

progress

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# Chapter 1

## README

### A library for quantum chemistry solvers.

PROGRESS: Parallel, Rapid  $O(N)$  and Graph-based Recursive Electronic Structure Solver. **LA-CC-16-068**

- This library is focused on the development of general solvers that are commonly used in *quantum chemistry packages*.
- This library has to be compiled with the *Basic Matrix Library* (BML).
- Our webpage can be found at <https://lanl.github.io/qmd-progress/>

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## Build Dependencies

- `>=OpenMP-3.1`
- `>=metis-5.0` if building with `PROGRESS_GRAPHLIB`

(On some distributions, metis is available as a package. Make sure you install the `-dev` package. For example, Ubuntu requires `libmetis-dev`.)

## Build and Install Instructions

### How to build

```
$ CMAKE_PREFIX_PATH=<BML install path> ./build.sh
```

### How to install

```
$ cd build
$ sudo make install
```

To specify the Intel Fortran compiler:

```
$ FC=ifort PKG_CONFIG_PATH=<BML install path>/lib/pkgconfig ./build.sh
```

To build with the gfortran compiler and OpenMP:

```
$ CC=gcc FC=gfortran \
  CMAKE_BUILD_TYPE=Release \
  PROGRESS_OPENMP=yes \
  CMAKE_PREFIX_PATH=<BML install path> \
  CMAKE_INSTALL_PREFIX=<PROGRESS install path> \
  ./build.sh configure
```

To build with OpenMP, MPI and testing enabled:

```
$ CC=mpicc FC=mpif90 \
  CMAKE_BUILD_TYPE=Release \
  PROGRESS_OPENMP=yes \
  PROGRESS_MPI=yes \
  PROGRESS_TESTING=yes \
  CMAKE_PREFIX_PATH=<BML install path> \
  CMAKE_INSTALL_PREFIX=<PROGRESS install path> \
  ./build.sh configure
```

To build with OpenMP, MPI, testing enabled and example programs built:

```
$ CC=mpicc FC=mpif90 \
  CMAKE_BUILD_TYPE=Release \
  PROGRESS_OPENMP=yes \
  PROGRESS_MPI=yes \
  PROGRESS_TESTING=yes \
  PROGRESS_EXAMPLES=yes \
  CMAKE_PREFIX_PATH=<BML install path> \
  CMAKE_INSTALL_PREFIX=<PROGRESS install path> \
  ./build.sh configure
```

To build with OpenMP and MPI and testing enabled and example programs built and the METIS graph partitioning library:

```
$ CC=mpicc FC=mpif90 \
  CMAKE_BUILD_TYPE=Release \
  PROGRESS_OPENMP=yes \
  PROGRESS_MPI=yes \
  PROGRESS_GRAPHLIB=yes \
  PROGRESS_TESTING=yes \
  PROGRESS_EXAMPLES=yes \
  CMAKE_PREFIX_PATH=<BML install path> \
  CMAKE_INSTALL_PREFIX=<PROGRESS install path> \
  ./build.sh configure
```



---

## Citing

```
@misc{2016progress,  
  title={\textrm{PROGRESS} Version 1.0},  
  author={Niklasson, Anders M. and Mniszewski, Susan M and Negre, Christian F. A. and Wall, Michael E. and C},  
  year={2016},  
  url = {https://github.com/lanl/qmd-progress},  
  institution={Los Alamos National Laboratory (LANL), Los Alamos, NM (United States)}  
}
```



## Chapter 2

# Testing the Progress library

### Testing program for the progress library

#### To run the tests:

Go into the build folder and type:

```
make test
```

To run the tests in verbose mode:

```
make test ARGS="-V"
```

#### To run a single test:

To run a test on its own (in build) we just need to type:

```
/qmd-progress/build/main <test_name>
```

, where "test\_name" is the name of the test we want to run. Right now the keywords (test\_name) we can pass are the following:

- density : Tests the diagonalization routine to build the density.
- sp2\_short : Tests the first version of sp2
- sp2\_alg1 : Algorithm 1 for sp2
- sp2\_alg2 : Algorithm 2 for sp2
- sp2\_alg2\_ellpack : Algorithm 2 for sp2 with ellpack
- sp2\_alg1\_seq : See sp2\_mod.F90 source file
- sp2\_alg2\_seq : See sp2\_mod.F90 source file
- deorthogonalize\_dense: See nonortho.F90 source file
- orthogonalize\_dense: See nonortho.F90 source file
- buildzdiag: See genz\_mod.F90 source file

**To add a test:**

- add the corresponding name of the test in `/progress/tests/CMakeLists.txt`
- add the corresponding keyword and test in `/progress/tests/src/main.F90`
- Copy any file that is necessary to run (data) in `/progress/tests/tests_data/`
- reconfigure and recompile

## Chapter 3

# Todo List

### Module `prg_dos_mod`

Add LDOS.

Subprogram `prg_pulaycomponent_mod::prg_pulaycomponent0` (rho\_bml, ham\_bml, pcm\_bml, threshold, M, bml\_type, verbose)

M and bml\_type will have to be removed from the input parameter.

Subprogram `prg_pulaycomponent_mod::prg_pulaycomponentt` (rho\_bml, ham\_bml, zmat\_bml, pcm\_bml, threshold, M, bml\_type, verbose)

M and bml\_type will have to be removed from the input parameter.

### Module `prg_pulaymixer_mod`

add the density matrix mixer.

### Module `prg_response_mod`

Add the response scf

Change name response\_SP2 to dm\_prt\_response

Change name response\_rs to rs\_prt\_response

Subprogram `prg_response_mod::prg_pert_from_file` (prt\_bml, norb)

Add read perturbation from file

Subprogram `prg_system_mod::prg_parse_system` (system, filename, extin)

Integrate this loop in the loop for building the splist.



## Chapter 4

# Module Index

### 4.1 Modules

Here is a list of all modules:

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| (PROGRESS related routines) . . . . .                     | <a href="#">18</a> |
| (EXTERNAL related routines) . . . . .                     | <a href="#">20</a> |
| (High-level codes using PROGRESS/LATTE modules) . . . . . | <a href="#">21</a> |





## Chapter 5

# Modules Index

### 5.1 Modules List

Here is a list of all modules with brief descriptions:

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| <a href="#">prg_charges_mod</a>        | A module to compute the Mulliken charges of a chemical system . . . . .                          | 23  |
| <a href="#">prg_chebyshev_mod</a>      | Module to obtain the density matrix by applying a Chebyshev polynomial expansion . . . . .       | 25  |
| <a href="#">prg_densitymatrix_mod</a>  | Module to obtain the density matrix by diagonalizing an prg_orthogonalized Hamiltonian . . . . . | 33  |
| <a href="#">prg_dos_mod</a>            | A module to compute the Density of state (DOS) and IDOS . . . . .                                | 39  |
| <a href="#">prg_extras_mod</a>         | Extra routines: . . . . .  | 41  |
| <a href="#">prg_genz_mod</a>           | To produce a matrix $Z$ which is needed to orthogonalize $H$ . . . . .                           | 45  |
| <a href="#">prg_graph_mod</a>          | The graph module . . . . .   | 51  |
| <a href="#">prg_graphsp2parser_mod</a> | Graph partitioning SP2 parser . . . . .  | 59  |
| <a href="#">prg_homolumo_mod</a>       | The homolumo module . . . . .  | 61  |
| <a href="#">prg_implicit_fermi_mod</a> |  | 61  |
| <a href="#">prg_initmatrices_mod</a>   | Initialization module . . . . .  | 62  |
| <a href="#">prg_kernelparser_mod</a>   | Some general parsing functions . . . . .   | 64  |
| <a href="#">prg_nonortho_mod</a>       | Module to prg_orthogonalize and prg_deorthogonalize any operator . . . . .                       | 67  |
| <a href="#">prg_normalize_mod</a>      | The prg_normalize module . . . . .   | 69  |
| <a href="#">prg_openfiles_mod</a>      | Module to handle input output files for the PROGRESS lib . . . . .                               | 74  |
| <a href="#">prg_parallel_mod</a>       | The parallel module . . . . .  | 77  |
| <a href="#">prg_partition_mod</a>      | The partition module . . . . .   | 93  |
| <a href="#">prg_progress_mod</a>       | The progress module . . . . .  | 108 |

|   |     |
|---|-----|
| <a href="#">prg_ptable_mod</a>  |     |
| Periodic table of elements  | 110 |
| <a href="#">prg_pulaycomponent_mod</a>                                |     |
| Produces a matrix to get the Pulay Component of the forces            | 117 |
| <a href="#">prg_pulaymixer_mod</a>                                    |     |
| Pulay mixer mode  | 119 |
| <a href="#">prg_quantumdynamics_mod</a>                               |     |
| A module to add in common quantum dynamical operations                | 121 |
| <a href="#">prg_response_mod</a>                                      |     |
| Module to compute the density matrix response and related quantities  | 125 |
| <a href="#">prg_sp2_fermi_mod</a>                                     |     |
| The SP2 Fermi module  | 132 |
| <a href="#">prg_sp2_mod</a>   |     |
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| SP2 parser  | 144 |
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| The subgraphloop module   | 145 |
| <a href="#">prg_syrotation_mod</a>                                    |     |
| A module to rotate the coordinates of a sybsystem in chemical systems | 149 |
| <a href="#">prg_system_mod</a>  |     |
| A module to read and handle chemical systems                          | 151 |
| <a href="#">prg_timer_mod</a>   |     |
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| A module to perform XLBO integration                                  | 175 |
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## Chapter 6

# Data Type Index

### 6.1 Data Types List

Here are the data types with brief descriptions:

|  |     |
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| <a href="#">prg_chebyshev_mod::chebdata_type</a>       |     |
| General Cheb solver type . . . . .                     | 183 |
| <a href="#">prg_system_mod::estruct_type</a>           |     |
| Electronic structure type . . . . .                    | 185 |
| <a href="#">prg_genz_mod::genzspdata</a>               |     |
| Data for the genZ driver . . . . .                     | 189 |
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| Input for the genz driver . . . . .                    | 190 |
| <a href="#">prg_graph_mod::graph_partitioning_t</a>    |     |
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| System type . . . . .                                  | 211 |
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| Timer status type . . . . .                            | 217 |
| <a href="#">prg_extras_mod::to_string</a>              | 219 |
| <a href="#">prg_xlbo_mod::xlbo_type</a>                |     |
| General xlbo solver type . . . . .                     | 220 |
| <a href="#">prg_xlkernel_mod::xlk_type</a>             | 222 |



## Chapter 7

# File Index

### 7.1 File List

Here is a list of all files with brief descriptions:

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| /home/christian/qmd-progress/src/prg_densitymatrix_mod.F90   | 226 |
| /home/christian/qmd-progress/src/prg_dos_mod.F90             | 227 |
| /home/christian/qmd-progress/src/prg_doxy_mod.F90            | 228 |
| /home/christian/qmd-progress/src/prg_extras_mod.F90          | 228 |
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| /home/christian/qmd-progress/src/prg_xlbo_mod.F90            | 248 |
| /home/christian/qmd-progress/src/prg_xlkernel_mod.F90        | 249 |



## **Chapter 8**

# **Module Documentation**

### **8.1 (LATTE related routines)**

## 8.2 (PROGRESS related routines)

### Modules

- module [prg\\_charges\\_mod](#)  
*A module to compute the Mulliken charges of a chemical system.*
- module [prg\\_chebyshev\\_mod](#)  
*Module to obtain the density matrix by applying a Chebyshev polynomial expansion.*
- module [prg\\_densitymatrix\\_mod](#)  
*Module to obtain the density matrix by diagonalizing an `prg_orthogonalized` Hamiltonian.*
- module [prg\\_extras\\_mod](#)  
*Extra routines:*
- module [prg\\_genz\\_mod](#)  
*To produce a matrix  $Z$  which is needed to orthogonalize  $H$ .*
- module [prg\\_graph\\_mod](#)  
*The graph module.*
- module [prg\\_graphsp2parser\\_mod](#)  
*Graph partitioning SP2 parser.*
- module [prg\\_homolumo\\_mod](#)  
*The homolumo module.*
- module [prg\\_initmatrices\\_mod](#)  
*Initialization module.*
- module [prg\\_kernelparser\\_mod](#)  
*Some general parsing functions.*
- module [prg\\_nonortho\\_mod](#)  
*Module to `prg_orthogonalize` and `prg_deorthogonalize` any operator.*
- module [prg\\_openfiles\\_mod](#)  
*Module to handle input output files for the PROGRESS lib.*
- module [prg\\_parallel\\_mod](#)  
*The parallel module.*
- module [prg\\_progress\\_mod](#)  
*The progress module.*
- module [prg\\_ptable\\_mod](#)  
*Periodic table of elements.*
- module [prg\\_pulaycomponent\\_mod](#)  
*Produces a matrix to get the Pulay Component of the forces.*
- module [prg\\_pulaymixer\\_mod](#)  
*Pulay mixer mode.*
- module [prg\\_quantumdynamics\\_mod](#)  
*A module to add in common quantum dynamical operations.*
- module [prg\\_response\\_mod](#)  
*Module to compute the density matrix response and related quantities.*
- module [prg\\_sp2\\_fermi\\_mod](#)  
*The SP2 Fermi module.*
- module [prg\\_sp2\\_mod](#)  
*The SP2 module.*
- module [prg\\_sp2parser\\_mod](#)  
*SP2 parser.*
- module [prg\\_syrotation\\_mod](#)  
*A module to rotate the coordinates of a subsystem in chemical systems.*



- module `prg_system_mod`  
*A module to read and handle chemical systems.*
- module `prg_timer_mod`  
*The timer module.*
- module `prg_xlbo_mod`  
*A module to perform XLBO integration.*
- module `prg_xlkernel_mod`  
*Add name.*

### 8.2.1 Detailed Description

### 8.3 (EXTERNAL related routines)

## 8.4 (High-level codes using PROGRESS/LATTE modules)



## Chapter 9

# Module Documentation

### 9.1 prg\_charges\_mod Module Reference

A module to compute the Mulliken charges of a chemical system.

#### Functions/Subroutines

- subroutine, public [prg\\_get\\_charges](#) (rho\_bml, over\_bml, hindex, charges, numel, spindex, mdimin, threshold)  
*Constructs the charges from the density matrix.*
- subroutine, public [prg\\_get\\_hscf](#) (ham0\_bml, over\_bml, ham\_bml, spindex, hindex, hubbardu, charges, coulomb\_pot\_r, coulomb\_pot\_k, mdimin, threshold)  
*Constructs the SCF hamiltonian given H0, HubbardU and charges. This routine does:  $H = \sum_i U_i q_i + V_i$ , where  $U$  is the Hubbard parameter for every atom  $i$ .  $V$  is the coulombic potential for every atom  $i$ .*

#### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.1.1 Detailed Description

A module to compute the Mulliken charges of a chemical system.

This module contains routines that compute properties related to charges.

#### 9.1.2 Function/Subroutine Documentation

9.1.2.1 subroutine, public prg\_charges\_mod::prg\_get\_charges ( type(bml\_matrix\_t), intent(inout) rho\_bml, type(bml\_matrix\_t), intent(inout) over\_bml, integer, dimension(:, :), intent(in) hindex, real(dp), dimension(:), intent(inout), allocatable charges, real(dp), dimension(:), intent(in) numel, integer, dimension(:), intent(in) spindex, integer, intent(in) mdimin, real(dp), intent(in) threshold )

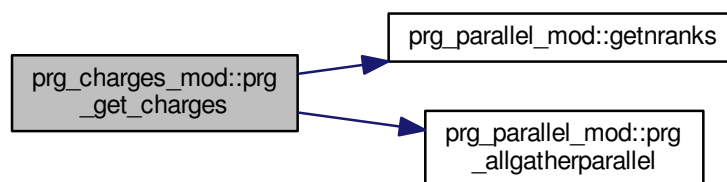
Constructs the charges from the density matrix.

## Parameters

|                  |   |
|------------------|---|
| <i>rho_bml</i>   | Density matrix in bml format.                       |
| <i>over_bml</i>  | Overlap matrix in bml format.                       |
| <i>hindex</i>    | Start and end index for every atom in the system.   |
| <i>charges</i>   | Output parameter that gives the vectorized charges. |
| <i>threshold</i> | Threshold value for matrix elements.                |

Definition at line 31 of file prg\_charges\_mod.F90.

Here is the call graph for this function:



9.1.2.2 subroutine, public prg\_charges\_mod::prg\_get\_hscf ( type(bml\_matrix\_t), intent(in) *ham0\_bml*, type(bml\_matrix\_t), intent(in) *over\_bml*, type(bml\_matrix\_t), intent(inout) *ham\_bml*, integer, dimension(:), intent(in) *spindex*, integer, dimension(:,:), intent(in) *hindex*, real(dp), dimension(:), intent(in) *hubbardu*, real(dp), dimension(:), intent(in) *charges*, real(dp), dimension(:), intent(in) *coulomb\_pot\_r*, real(dp), dimension(:), intent(in) *coulomb\_pot\_k*, integer, intent(in) *mdimin*, real(dp), intent(in) *threshold* )

Constructs the SCF hamiltonian given H0, HubbardU and charges. This routine does:  $H = \sum_i U_i q_i + V_i$ , where  $U$  is the Hubbard parameter for every atom  $i$ .  $V$  is the coulombic potential for every atom  $i$ .

## Parameters

|                                   |  |
|-----------------------------------|--|
| <i>ham_bml</i>                    | Hamiltonian in bml format.                         |
| <i>over_bml</i>                   | Overlap in bml format.                             |
| <i>hindex</i>                     | Start and end index for every atom in the system.  |
| <i>hubbardu</i>                   | Hubbard parameter for every atom.                  |
| <i>charges</i>                    | Charges for every atom.                            |
| <i>coulomb_pot</i> ↔<br><i>_r</i> | Coulombic potential (r contribution)               |
| <i>coulomb_pot</i> ↔<br><i>_k</i> | Coulombic potential (k contribution)               |
| <i>mdim</i>                       | Maximum non zeroes elements per row for every row. |
| <i>threshold</i>                  | Threshold value for matrix elements.               |

Definition at line 101 of file prg\_charges\_mod.F90.

### 9.1.3 Variable Documentation

#### 9.1.3.1 integer, parameter prg\_charges\_mod::dp = kind(1.0d0) [private]

Definition at line 17 of file prg\_charges\_mod.F90.

## 9.2 prg\_chebyshev\_mod Module Reference

Module to obtain the density matrix by applying a Chebyshev polynomial expansion.

### Data Types

- type [chebdata\\_type](#)  
General Cheb solver type.

### Functions/Subroutines

- subroutine, public [prg\\_parse\\_cheb](#) (chebdata, filename)  
*Chebyshev parser. This module is used to parse all the input variables for the cheb electronic structure solver. Adding a new input keyword to the parser:*
- subroutine, public [prg\\_build\\_density\\_cheb](#) (ham\_bml, rho\_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, jon, verbose)  
*Builds the density matrix from  $H_0$  for a Fermi function approximated with a Chebyshev polynomial expansion.*
- subroutine, public [prg\\_build\\_density\\_cheb\\_fermi](#) (ham\_bml, rho\_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, getef, fermitol, jon, npts, trkfunc, verbose)  
*Builds the density matrix from  $H_0$  for a Fermi function approximated with a Chebyshev polynomial expansion. In this case the self-consistent recursion is applied to converge to the correct number of electrons and obtain the Fermi level.*
- real(dp) function [jackson](#) (ncoeffs, i, jon)  
*Evaluates the Jackson Kernel Coefficients.*
- subroutine [prg\\_get\\_chebcoeffs](#) (npts, kbt, ef, ncoeffs, coeffs, emin, emax)  
*Gets the coefficients of the Chebyshev expansion.*
- subroutine [prg\\_get\\_chebcoeffs\\_fermi\\_bs](#) (npts, kbt, ef, tracesT, ncoeffs, coeffs, emin, emax, bndfil, norb, tol, jon, verbose)  
*Gets the coefficients of the Chebyshev expansion with Ef computation.*
- subroutine [prg\\_get\\_chebcoeffs\\_fermi\\_nt](#) (npts, kbt, ef, tracesT, ncoeffs, coeffs, emin, emax, bndfil, norb, tol, jon, verbose)  
*Gets the coefficients of the Chebyshev expansion with Ef computation.*
- real(dp) function [tr](#) (r, x)  
*Chebyshev polynomial obtained by recursion.*
- real(dp) function [fermi](#) (e, ef, kbt)  
*Gives the Fermi distribution value for energy e.*
- real(dp) function [absmaxderivative](#) (func, de)  
*Gets the absolute maximum of the derivative of a function.*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)
- real(dp), parameter [pi](#) = 3.14159265358979323846264338327950\_dp

### 9.2.1 Detailed Description

Module to obtain the density matrix by applying a Chebyshev polynomial expansion.

See Amparo Gil 2007 [**Amparo2007**] , See Silver et al [**Silver1996**] , See Weisse et al [**Weisse2006**]

### 9.2.2 Function/Subroutine Documentation

**9.2.2.1** `real(dp) function prg_chebyshev_mod::absmaxderivative ( real(dp), dimension(:), intent(in) func, real(dp), intent(in) de ) [private]`

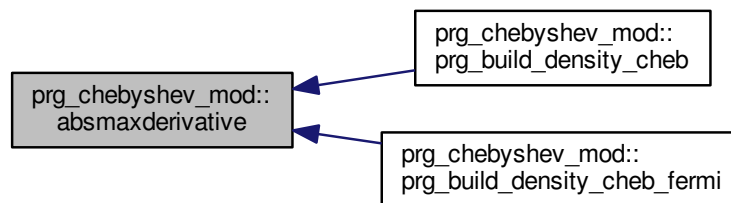
Gets the absolute maximum of the derivative of a function.

Parameters

|               |              |
|---------------|--------------|
| <i>func</i> . |              |
| <i>de</i>     | Energy step. |

Definition at line 802 of file prg\_chebyshev\_mod.F90.

Here is the caller graph for this function:



**9.2.2.2** `real(dp) function prg_chebyshev_mod::fermi ( real(dp), intent(in) e, real(dp), intent(in) ef, real(dp), intent(in) kbt ) [private]`

Gives the Fermi distribution value for energy *e*.

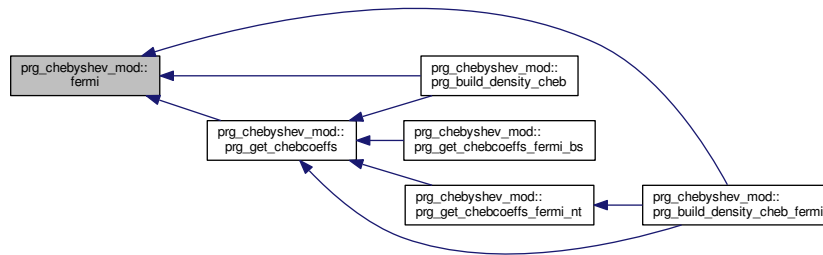
Parameters

|           |               |
|-----------|---------------|
| <i>e</i>  | Energy.       |
| <i>ef</i> | Fermi energy. |

Definition at line 790 of file prg\_chebyshev\_mod.F90.



Here is the caller graph for this function:



### 9.2.2.3 real(dp) function prg\_chebyshev\_mod::jackson ( integer, intent(in) *ncoeffs*, integer, intent(in) *i*, logical, intent(in) *jon* ) [private]

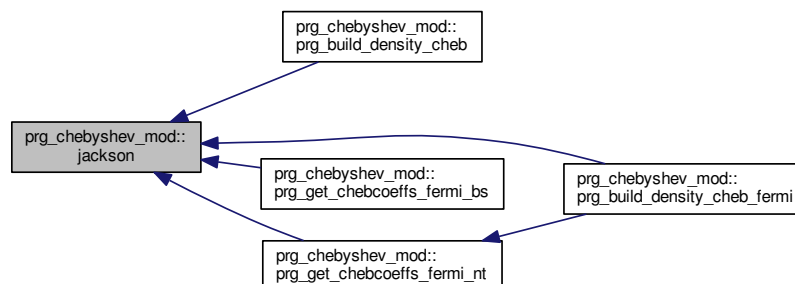
Evaluates the Jackson Kernel Coefficients.

#### Parameters

|                |                                 |
|----------------|---------------------------------|
| <i>ncoeffs</i> | Number of Chebyshev polynomial. |
| <i>i</i>       | Coefficient number i.           |

Definition at line 532 of file prg\_chebyshev\_mod.F90.

Here is the caller graph for this function:



### 9.2.2.4 subroutine, public prg\_chebyshev\_mod::prg\_build\_density\_cheb ( type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(inout) *rho\_bml*, real(dp), intent(in) *athr*, real(dp), intent(in) *threshold*, integer, intent(in) *ncoeffs*, real(dp), intent(in) *kbt*, real(dp), intent(in) *ef*, real(dp), intent(in) *bndfil*, logical, intent(in) *jon*, integer, intent(in) *verbose* )

Builds the density matrix from  $H_0$  for a Fermi function approximated with a Chebyshev polynomial expansion.

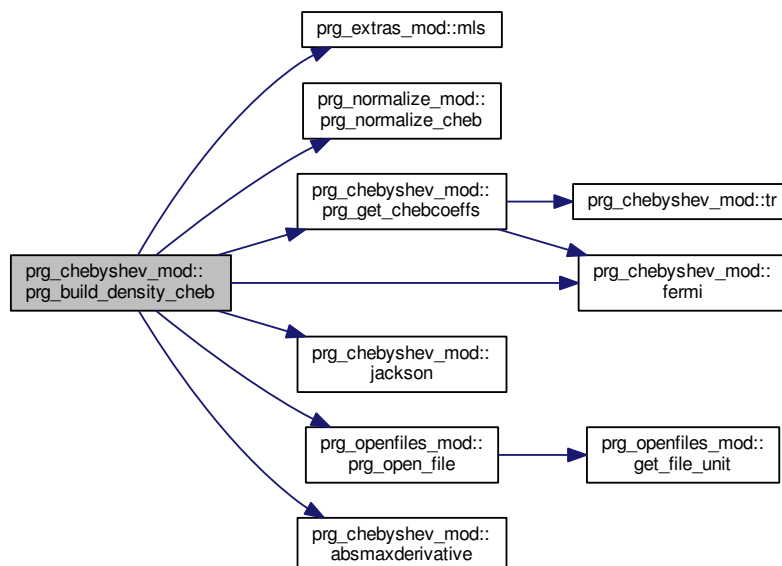
$\rho_{n+1} = b_{n+1}T_{n+1} + \rho_n$  Where,  $T_n$  is the nth Chebyshev polynomial and  $b_n$  is the nth coefficient of the expansion for the Fermi function. In the sparse version (when ellpack is used) the threshold can be varied linearly with the polynomial degree. The function is the following:  $Thresh(n) = Thresh_0[a_{thr}(n - 1) + (1 - a_{thr})]$

## Parameters

|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Input Orthogonalized Hamiltonian matrix.                       |
| <i>rho_bml</i>   | Output density matrix.   |
| <i>athr</i>      | Threshold linear increasing constant.                          |
| <i>threshold</i> | Threshold for sparse matrix algebra.                           |
| <i>ncoeffs</i>   | Number of Chebyshev coefficients.                              |
| <i>kbt</i>       | Electronic temperature in the energy units of the Hamiltonian. |
| <i>ef</i>        | Fermi level in the energy units of the Hamiltonian.            |
| <i>bndfil</i>    | Band filing factor.  |
| <i>verbose</i>   | Verbosity level.   |

Definition at line 143 of file prg\_chebyshev\_mod.F90.

