h"
#include "psi4/libmints/matrix.h"
#include "psi4/libmints/oeprop.h"
#include "psi4/libmints/local.h"
#include "psi4/libfunctional/superfunctional.h"
#include "psi4/libtrans/mospace.h"
#include "psi4/libtrans/integraltransform.h"
#include "psi4/libscf_solver/rhf.h"
#include "psi4/libdpd/dpd.h"
```

Namespaces

- [oepdev](#)

OEPEDev module namespace.

Typedefs

- using **oepdev::SharedMolecule** = std::shared_ptr< Molecule >
- using **oepdev::SharedSuperFunctional** = std::shared_ptr< SuperFunctional >
- using **oepdev::SharedMOSpace** = std::shared_ptr< MOSpace >
- using **oepdev::SharedMOSpaceVector** = std::vector< std::shared_ptr< MOSpace >>
- using **oepdev::SharedIntegralTransform** = std::shared_ptr< IntegralTransform >
- using **oepdev::SharedLocalizer** = std::shared_ptr< Localizer >

Functions

- void **oepdev::preamble** (void)
Print preamble for module OEPDEV.
- std::shared_ptr< SuperFunctional > **oepdev::create_superfunctional** (std::string name, Options &options)
Set up DFT functional.
- std::shared_ptr< Molecule > **oepdev::extract_monomer** (std::shared_ptr< const Molecule > molecule_dimer, int id)
Extract molecule from dimer.
- std::shared_ptr< Wavefunction > **oepdev::solve_scf** (std::shared_ptr< Molecule > molecule, std::shared_ptr< BasisSet > primary, std::shared_ptr< SuperFunctional > functional, Options &options, std::shared_ptr< PSIO > psio)
Solve RHF-SCF equations for a given molecule in a given basis set.

18.14 oepdev/libutil/wavefunction_union.h File Reference

```
#include <cstdio>
#include <string>
#include <map>
#include "psi4/psi4-dec.h"
#include "psi4/libparallel/parallel.h"
#include "psi4/liboptions/liboptions.h"
#include "psi4/libpsio/psio.h"
#include "psi4/libciomr/libciomr.h"
#include "psi4/libpsio/psio.hpp"
#include "psi4/libqt/qt.h"
#include "psi4/libmints/molecule.h"
#include "psi4/libmints/writer.h"
#include "psi4/libmints/writer_file_prefix.h"
#include "psi4/libmints/wavefunction.h"
#include "psi4/libmints/basisset.h"
#include "psi4/libmints/vector.h"
#include "psi4/libmints/matrix.h"
#include "psi4/libmints/oeprop.h"
#include "psi4/libmints/local.h"
#include "psi4/libfunctional/superfunctional.h"
#include "psi4/libtrans/mospace.h"
#include "psi4/libtrans/integraltransform.h"
#include "psi4/libscf_solver/rhf.h"
#include "psi4/libdpd/dpd.h"
```

Classes

- class **oepdev::WavefunctionUnion**

Union of two Wavefunction objects.

Namespaces

- [oepdev](#)

OEPEv module namespace.

Chapter 19

Example Documentation

19.1 example_integrals_iter.cc

Iterations over electron repulsion integrals in AO basis. This is an example of how to use

- the AllAOShellCombinationsIterator class
- the AllAOIntegralsIterator class.

```
void iterate(std::shared_ptr<oeplib::IntegralFactory> ints)
{
    // Prepare for direct calculation of ERI's (shell by shell)
    std::shared_ptr<psi::TwoBodyAOInt> tei(ints->eri());

    // Grab the buffer where the integrals for a current shell will be placed
    const double* buffer = tei->buffer();

    // Create iterator to go through all shell quartet combinations
    oeplib::AllAOShellCombinationsIterator shellIter(ints);

    // Iterate over shells, and then over all integrals in each shell quartet
    for (shellIter.first(); shellIter.is_done() == false; shellIter.
        next())
    {
        // Compute all integrals between shells in the current quartet
        shellIter.compute_shell(tei);

        // Create iterator to go through all integrals within a shell quartet
        oeplib::AllAOIntegralsIterator intsIter(shellIter);

        for (intsIter.first(); intsIter.is_done() == false; intsIter.
            next())
        {
            // Grab current (ij|kl) indices here
            int i = intsIter.i();
            int j = intsIter.j();
            int k = intsIter.k();
            int l = intsIter.l();

            // Grab the (ij|kl) integral
            double integral = buffer[intsIter.index()];
        }
    }
}
```

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