Here is the call graph for this function:



**9.2.2.5** subroutine, public `prg_chebyshev_mod::prg_build_density_cheb_fermi` ( `type(bml_matrix_t)`, intent(in) *ham\_bml*, `type(bml_matrix_t)`, intent(inout) *rho\_bml*, `real(dp)`, intent(in) *athr*, `real(dp)`, intent(in) *threshold*, integer, intent(in) *ncoeffs*, `real(dp)`, intent(in) *kbt*, `real(dp)`, intent(inout) *ef*, `real(dp)`, intent(in) *bndfil*, logical, intent(in) *getef*, `real(dp)` *fermitol*, logical, intent(in) *jon*, integer *npts*, logical, intent(in) *trkfunc*, integer, intent(in) *verbose* )

Builds the density matrix from  $H_0$  for a Fermi function approximated with a Chebyshev polynomial expansion. In this case the self-consistent recursion is applied to converge to the correct number of electrons and obtain the Fermi level.

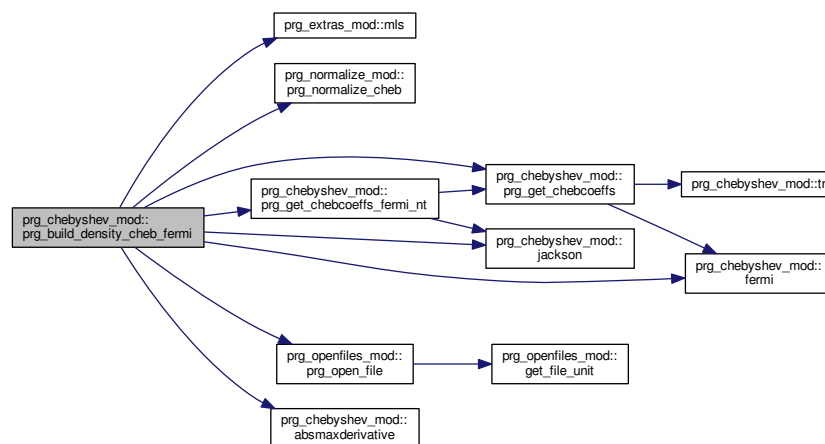
$\rho_{n+1} = b_{n+1}T_{n+1} + \rho_n$  Where,  $T_n$  is the  $n$ th Chebyshev polynomial and  $b_n$  is the  $n$ th coefficient of the expansion for the Fermi function. In the sparse version (when ellpack is used) the threshold can be varied linearly with the polynomial degree. The function is the following:  $Thresh(n) = Thresh_0[a_{thr}(n - 1) + (1 - a_{thr})]$

## Parameters

|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Input Orthogonalized Hamiltonian matrix.                       |
| <i>rho_bml</i>   | Output density matrix.   |
| <i>athr</i>      | Threshold linear increasing constant.                          |
| <i>threshold</i> | Threshold for sparse matrix algebra.                           |
| <i>ncoeffs</i>   | Number of Chebyshev coefficients.                              |
| <i>kbt</i>       | Electronic temperature in the energy units of the Hamiltonian. |
| <i>ef</i>        | Fermi level in the energy units of the Hamiltonian.            |
| <i>bndfil</i>    | Band filing factor.  |
| <i>npts</i>      | Number of energy point to compute the coefficients             |
| <i>verbose</i>   | Verbosity level.   |

Definition at line 310 of file prg\_chebyshev\_mod.F90.

Here is the call graph for this function:



**9.2.2.6** subroutine prg\_chebyshev\_mod::prg\_get\_chebcoeffs ( integer, intent(in) *npts*, real(dp), intent(in) *kbt*, real(dp), intent(in) *ef*, integer, intent(in) *ncoeffs*, real(dp), dimension(:), intent(inout) *coeffs*, real(dp), intent(in) *emin*, real(dp), intent(in) *emax* ) [private]

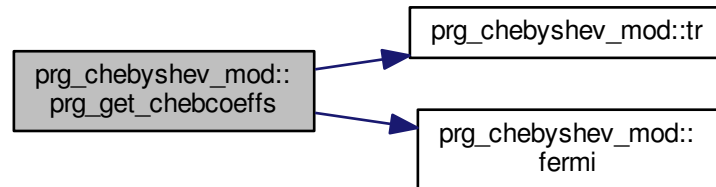
Gets the coefficients of the Chebyshev expansion.

## Parameters

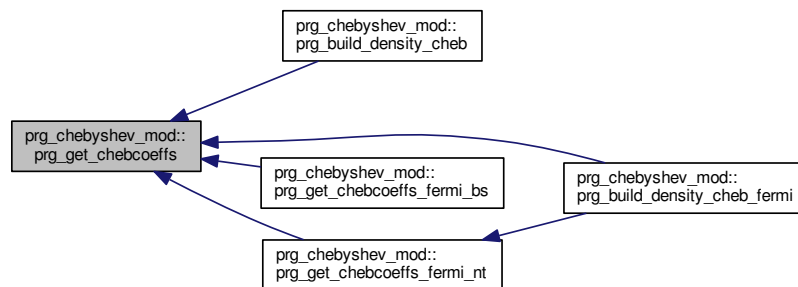
|                |   |
|----------------|---|
| <i>npts</i>    | Number of points for discretization.          |
| <i>kbt</i>     | Electronic temperature.                       |
| <i>ef</i>      | Fermi level.                                  |
| <i>ncoeffs</i> | Number of Chebyshev coefficients.             |
| <i>coeffs</i>  | Output vector for the Chebyshev coefficients. |
| <i>emin</i>    | lowest boundary for the eigenvalues of H.     |
| <i>emax</i>    | highest boundary for the eigenvalues of H.    |

Definition at line 568 of file prg\_chebyshev\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



**9.2.2.7** subroutine `prg_chebyshev_mod::prg_get_chebcoeffs_fermi_bs` ( integer, intent(in) *npts*, real(dp), intent(in) *kbt*, real(dp), intent(inout) *ef*, real(dp), dimension(:), intent(in) *tracesT*, integer, intent(in) *ncoeffs*, real(dp), dimension(:), intent(inout) *coeffs*, real(dp), intent(in) *emin*, real(dp), intent(in) *emax*, real(dp), intent(in) *bndfil*, integer, intent(in) *norb*, real(dp), intent(in) *tol*, logical, intent(in) *jon*, integer, intent(in) *verbose* ) [private]

Gets the coefficients of the Chebyshev expansion with Ef computation.

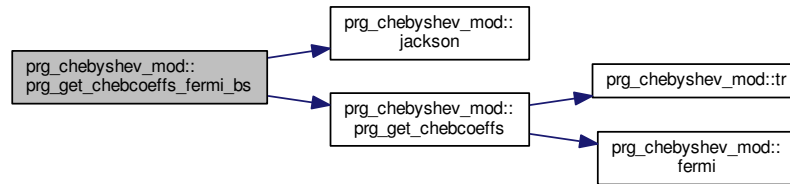
In this case we are applying the bisection method to find the root.

#### Parameters

|                |   |
|----------------|---|
| <i>npts</i>    | Number of points for the discretization.      |
| <i>kbt</i>     | Electronic temperature.                       |
| <i>ef</i>      | Fermi level.                                  |
| <i>tracesT</i> | Input traces for matrix polynomials.          |
| <i>ncoeffs</i> | Number of Chebyshev coefficients.             |
| <i>coeffs</i>  | Output vector for the Chebyshev coefficients. |
| <i>emin</i>    | lowest boundary for the eigenvalues of H.     |
| <i>emax</i>    | highest boundary for the eigenvalues of H.    |
| <i>tol</i>     | Tolerance for the bisection method.           |
| <i>verbose</i> | Verbosity level.                              |

Definition at line 620 of file prg\_chebyshev\_mod.F90.

Here is the call graph for this function:



**9.2.2.8** subroutine prg\_chebyshev\_mod::prg\_get\_chebcoeffs\_fermi\_nt ( integer, intent(in) *npts*, real(dp), intent(in) *kbt*, real(dp), intent(inout) *ef*, real(dp), dimension(:), intent(in) *tracesT*, integer, intent(in) *ncoeffs*, real(dp), dimension(:), intent(inout) *coeffs*, real(dp), intent(in) *emin*, real(dp), intent(in) *emax*, real(dp), intent(in) *bndfil*, integer, intent(in) *norb*, real(dp), intent(in) *tol*, logical, intent(in) *jon*, integer, intent(in) *verbose* ) [private]

Gets the coefficients of the Chebyshev expansion with Ef computation.

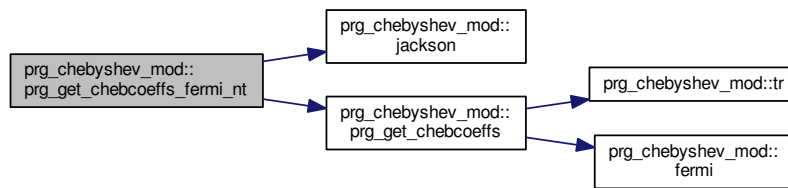
In this case the Newton-Raphson method is applied to find the root.

#### Parameters

|                |   |
|----------------|---|
| <i>npst</i>    | Number of points for the discretization.      |
| <i>kbt</i>     | Electronic temperature.                       |
| <i>ef</i>      | Fermi level.                                  |
| <i>tracesT</i> | Input traces for matrix polynomials.          |
| <i>ncoeffs</i> | Number of Chebyshev coefficients.             |
| <i>coeffs</i>  | Output vector for the Chebyshev coefficients. |
| <i>emin</i>    | lowest boundary for the eigenvalues of H.     |
| <i>emax</i>    | highest boundary for the eigenvalues of H.    |
| <i>bndfil</i>  | Band filling factor.                          |
| <i>norb</i>    | Number of orbitals.                           |
| <i>tol</i>     | Tolerance for NR method.                      |
| <i>verbose</i> | Verbosity level.                              |

Definition at line 697 of file prg\_chebyshev\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



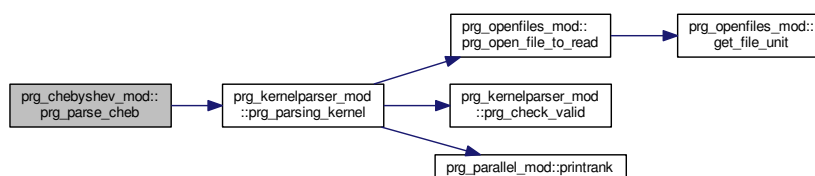
9.2.2.9 subroutine, public `prg_chebyshev_mod::prg_parse_cheb ( type(chebdata_type), intent(inout) chebdata, character(len=*) filename )`

Chebyshev parser. This module is used to parse all the input variables for the cheb electronic structure solver. Adding a new input keyword to the parser:

- If the variable is real, we have to increase `nkey_re`.
- Add the keyword (character type) in the `keyvector_re` vector.
- Add a default value (real type) in the `valvector_re`.
- Define a new variable and pass the value through `valvector_re(num)` where `num` is the position of the new keyword in the vector.

Definition at line 54 of file `prg_chebyshev_mod.F90`.

Here is the call graph for this function:



9.2.2.10 `real(dp) function prg_chebyshev_mod::tr ( integer, intent(in) r, real(dp), intent(in) x ) [private]`

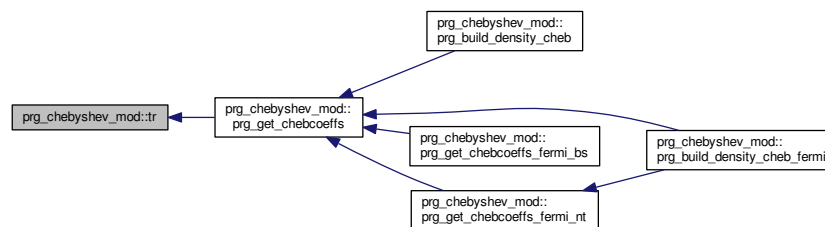
Chebyshev polynomial obtained by recursion.

#### Parameters

|          |                                       |
|----------|---------------------------------------|
| <i>r</i> | rth polynomial.                       |
| <i>x</i> | argument the evaluate the polynomial. |

Definition at line 777 of file prg\_chebyshev\_mod.F90.

Here is the caller graph for this function:



## 9.2.3 Variable Documentation

9.2.3.1 `integer, parameter prg_chebyshev_mod::dp = kind(1.0d0) [private]`

Definition at line 23 of file prg\_chebyshev\_mod.F90.

9.2.3.2 `real(dp), parameter prg_chebyshev_mod::pi = 3.14159265358979323846264338327950_dp [private]`

Definition at line 24 of file prg\_chebyshev\_mod.F90.

## 9.3 prg\_densitymatrix\_mod Module Reference

Module to obtain the density matrix by diagonalizing an prg\_orthogonalized Hamiltonian.

## Functions/Subroutines

- subroutine, public [prg\\_build\\_density\\_t0](#) (ham\_bml, rho\_bml, threshold, bndfil)  
*Builds the density matrix from  $H_0$  for zero electronic temperature.  $\rho = C\Theta(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $\Theta()$  is the Heaviside function.*
- subroutine, public [prg\\_build\\_density\\_t](#) (ham\_bml, rho\_bml, threshold, bndfil, kbt, ef)  
*Builds the density matrix from  $H_0$  for electronic temperature  $T$ .  $\rho = Cf(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $f$  is the Fermi function.*
- subroutine, public [prg\\_build\\_density\\_t\\_fermi](#) (ham\_bml, rho\_bml, threshold, kbt, ef, verbose)  
*Builds the density matrix from  $H_0$  for electronic temperature  $T$ .  $\rho = Cf(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $f$  is the Fermi function. In this routine the Fermi level is passed as an argument.*
- subroutine, public [prg\\_build\\_atomic\\_density](#) (rhoat\_bml, numel, hindex, spindex, norb, bml\_type)  
*Builds the atomic density matrix.  $\rho_{ii} = \text{mathcal{Z}}_{ii}$  Where,  $\text{mathcal{Z}}_{ii}$  is the number of electrons for orbital  $i$ .*
- subroutine, public [prg\\_get\\_flevel](#) (eigenvalues, kbt, bndfil, tol, Ef)  
*Routine to compute the Fermi level given a set of eigenvalues and a temperature. It applies the Bisection method over the function:  $g(\mu) = \sum_k 2f(\epsilon_k - \mu) - N = 0$  Where  $f(\epsilon_k - \mu) = \frac{1}{1 + \exp((\epsilon_k - \mu)/(k_b T))}$ .*
- subroutine, public [prg\\_get\\_eigenvalues](#) (ham\_bml, eigenvalues, verbose)  
*Gets the eigenvalues of the Orthogonalized Hamiltonian.*
- subroutine, public [prg\\_check\\_idempotency](#) (mat\_bml, threshold, idempotency)  
*To check the idempotency error of a matrix. This is calculated as the Frobenius norm of  $(A - A^2)$ .*
- real(dp) function [fermi](#) (e, ef, kbt)  
*Gives the Fermi distribution value for energy  $e$ .*

## Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.3.1 Detailed Description

Module to obtain the density matrix by diagonalizing an prg\_orthogonalized Hamiltonian.

### 9.3.2 Function/Subroutine Documentation

**9.3.2.1** [real\(dp\) function prg\\_densitymatrix\\_mod::fermi \( real\(dp\), intent\(in\) e, real\(dp\), intent\(in\) ef, real\(dp\), intent\(in\) kbt \)](#)  
[private]

Gives the Fermi distribution value for energy  $e$ .

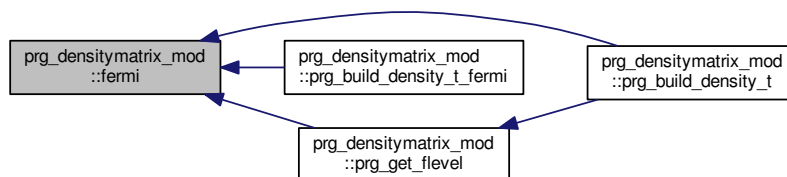
#### Parameters

|           |               |
|-----------|---------------|
| <i>e</i>  | Energy.       |
| <i>ef</i> | Fermi energy. |

Definition at line 413 of file prg\_densitymatrix\_mod.F90.



Here is the caller graph for this function:



9.3.2.2 subroutine, public prg\_densitymatrix\_mod::prg\_build\_atomic\_density ( type(bml\_matrix\_t), intent(inout) rhoat\_bml, real(dp), dimension(:), intent(in) numel, integer, dimension(:,:), intent(in) hindex, integer, dimension(:), intent(in) spindex, integer, intent(in) norb, character(len=\*), intent(in) bml\_type )

Builds the atomic density matrix.  $\rho_{ii} = \text{mathcal{Z}}_{ii}$  Where,  $\text{mathcal{Z}}_{ii}$  is the number of electrons for orbital i.

#### Parameters

|                |  |
|----------------|--|
| <i>rhoat</i>   | Output atomic diagonal density matrix,                         |
| <i>hindex</i>  | Start and end index for every atom in the system.              |
| <i>numel</i>   | Number of electrons per specie. It runs over the specie index. |
| <i>spindex</i> | Specie index.  |
| <i>norbs</i>   | Number of orbitals.  |

Definition at line 215 of file prg\_densitymatrix\_mod.F90.

9.3.2.3 subroutine, public prg\_densitymatrix\_mod::prg\_build\_density\_t ( type(bml\_matrix\_t), intent(in) ham\_bml, type(bml\_matrix\_t), intent(inout) rho\_bml, real(8), intent(in) threshold, real(8), intent(in) bndfil, real(8), intent(in) kbt, real(8), intent(inout) ef )

Builds the density matrix from  $H_0$  for electronic temperature T.  $\rho = Cf(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $f$  is the Fermi function.

#### Parameters

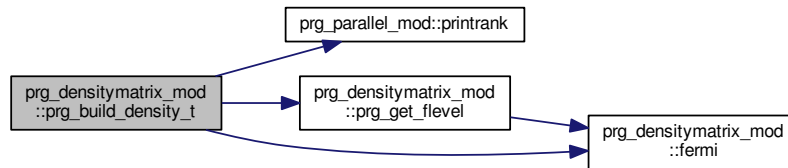
|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Input Orthogonalized Hamiltonian matrix. |
| <i>rho_bml</i>   | Output density matrix,                   |
| <i>threshold</i> | Threshold for sparse matrix algebra.     |
| <i>bndfil</i>    | Filing factor.                           |

#### Warning

This does not solve the generalized eigenvalue problem. The Hamiltonian that comes in has to be preprg\_↔ orthogonalized.

Definition at line 94 of file prg\_densitymatrix\_mod.F90.

Here is the call graph for this function:



**9.3.2.4** subroutine, public prg\_densitymatrix\_mod::prg\_build\_density\_t0 ( type(bml\_matrix\_t), intent(in) ham\_bml, type(bml\_matrix\_t), intent(inout) rho\_bml, real(8), intent(in) threshold, real(8), intent(in) bndfil )

Builds the density matrix from  $H_0$  for zero electronic temperature.  $\rho = C\Theta(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $\Theta()$  is the Heaviside function.

#### Parameters

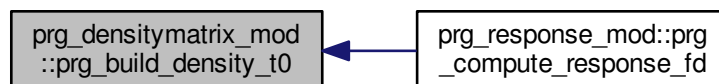
|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Input Orthogonalized Hamiltonian matrix. |
| <i>rho_bml</i>   | Output density matrix,                   |
| <i>threshold</i> | Threshold for sparse matrix algebra.     |
| <i>bndfil</i>    | Filing factor.                           |

#### Warning

This does not solve the generalized eigenvalue problem. The Hamiltonian that comes in has to be preprg\_orthogonalized.

Definition at line 33 of file prg\_densitymatrix\_mod.F90.

Here is the caller graph for this function:



**9.3.2.5** subroutine, public prg\_densitymatrix\_mod::prg\_build\_density\_t\_fermi ( type(bml\_matrix\_t), intent(in) ham\_bml, type(bml\_matrix\_t), intent(inout) rho\_bml, real(8), intent(in) threshold, real(8), intent(in) kbt, real(8), intent(in) ef, integer, intent(in), optional verbose )

Builds the density matrix from  $H_0$  for electronic temperature  $T$ .  $\rho = Cf(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $f$  is the Fermi function. In this routine the Fermi level is passed as an argument.

## Parameters

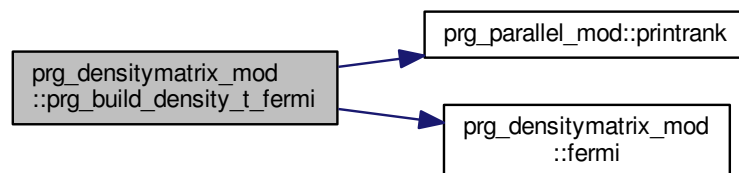
|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Input Orthogonalized Hamiltonian matrix. |
| <i>rho_bml</i>   | Output density matrix,                   |
| <i>threshold</i> | Threshold for sparse matrix algebra.     |

## Warning

This does not solve the generalized eigenvalue problem. The Hamiltonian that comes in has to be preprg\_orthogonalized.

Definition at line 156 of file prg\_densitymatrix\_mod.F90.

Here is the call graph for this function:



9.3.2.6 subroutine, public prg\_densitymatrix\_mod::prg\_check\_idempotency ( type(bml\_matrix\_t), intent(in) *mat\_bml*, real(dp), intent(in) *threshold*, real(dp), intent(out) *idempotency* )

To check the idempotency error of a matrix. This is calculated as the Frobenius norm of  $(A - A^2)$ .

## Parameters

|                    |   |
|--------------------|---|
| <i>mat_bml</i>     | Some bml matrix                         |
| <i>idempotency</i> | (Output value of the idempotency error) |

Definition at line 389 of file prg\_densitymatrix\_mod.F90.

9.3.2.7 subroutine, public prg\_densitymatrix\_mod::prg\_get\_eigenvalues ( type(bml\_matrix\_t), intent(in) *ham\_bml*, real(dp), dimension(:), intent(inout), allocatable *eigenvalues*, integer, intent(in) *verbose* )

Gets the eigenvalues of the Orthogonalized Hamiltonian.

## Parameters

|                    |  |
|--------------------|--|
| <i>ham_bml</i>     | Input Orthogonalized Hamiltonian matrix. |
| <i>eigenvalues</i> | Output eigenvalues of the system.        |
| <i>verbose</i>     | Verbosity level.                         |

Definition at line 344 of file prg\_densitymatrix\_mod.F90.

**9.3.2.8** subroutine, public prg\_densitymatrix\_mod::prg\_get\_flevel ( real(dp), dimension(:), intent(in) *eigenvalues*, real(dp), intent(in) *kbt*, real(dp), intent(in) *bndfil*, real(dp) *tol*, real(dp), intent(inout) *Ef* )

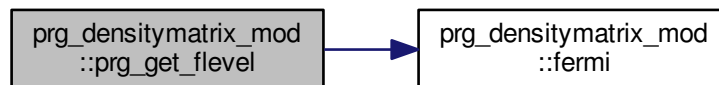
Routine to compute the Fermi level given a set of eigenvalues and a temperature. It applies the Bisection method over the function:  $g(\mu) = \sum_k 2f(\epsilon_k - \mu) - N = 0$  Where  $f(\epsilon_k - \mu) = \frac{1}{1 + \exp((\epsilon_k - \mu)/(k_b T))}$ .

#### Parameters

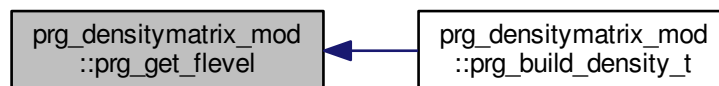
|                    |   |
|--------------------|---|
| <i>eigenvalues</i> | Eigenvalues of the system ( $\{\epsilon_k\}$ ).         |
| <i>kbt</i>         | Temperature times the Boltzmann's constant ( $k_b T$ ). |
| <i>bndfil</i>      | Filing factor ( $N_{el}/(2 * N_{orbs})$ ).              |
| <i>tol</i>         | Tolerance for the bisection method.                     |
| <i>Ef</i>          | Fermi level ( $\mu$ ).                                  |

Definition at line 280 of file prg\_densitymatrix\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



### 9.3.3 Variable Documentation

**9.3.3.1** integer, parameter prg\_densitymatrix\_mod::dp = kind(1.0d0) [private]

Definition at line 14 of file prg\_densitymatrix\_mod.F90.

## 9.4 prg\_dos\_mod Module Reference

A module to compute the Density of state (DOS) and IDOS.

### Functions/Subroutines

- subroutine, public [prg\\_write\\_tdos](#) (eigenvals, gamma, npts, emin, emax, filename)  
*Writes the total DOS into a file.  $DOS(\epsilon) = \sum_k L(\epsilon - \epsilon_k)$  Where  $\int_{-\infty}^{\infty} DOS(\epsilon) = Nstates$ .*
- real(dp) function [lorentz](#) (energy, eigenvals, loads, Gamma)  
*Lorentzian Function.*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.4.1 Detailed Description

A module to compute the Density of state (DOS) and IDOS.

This module will be used to compute DOS and IDOS.

**Todo** Add LDOS.

#### 9.4.2 Function/Subroutine Documentation

**9.4.2.1** real(dp) function prg\_dos\_mod::lorentz ( real(dp), intent(in) *energy*, real(dp), dimension(:), intent(in) *eigenvals*, real(dp), dimension(:), intent(in) *loads*, real(dp), intent(in) *Gamma* ) [private]

Lorentzian Function.

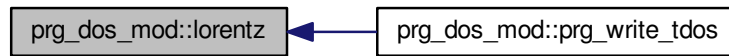
Computes:  $L(\epsilon) = \sum_k \frac{\omega(k)\Gamma}{2\pi} \frac{1}{(\epsilon - \epsilon_k)^2 + (\Gamma/2)^2}$

##### Parameters

|                  |                              |
|------------------|------------------------------|
| <i>energy</i>    | Energy point.                |
| <i>eigenvals</i> | Eigenvalues of the system.   |
| <i>Gamma</i>     | Lorentz function broadening. |

Definition at line 78 of file prg\_dos\_mod.F90.

Here is the caller graph for this function:



9.4.2.2 subroutine, public `prg_dos_mod::prg_write_tdos` ( `real(dp)`, `dimension(:)`, `intent(in)` *eigenvals*, `real(dp)`, `intent(in)` *gamma*, `integer`, `intent(in)` *npts*, `real(dp)`, `intent(in)` *emin*, `real(dp)`, `intent(in)` *emax*, `character(len=*)`, `intent(in)` *filename* )

Writes the total DOS into a file.  $DOS(\epsilon) = \sum_k L(\epsilon - \epsilon_k)$  Where  $\int_{-\infty}^{\infty} DOS(\epsilon) = Nstates$ .

#### Note

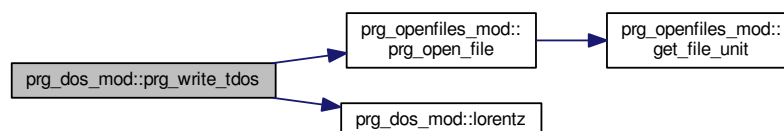
DOS is NOT shifted respect to Ef.

#### Parameters

|                  |  |
|------------------|--|
| <i>eigenvals</i> | Eigenvalues of the system. gamma Lorentzian width. |
| <i>npts</i>      | Number of energy points.                           |
| <i>emin</i>      | Minimum energy value.                              |
| <i>emax</i>      | Maximum energy value.                              |
| <i>filename</i>  | Filename to write the DOS.                         |

Definition at line 36 of file `prg_dos_mod.F90`.

Here is the call graph for this function:



### 9.4.3 Variable Documentation

9.4.3.1 integer, parameter `prg_dos_mod::dp = kind(1.0d0)` [private]

Definition at line 17 of file `prg_dos_mod.F90`.

## 9.5 prg\_extras\_mod Module Reference

Extra routines:

### Data Types

- interface [prg\\_memory\\_consumption](#)
- interface [to\\_string](#)

### Functions/Subroutines

- character(len=:) function, allocatable [to\\_string\\_integer](#) (i)  
*Convert integer to string.*
- character(len=:) function, allocatable [to\\_string\\_long\\_long](#) (i)  
*Convert integer to string.*
- character(len=:) function, allocatable [to\\_string\\_double](#) (x)  
*Convert double to string.*
- subroutine, public [prg\\_print\\_matrix](#) (matname, amat, i1, i2, j1, j2)  
*To write a dense matrix to screen.*
- real(dp) function, public [mls](#) ()  
*To get the actual time in milliseconds.*
- subroutine, public [prg\\_delta](#) (x, s, nn, dta)  
*Delta function  $\|X^tSX - I\|$ . CFAN, March 2015.*
- subroutine, public [prg\\_get\\_mem](#) (procname, tag)  
*Get proc memory.*
- subroutine [prg\\_twonorm](#) (a, nn, norm2)

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.5.1 Detailed Description

Extra routines:

A module to add any extra routine considered necessary but which is NOT essential for any other PROGRESS routines.

#### 9.5.2 Function/Subroutine Documentation

##### 9.5.2.1 real(dp) function, public prg\_extras\_mod::mls ( )

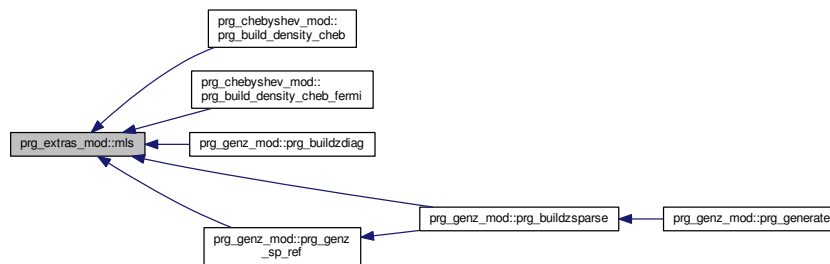
To get the actual time in milliseconds.

## Parameters

|            |   |
|------------|---|
| <i>m/s</i> | Output value with the machine time in milliseconds. |
|------------|---|

Definition at line 139 of file prg\_extras\_mod.F90.

Here is the caller graph for this function:



**9.5.2.2** subroutine, public prg\_extras\_mod::prg\_delta ( real(dp), dimension(nn,nn) *x*, real(dp), dimension(nn,nn) *s*, integer *nn*, real(dp) *dta* )

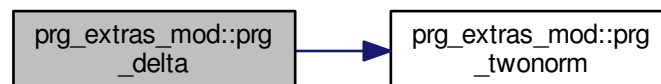
Delta function  $\|X^t S X - I\|$ . CFAN, March 2015.

## Parameters

|            |                     |
|------------|---------------------|
| <i>x</i>   | input matrix.       |
| <i>s</i>   | overlap matrix.     |
| <i>dta</i> | Delta output value. |

Definition at line 155 of file prg\_extras\_mod.F90.

Here is the call graph for this function:



**9.5.2.3** subroutine, public prg\_extras\_mod::prg\_get\_mem ( character(\*) , intent(in) *procname*, character(\*) , intent(in) *tag* )

Get proc memory.



## Parameters

|                 |  |
|-----------------|--|
| <i>procname</i> | Process name to get the mem usage.     |
| <i>tag</i>      | Tag to pprint the processor mem usage. |

Definition at line 191 of file prg\_extras\_mod.F90.

**9.5.2.4** subroutine, public prg\_extras\_mod::prg\_print\_matrix ( character(len=\*) *matname*, real(dp), dimension(:, :), intent(in) *amat*, integer, intent(in) *i1*, integer, intent(in) *i2*, integer, intent(in) *j1*, integer, intent(in) *j2* )

To write a dense matrix to screen.

## Parameters

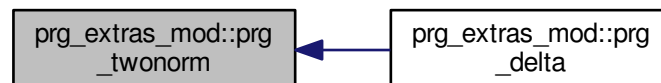
|                |                          |
|----------------|--------------------------|
| <i>matname</i> | Matrix name.             |
| <i>amat</i>    | Matrix to be printed.    |
| <i>i1</i>      | Print from row i1.       |
| <i>i2</i>      | Print up to from row i2. |
| <i>j1</i>      | Print from column j1.    |
| <i>j2</i>      | Print up to column j2.   |

Definition at line 100 of file prg\_extras\_mod.F90.

**9.5.2.5** subroutine prg\_extras\_mod::prg\_twonorm ( real(dp), dimension(nn,nn) *a*, integer *nn*, real(dp) *norm2* )  
[private]

Definition at line 211 of file prg\_extras\_mod.F90.

Here is the caller graph for this function:



**9.5.2.6** character(len=:) function, allocatable prg\_extras\_mod::to\_string\_double ( double precision, intent(in) *x* )  
[private]

Convert double to string.

**Parameters**

|          |            |
|----------|------------|
| <i>x</i> | The double |
|----------|------------|

**Returns**

The string

Definition at line 80 of file prg\_extras\_mod.F90.

#### 9.5.2.7 `character(len=:)` function, allocatable `prg_extras_mod::to_string_integer ( integer, intent(in) i )` `[private]`

Convert integer to string.

**Parameters**

|          |             |
|----------|-------------|
| <i>i</i> | The integer |
|----------|-------------|

**Returns**

The string

Definition at line 46 of file prg\_extras\_mod.F90.

#### 9.5.2.8 `character(len=:)` function, allocatable `prg_extras_mod::to_string_long_long ( integer(kind=c_long_long), intent(in) i )` `[private]`

Convert integer to string.

**Parameters**

|          |             |
|----------|-------------|
| <i>i</i> | The integer |
|----------|-------------|

**Returns**

The string

Definition at line 62 of file prg\_extras\_mod.F90.

### 9.5.3 Variable Documentation

#### 9.5.3.1 `integer, parameter prg_extras_mod::dp = kind(1.0d0)` `[private]`

Definition at line 31 of file prg\_extras\_mod.F90.

## 9.6 prg\_genz\_mod Module Reference

To produce a matrix  $Z$  which is needed to orthogonalize  $H$ .

### Data Types

- type `genzspdata`  
*contains the data for the genZ driver.*
- type `genzspinp`  
*Input for the genz driver.*

### Functions/Subroutines

- subroutine, public `prg_parse_zsp` (input, filename)  
*The parser for genz solver.*
- subroutine `prg_init` (self, input)  
*Initializes the genz input variables.*
- subroutine `prg_allocatezspmat` (self, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, norb, bml\_type)  
*Allocates the matrices for the XI integration of Z.*
- subroutine, public `prg_init_zspmat` (igenz, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, norb, bml\_type)  
*Initiates the matrices for the XI integration of Z.*
- subroutine `prg_generate` (self, over\_bml, zmat\_bml, igenz, mdim, bml\_type, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml)  
*Generates the Z matrix.*
- subroutine, public `prg_buildzdiag` (smat\_bml, zmat\_bml, threshold, mdimin, bml\_type, verbose)  
*Usual subroutine involving diagonalization.*
- subroutine, public `prg_buildzsparse` (smat\_bml, zmat\_bml, igenz, mdim, bml\_type, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, nfirst, nrefi, nreff, thresholdi, thresholdf, integration, verbose)  
*Inverse factorization using niklasson's algorithm.*
- subroutine, public `prg_genz_sp_initialz0` (smat\_bml, zmat\_bml, norb, mdim, bml\_type\_f, threshold)
- subroutine, public `prg_genz_sp_initial_zmat` (smat\_bml, zmat\_bml, norb, mdim, bml\_type\_f, threshold)  
*Estimate Z matrix.*
- subroutine `prg_genz_sp_int` (zmat\_bml, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, igenz, norb, bml\_type, threshold)
- subroutine, public `prg_genz_sp_ref` (smat\_bml, zmat\_bml, nref, norb, bml\_type, threshold)

### Variables

- integer, parameter `dp` = kind(1.0d0)

#### 9.6.1 Detailed Description

To produce a matrix  $Z$  which is needed to orthogonalize  $H$ .

$$H_{orth} = Z^\dagger H Z \text{ See Negre 2016 [2]}$$

#### 9.6.2 Function/Subroutine Documentation

**9.6.2.1** subroutine `prg_genz_mod::prg_allocatezspmat` ( class(`genzspdata`), intent(in) *self*, type(`bml_matrix_t`) *zk1\_bml*, type(`bml_matrix_t`) *zk2\_bml*, type(`bml_matrix_t`) *zk3\_bml*, type(`bml_matrix_t`) *zk4\_bml*, type(`bml_matrix_t`) *zk5\_bml*, type(`bml_matrix_t`) *zk6\_bml*, integer *norb*, character(20) *bml\_type* ) [private]

Allocates the matrices for the XI integration of Z.

## Parameters

|                        |  |
|------------------------|--|
| <i>self</i>            | input zsp variables                        |
| <i>zk1_bml-zk6_bml</i> | history record of the previous Z matrices. |
| <i>norb</i>            | number of orbitals.                        |
| <i>bml_type</i>        | the bml format we are passing.             |

Definition at line 174 of file prg\_genz\_mod.F90.

9.6.2.2 subroutine, public prg\_genz\_mod::prg\_buildzdiag ( type(bml\_matrix\_t), intent(inout) *smat\_bml*, type(bml\_matrix\_t) *zmat\_bml*, real(dp) *threshold*, integer, intent(in) *mdimin*, character(len=\*) *bml\_type*, integer, intent(in), optional *verbose* )

Usual subroutine involving diagonalization.

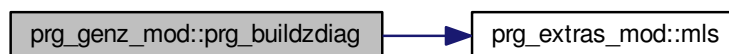
$Z = U\sqrt{s}U^\dagger$ , where  $U$  = eigenvectors and  $s$  = eigenvalues. The purpose of this subroutine is to have an exact way of computing  $z$  for comparing with the sparse approach.

## Parameters

|                  |   |
|------------------|---|
| <i>smat_bml</i>  | Overlap matrix in bml format.   |
| <i>zmat_bml</i>  | Congruence transform in bml format.   |
| <i>threshold</i> | Threshold value to use, in this case, only in the backtransformation to ellpack format. |
| <i>mdim</i>      | Maximun nonzero to use, in this case, only in the backtransformation to ellpack format. |
| <i>bml_type</i>  | the bml type we are passing.  |

Definition at line 281 of file prg\_genz\_mod.F90.

Here is the call graph for this function:



9.6.2.3 subroutine, public prg\_genz\_mod::prg\_buildzsparse ( type(bml\_matrix\_t) *smat\_bml*, type(bml\_matrix\_t) *zmat\_bml*, integer *igenz*, integer *mdim*, character(20) *bml\_type*, type(bml\_matrix\_t) *zk1\_bml*, type(bml\_matrix\_t) *zk2\_bml*, type(bml\_matrix\_t) *zk3\_bml*, type(bml\_matrix\_t) *zk4\_bml*, type(bml\_matrix\_t) *zk5\_bml*, type(bml\_matrix\_t) *zk6\_bml*, integer *nfirst*, integer *nrefi*, integer *nreff*, real(dp) *thresholdi*, real(dp) *thresholdf*, logical *integration*, integer *verbose* )

Inverse factorization using niklasson's algorithm.

## Parameters

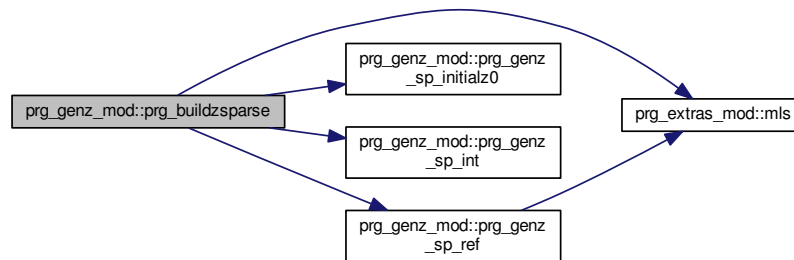
|                 |                |
|-----------------|----------------|
| <i>smat_bml</i> | overlap matrix |
|-----------------|----------------|

## Parameters

|                        |  |
|------------------------|--|
| <i>zmat_bml</i>        | congruence transform to be updated or computed. (bml format)               |
| <i>igenz</i>           | counter to keep track of the calls to this subroutine.                     |
| <i>mdim</i>            | dimension of the maxnonzero per row.                                       |
| <i>zk1_bml-zk6_bml</i> | history of the past congruence transforms.                                 |
| <i>nfirst</i>          | first pre septs with nrefi and thresholdi.                                 |
| <i>nrefi</i>           | number of refinement iterations for the firsts "nfirst" steps.             |
| <i>nreff</i>           | number of refinement iterations for the rest of the steps.                 |
| <i>integration</i>     | if we want to apply xl integration scheme for z (default is always .true.) |
| <i>verbose</i>         | to print extra information.  |

Definition at line 421 of file prg\_genz\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



```

9.6.2.4 subroutine prg_genz_mod::prg_generate ( class(genzspdata), intent(in) self, type(bml_matrix_t), intent(in) over_bml,
type(bml_matrix_t), intent(inout) zmat_bml, integer igenz, integer mdim, character(20) bml_type, type(bml_matrix_t),
intent(inout) zk1_bml, type(bml_matrix_t), intent(inout) zk2_bml, type(bml_matrix_t), intent(inout) zk3_bml,
type(bml_matrix_t), intent(inout) zk4_bml, type(bml_matrix_t), intent(inout) zk5_bml, type(bml_matrix_t), intent(inout)
zk6_bml ) [private]

```

Generates the Z matrix.

## Parameters

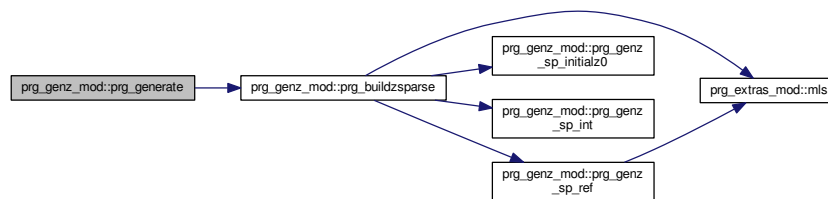
|                 |                 |
|-----------------|-----------------|
| <i>over_bml</i> | Overlap matrix. |
|-----------------|-----------------|

## Parameters

|                        |  |
|------------------------|--|
| <i>zmat_bml</i>        | Congruence transform to be computed. (bml format)      |
| <i>igenz</i>           | Counter to keep track of the calls to this subroutine. |
| <i>mdim</i>            | dimension of the maxnonzero per row.                   |
| <i>zk1_bml-zk6_bml</i> | history of the past congruence transforms.             |

Definition at line 242 of file prg\_genz\_mod.F90.

Here is the call graph for this function:



9.6.2.5 subroutine, public `prg_genz_mod::prg_genz_sp_initial_zmat` ( `type(bml_matrix_t)`, intent(in) *smat\_bml*, `type(bml_matrix_t)` *zmat\_bml*, integer *norb*, integer *mdim*, character(20) *bml\_type\_f*, `real(dp)`, intent(in) *threshold* )

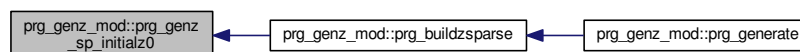
Estimate Z matrix.

Definition at line 600 of file prg\_genz\_mod.F90.

9.6.2.6 subroutine, public `prg_genz_mod::prg_genz_sp_initialz0` ( `type(bml_matrix_t)`, intent(in) *smat\_bml*, `type(bml_matrix_t)` *zmat\_bml*, integer *norb*, integer *mdim*, character(20) *bml\_type\_f*, `real(dp)` *threshold* )

Definition at line 476 of file prg\_genz\_mod.F90.

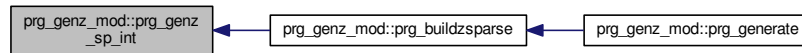
Here is the caller graph for this function:



9.6.2.7 subroutine prg\_genz\_mod::prg\_genz\_sp\_int ( type(bml\_matrix\_t) *zmat\_bml*, type(bml\_matrix\_t) *zk1\_bml*, type(bml\_matrix\_t) *zk2\_bml*, type(bml\_matrix\_t) *zk3\_bml*, type(bml\_matrix\_t) *zk4\_bml*, type(bml\_matrix\_t) *zk5\_bml*, type(bml\_matrix\_t) *zk6\_bml*, integer *igenz*, integer *norb*, character(20) *bml\_type*, real(dp) *threshold* ) [private]

Definition at line 739 of file prg\_genz\_mod.F90.

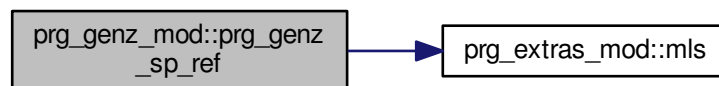
Here is the caller graph for this function:



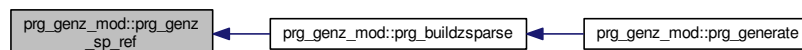
9.6.2.8 subroutine, public prg\_genz\_mod::prg\_genz\_sp\_ref ( type(bml\_matrix\_t), intent(in) *smat\_bml*, type(bml\_matrix\_t), intent(inout) *zmat\_bml*, integer, intent(in) *nref*, integer, intent(inout) *norb*, character(20), intent(in) *bml\_type*, real(dp), intent(in) *threshold* )

Definition at line 806 of file prg\_genz\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.6.2.9 subroutine prg\_genz\_mod::prg\_init ( class(genzspdata), intent(out) *self*, type(genzspinp), intent(in) *input* ) [private]

Initializes the genz input variables.

## Parameters

|              |   |
|--------------|---|
| <i>self</i>  | basic input parameters.                 |
| <i>input</i> | basic input parameters from the parser. |

Definition at line 152 of file prg\_genz\_mod.F90.

9.6.2.10 subroutine, public prg\_genz\_mod::prg\_init\_zspmat ( integer *igenz*, type(bml\_matrix\_t) *zk1\_bml*, type(bml\_matrix\_t) *zk2\_bml*, type(bml\_matrix\_t) *zk3\_bml*, type(bml\_matrix\_t) *zk4\_bml*, type(bml\_matrix\_t) *zk5\_bml*, type(bml\_matrix\_t) *zk6\_bml*, integer *norb*, character(20) *bml\_type* )

Initiates the matrices for the XI integration of Z.

## Parameters

|                                 |  |
|---------------------------------|--|
| <i>self</i>                     | input zsp variables                        |
| <i>zk1_bml</i> - <i>zk6_bml</i> | history record of the previous Z matrices. |
| <i>norb</i>                     | number of orbitals.                        |
| <i>bml_type</i>                 | the bml format we are passing.             |

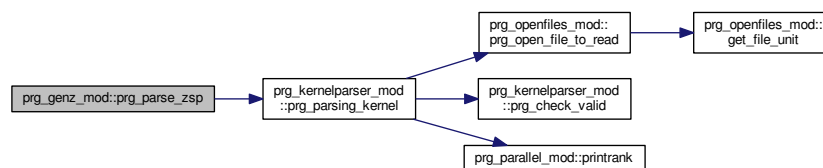
Definition at line 207 of file prg\_genz\_mod.F90.

9.6.2.11 subroutine, public prg\_genz\_mod::prg\_parse\_zsp ( type(genzspinp), intent(inout) *input*, character(len=\*) *filename* )

The parser for genz solver.

Definition at line 88 of file prg\_genz\_mod.F90.

Here is the call graph for this function:



## 9.6.3 Variable Documentation

9.6.3.1 integer, parameter prg\_genz\_mod::dp = kind(1.0d0) [private]

Definition at line 20 of file prg\_genz\_mod.F90.



## 9.7 prg\_graph\_mod Module Reference

The graph module.

### Data Types

- type [graph\\_partitioning\\_t](#)  
*Trace per iteration.*
- type [subgraph\\_t](#)  
*Subgraph type.*

### Functions/Subroutines

- subroutine, public [prg\\_initsubgraph](#) (sg, pnum, hsize)  
*Initialize subgraph.*
- subroutine, public [prg\\_destroysubgraph](#) (sg)  
*Destroy subgraph.*
- subroutine, public [prg\\_initgraphpartitioning](#) (gp, pname, np, nnodes, nnodes2)  
*Initialize graph partitioning.*
- subroutine, public [prg\\_destroygraphpartitioning](#) (gp)  
*Destroy graph partitioning.*
- subroutine, public [prg\\_printgraphpartitioning](#) (gp)  
*Print graph partitioning structure data.*
- subroutine, public [prg\\_equalpartition](#) (gp, nodesPerPart, nnodes)  
*Create equal graph partitions, based on number of rows/orbitals.*
- subroutine, public [prg\\_equalgrouppartition](#) (gp, hindex, ngroup, nodesPerPart, nnodes)  
*Create equal group graph partitions, based on number of atoms/groups.*
- subroutine, public [prg\\_filepartition](#) (gp, partFile)  
*Read graph partitions from a file, based on number of rows/orbitals.*
- subroutine [prg\\_readpart](#) (gp, partFile)  
*Read parts (core) from part file.*
- subroutine, public [prg\\_fnormgraph](#) (gp)  
*Accumulate trace norm across all subgraphs.*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.7.1 Detailed Description

The graph module.

#### 9.7.2 Function/Subroutine Documentation

9.7.2.1 subroutine, public [prg\\_graph\\_mod::prg\\_destroygraphpartitioning](#) ( type ([graph\\_partitioning\\_t](#)), intent(inout) *gp* )

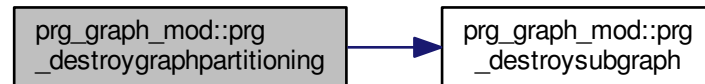
Destroy graph partitioning.

## Parameters

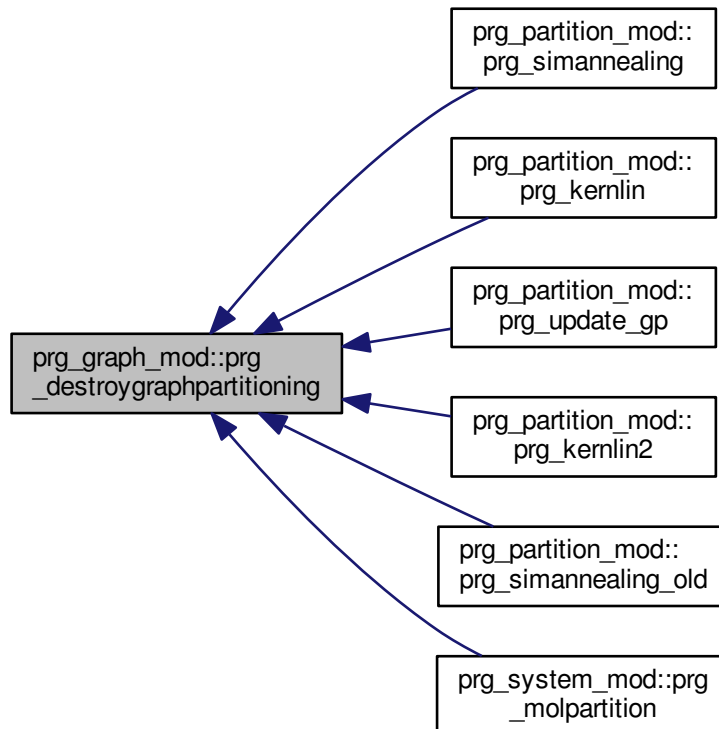
|                 |          |
|-----------------|----------|
| <code>sg</code> | Subgraph |
|-----------------|----------|

Definition at line 263 of file `prg_graph_mod.F90`.

Here is the call graph for this function:



Here is the caller graph for this function:



9.7.2.2 subroutine, public `prg_graph_mod::prg_destroysubgraph ( type (subgraph_t), intent(inout) sg )`

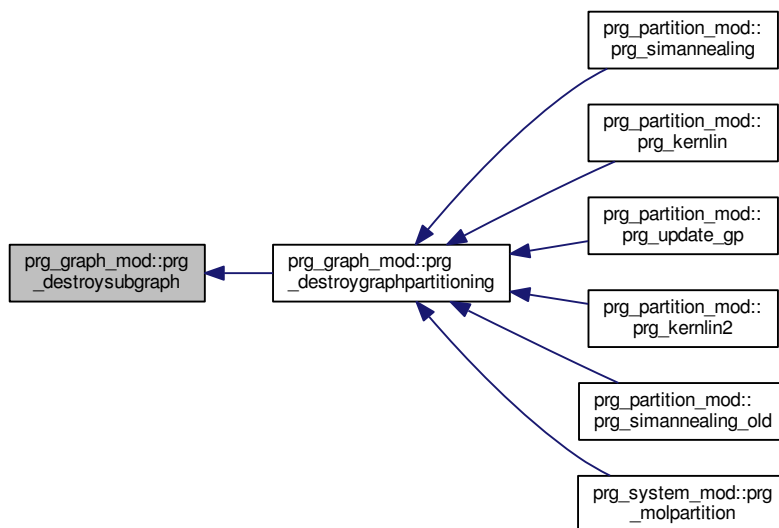
Destroy subgraph.

## Parameters

|           |          |
|-----------|----------|
| <i>sg</i> | Subgraph |
|-----------|----------|

Definition at line 159 of file prg\_graph\_mod.F90.

Here is the caller graph for this function:



**9.7.2.3** subroutine, public `prg_graph_mod::prg_equalgrouppartition` ( `type (graph_partitioning_t)`, intent(inout) *gp*, integer, dimension(2,ngroup), intent(in) *hindex*, integer, intent(in) *ngroup*, integer, intent(in) *nodesPerPart*, integer, intent(in) *nnodes* )

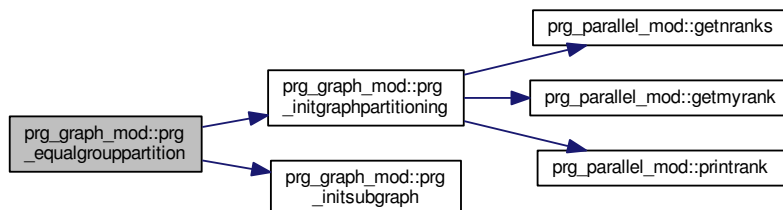
Create equal group graph partitions, based on number of atoms/groups.

## Parameters

|                     |  |
|---------------------|--|
| <i>gp</i>           | Graph partitioning                                 |
| <i>hindex</i>       | Node indeces that represent ranges of atoms/groups |
| <i>ngroup</i>       | Number of group nodes                              |
| <i>nodesPerPart</i> | Number of core nodes per partition                 |
| <i>nnodes</i>       | Total nodes in Hamiltonian matrix                  |

Definition at line 402 of file prg\_graph\_mod.F90.

Here is the call graph for this function:



9.7.2.4 subroutine, public `prg_graph_mod::prg_equalpartition ( type (graph_partitioning_t), intent(inout) gp, integer, intent(in) nodesPerPart, integer, intent(in) nnodes )`

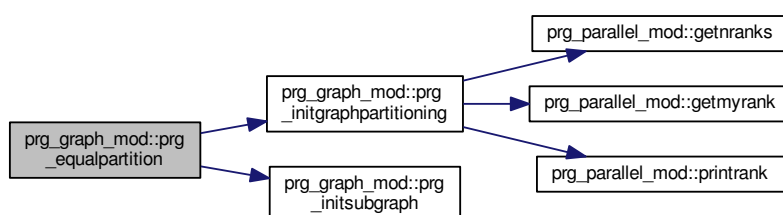
Create equal graph partitions, based on number of rows/orbitals.

#### Parameters

|                     |                                    |
|---------------------|------------------------------------|
| <i>gp</i>           | Graph partitioning'                |
| <i>nodesPerPart</i> | Number of core nodes per partition |
| <i>nnodes</i>       | Total nodes in Hamiltonian matrix  |

Definition at line 355 of file `prg_graph_mod.F90`.

Here is the call graph for this function:



9.7.2.5 subroutine, public `prg_graph_mod::prg_filepartition ( type (graph_partitioning_t), intent(inout) gp, character(len=*), intent(in) partFile )`

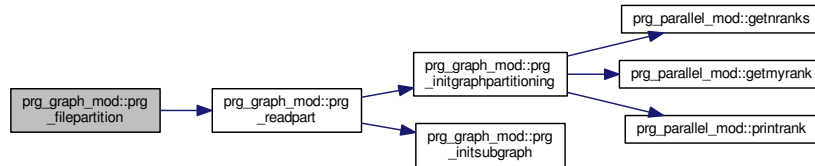
Read graph partitions from a file, based on number of rows/orbitals.

#### Parameters

|                 |   |
|-----------------|---|
| <i>partFile</i> | File containing core nodes for each partition |
| <i>gp</i>       | Graph partitioning                            |

Definition at line 463 of file prg\_graph\_mod.F90.

Here is the call graph for this function:



#### 9.7.2.6 subroutine, public `prg_graph_mod::prg_fnormgraph ( type(graph_partitioning_t), intent(inout) gp )`

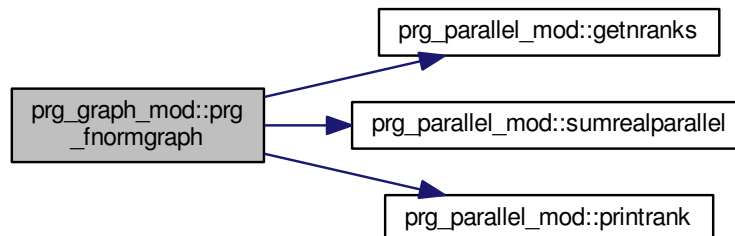
Accumulate trace norm across all subgraphs.

##### Parameters

|           |                    |
|-----------|--------------------|
| <i>gp</i> | Graph partitioning |
|-----------|--------------------|

Definition at line 516 of file prg\_graph\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.7.2.7 subroutine, public prg\_graph\_mod::prg\_initgraphpartitioning ( type (graph\_partitioning\_t), intent(inout) *gp*, character(len=\*), intent(in) *pname*, integer, intent(in) *np*, integer, intent(in) *nnodes*, integer, intent(in) *nnodes2* )

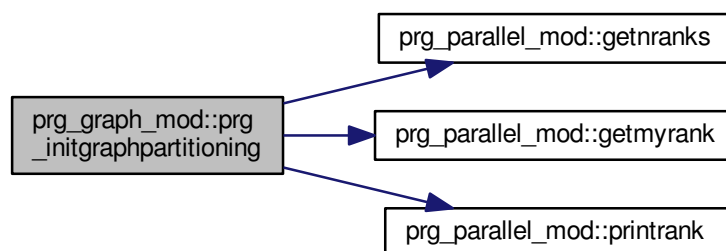
Initialize graph partitioning.

#### Parameters

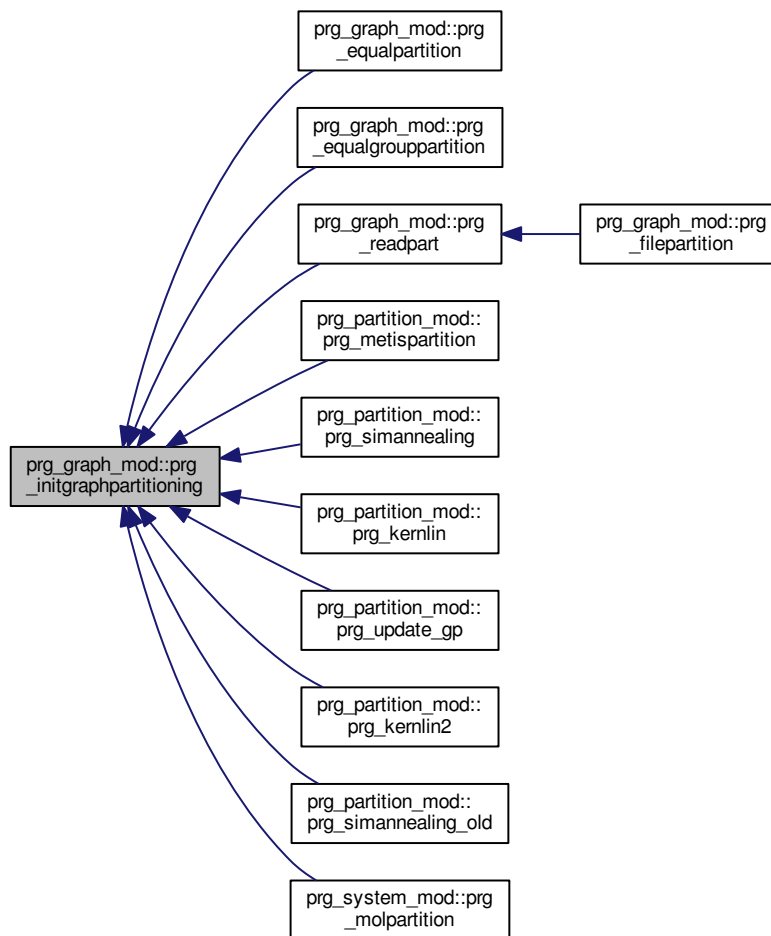
|                |                        |
|----------------|------------------------|
| <i>gp</i>      | Graph partitioning     |
| <i>pname</i>   | Partitioning name      |
| <i>np</i>      | Number of partitions   |
| <i>nnodes</i>  | Number of groups/nodes |
| <i>nnodes2</i> | Number of nodes        |

Definition at line 175 of file prg\_graph\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.7.2.8 subroutine, public `prg_graph_mod::prg_initsubgraph ( type (subgraph_t), intent(inout) sg, integer, intent(in) pnum, integer, intent(in) hsize )`

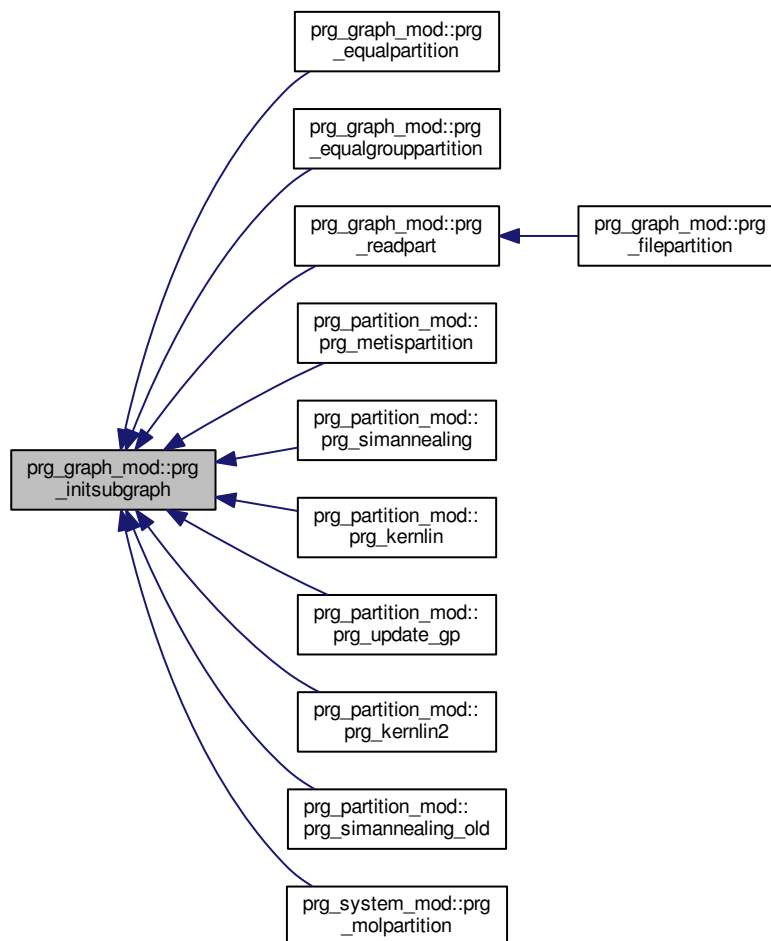
Initialize subgraph.

#### Parameters

|              |                     |
|--------------|---------------------|
| <i>sg</i>    | Subgraph            |
| <i>pnum</i>  | Part number         |
| <i>hsize</i> | Size of full matrix |

Definition at line 143 of file `prg_graph_mod.F90`.

Here is the caller graph for this function:



#### 9.7.2.9 subroutine, public prg\_graph\_mod::prg\_printgraphpartitioning ( type (graph\_partitioning\_t), intent(in) gp )

Print graph partitioning structure data.

##### Parameters

|           |                    |
|-----------|--------------------|
| <i>gp</i> | Graph partitioning |
|-----------|--------------------|

Definition at line 292 of file prg\_graph\_mod.F90.

#### 9.7.2.10 subroutine prg\_graph\_mod::prg\_readpart ( type (graph\_partitioning\_t), intent(inout) gp, character(len=\*) intent(in) partFile ) [private]

Read parts (core) from part file.

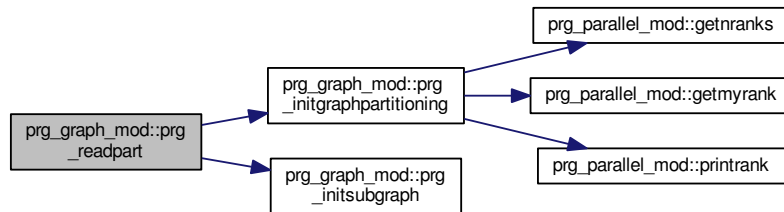


## Parameters

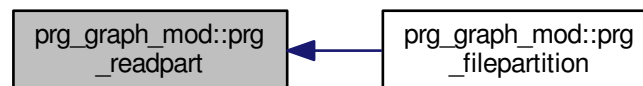
|                 |                    |
|-----------------|--------------------|
| <i>gp</i>       | Graph partitioning |
| <i>partFile</i> | Partition file     |

Definition at line 475 of file prg\_graph\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



### 9.7.3 Variable Documentation

9.7.3.1 integer, parameter `prg_graph_mod::dp = kind(1.0d0)` `[private]`

Definition at line 16 of file prg\_graph\_mod.F90.

## 9.8 prg\_graphsp2parser\_mod Module Reference

Graph partitioning SP2 parser.

### Data Types

- type [gsp2data\\_type](#)  
*General SP2 solver type.*

## Functions/Subroutines

- subroutine, public `prg_parse_gsp2` (gsp2data, filename)  
*The parser for SP2 solver.*

## Variables

- integer, parameter `dp = kind(1.0d0)`

### 9.8.1 Detailed Description

Graph partitioning SP2 parser.

This module is used to parse all the necessary input variables for graph-based SP2 electronic structure solver. Adding a new input keyword to the parser:

- If the variable is real, we have to increase `nkey_re`.
- Add the keyword (character type) in the `keyvector_re` vector.
- Add a default value (real type) in the `valvector_re`.
- Define a new variable and pass the value through `valvector_re(num)` where `num` is the position of the new keyword in the vector.

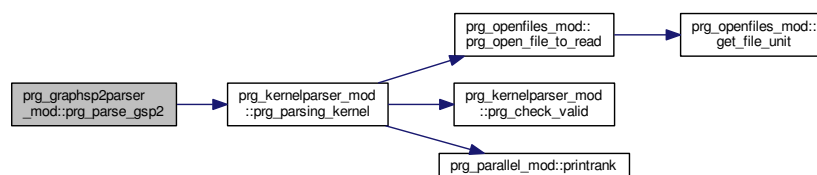
### 9.8.2 Function/Subroutine Documentation

9.8.2.1 subroutine, public `prg_graphsp2parser_mod::prg_parse_gsp2` ( `type(gsp2data_type)`, intent(inout) `gsp2data`, character(len=\*) `filename` )

The parser for SP2 solver.

Definition at line 62 of file `prg_graphsp2parser_mod.F90`.

Here is the call graph for this function:



### 9.8.3 Variable Documentation

9.8.3.1 integer, parameter `prg_graphsp2parser_mod::dp = kind(1.0d0)` [private]

Definition at line 22 of file `prg_graphsp2parser_mod.F90`.

## 9.9 prg\_homolumo\_mod Module Reference

The homolumo module.

### Functions/Subroutines

- subroutine, public [prg\\_homolumogap](#) (vv, imax, pp, mineval, maxeval, ehomo, elumo, egap, verbose)
- subroutine, public [prg\\_sp2sequence](#) (pp, imax, mineval, maxeval, ehomo, elumo, errlimit, verbose)

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.9.1 Detailed Description

The homolumo module.

### 9.9.2 Function/Subroutine Documentation

**9.9.2.1** subroutine, public `prg_homolumo_mod::prg_homolumogap` ( `real(dp)`, `dimension(:)`, `intent(in)` `vv`, `integer`, `intent(in)` `imax`, `integer`, `dimension(:)`, `intent(in)` `pp`, `real(dp)`, `intent(in)` `mineval`, `real(dp)`, `intent(in)` `maxeval`, `real(dp)`, `intent(inout)` `ehomo`, `real(dp)`, `intent(inout)` `elumo`, `real(dp)`, `intent(inout)` `egap`, `integer`, `intent(in)`, optional `verbose` )

Definition at line 24 of file `prg_homolumo_mod.F90`.

**9.9.2.2** subroutine, public `prg_homolumo_mod::prg_sp2sequence` ( `integer`, `dimension(:)`, `intent(inout)` `pp`, `integer`, `intent(inout)` `imax`, `real(dp)`, `intent(in)` `mineval`, `real(dp)`, `intent(in)` `maxeval`, `real(dp)`, `intent(in)` `ehomo`, `real(dp)`, `intent(in)` `elumo`, `real(dp)`, `intent(in)` `errlimit`, `integer`, `intent(in)`, optional `verbose` )

Definition at line 94 of file `prg_homolumo_mod.F90`.

### 9.9.3 Variable Documentation

**9.9.3.1** integer, parameter `prg_homolumo_mod::dp` = kind(1.0d0) [private]

Definition at line 14 of file `prg_homolumo_mod.F90`.

## 9.10 prg\_implicit\_fermi\_mod Module Reference

### Functions/Subroutines

- subroutine, public [prg\\_implicit\\_fermi](#) (h\_bml, xi0\_bml, p\_bml, nsteps, nocc, mu, beta, osteps, occErrLimit, threshold)  
*Recursive Implicit Fermi Dirac.*

## Variables

- integer, parameter `dp = kind(1.0d0)`

### 9.10.1 Function/Subroutine Documentation

9.10.1.1 subroutine, public `prg_implicit_fermi_mod::prg_implicit_fermi` ( `type(bml_matrix_t)`, `intent(in) h_bml`, `type(bml_matrix_t)`, `intent(inout) xi0_bml`, `type(bml_matrix_t)`, `intent(inout) p_bml`, `integer`, `intent(in) nsteps`, `real(dp)`, `intent(in) nocc`, `real(dp)`, `intent(inout) mu`, `real(dp)`, `intent(in) beta`, `integer`, `intent(in) osteps`, `real(dp)`, `intent(in) occErrLimit`, `real(dp)`, `intent(in) threshold` )

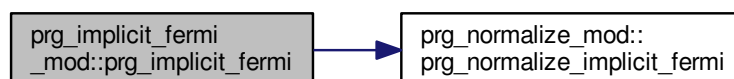
Recursive Implicit Fermi Dirac.

#### Parameters

|                    |   |
|--------------------|---|
| <i>h_bml</i>       | Input Hamiltonian matrix.                       |
| <i>xi0_bml</i>     | Initial guess of first inverse.                 |
| <i>p_bml</i>       | Output density matrix.                          |
| <i>nsteps</i>      | Number of sp2 iterations.                       |
| <i>nocc</i>        | Number of occupied states.                      |
| <i>mu</i>          | Shifted chemical potential                      |
| <i>beta</i>        | Input inverse temperature.                      |
| <i>osteps</i>      | Outer loop steps to converge chemical potential |
| <i>occErrLimit</i> | Occupation error limit.                         |
| <i>threshold</i>   | Threshold for multiplication.                   |

Definition at line 39 of file `prg_implicit_fermi_mod.F90`.

Here is the call graph for this function:



### 9.10.2 Variable Documentation

9.10.2.1 integer, parameter `prg_implicit_fermi_mod::dp = kind(1.0d0)` [`private`]

Definition at line 20 of file `prg_implicit_fermi_mod.F90`.

## 9.11 prg\_initmatrices\_mod Module Reference

Initialization module.

## Functions/Subroutines

- subroutine, public [prg\\_init\\_hsmat](#) (ham\_bml, over\_bml, bml\_type, mdim, norb)  
*Initialize Hamiltonian and Overlap Matrix.*
- subroutine, public [prg\\_init\\_pzmat](#) (rho\_bml, zmat\_bml, bml\_type, mdim, norb)  
*Initialize Density matrix and Inverse square root Overlap.*
- subroutine, public [prg\\_init\\_ortho](#) (orthoh\_bml, orthop\_bml, bml\_type, mdim, norb)  
*Initialize The orthogonal versions of Hamiltonian and Density Matrix.*

## Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.11.1 Detailed Description

Initialization module.

Routines in this module are used to prg\_initialize several matrices that will be used in the code.

### 9.11.2 Function/Subroutine Documentation

9.11.2.1 subroutine, public prg\_initmatrices\_mod::prg\_init\_hsmat ( type(bml\_matrix\_t), intent(inout) ham\_bml, type(bml\_matrix\_t), intent(inout) over\_bml, character(20) bml\_type, integer, intent(inout) mdim, integer, intent(in) norb )

Initialize Hamiltonian and Overlap Matrix.

Allocation of the Hamiltonian and Overlap matrix into bml formats.

#### Parameters

|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Hamiltonian in bml format.                           |
| <i>over_bml</i>  | Overlap in bml format.                               |
| <i>threshold</i> | Threshold value for matrix elements.                 |
| <i>mdim</i>      | Max nonzero elements per row for every row see [1] . |
| <i>norb</i>      | Total number of orbitals.                            |

Definition at line 28 of file prg\_initmatrices\_mod.F90.

9.11.2.2 subroutine, public prg\_initmatrices\_mod::prg\_init\_ortho ( type(bml\_matrix\_t), intent(inout) orthoh\_bml, type(bml\_matrix\_t), intent(inout) orthop\_bml, character(20) bml\_type, integer, intent(inout) mdim, integer, intent(in) norb )

Initialize The orthogonal versions of Hamiltonian and Density Matrix.

Allocation of the orthogonal Hamiltonian and Density matrix into bml formats.

## Parameters

|                   |  |
|-------------------|--|
| <i>orthoh_bml</i> | Orthogonal Hamiltonian in bml format.                |
| <i>orthop_bml</i> | Orthogonal Density Matrix in bml format.             |
| <i>threshold</i>  | Threshold value for matrix elements.                 |
| <i>mdim</i>       | Max nonzero elements per row for every row see [1] . |
| <i>norb</i>       | Total number of orbitals.                            |

Definition at line 70 of file prg\_initmatrices\_mod.F90.

```
9.11.2.3  subroutine, public prg_initmatrices_mod::prg_init_pzmat ( type(bml_matrix_t), intent(inout) rho_bml,
                                type(bml_matrix_t), intent(inout) zmat_bml, character(20) bml_type, integer, intent(inout) mdim, integer, intent(in) norb
                                )
```

Initialize Density matrix and Inverse square root Overlap.

Allocation of the Density matrix and Inverse square root Overlap matrix into bml formats.

## Parameters

|                  |  |
|------------------|--|
| <i>rho_bml</i>   | Density matrix in bml format.                        |
| <i>zmat_bml</i>  | Inverse square root Overlap in bml format.           |
| <i>threshold</i> | Threshold value for matrix elements.                 |
| <i>mdim</i>      | Max nonzero elements per row for every row see [1] . |
| <i>norb</i>      | Total number of orbitals.                            |

Definition at line 49 of file prg\_initmatrices\_mod.F90.

### 9.11.3 Variable Documentation

```
9.11.3.1  integer, parameter prg_initmatrices_mod::dp = kind(1.0d0)  [private]
```

Definition at line 14 of file prg\_initmatrices\_mod.F90.

## 9.12 prg\_kernelparser\_mod Module Reference

Some general parsing functions.

### Functions/Subroutines

- subroutine, public [prg\\_parsing\\_kernel](#) (keyvector\_char, valvector\_char, keyvector\_int, valvector\_int, keyvector\_re, valvector\_re, keyvector\_log, valvector\_log, filename, startstop)  
*The general parsing function. It is used to vectorize a set of "keywords" "value" pairs as included in a general input file.*
- subroutine [prg\\_check\\_valid](#) (invalidc)  
*Check for valid keywords (checks for an = sign)*

## Variables

- integer, parameter `dp` = kind(1.0d0)

### 9.12.1 Detailed Description

Some general parsing functions.

#### Author

C. F. A. Negre ([cnegre@lanl.gov](mailto:cnegre@lanl.gov))

### 9.12.2 Function/Subroutine Documentation

9.12.2.1 subroutine `prg_kernelparser_mod::prg_check_valid` ( `character(len=*)`, `intent(in) invalidc` ) [private]

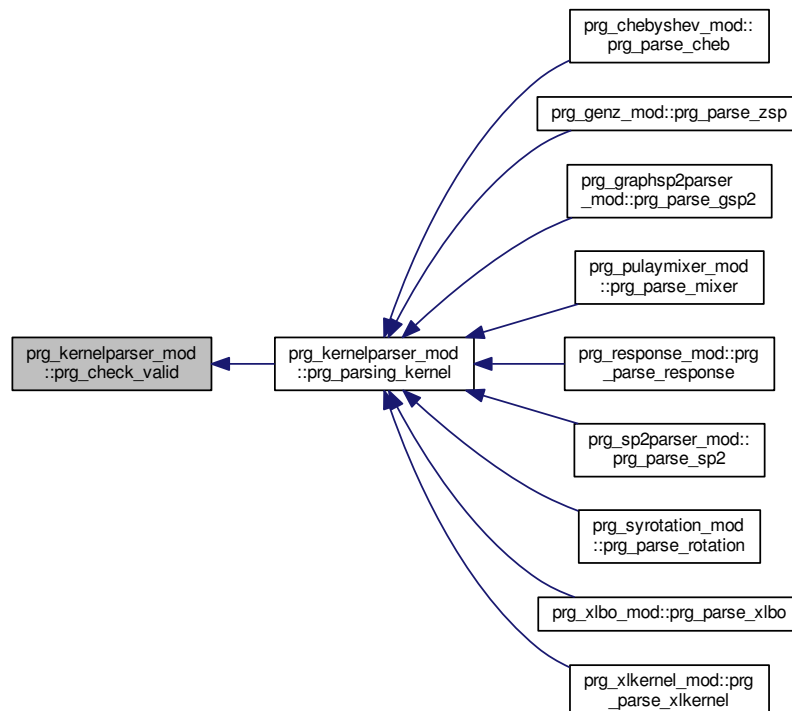
Check for valid keywords (checks for an = sign)

#### Parameters

|                       |                   |
|-----------------------|-------------------|
| <code>invalidc</code> | Keyword to check. |
|-----------------------|-------------------|

Definition at line 396 of file `prg_kernelparser_mod.F90`.

Here is the caller graph for this function:



9.12.2.2 subroutine, public prg\_kernelparser\_mod::prg\_parsing\_kernel ( character(50), dimension(:) *keyvector\_char*, character(100), dimension(:) *valvector\_char*, character(50), dimension(:) *keyvector\_int*, integer, dimension(:) *valvector\_int*, character(50), dimension(:) *keyvector\_re*, real(dp), dimension(:) *valvector\_re*, character(50), dimension(:) *keyvector\_log*, logical, dimension(:) *valvector\_log*, character(len=\*) *filename*, character(len=\*) , dimension(2), intent(in), optional *startstop* )

The general parsing function. It is used to vectorize a set of "keywords" "value" pairs as included in a general input file.

#### Note

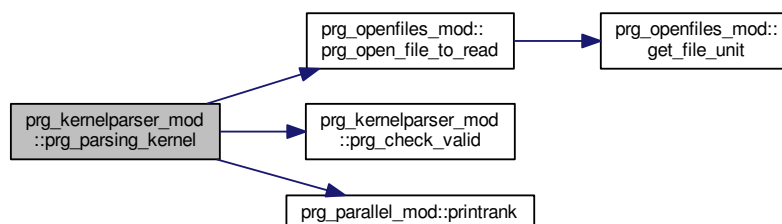
This parsing strategy can only parse a file of 500 lines by 500 words.

#### Warning

If the length of variable vect is changed, this could produce a segmentation fault.

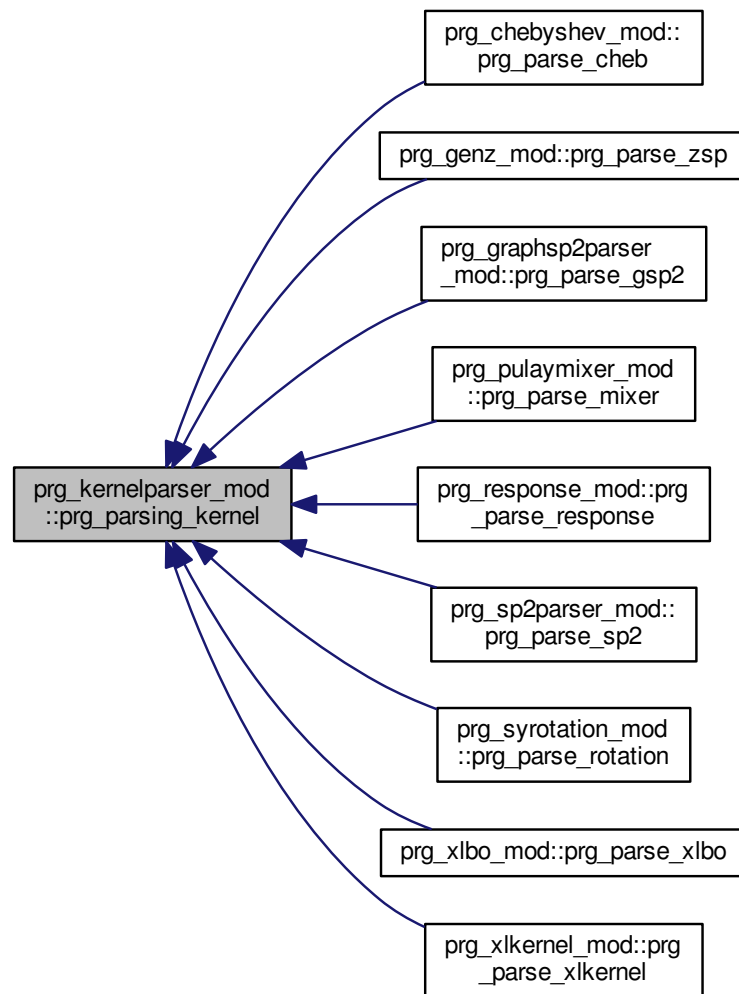
Definition at line 33 of file prg\_kernelparser\_mod.F90.

Here is the call graph for this function:





Here is the caller graph for this function:



### 9.12.3 Variable Documentation

9.12.3.1 integer, parameter `prg_kernelparser_mod::dp = kind(1.0d0)` `[private]`

Definition at line 16 of file `prg_kernelparser_mod.F90`.

## 9.13 prg\_nonortho\_mod Module Reference

Module to `prg_orthogonalize` and `prg_deorthogonalize` any operator.

## Functions/Subroutines

- subroutine, public `prg_orthogonalize` (`A_bml`, `zmat_bml`, `orthoA_bml`, `threshold`, `bml_type`, `verbose`)  
*This routine performs:  $A_{ortho} = Z^\dagger A Z$ .*
- subroutine, public `prg_deorthogonalize` (`orthoA_bml`, `zmat_bml`, `a_bml`, `threshold`, `bml_type`, `verbose`)  
*This routine performs:  $A = Z A_{ortho} Z^\dagger$ .*

## Variables

- integer, parameter `dp` = kind(1.0d0)

### 9.13.1 Detailed Description

Module to `prg_orthogonalize` and `prg_deorthogonalize` any operator.

Typically the Hamiltonian needs to be `prg_orthogonalized`:  $H_{ortho} = Z^\dagger H Z$

Also, if the density matrix was obtained from the `prg_orthogonalized` Hamiltonian, it can be `prg_deorthogonalized` as:  $\rho = Z \rho_{ortho} Z^\dagger$

### 9.13.2 Function/Subroutine Documentation

- 9.13.2.1 subroutine, public `prg_nonortho_mod::prg_deorthogonalize` ( `type(bml_matrix_t)`, `intent(in) orthoA_bml`, `type(bml_matrix_t)`, `intent(in) zmat_bml`, `type(bml_matrix_t)`, `intent(inout) a_bml`, `real(dp) threshold`, `character(len=*) bml_type`, `integer verbose` )

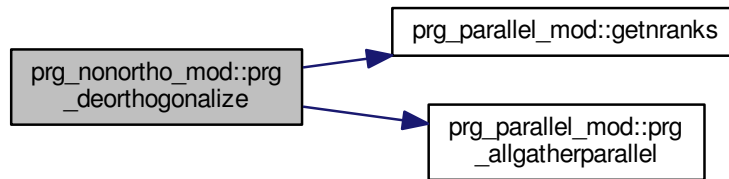
This routine performs:  $A = Z A_{ortho} Z^\dagger$ .

#### Parameters

|                         |   |
|-------------------------|---|
| <code>orthoA_bml</code> | Matrix to be <code>prg_deorthogonalized</code> .  |
| <code>zmat_bml</code>   | Congruence transform to be used.  |
| <code>A_bml</code>      | Matrix resulting from the <code>prg_deorthogonalized</code> in <code>bml</code> format. |
| <code>threshold</code>  | Threshold value to be used in the matrix-matrix operations.                             |
| <code>bml_type</code>   | <code>bml</code> format to be used.   |
| <code>verbose</code>    | Verbosity level.  |

Definition at line 82 of file `prg_nonortho_mod.F90`.

Here is the call graph for this function:



9.13.2.2 subroutine, public `prg_nonortho_mod::prg_orthogonalize` ( `type(bml_matrix_t)`, `intent(inout)` *A\_bml*, `type(bml_matrix_t)`, `intent(inout)` *zmat\_bml*, `type(bml_matrix_t)`, `intent(inout)` *orthoA\_bml*, `real(dp)`, `intent(in)` *threshold*, `character(len=*)`, `intent(in)` *bml\_type*, `integer`, `intent(in)` *verbose* )

This routine performs:  $A_{ortho} = Z^{\dagger} A Z$ .

#### Parameters

|                   |   |
|-------------------|---|
| <i>A_bml</i>      | Matrix to be <code>prg_orthogonalized</code> in bml format. |
| <i>zmat_bml</i>   | Congruence transform to be used.                            |
| <i>orthoA_bml</i> | Matrix resulting from the orthogonalization.                |
| <i>threshold</i>  | Threshold value to be used in the matrix-matrix operations. |
| <i>bml_type</i>   | bml format to be used.                                      |
| <i>verbose</i>    | Verbosity level.  |

Definition at line 36 of file `prg_nonortho_mod.F90`.

### 9.13.3 Variable Documentation

9.13.3.1 `integer`, parameter `prg_nonortho_mod::dp = kind(1.0d0)` [`private`]

Definition at line 19 of file `prg_nonortho_mod.F90`.

## 9.14 prg\_normalize\_mod Module Reference

The `prg_normalize` module.

## Functions/Subroutines

- subroutine, public [prg\\_normalize](#) (h\_bml)  
*Normalize a Hamiltonian matrix prior to running the SP2 algorithm.*
- subroutine, public [prg\\_normalize\\_fermi](#) (h\_bml, h1, hN, mu)  
*Normalize a Hamiltonian matrix prior to running the truncated SP2 algorithm.*
- subroutine, public [prg\\_normalize\\_implicit\\_fermi](#) (h\_bml, cnst, mu)  
*Normalize a Hamiltonian matrix prior to running the implicit fermi dirac algorithm.*
- subroutine, public [prg\\_gershgorinreduction](#) (gp)  
*Determine gershgorin bounds across all parts, local and distributed.*
- subroutine, public [prg\\_normalize\\_cheb](#) (h\_bml, mu, emin, emax, alpha, scaledmu)  
*Normalize a Hamiltonian matrix prior to running the Chebyshev algorithm.*

## Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.14.1 Detailed Description

The prg\_normalize module.

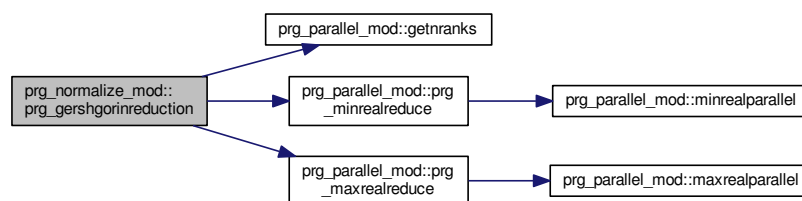
### 9.14.2 Function/Subroutine Documentation

9.14.2.1 subroutine, public `prg_normalize_mod::prg_gershgorinreduction ( type(graph_partitioning_t), intent(inout) gp )`

Determine gershgorin bounds across all parts, local and distributed.

Definition at line 101 of file prg\_normalize\_mod.F90.

Here is the call graph for this function:



9.14.2.2 subroutine, public `prg_normalize_mod::prg_normalize ( type(bml_matrix_t), intent(inout) h_bml )`

Normalize a Hamiltonian matrix prior to running the SP2 algorithm.

$$X0 = (e\_max * I - H) / (e\_max - e\_min)$$

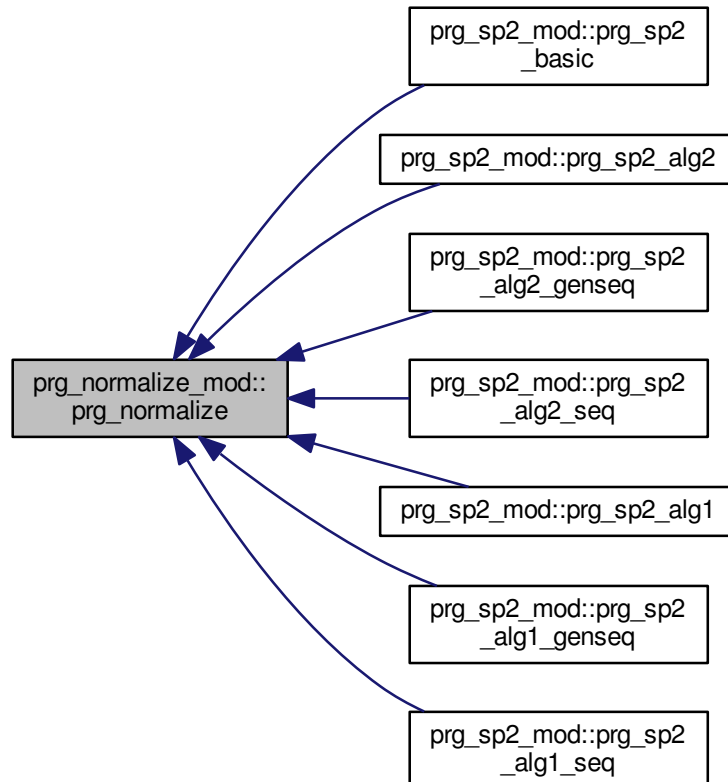
where `e_max` and `e_min` are obtained sing the Gershgorin circle theorem.

## Parameters

|              |                                 |
|--------------|---------------------------------|
| <i>h_bml</i> | Input/Output Hamiltonian matrix |
|--------------|---------------------------------|

Definition at line 33 of file prg\_normalize\_mod.F90.

Here is the caller graph for this function:



```

9.14.2.3  subroutine, public prg_normalize_mod::prg_normalize_cheb ( type(bml_matrix_t), intent(inout) h_bml, real(dp),
intent(in) mu, real(dp), intent(in) emin, real(dp), intent(in) emax, real(dp), intent(inout) alpha, real(dp), intent(inout)
scaledmu )
  
```

Normalize a Hamiltonian matrix prior to running the Chebyshev algorithm.

$$X0 = 2*(H - e\_min*I) / (e\_max - e\_min) - I$$

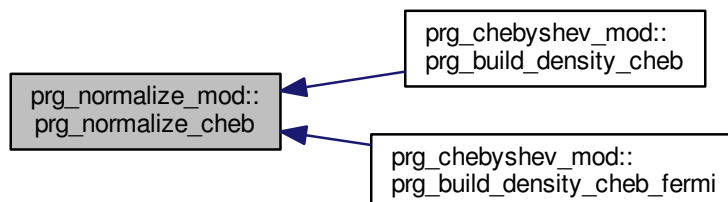
where `e_max` and `e_min` are obtained sing the Gershgorin circle theorem.

## Parameters

|              |                                 |
|--------------|---------------------------------|
| <i>h_bml</i> | Input/Output Hamiltonian matrix |
|--------------|---------------------------------|

Definition at line 130 of file prg\_normalize\_mod.F90.

Here is the caller graph for this function:



9.14.2.4 subroutine, public prg\_normalize\_mod::prg\_normalize\_fermi ( type(bml\_matrix\_t), intent(inout) *h\_bml*, real(dp), intent(in) *h1*, real(dp), intent(in) *hN*, real(dp), intent(in) *mu* )

Normalize a Hamiltonian matrix prior to running the truncated SP2 algorithm.

$X0 = ((hN - \mu) * I - H) / (hN - h1)$  or  $X0 = (hN * I - H0 - \mu * I) / (hN - h1)$

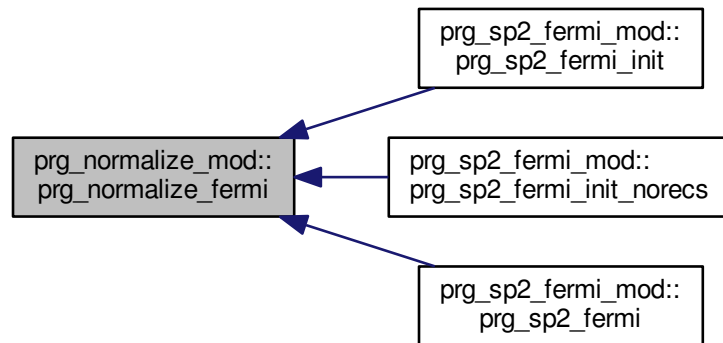
where *h1* and *hN* are scaled Gershgorin bounds.

#### Parameters

|              |                                  |
|--------------|----------------------------------|
| <i>H_bml</i> | Hamiltonian matrix               |
| <i>h1</i>    | Scaled minimum Gershgorin bound. |
| <i>hN</i>    | Scaled maximum Gershgorin bound. |
| <i>mu</i>    | Chemical potential               |

Definition at line 63 of file prg\_normalize\_mod.F90.

Here is the caller graph for this function:



9.14.2.5 subroutine, public prg\_normalize\_mod::prg\_normalize\_implicit\_fermi ( type(bml\_matrix\_t), intent(inout) *h\_bml*, real(dp), intent(in) *cnst*, real(dp), intent(in) *mu* )

Normalize a Hamiltonian matrix prior to running the implicit fermi dirac algorithm.

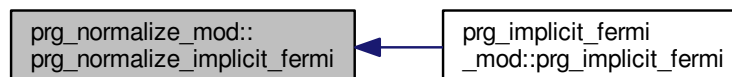
$X0 = 0.5 * I - cnst * (H0 - \mu_0 * I)$  or  $X0 = (0.5 + cnst * \mu_0) * I - cnst * H0$

#### Parameters

|              |                                  |
|--------------|----------------------------------|
| <i>H_bml</i> | Hamiltonian matrix               |
| <i>cnst</i>  | Constant based on beta and steps |
| <i>mu</i>    | Chemical potential               |

Definition at line 87 of file prg\_normalize\_mod.F90.

Here is the caller graph for this function:



### 9.14.3 Variable Documentation

9.14.3.1 integer, parameter prg\_normalize\_mod::dp = kind(1.0d0) [private]

Definition at line 15 of file prg\_normalize\_mod.F90.

## 9.15 prg\_openfiles\_mod Module Reference

Module to handle input output files for the PROGRESS lib.

### Functions/Subroutines

- integer function, public [get\\_file\\_unit](#) (io\_max)  
*Returns a unit number that is not in use.*
- subroutine, public [prg\\_open\\_file](#) (io, name)  
*Opens a file to write.*
- subroutine, public [prg\\_open\\_file\\_to\\_read](#) (io, name)  
*Opens a file to read.*

### 9.15.1 Detailed Description

Module to handle input output files for the PROGRESS lib.

### 9.15.2 Function/Subroutine Documentation

#### 9.15.2.1 integer function, public prg\_openfiles\_mod::get\_file\_unit ( integer io\_max )

Returns a unit number that is not in use.

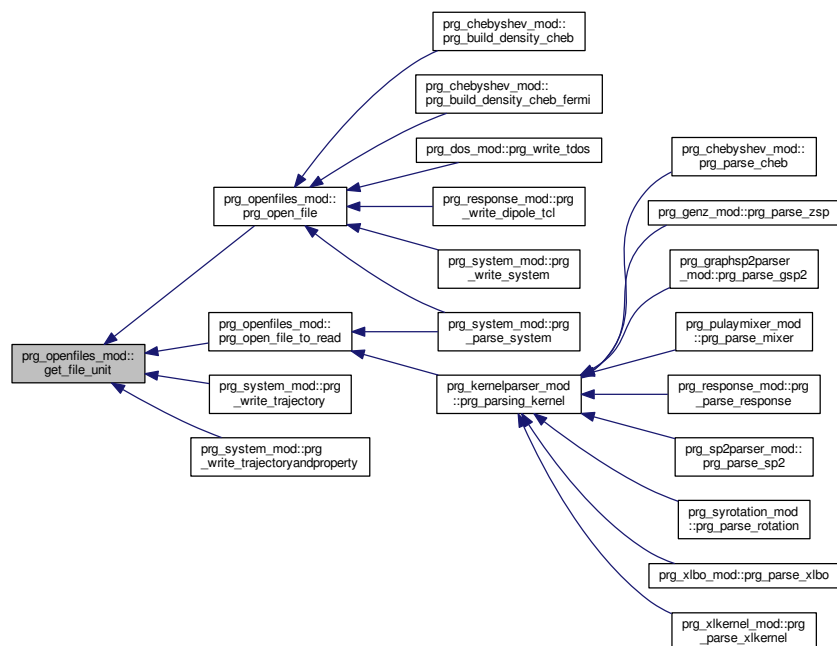
#### Parameters

|                      |                                  |
|----------------------|----------------------------------|
| <i>io_max</i>        | Maximum units to search.         |
| <i>get_file_unit</i> | Unit return to use for the file. |

Definition at line 19 of file prg\_openfiles\_mod.F90.



Here is the caller graph for this function:



### 9.15.2.2 subroutine, public prg\_openfiles\_mod::prg\_open\_file ( integer *io*, character(len=\*) *name* )

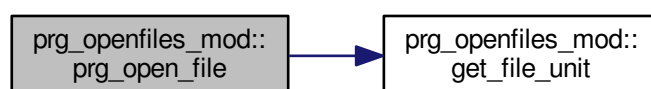
Opens a file to write.

### Parameters

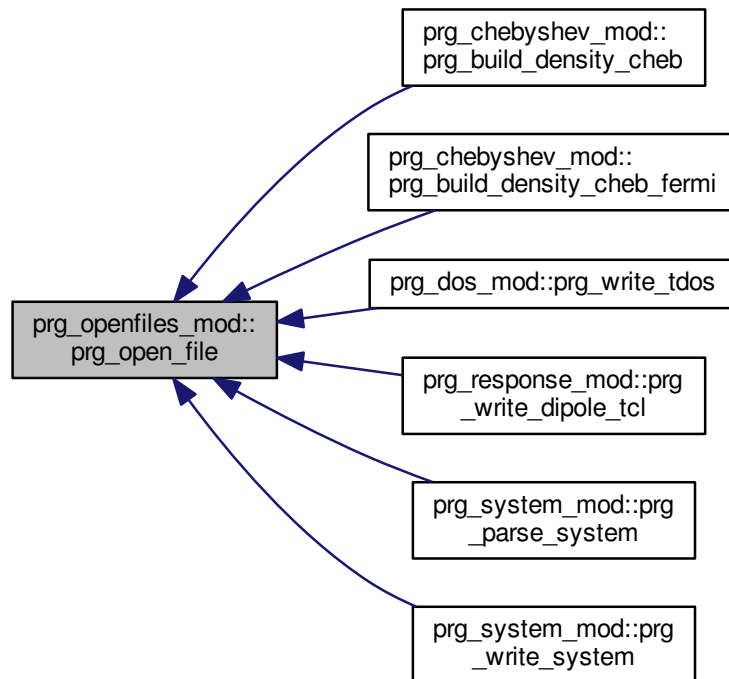
|             |                    |
|-------------|--------------------|
| <i>io</i>   | Unit for the file. |
| <i>name</i> | Name of the file.  |

Definition at line 38 of file prg\_openfiles\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



#### 9.15.2.3 subroutine, public `prg_openfiles_mod::prg_open_file_to_read ( integer io, character(len=*) name )`

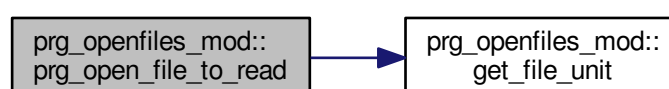
Opens a file to read.

##### Parameters

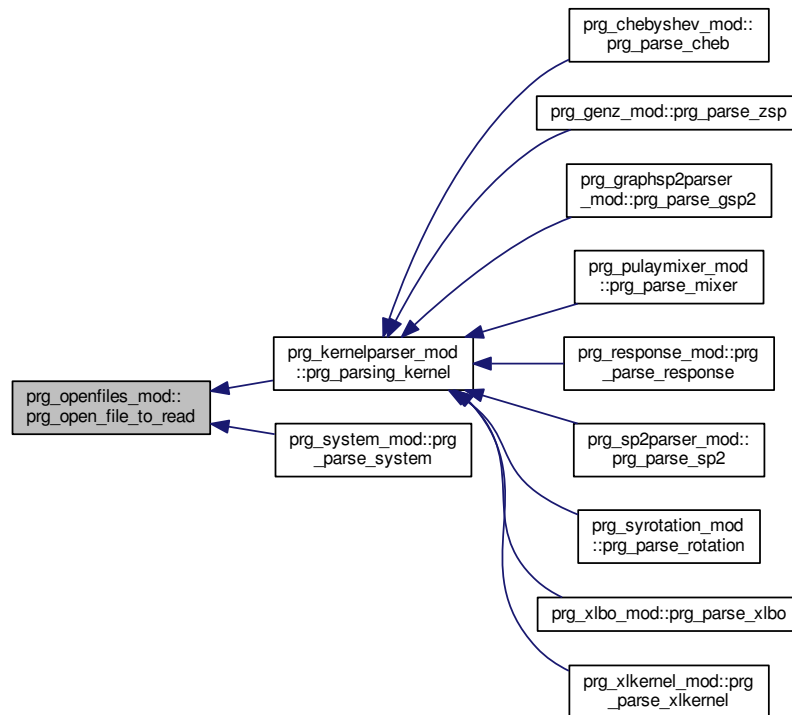
|             |                    |
|-------------|--------------------|
| <i>io</i>   | Unit for the file. |
| <i>name</i> | Name of the file.  |

Definition at line 54 of file `prg_openfiles_mod.F90`.

Here is the call graph for this function:



Here is the caller graph for this function:



## 9.16 prg\_parallel\_mod Module Reference

The parallel module.

### Data Types

- type `rankreducedata_t`  
*Data structure for rection over MPI ranks.*

### Functions/Subroutines

- integer function, public `getnranks` ()
- integer function, public `getmyrank` ()
- integer function, public `printrank` ()
- subroutine, public `prg_initparallel` ()
- subroutine, public `prg_shutdownparallel` ()
- integer function `saverequest` (irequest)
- subroutine, public `prg_barrierparallel` ()
- subroutine, public `sendreceiveparallel` (sendBuf, sendLen, dest, recvBuf, recvLen, source, nreceived)
- subroutine, public `isendparallel` (sendBuf, sendLen, dest)
- subroutine, public `sendparallel` (sendBuf, sendLen, dest)

- subroutine, public [prg\\_iprg\\_recvparallel](#) (recvBuf, recvLen, rind)
- subroutine, public [prg\\_recvparallel](#) (recvBuf, recvLen)
- subroutine, public [sumintparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [sumrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [maxintparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [maxrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [minintparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [minrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_minrealreduce](#) (rvalue)
- subroutine, public [prg\\_maxrealreduce](#) (rvalue)
- subroutine, public [prg\\_maxintreduce2](#) (value1, value2)
- subroutine, public [prg\\_sumintreduce2](#) (value1, value2)
- subroutine, public [prg\\_sumrealreduce](#) (value1)
- subroutine, public [prg\\_sumrealreduce2](#) (value1, value2)
- subroutine, public [prg\\_sumrealreduce3](#) (value1, value2, value3)
- subroutine, public [prg\\_sumrealreducen](#) (valueVec, N)
- subroutine, public [prg\\_sumintreducen](#) (valueVec, N)
- subroutine, public [minrankrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [maxrankrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_bcastparallel](#) (buf, blen, root)
- subroutine, public [allgatherrealparallel](#) (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public [allgatherintparallel](#) (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public [allgathervrealparallel](#) (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public [allgathervintparallel](#) (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public [prg\\_allsumrealreduceparallel](#) (buf, buflen)
- subroutine, public [prg\\_allsumintreduceparallel](#) (buf, buflen)
- subroutine, public [prg\\_allgatherparallel](#) (a)
- subroutine, public [prg\\_wait](#) ()

## Variables

- integer, parameter [dp](#) = kind(1.0d0)
- integer [myrank](#)
- integer [nranks](#)
- integer [ierr](#)
- integer [reqcount](#)
- integer, dimension(:), allocatable [requestlist](#)
- integer, dimension(:), allocatable [rused](#)

## 9.16.1 Detailed Description

The parallel module.

## 9.16.2 Function/Subroutine Documentation

- 9.16.2.1 subroutine, public [prg\\_parallel\\_mod::allgatherintparallel](#) ( integer, dimension(\*), intent(in) *sendBuf*, integer, intent(in) *sendLen*, integer, dimension(\*), intent(out) *recvBuf*, integer, intent(in) *recvLen* )

Definition at line 660 of file [prg\\_parallel\\_mod.F90](#).

9.16.2.2 subroutine, public prg\_parallel\_mod::allgatherrealparallel ( real(dp), dimension(\*), intent(in) *sendBuf*, integer, intent(in) *sendLen*, real(dp), dimension(\*), intent(out) *recvBuf*, integer, intent(in) *recvLen* )

Definition at line 644 of file prg\_parallel\_mod.F90.

9.16.2.3 subroutine, public prg\_parallel\_mod::allgathervintparallel ( integer, dimension(\*), intent(in) *sendBuf*, integer, intent(in) *sendLen*, integer, dimension(\*), intent(out) *recvBuf*, integer, dimension(\*), intent(in) *recvLen*, integer, dimension(\*), intent(in) *recvDispl* )

Definition at line 696 of file prg\_parallel\_mod.F90.

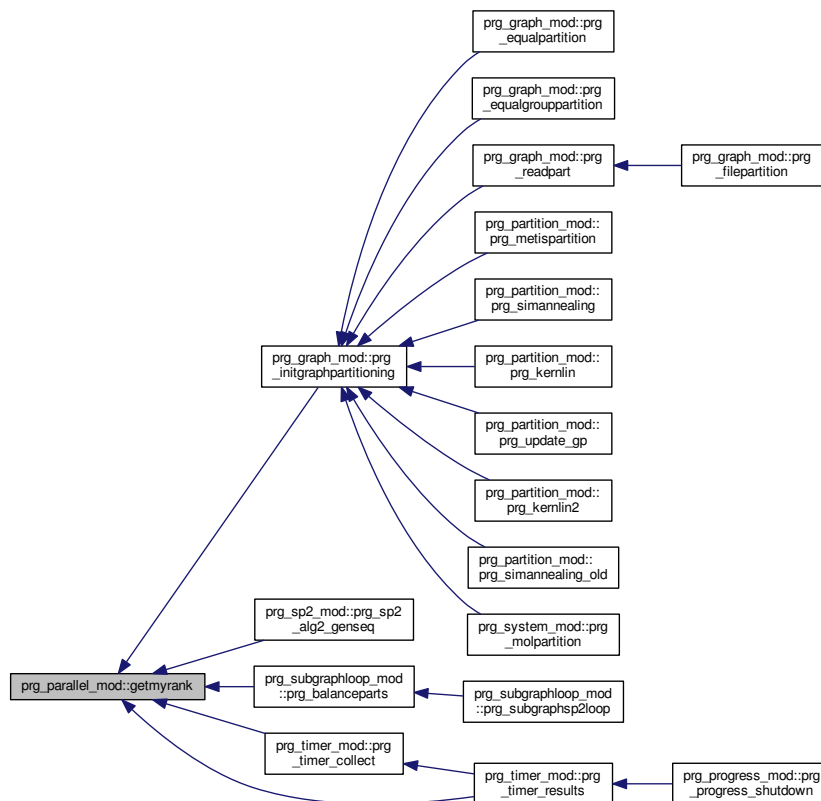
9.16.2.4 subroutine, public prg\_parallel\_mod::allgathervrealparallel ( real(dp), dimension(\*), intent(in) *sendBuf*, integer, intent(in) *sendLen*, real(dp), dimension(\*), intent(out) *recvBuf*, integer, dimension(\*), intent(in) *recvLen*, integer, dimension(\*), intent(in) *recvDispl* )

Definition at line 676 of file prg\_parallel\_mod.F90.

9.16.2.5 integer function, public prg\_parallel\_mod::getmyrank ( )

Definition at line 99 of file prg\_parallel\_mod.F90.

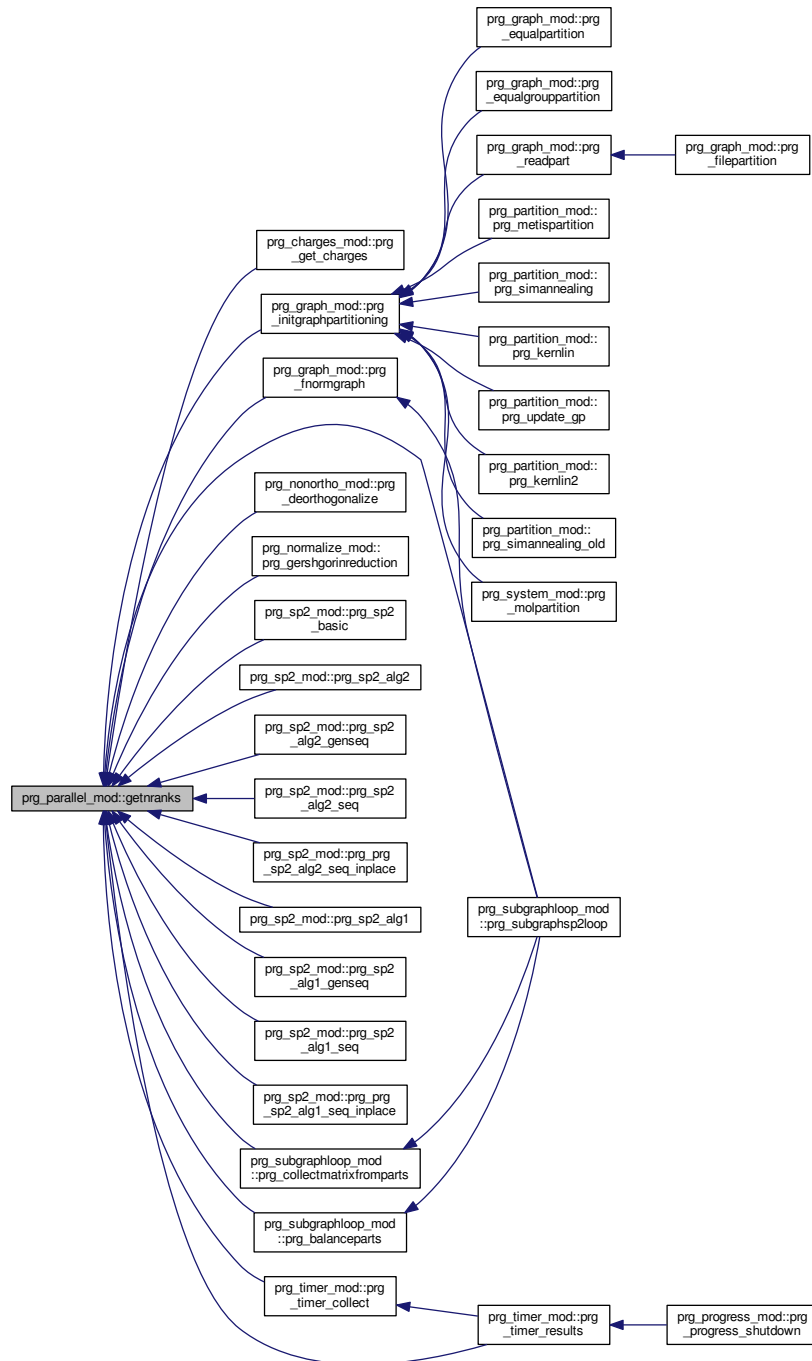
Here is the caller graph for this function:



### 9.16.2.6 integer function, public prg\_parallel\_mod::getnranks ( )

Definition at line 88 of file prg\_parallel\_mod.F90.

Here is the caller graph for this function:



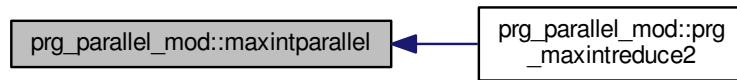
### 9.16.2.7 subroutine, public prg\_parallel\_mod::isendparallel ( real(dp), dimension(\*), intent(in) sendBuf, integer, intent(in) sendLen, integer, intent(in) dest )

Definition at line 230 of file prg\_parallel\_mod.F90.

9.16.2.8 subroutine, public prg\_parallel\_mod::maxintparallel ( integer, dimension(\*), intent(in) *sendBuf*, integer, dimension(\*), intent(out) *recvBuf*, integer, intent(in) *icount* )

Definition at line 337 of file prg\_parallel\_mod.F90.

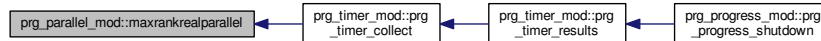
Here is the caller graph for this function:



9.16.2.9 subroutine, public prg\_parallel\_mod::maxrankrealparallel ( type(rankreducedata\_t), dimension(\*), intent(in) *sendBuf*, type(rankreducedata\_t), dimension(\*), intent(out) *recvBuf*, integer, intent(in) *icount* )

Definition at line 607 of file prg\_parallel\_mod.F90.

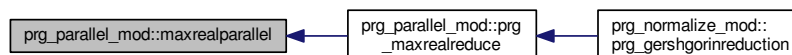
Here is the caller graph for this function:



9.16.2.10 subroutine, public prg\_parallel\_mod::maxrealparallel ( real(dp), dimension(\*), intent(in) *sendBuf*, real(dp), dimension(\*), intent(out) *recvBuf*, integer, intent(in) *icount* )

Definition at line 358 of file prg\_parallel\_mod.F90.

Here is the caller graph for this function:



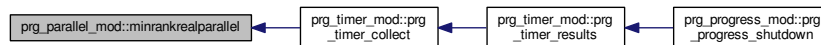
9.16.2.11 subroutine, public prg\_parallel\_mod::minintparallel ( integer, dimension(\*), intent(in) *sendBuf*, integer, dimension(\*), intent(out) *recvBuf*, integer, intent(in) *icount* )

Definition at line 379 of file prg\_parallel\_mod.F90.

9.16.2.12 subroutine, public prg\_parallel\_mod::minrankrealparallel ( type(rankreducedata\_t), dimension(\*), intent(in) *sendBuf*, type(rankreducedata\_t), dimension(\*), intent(out) *recvBuf*, integer, intent(in) *icount* )

Definition at line 584 of file prg\_parallel\_mod.F90.

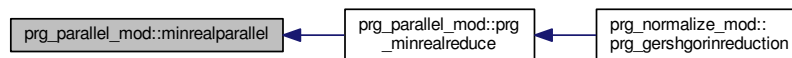
Here is the caller graph for this function:



9.16.2.13 subroutine, public prg\_parallel\_mod::minrealparallel ( real(dp), dimension(\*), intent(in) *sendBuf*, real(dp), dimension(\*), intent(out) *recvBuf*, integer, intent(in) *icount* )

Definition at line 400 of file prg\_parallel\_mod.F90.

Here is the caller graph for this function:

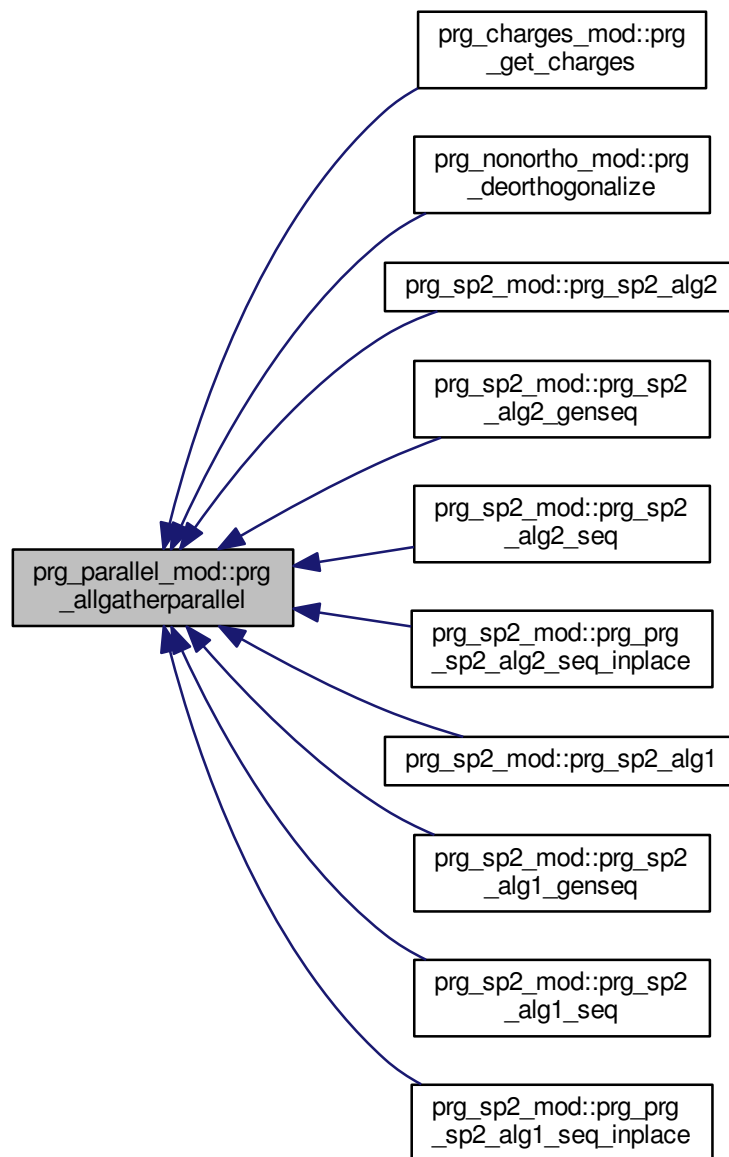


9.16.2.14 subroutine, public prg\_parallel\_mod::prg\_allgatherparallel ( type (bml\_matrix\_t), intent(inout) *a* )

Definition at line 744 of file prg\_parallel\_mod.F90.



Here is the caller graph for this function:



9.16.2.15 subroutine, public `prg_parallel_mod::prg_allsumintreduceparallel` ( integer, dimension(\*), intent(inout) *buf*, integer, intent(in) *buflen* )

Definition at line 729 of file `prg_parallel_mod.F90`.

9.16.2.16 subroutine, public `prg_parallel_mod::prg_allsumrealreduceparallel` ( real(dp), dimension(\*), intent(inout) *buf*, integer, intent(in) *buflen* )

Definition at line 714 of file `prg_parallel_mod.F90`.

9.16.2.17 subroutine, public prg\_parallel\_mod::prg\_barrierparallel ( )

Definition at line 196 of file prg\_parallel\_mod.F90.

9.16.2.18 subroutine, public prg\_parallel\_mod::prg\_bcastparallel ( character, dimension(\*), intent(in) *buf*, integer, intent(in) *blen*, integer, intent(in) *root* )

Definition at line 630 of file prg\_parallel\_mod.F90.

9.16.2.19 subroutine, public prg\_parallel\_mod::prg\_initparallel ( )

Definition at line 127 of file prg\_parallel\_mod.F90.

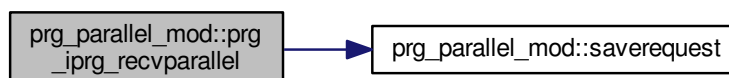
Here is the caller graph for this function:



9.16.2.20 subroutine, public prg\_parallel\_mod::prg\_iprg\_recvparallel ( real(dp), dimension(\*) *recvBuf*, integer, intent(in) *recvLen*, integer *rind* )

Definition at line 261 of file prg\_parallel\_mod.F90.

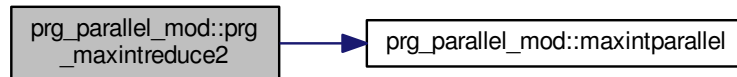
Here is the call graph for this function:



9.16.2.21 subroutine, public prg\_parallel\_mod::prg\_maxintreduce2 ( integer, intent(inout) *value1*, integer, intent(inout) *value2* )

Definition at line 453 of file prg\_parallel\_mod.F90.

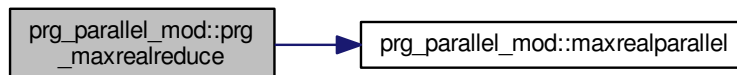
Here is the call graph for this function:



9.16.2.22 subroutine, public prg\_parallel\_mod::prg\_maxrealreduce ( real(dp), intent(inout) *rvalue* )

Definition at line 437 of file prg\_parallel\_mod.F90.

Here is the call graph for this function:



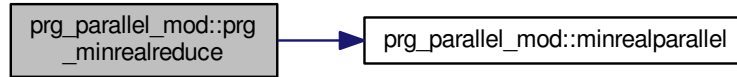
Here is the caller graph for this function:



9.16.2.23 subroutine, public prg\_parallel\_mod::prg\_minrealreduce ( real(dp), intent(inout) *rvalue* )

Definition at line 421 of file prg\_parallel\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.16.2.24 subroutine, public prg\_parallel\_mod::prg\_recvparallel ( real(dp), dimension(\*) *recvBuf*, integer, intent(in) *recvLen* )

Definition at line 279 of file prg\_parallel\_mod.F90.

9.16.2.25 subroutine, public prg\_parallel\_mod::prg\_shutdownparallel ( )

Definition at line 154 of file prg\_parallel\_mod.F90.

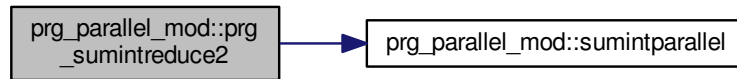
Here is the caller graph for this function:



9.16.2.26 subroutine, public prg\_parallel\_mod::prg\_sumintreduce2 ( integer, intent(inout) *value1*, integer, intent(inout) *value2* )

Definition at line 471 of file prg\_parallel\_mod.F90.

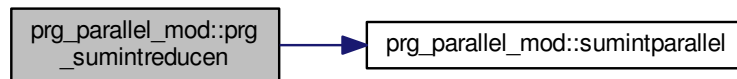
Here is the call graph for this function:



9.16.2.27 subroutine, public prg\_parallel\_mod::prg\_sumintreducen ( integer, dimension(n), intent(inout) *valueVec*, integer, intent(in) *N* )

Definition at line 564 of file prg\_parallel\_mod.F90.

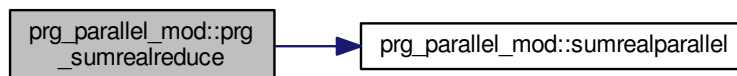
Here is the call graph for this function:



9.16.2.28 subroutine, public prg\_parallel\_mod::prg\_sumrealreduce ( real(dp), intent(inout) *value1* )

Definition at line 489 of file prg\_parallel\_mod.F90.

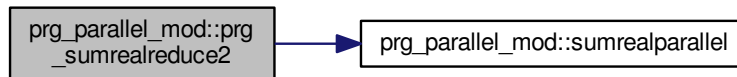
Here is the call graph for this function:



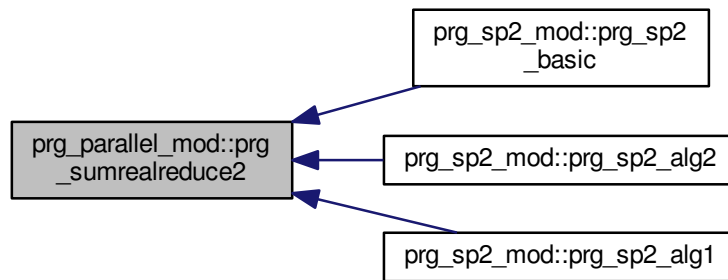
9.16.2.29 subroutine, public prg\_parallel\_mod::prg\_sumrealreduce2 ( real(dp), intent(inout) *value1*, real(dp), intent(inout) *value2* )

Definition at line 505 of file prg\_parallel\_mod.F90.

Here is the call graph for this function:



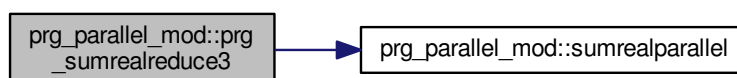
Here is the caller graph for this function:



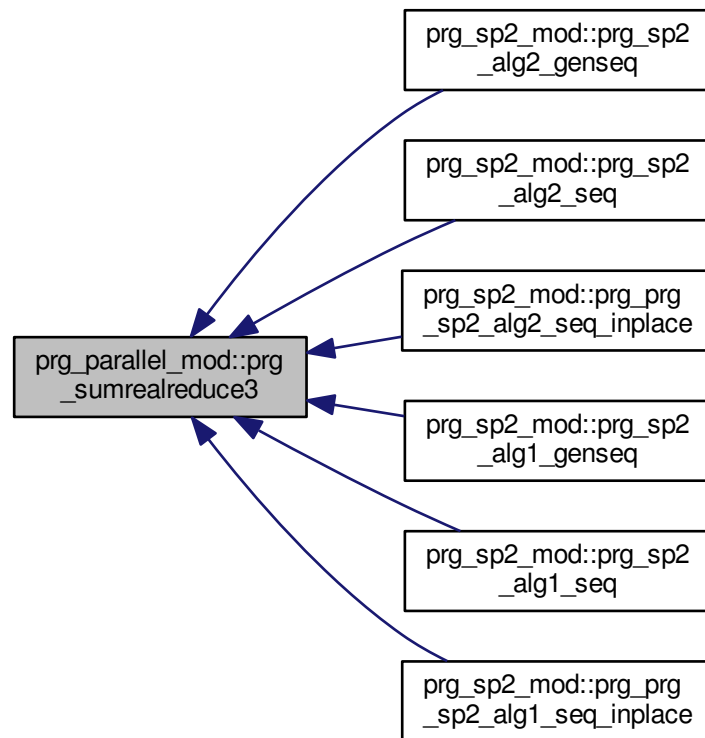
9.16.2.30 subroutine, public prg\_parallel\_mod::prg\_sumrealreduce3 ( real(dp), intent(inout) *value1*, real(dp), intent(inout) *value2*, real(dp), intent(inout) *value3* )

Definition at line 523 of file prg\_parallel\_mod.F90.

Here is the call graph for this function:



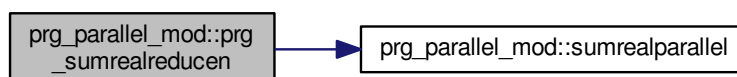
Here is the caller graph for this function:



**9.16.2.31** subroutine, public `prg_parallel_mod::prg_sumrealreducen` ( `real(dp)`, `dimension(n)`, `intent(inout) valueVec`, `integer`, `intent(in) N` )

Definition at line 543 of file `prg_parallel_mod.F90`.

Here is the call graph for this function:



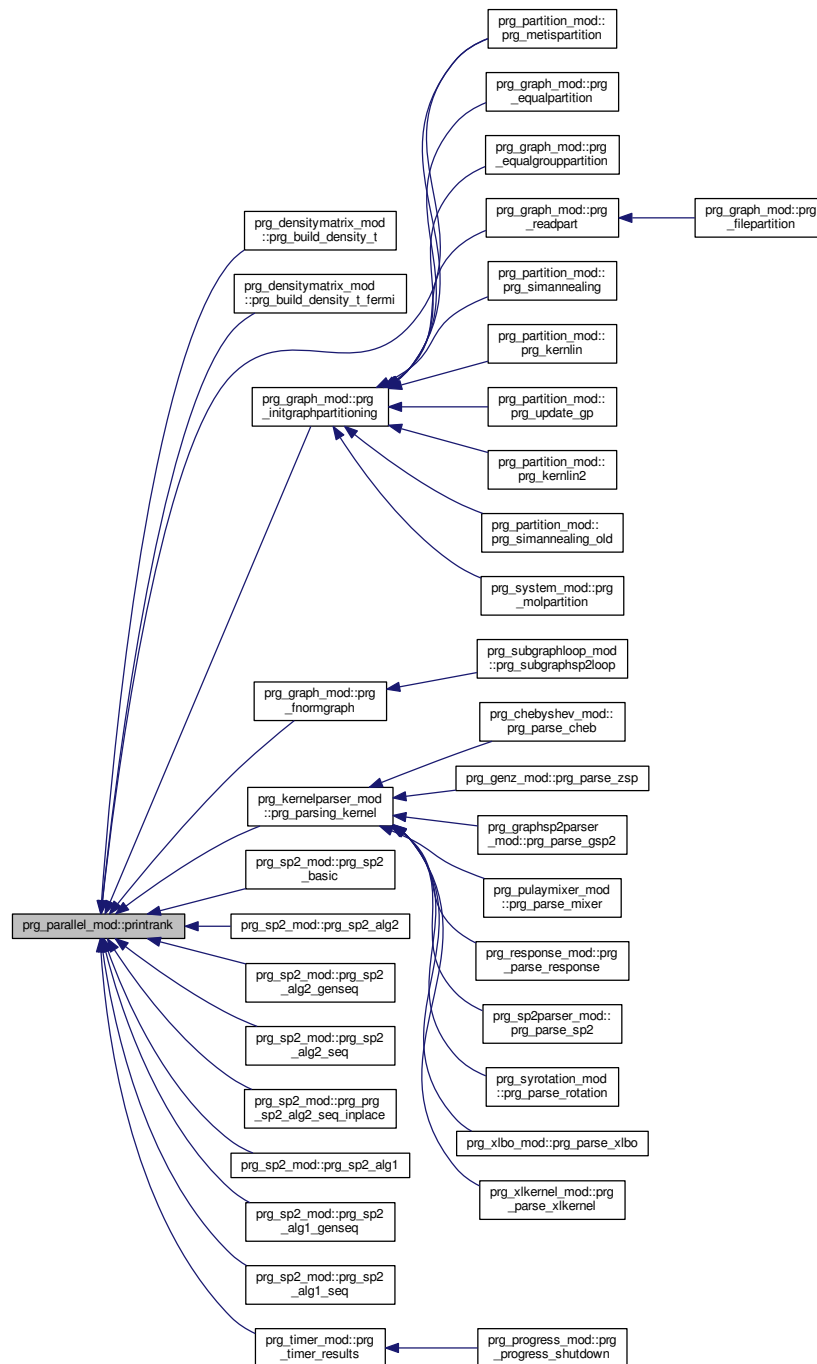
**9.16.2.32** subroutine, public `prg_parallel_mod::prg_wait` ( )

Definition at line 758 of file `prg_parallel_mod.F90`.

### 9.16.2.33 integer function, public prg\_parallel\_mod::printrank ( )

Definition at line 111 of file prg\_parallel\_mod.F90.

Here is the caller graph for this function:



### 9.16.2.34 integer function prg\_parallel\_mod::saverequest ( integer, intent(in) irequest ) [private]

Definition at line 170 of file prg\_parallel\_mod.F90.



Here is the caller graph for this function:



9.16.2.35 subroutine, public `prg_parallel_mod::sendparallel ( real(dp), dimension(*), intent(in) sendBuf, integer, intent(in) sendLen, integer, intent(in) dest )`

Definition at line 246 of file `prg_parallel_mod.F90`.

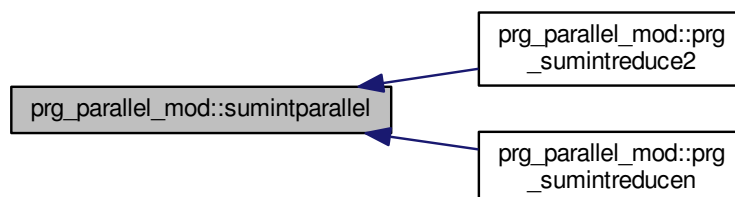
9.16.2.36 subroutine, public `prg_parallel_mod::sendreceiveparallel ( real(dp), dimension(*), intent(in) sendBuf, integer, intent(in) sendLen, integer, intent(in) dest, real(dp), dimension(*), intent(out) recvBuf, integer, intent(in) recvLen, integer, intent(in) source, integer, intent(out) nreceived )`

Definition at line 207 of file `prg_parallel_mod.F90`.

9.16.2.37 subroutine, public `prg_parallel_mod::sumintparallel ( integer, dimension(*), intent(in) sendBuf, integer, dimension(*) recvBuf, integer, intent(in) icount )`

Definition at line 295 of file `prg_parallel_mod.F90`.

Here is the caller graph for this function:





### 9.16.3.5 integer prg\_parallel\_mod::reqcount [private]

Definition at line 29 of file prg\_parallel\_mod.F90.

### 9.16.3.6 integer, dimension(:), allocatable prg\_parallel\_mod::requestlist [private]

Definition at line 30 of file prg\_parallel\_mod.F90.

### 9.16.3.7 integer, dimension(:), allocatable prg\_parallel\_mod::rused [private]

Definition at line 30 of file prg\_parallel\_mod.F90.

## 9.17 prg\_partition\_mod Module Reference

The partition module.

### Functions/Subroutines

- subroutine, public [prg\\_metispartition](#) (gp, ngroups, nnodes, xadj, adjncy, nparts, part, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)  
*Create graph partitions minizing number of cut edges.*
- subroutine, public [prg\\_costpartition](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)  
*Compute cost of a partition.*
- subroutine, public [update\\_prg\\_costpartition](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, node, new\_part)  
*Update cost of partition and the different parameters node is moves into new\_part For each neighbor of node, the following cases hold: Case 1: neighbor is in old\_part Case 2: neighbor is in new\_part Case 3: neighbor is neither in old\_ or new\_part.*
- subroutine [prg\\_accept\\_prob](#) (it, prg\_delta, r)  
*Compute acceptance probability for simulated annealing.*
- subroutine [prg\\_costindex](#) (cost, sumCubes, maxCH, smooth\_maxCH, obj\_fun)  
*Choose objective function to work with.*
- subroutine [prg\\_rand\\_node](#) (gp, node, seed)  
*Pick a random node.*
- subroutine, public [prg\\_simannealing](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, niter, seed)  
*Graph partitioning based on Simulated Annealing.*
- subroutine, public [prg\\_kernlin](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, nconverg, seed)  
*Graph partitioning based on inspired by Kernighan-Lin Review METiS manual for description of k-way implementation of KL Pick a core together with its halos Place free vertices on a priority queue with (key, value) =(prg\_delta, best\_part), with prg\_delta = change in obj\_value Dequeue and allow hill climbing.*
- subroutine, public [prg\\_update\\_gp](#) (gp, partNumber, core\_count)
- subroutine [prg\\_rand\\_shuffle](#) (array, seed)  
*Randomly shuffle array.*
- subroutine, public [prg\\_check\\_arrays](#) (gp, core\_count, CH\_count, Halo\_count)

*Error checking Checking that core\_count, CH\_count, Halo\_count match.*

- subroutine, public [prg\\_kernlin\\_queue](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)

*Greedy algorithm. At each step it chooses the (vertex, new\_part) pair with highest gain Currently implementation is very slow.*

- subroutine [prg\\_find\\_best\\_move](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, best\_node, best\_part)

*For kernlin\_queue to find (vertex, new\_part) pair with highest gain.*

- subroutine, public [prg\\_kernlin2](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)
- subroutine [prg\\_get\\_largest\\_hedge\\_in\\_part](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, search\_part, largest\_Hedge)
- subroutine, public [prg\\_simannealing\\_old](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, niter, seed)

## Variables

- integer, parameter [dp](#) = kind(1.0d0)
- integer, parameter [metis\\_index\\_kind](#) = METIS\_INDEX\_KIND  
*From /usr/include/metis.h.*
- integer, parameter [metis\\_real\\_kind](#) = kind(METIS\_REAL\_KIND)  
*From /usr/include/metis.h.*

### 9.17.1 Detailed Description

The partition module.

Contains different partitioning algorithms such as Metis, Simulated Annealing etc. Also contains optimization routines to improve upon existing partitioning, such as simulated annealing, etc.

### 9.17.2 Function/Subroutine Documentation

- 9.17.2.1 subroutine [prg\\_partition\\_mod::prg\\_accept\\_prob](#) ( integer, intent(in) *it*, real(dp), intent(in) *prg\_delta*, real, intent(inout) *r* ) [private]

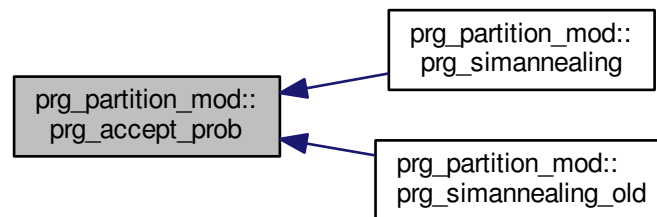
Compute acceptance probability for simulated annealing.

#### Parameters

|                  |                                 |
|------------------|---------------------------------|
| <i>it</i>        | iteration                       |
| <i>prg_delta</i> | (new_obj_value - old_obj_value) |
| <i>r</i>         | acceptance probability          |

Definition at line 489 of file prg\_partition\_mod.F90.

Here is the caller graph for this function:



9.17.2.2 subroutine, public prg\_partition\_mod::prg\_check\_arrays ( type (graph\_partitioning\_t), intent(inout) *gp*, integer, dimension(:), intent(inout), allocatable *core\_count*, integer, dimension(:), intent(inout), allocatable *CH\_count*, integer, dimension(:,:), intent(inout), allocatable *Halo\_count* )

Error checking Checking that core\_count, CH\_count, Halo\_count match.

Definition at line 1146 of file prg\_partition\_mod.F90.

9.17.2.3 subroutine prg\_partition\_mod::prg\_costindex ( real(dp), intent(inout) *cost*, real(dp), intent(inout) *sumCubes*, real(dp), intent(inout) *maxCH*, real(dp), intent(inout) *smooth\_maxCH*, integer, intent(inout) *obj\_fun* ) [private]

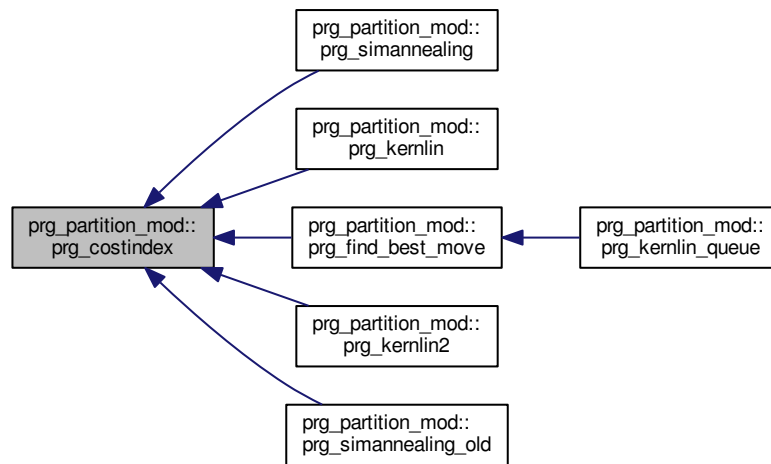
Choose objective function to work with.

#### Parameters

|                 |   |
|-----------------|---|
| <i>cost</i>     | output according to chosen obj_fun          |
| <i>sumCubes</i> | Sum of cubes obj value                      |
| <i>maxCH</i>    | maximum core-halo part size objective value |
| <i>obj_fun</i>  | 0=sumcubes, 1=maxCH                         |

Definition at line 507 of file prg\_partition\_mod.F90.

Here is the caller graph for this function:



9.17.2.4 subroutine, public `prg_partition_mod::prg_costpartition` ( `type (graph_partitioning_t)`, `intent(inout) gp`, `integer, dimension(:), intent(inout), allocatable xadj`, `integer, dimension(:), intent(inout), allocatable adjncy`, `integer, dimension(:), intent(in), allocatable partNumber`, `integer, dimension(:), intent(inout), allocatable core_count`, `integer, dimension(:), intent(inout), allocatable CH_count`, `integer, dimension(:, :), intent(inout), allocatable Halo_count`, `real(dp), intent(inout) sumCubes`, `real(dp), intent(inout) maxCH`, `real(dp), intent(inout) smooth_maxCH`, `real(dp), intent(inout) pnorm` )

Compute cost of a partition.

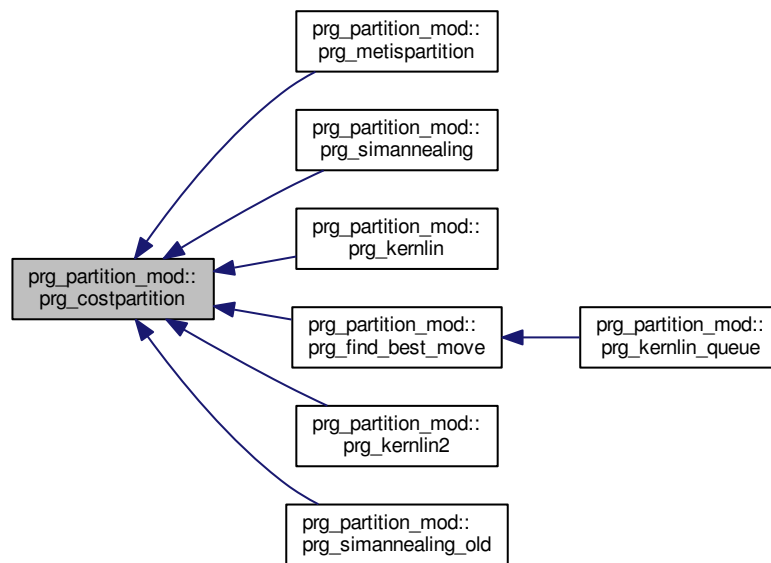
#### Parameters

|                   |   |
|-------------------|---|
| <i>gp</i>         | Graph partitioning  |
| <i>xadj</i>       | CSR array of graph nodes  |
| <i>adjncy</i>     | CSR array of graph neighbors  |
| <i>nparts</i>     | Number of Parts   |
| <i>partNumber</i> | Partition vector  |
| <i>core_count</i> | Array: number of core vertices in each part   |
| <i>CH_count</i>   | Array: number of core+halo vertices in each part  |
| <i>Halo_count</i> | 2D Array of size nparts by totalNodes: $Halo\_count(i,j) = k$ , node $j$ is a halo of part $i$ with $k$ connections |
| <i>sumCubes</i>   | Sum of cubes objective value  |
| <i>maxCh</i>      | maximum core-halo part size objective value   |

`prg_initialize`

Definition at line 327 of file `prg_partition_mod.F90`.

Here is the caller graph for this function:

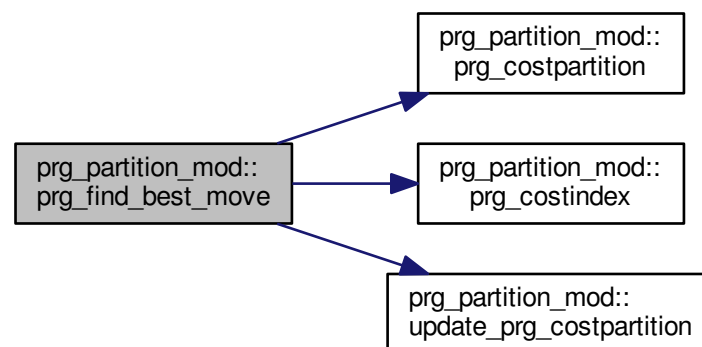


9.17.2.5 subroutine `prg_partition_mod::prg_find_best_move` ( type(`graph_partitioning_t`), intent(inout) *gp*, integer, dimension(:), intent(inout), allocatable *xadj*, integer, dimension(:), intent(inout), allocatable *adjncy*, integer, dimension(:), intent(inout), allocatable *partNumber*, integer, dimension(:), intent(inout), allocatable *core\_count*, integer, dimension(:), intent(inout), allocatable *CH\_count*, integer, dimension(:,:), intent(inout), allocatable *Halo\_count*, real(dp), intent(inout) *sumCubes*, real(dp), intent(inout) *maxCH*, real(dp), intent(inout) *smooth\_maxCH*, real(dp), intent(inout) *pnorm*, integer, intent(inout) *best\_node*, integer, intent(inout) *best\_part* ) [private]

For `kerlin_queue` to find (vertex, new\_part) pair with highest gain.

Definition at line 1209 of file `prg_partition_mod.F90`.

Here is the call graph for this function:



Here is the caller graph for this function:

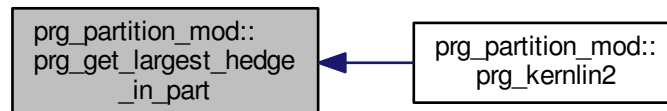


9.17.2.6 subroutine `prg_partition_mod::prg_get_largest_hedge_in_part` ( type (`graph_partitioning_t`), intent(inout) `gp`, integer, dimension(:), intent(inout), allocatable `xadj`, integer, dimension(:), intent(inout), allocatable `adjncy`, integer, dimension(:), intent(inout), allocatable `partNumber`, integer, dimension(:), intent(inout), allocatable `core_count`, integer, dimension(:), intent(inout), allocatable `CH_count`, integer, dimension(:,,:), intent(inout), allocatable `Halo_count`, real(dp), intent(inout) `sumCubes`, real(dp), intent(inout) `maxCH`, real(dp), intent(inout) `smooth_maxCH`, real(dp), intent(inout) `pnorm`, integer, intent(inout) `search_part`, integer, intent(inout) `largest_Hedge` ) [private]

i can be viewed as a hyperedge for all hyperedges in `search_part`, pick the one with largest size

Definition at line 1420 of file `prg_partition_mod.F90`.

Here is the caller graph for this function:



9.17.2.7 subroutine, public `prg_partition_mod::prg_kernlin` ( type (`graph_partitioning_t`), intent(inout) `gp`, integer, dimension(:), intent(inout), allocatable `xadj`, integer, dimension(:), intent(inout), allocatable `adjncy`, integer, dimension(:), intent(inout), allocatable `partNumber`, integer, dimension(:), intent(inout), allocatable `core_count`, integer, dimension(:), intent(inout), allocatable `CH_count`, integer, dimension(:,,:), intent(inout), allocatable `Halo_count`, real(dp), intent(inout) `sumCubes`, real(dp), intent(inout) `maxCH`, real(dp), intent(inout) `smooth_maxCH`, real(dp), intent(inout) `pnorm`, integer, intent(in) `nconverg`, integer, intent(inout) `seed` )

Graph partitioning based on inspired by Kernighan-Lin Review METIS manual for description of k-way implementation of KL Pick a core together with its halos Place free vertices on a priority queue with (key, value) =(prg\_delta, best\_part), with prg\_delta = change in obj\_value Dequeue and allow hill climbing.

#### Parameters

|                 |                    |
|-----------------|--------------------|
| <code>gp</code> | Graph partitioning |
|-----------------|--------------------|



## Parameters

|                   |   |
|-------------------|---|
| <i>xadj</i>       | CSR array of graph nodes  |
| <i>adjncy</i>     | CSR array of graph neighbors  |
| <i>nparts</i>     | Number of Parts   |
| <i>partNumber</i> | Partition vector  |
| <i>core_count</i> | Array: number of core vertices in each part   |
| <i>CH_count</i>   | Array: number of core+halo vertices in each part  |
| <i>Halo_count</i> | 2D Array of size nparts by totalNodes: $Halo\_count(i,j) = k$ , node $j$ is a halo of part $i$ with $k$ connections |
| <i>sumCubes</i>   | Sum of cubes objective value  |
| <i>maxCh</i>      | maximum core-halo part size objective value   |
| <i>nconverg</i>   | number of before convergence  |
| <i>seed</i>       | random number generator seed  |

Allocate arrays

Initialize variables

Initialize array of nodes

Randomize nodes

Compute current cost of partition

Choose objective function to minimize

iterate over the columns of the matrix, ie the hyperedges

KL iteration

let min\_part be the smallest CH\_part

Try and move free nodes to min\_part

lock vertices (climb\_counter) vertices have been accepted need to lock (climb\_counter) vertices Last vertex to be moved is node\_backup(climb\_counter)

reset

If all vertices locked, go to next iteration

If empty parts exist, place a vertex in max\_part there

Place  $j$  and it's neighbors that are in the max part into the empty part

Check Convergence

Check empty part exist move nodes from maxpart to empty part

move it neighbor in the max parts to the newpart

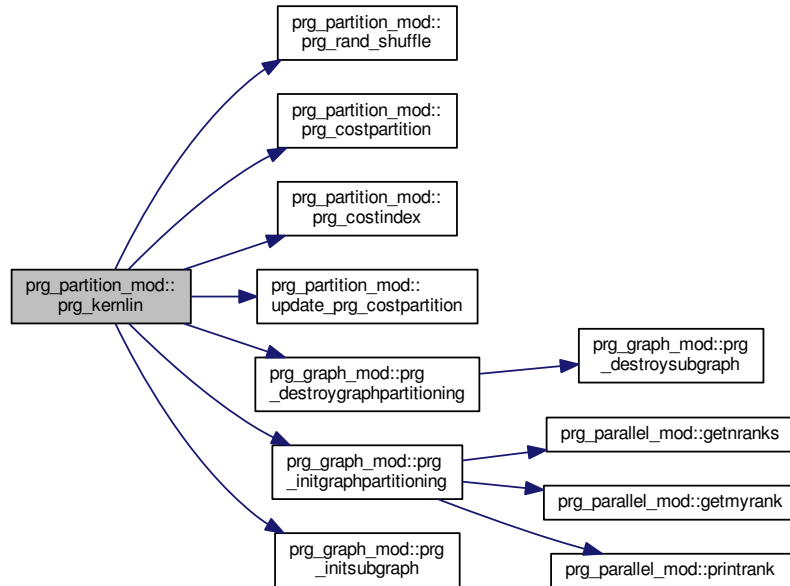
Update graph structure

Allocate subgraph structure

Assign node ids to sgraph

Definition at line 758 of file prg\_partition\_mod.F90.

Here is the call graph for this function:



**9.17.2.8** subroutine, public prg\_partition\_mod::prg\_kernlin2 ( type (graph\_partitioning\_t), intent(inout) gp, integer, dimension(:), intent(inout), allocatable xadj, integer, dimension(:), intent(inout), allocatable adjncy, integer, dimension(:), intent(inout), allocatable partNumber, integer, dimension(:), intent(inout), allocatable core\_count, integer, dimension(:), intent(inout), allocatable CH\_count, integer, dimension(:,:), intent(inout), allocatable Halo\_count, real(dp), intent(inout) sumCubes, real(dp), intent(inout) maxCH, real(dp), intent(inout) smooth\_maxCH, real(dp), intent(inout) pnorm )

Allocate arrays

Pick hyperedge with largest size or random hyperedge with probability 0.5 We will change it to pick hyperedge with highest priority, where priority will be defined according to different metrics

Find part with smallest size (should be included in update\_prg\_costPartition)

if current part is max, move to min\_part then move subsets (neighbors)

Move hyperedges to minCH part

Try and move intersecting hyperedges

Move k number of vertices. k should be small i.e k <=20, k set in prg\_Kernlin\_queue Only use this for small systems

Check empty part exist move nodes from maxpart to empty part

move it neighbor in the max parts to the newpart

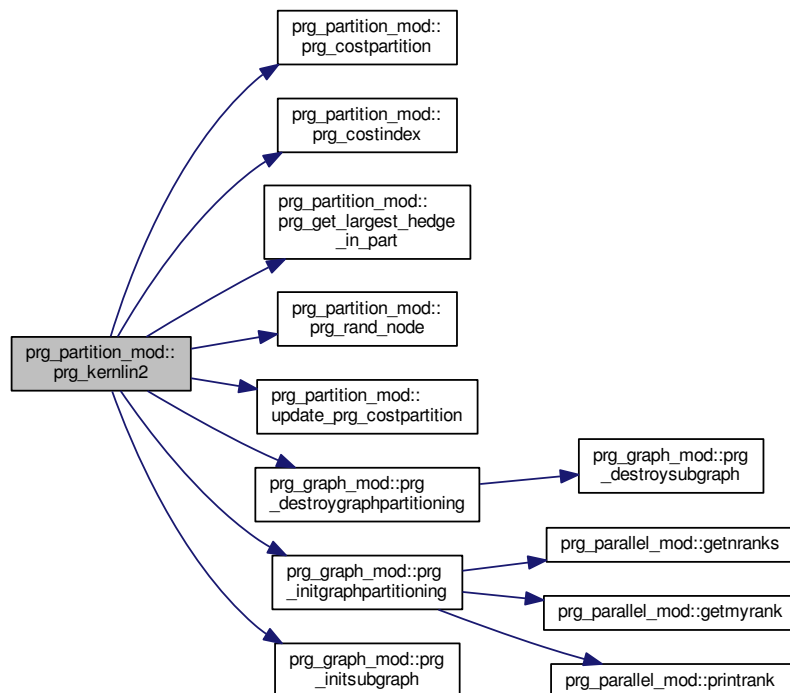
Update graph structure

Allocate subgraph structure

Assign node ids to sgraph

Definition at line 1257 of file prg\_partition\_mod.F90.

Here is the call graph for this function:

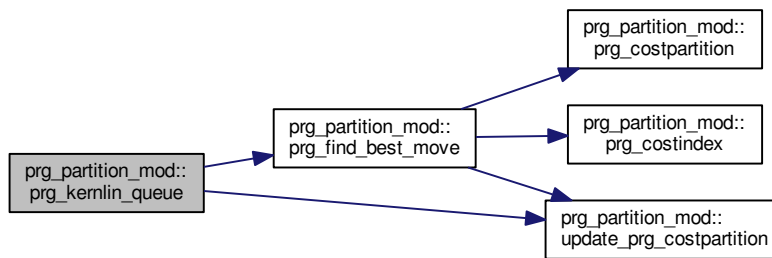


9.17.2.9 subroutine, public prg\_partition\_mod::prg\_kernlin\_queue ( type (graph\_partitioning\_t), intent(inout) gp, integer, dimension(:), intent(inout), allocatable xadj, integer, dimension(:), intent(inout), allocatable adjncy, integer, dimension(:), intent(inout), allocatable partNumber, integer, dimension(:), intent(inout), allocatable core\_count, integer, dimension(:), intent(inout), allocatable CH\_count, integer, dimension(:,:), intent(inout), allocatable Halo\_count, real(dp), intent(inout) sumCubes, real(dp), intent(inout) maxCH, real(dp), intent(inout) smooth\_maxCH, real(dp), intent(inout) pnorm )

Greedy algorithm. At each step it chooses the (vertex, new\_part) pair with highest gain. Currently implementation is very slow.

Definition at line 1173 of file prg\_partition\_mod.F90.

Here is the call graph for this function:



9.17.2.10 subroutine, public `prg_partition_mod::prg_metispartition` ( type (`graph_partitioning_t`), intent(inout) `gp`, integer, intent(in) `ngroups`, integer, intent(in) `nnodes`, integer, dimension(:), intent(inout), allocatable `xadj`, integer, dimension(:), intent(inout), allocatable `adjncy`, integer, intent(inout) `nparts`, integer, dimension(:), intent(inout), allocatable `part`, integer, dimension(:), intent(inout), allocatable `core_count`, integer, dimension(:), intent(inout), allocatable `CH_count`, integer, dimension(:, :), intent(inout), allocatable `Halo_count`, real(dp), intent(inout) `sumCubes`, real(dp), intent(inout) `maxCH`, real(dp), intent(inout) `smooth_maxCH`, real(dp), intent(inout) `pnorm` )

Create graph partitions minizing number of cut edges.

#### Parameters

|                   |   |
|-------------------|---|
| <i>gp</i>         | Graph partitioning'   |
| <i>ngroups</i>    | Number of groups/nodes  |
| <i>nnodes</i>     | Number of nodes   |
| <i>xadj</i>       | CSR array of graph nodes  |
| <i>adjncy</i>     | CSR array of graph neighbors  |
| <i>nparts</i>     | Number of Parts   |
| <i>part</i>       | Partition vector  |
| <i>core_count</i> | Array: number of core vertices in each part   |
| <i>CH_count</i>   | Array: number of core+halo vertices in each part  |
| <i>Halo_count</i> | 2D Array of size nparts by totalNodes: Halo_count(i,j) = k, node j is a halo of part i with k connections |
| <i>sumCubes</i>   | Sum of cubes objective value  |
| <i>maxCh</i>      | maximum core-halo part size obective value  |

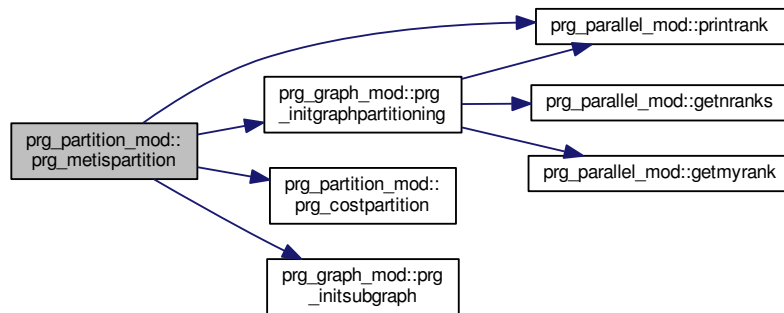
`prg_initialize`

Partition graph into nparts'

Compute cost of partition

Definition at line 217 of file `prg_partition_mod.F90`.

Here is the call graph for this function:



9.17.2.11 subroutine `prg_partition_mod::prg_rand_node` ( type (graph\_partitioning\_t), intent(inout) *gp*, integer, intent(inout) *node*, integer, intent(inout) *seed* ) [private]

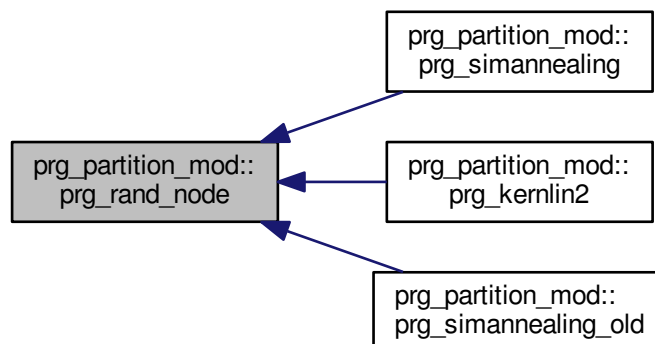
Pick a random node.

#### Parameters

|             |                              |
|-------------|------------------------------|
| <i>gp</i>   | graph partitioning structure |
| <i>node</i> | output node                  |
| <i>seed</i> | random seed                  |

Definition at line 527 of file `prg_partition_mod.F90`.

Here is the caller graph for this function:



9.17.2.12 subroutine `prg_partition_mod::prg_rand_shuffle` ( integer, dimension(:), intent(inout) *array*, integer, intent(inout) *seed* ) [private]

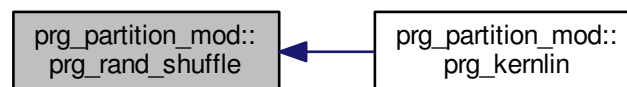
Randomly shuffle array.

Random seed

Shuffle array

Definition at line 1123 of file `prg_partition_mod.F90`.

Here is the caller graph for this function:



9.17.2.13 subroutine, public `prg_partition_mod::prg_simannealing` ( type (graph\_partitioning\_t), intent(inout) *gp*, integer, dimension(:), intent(inout), allocatable *xadj*, integer, dimension(:), intent(inout), allocatable *adjncy*, integer, dimension(:), intent(inout), allocatable *partNumber*, integer, dimension(:), intent(inout), allocatable *core\_count*, integer, dimension(:), intent(inout), allocatable *CH\_count*, integer, dimension(:, :), intent(inout), allocatable *Halo\_count*, real(dp), intent(inout) *sumCubes*, real(dp), intent(inout) *maxCH*, real(dp), intent(inout) *smooth\_maxCH*, real(dp), intent(inout) *pnorm*, integer, intent(in) *niter*, integer, intent(inout) *seed* )

Graph partitioning based on Simulated Annealing.

#### Parameters

|                   |  |
|-------------------|--|
| <i>gp</i>         | Graph partitioning   |
| <i>xadj</i>       | CSR array of graph nodes   |
| <i>adjncy</i>     | CSR array of graph neighbors   |
| <i>nparts</i>     | Number of Parts  |
| <i>partNumber</i> | Partition vector   |
| <i>core_count</i> | Array: number of core vertices in each part  |
| <i>CH_count</i>   | Array: number of core+halo vertices in each part   |
| <i>Halo_count</i> | 2D Array of size nparts by totalNodes: $Halo\_count(i,j) = k$ , node <i>j</i> is a halo of part <i>i</i> with <i>k</i> connections |
| <i>sumCubes</i>   | Sum of cubes objective value   |
| <i>maxCh</i>      | maximum core-halo part size objective value  |
| <i>niter</i>      | Number of iterations   |
| <i>seed</i>       | Random seed  |

Compute current cost of partition

Choose objective function to minimize

Perform SA

Find part with smallest size (should be included in update\_prg\_costPartition

if part(node) == max\_ch\_part, try to move node and its neighbors to min\_ch\_part else move neighbors to part(node)

Check empty part exist move nodes from maxpart to empty part

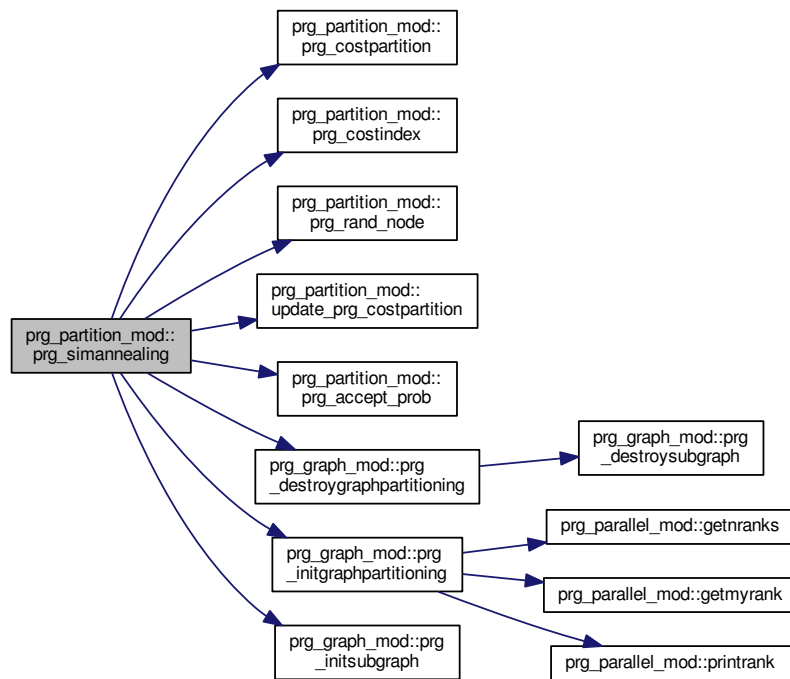
move it neighbor in the max parts to the newpart

Update graph structure

For debugging

Definition at line 552 of file prg\_partition\_mod.F90.

Here is the call graph for this function:



9.17.2.14 subroutine, public `prg_partition_mod::prg_simannealing_old` ( type (graph\_partitioning\_t), intent(inout) *gp*, integer, dimension(:), intent(inout), allocatable *xadj*, integer, dimension(:), intent(inout), allocatable *adjncy*, integer, dimension(:), intent(inout), allocatable *partNumber*, integer, dimension(:), intent(inout), allocatable *core\_count*, integer, dimension(:), intent(inout), allocatable *CH\_count*, integer, dimension(:, :), intent(inout), allocatable *Halo\_count*, real(dp), intent(inout) *sumCubes*, real(dp), intent(inout) *maxCH*, real(dp), intent(inout) *smooth\_maxCH*, real(dp), intent(inout) *pnorm*, integer, intent(in) *niter*, integer, intent(inout) *seed* )

Compute current cost of partition

Choose objective function to minimize

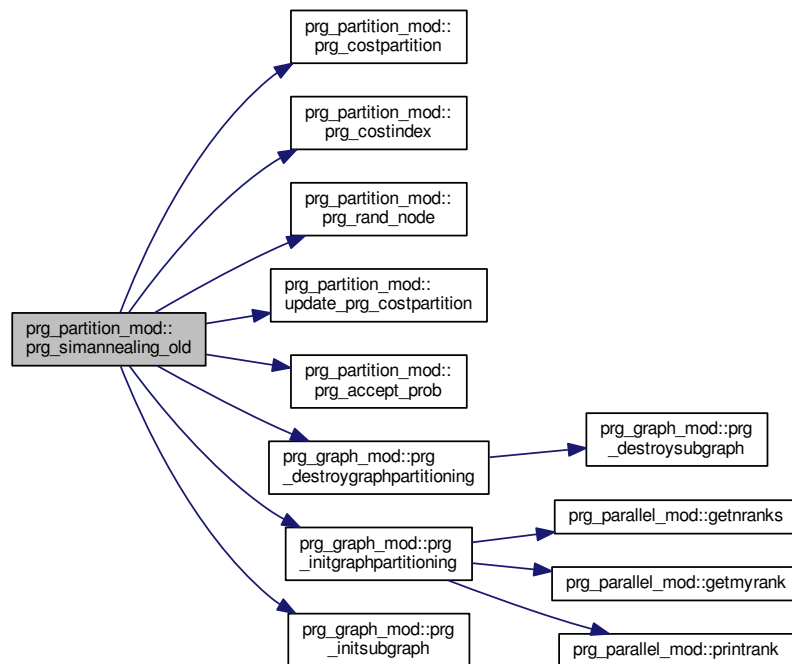
Perform SA

Update graph structure

For debugging

Definition at line 1453 of file prg\_partition\_mod.F90.

Here is the call graph for this function:



9.17.2.15 subroutine, public `prg_partition_mod::prg_update_gp ( type (graph_partitioning_t), intent(inout) gp, integer, dimension(:), intent(inout), allocatable partNumber, integer, dimension(:), intent(inout), allocatable core_count )`

Update graph structure

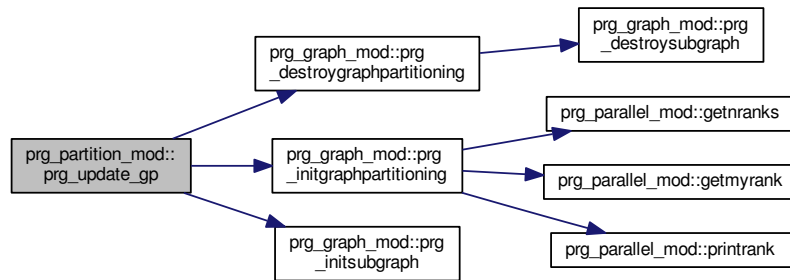
Allocate subgraph structure

Assign node ids to sgraph

Definition at line 1082 of file prg\_partition\_mod.F90.



Here is the call graph for this function:



**9.17.2.16** subroutine, public prg\_partition\_mod::update\_prg\_costpartition ( type (graph\_partitioning\_t), intent(inout) *gp*, integer, dimension(:), intent(inout), allocatable *xadj*, integer, dimension(:), intent(inout), allocatable *adjncy*, integer, dimension(:), intent(inout), allocatable *partNumber*, integer, dimension(:), intent(inout), allocatable *core\_count*, integer, dimension(:), intent(inout), allocatable *CH\_count*, integer, dimension(:, :), intent(inout), allocatable *Halo\_count*, real(dp), intent(inout) *sumCubes*, real(dp), intent(inout) *maxCH*, real(dp), intent(inout) *smooth\_maxCH*, real(dp), intent(inout) *pnorm*, integer, intent(in) *node*, integer, intent(in) *new\_part* )

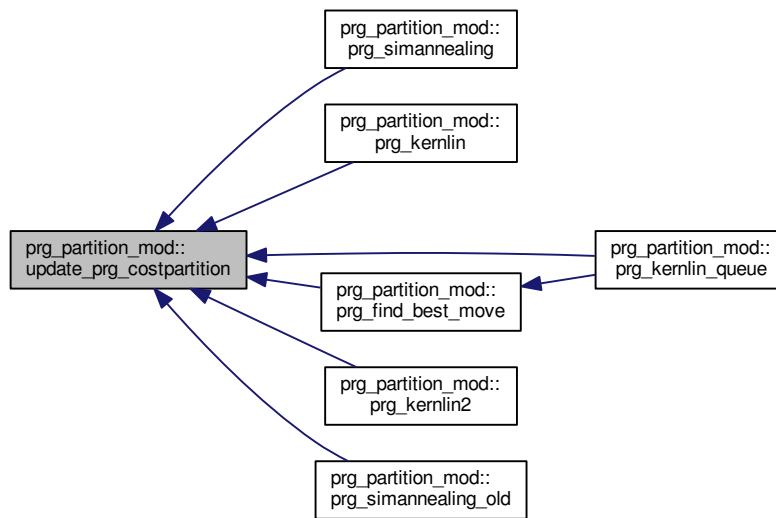
Update cost of partition and the different parameters node is moves into new\_part For each neighbor of node, the following cases hold: Case 1: neighbor is in old\_part Case 2: neighbor is in new\_part Case 3: neighbor is neither in old\_ or new\_part.

#### Parameters

|                   |   |
|-------------------|---|
| <i>gp</i>         | Graph partitioning  |
| <i>xadj</i>       | CSR array of graph nodes  |
| <i>adjncy</i>     | CSR array of 1043365660.0000000graph neighbors  |
| <i>nparts</i>     | Number of Parts   |
| <i>partNumber</i> | Partition vector  |
| <i>core_count</i> | Array: number of core vertices in each part   |
| <i>CH_count</i>   | Array: number of core+halo vertices in each part  |
| <i>Halo_count</i> | 2D Array of size nparts by totalNodes: Halo_count(i,j) = k, node j is a halo of part i with k connections |
| <i>sumCubes</i>   | Sum of cubes objective value  |
| <i>maxCh</i>      | maximum core-halo part size obective value  |
| <i>node</i>       | Vertex that has moved to new_part   |
| <i>new_part</i>   | new part that node has moved to   |

Definition at line 401 of file prg\_partition\_mod.F90.

Here is the caller graph for this function:



### 9.17.3 Variable Documentation

9.17.3.1 integer, parameter `prg_partition_mod::dp = kind(1.0d0)` `[private]`

Definition at line 18 of file `prg_partition_mod.F90`.

9.17.3.2 integer, parameter `prg_partition_mod::metis_index_kind = METIS_INDEX_KIND` `[private]`

From `/usr/include/metis.h`.

`IDXTYPEWIDTH = 32 -> metis_index_kind = 4` `IDXTYPEWIDTH = 64 -> metis_index_kind = 8`

Definition at line 24 of file `prg_partition_mod.F90`.

9.17.3.3 integer, parameter `prg_partition_mod::metis_real_kind = kind(METIS_REAL_KIND)` `[private]`

From `/usr/include/metis.h`.

`REALTYPEWIDTH = 32 -> metis_real_kind = kind(0e0)` `REALTYPEWIDTH = 64 -> metis_real_kind = kind(0d0)`

Definition at line 30 of file `prg_partition_mod.F90`.

## 9.18 prg\_progress\_mod Module Reference

The progress module.

## Functions/Subroutines

- subroutine, public [prg\\_progress\\_init](#) ()  
*Initialize progress.*
- subroutine, public [prg\\_progress\\_shutdown](#) ()  
*Shutdown progress.*

## Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.18.1 Detailed Description

The progress module.

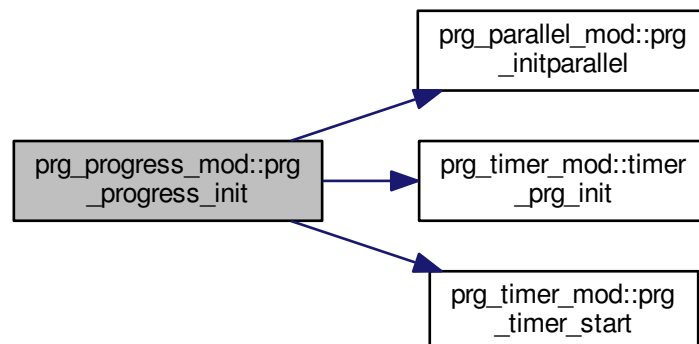
### 9.18.2 Function/Subroutine Documentation

#### 9.18.2.1 subroutine, public `prg_progress_mod::prg_progress_init` ( )

Initialize progress.

Definition at line 25 of file `prg_progress_mod.F90`.

Here is the call graph for this function:

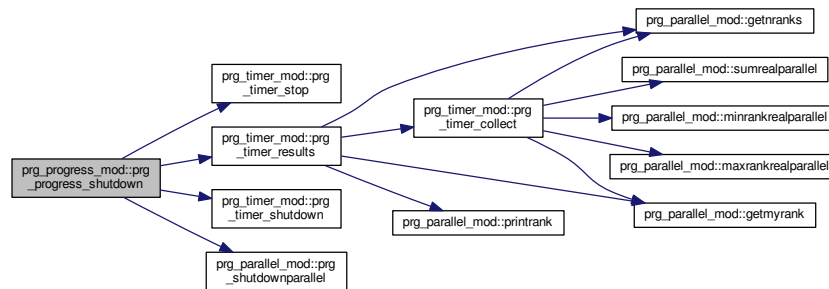


### 9.18.2.2 subroutine, public prg\_progress\_mod::prg\_progress\_shutdown ( )

Shutdown progress.

Definition at line 37 of file prg\_progress\_mod.F90.

Here is the call graph for this function:



## 9.18.3 Variable Documentation

### 9.18.3.1 integer, parameter prg\_progress\_mod::dp = kind(1.0d0) [private]

Definition at line 16 of file prg\_progress\_mod.F90.

## 9.19 prg\_ptable\_mod Module Reference

Periodic table of elements.

### Functions/Subroutines

- integer function, public [element\\_atomic\\_number](#) (symbol)
- integer function [element\\_atomic\\_number\\_upper](#) (symbol)

### Variables

- integer, parameter [nz](#) = 103
- integer, parameter, private [dp](#) = kind(1.0d0)
- character(2), dimension([nz](#)), parameter [element\\_symbol](#) = [character(2) :: "H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne", "Na", "Mg", "Al", "Si", "P", "S", "Cl", "Ar", "K", "Ca", "Sc", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn", "Ga", "Ge", "As", "Se", "Br", "Kr", "Rb", "Sr", "Y", "Zr", "Nb", "Mo", "Tc", "Ru", "Rh", "Pd", "Ag", "Cd", "In", "Sn", "Sb", "Te", "I", "Xe", "Cs", "Ba", "La", "Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb", "Lu", "Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg", "Tl", "Pb", "Bi", "Po", "At", "Rn", "Fr", "Ra", "Ac", "Th", "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk", "Cf", "Es", "Fm", "Md", "No", "Lr"]

*Element symbol.*

- `character(2)`, `dimension(nz)`, parameter `element_symbol_upper` = [`character(2)` :: "H", "HE", "LI", "BE", "B", "C", "N", "O", "F", "NE", "NA", "MG", "AL", "SI", "P", "S", "CL", "AR", "K", "CA", "SC", "TI", "V", "CR", "MN", "FE", "CO", "NI", "CU", "ZN", "GA", "GE", "AS", "SE", "BR", "KR", "RB", "SR", "Y", "ZR", "NB", "MO", "TC", "RU", "RH", "PD", "AG", "CD", "IN", "SN", "SB", "TE", "I", "XE", "CS", "BA", "LA", "CE", "PR", "ND", "PM", "SM", "EU", "GD", "TB", "DY", "HO", "ER", "TM", "YB", "LU", "HF", "TA", "W", "RE", "OS", "IR", "PT", "AU", "HG", "TL", "PB", "BI", "PO", "AT", "RN", "FR", "RA", "AC", "TH", "PA", "U", "NP", "PU", "AM", "CM", "BK", "CF", "ES", "FM", "MD", "NO", "LR"]

*Element symbol upper.*

- `character(20)`, `dimension(nz)`, parameter `element_name` = [`character(20)` :: "Hydrogen", "Helium", "Lithium", "Beryllium", "Boron", "Carbon", "Nitrogen", "Oxygen", "Fluorine", "Neon", "Sodium", "Magnesium", "Aluminium", "Silicon", "Phosphorus", "Sulfur", "Chlorine", "Argon", "Potassium", "Calcium", "Scandium", "Titanium", "Vanadium", "Chromium", "Manganese", "Iron", "Cobalt", "Nickel", "Copper", "Zinc", "Gallium", "Germanium", "Arsenic", "Selenium", "Bromine", "Krypton", "Rubidium", "Strontium", "Yttrium", "Zirconium", "Niobium", "Molybdenum", "Technetium", "Ruthenium", "Rhodium", "Palladium", "Silver", "Cadmium", "Indium", "Tin", "Antimony", "Tellurium", "Iodine", "Xenon", "Caesium", "Barium", "Lanthanum", "Cerium", "Praseodymium", "Neodymium", "Promethium", "Samarium", "Europium", "Gadolinium", "Terbium", "Dysprosium", "Holmium", "Erbium", "Thulium", "Ytterbium", "Lutetium", "Hafnium", "Tantalum", "Tungsten", "Rhenium", "Osmium", "Iridium", "Platinum", "Gold", "Mercury", "Thallium", "Lead", "Bismuth", "Polonium", "Astatine", "Radon", "Francium", "Radium", "Actinium", "Thorium", "Protactinium", "Uranium", "Neptunium", "Plutonium", "Americium", "Curium", "Berkelium", "Californium", "Einsteinium", "Fermium", "Mendelevium", "Nobelium", "Lawrencium"]

*Element name.*

- `real(dp)`, `dimension(nz)`, parameter `element_mass` = (/ 1.007825032, 4.002603254, 7.01600455, 9.0121822, 11.0093054, 12.0, 14.003074005, 15.99491462, 18.99840322, 19.992440175, 22.989769281, 23.↵ 9850417, 26.98153863, 27.976926532, 30.97376163, 31.972071, 34.96885268, 39.962383123, 38.↵ 96370668, 39.96259098, 44.9559119, 47.9479463, 50.9439595, 51.9405075, 54.9380451, 55.9349375, 58.933195, 57.9353429, 62.9295975, 63.929142, 68.925573, 73.921177, 74.921596, 79.916521, 78.↵ 918337, 83.911507, 84.911789, 87.905612, 88.905848, 89.904704, 92.906378, 97.905408, 97.907216, 101.904349, 102.905504, 105.903486, 106.905097, 113.903358, 114.903878, 119.902194, 120.↵ 903815, 129.906224, 126.904473, 131.904153, 132.905451, 137.905247, 138.906353, 139.905438, 140.907652, 141.907723, 144.912749, 151.919732, 152.92123, 157.924103, 158.925346, 163.929174, 164.930322, 165.930293, 168.934213, 173.938862, 174.940771, 179.94655, 180.947995, 183.950931, 186.955753, 191.96148, 192.962926, 194.964791, 196.966568, 201.970643, 204.974427, 207.976652, 208.980398, 208.98243, 209.987148, 222.017577, 223.019735, 226.025409, 227.027752, 232.038055, 231.035884, 238.050788, 237.048173, 244.064204, 243.061381, 247.070354, 247.070307, 251.079587, 252.08298, 257.095105, 258.098431, 259.10103, 262.10963 /)

*Element mass in atomic mass units (1.66 x 10<sup>-27</sup> kg)*

- `real(dp)`, `dimension(nz)`, parameter `element_vdwr` = (/ 1.1, 1.4, 1.81, 1.53, 1.92, 1.7, 1.55, 1.52, 1.47, 1.54, 2.27, 1.73, 1.84, 2.1, 1.8, 1.8, 1.75, 1.88, 2.75, 2.31, 2.3, 2.15, 2.05, 2.05, 2.05, 2.0, 2.0, 2.0, 2.1, 1.87, 2.11, 1.85, 1.9, 1.83, 2.02, 3.03, 2.49, 2.4, 2.3, 2.15, 2.1, 2.05, 2.05, 2.0, 2.05, 2.1, 2.2, 2.2, 1.93, 2.17, 2.06, 1.98, 2.16, 3.43, 2.68, 2.5, 2.48, 2.47, 2.45, 2.43, 2.42, 2.4, 2.38, 2.37, 2.35, 2.33, 2.32, 2.3, 2.28, 2.27, 2.25, 2.2, 2.1, 2.05, 2.0, 2.0, 2.05, 2.1, 2.05, 1.96, 2.02, 2.07, 1.97, 2.02, 2.2, 3.48, 2.83, 2.0, 2.4, 2.0, 2.3, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0 /)

*van der Waals radius (in Angstroms)*

- `real(dp)`, `dimension(nz)`, parameter `element_covr` = (/ 0.31, 0.28, 1.28, 0.96, 0.84, 0.76, 0.71, 0.66, 0.57, 0.58, 1.66, 1.41, 1.21, 1.11, 1.07, 1.05, 1.02, 1.06, 2.03, 1.76, 1.7, 1.6, 1.53, 1.39, 1.39, 1.32, 1.26, 1.24, 1.32, 1.22, 1.22, 1.2, 1.19, 1.2, 1.2, 1.16, 2.2, 1.95, 1.9, 1.75, 1.64, 1.54, 1.47, 1.46, 1.42, 1.39, 1.45, 1.44, 1.42, 1.39, 1.39, 1.38, 1.39, 1.4, 2.44, 2.15, 2.07, 2.04, 2.03, 2.01, 1.99, 1.98, 1.98, 1.96, 1.94, 1.92, 1.92, 1.89, 1.9, 1.87, 1.87, 1.75, 1.7, 1.62, 1.51, 1.44, 1.41, 1.36, 1.36, 1.32, 1.45, 1.46, 1.48, 1.4, 1.5, 1.5, 2.6, 2.21, 2.15, 2.06, 2.0, 1.96, 1.9, 1.87, 1.8, 1.69, 1.6, 1.6, 1.6, 1.6, 1.6, 1.6, 1.6 /)

*Covalent radius (in Angstroms)*

- `real(dp)`, `dimension(nz)`, parameter `element_ip` = (/ 13.5984, 24.5874, 5.3917, 9.3227, 8.298, 11.2603, 14.5341, 13.6181, 17.4228, 21.5645, 5.1391, 7.6462, 5.9858, 8.1517, 10.4867, 10.36, 12.9676, 15.7596, 4.3407, 6.1132, 6.5615, 6.8281, 6.7462, 6.7665, 7.434, 7.9024, 7.881, 7.6398, 7.7264, 9.3942, 5.9993, 7.8994, 9.7886, 9.7524, 11.8138, 13.9996, 4.1771, 5.6949, 6.2173, 6.6339, 6.7589

, 7.0924 , 7.28 , 7.3605 , 7.4589 , 8.3369 , 7.5762 , 8.9938 , 5.7864 , 7.3439 , 8.6084 , 9.0096 , 10.4513 , 12.1298 , 3.8939 , 5.2117 , 5.5769 , 5.5387 , 5.473 , 5.525 , 5.582 , 5.6437 , 5.6704 , 6.1498 , 5.8638 , 5.9389 , 6.0215 , 6.1077 , 6.1843 , 6.2542 , 5.4259 , 6.8251 , 7.5496 , 7.864 , 7.8335 , 8.4382 , 8.967 , 8.9588 , 9.2255 , 10.4375 , 6.1082 , 7.4167 , 7.2855 , 8.414 , 0.0 , 10.7485 , 4.0727 , 5.2784 , 5.17 , 6.3067 , 5.89 , 6.1941 , 6.2657 , 6.026 , 5.9738 , 5.9914 , 6.1979 , 6.2817 , 6.42 , 6.5 , 6.58 , 6.65 , 4.9 /)

*Ionization energy (in eV)*

- real(dp), dimension(nz), parameter `element_ea` = (/ 0.75420375 , 0.0 , 0.618049 , 0.0 , 0.279723 , 1.262118 , -0.07 , 1.461112 , 3.4011887 , 0.0 , 0.547926 , 0.0 , 0.43283 , 1.389521 , 0.7465 , 2.0771029 , 3.612724 , 0.0 , 0.501459 , 0.02455 , 0.188 , 0.084 , 0.525 , 0.67584 , 0.0 , 0.151 , 0.6633 , 1.15716 , 1.23578 , 0.0 , 0.41 , 1.232712 , 0.814 , 2.02067 , 3.363588 , 0.0 , 0.485916 , 0.05206 , 0.307 , 0.426 , 0.893 , 0.7472 , 0.55 , 1.04638 , 1.14289 , 0.56214 , 1.30447 , 0.0 , 0.404 , 1.112066 , 1.047401 , 1.970875 , 3.059038 , 0.0 , 0.471626 , 0.14462 , 0.47 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.0 , 0.322 , 0.815 , 0.15 , 1.0778 , 1.56436 , 2.1251 , 2.30861 , 0.0 , 0.377 , 0.364 , 0.942363 , 1.9 , 2.8 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 /)

*Electron affprg\_inity (in eV)*

- real(dp), dimension(nz), parameter `atom_en` = (/ 2.2 , 0.0 , 0.98 , 1.57 , 2.04 , 2.55 , 3.04 , 3.44 , 3.98 , 0.0 , 0.93 , 1.31 , 1.61 , 1.9 , 2.19 , 2.58 , 3.16 , 0.0 , 0.82 , 1.0 , 1.36 , 1.54 , 1.63 , 1.66 , 1.55 , 1.83 , 1.88 , 1.91 , 1.9 , 1.65 , 1.81 , 2.01 , 2.18 , 2.55 , 2.96 , 3.0 , 0.82 , 0.95 , 1.22 , 1.33 , 1.6 , 2.16 , 1.9 , 2.2 , 2.28 , 2.2 , 1.93 , 1.69 , 1.78 , 1.96 , 2.05 , 2.1 , 2.66 , 2.6 , 0.79 , 0.89 , 1.1 , 1.12 , 1.13 , 1.14 , 0.0 , 1.17 , 0.0 , 1.2 , 0.0 , 1.22 , 1.23 , 1.24 , 1.25 , 0.0 , 1.27 , 1.3 , 1.5 , 2.36 , 1.9 , 2.2 , 2.2 , 2.28 , 2.54 , 2.0 , 1.62 , 2.33 , 2.02 , 2.0 , 2.2 , 0.0 , 0.7 , 0.9 , 1.1 , 1.3 , 1.5 , 1.38 , 1.36 , 1.28 , 1.3 , 1.3 , 1.3 , 1.3 , 1.3 , 1.3 , 1.3 , 0.0 /)

*The Pauling electronegativity for this element.*

- integer, dimension(nz), parameter `element_maxbonds` = (/ 1 , 0 , 1 , 2 , 4 , 4 , 4 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 8 , 6 , 6 , 6 , 6 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 12 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 /)

*The maximum expected number of bonds to this element.*

- integer, dimension(nz), parameter `element_numel` = (/ 1 , 2 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 , 18 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 , 18 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 , 18 , 19 , 20 , 21 , 22 , 23 , 24 , 25 , 26 , 27 , 28 , 29 , 30 , 31 , 32 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 /)

*Last shell number of electrons.*

- character(50), dimension(nz), parameter `element_econf` = [character(50) :: "1s" , "1s2" , "1s22s" , "1s22s2" , "1s22s22p" , "1s22s22p2" , "1s22s22p3" , "1s22s22p4" , "1s22s22p5" , "1s22s22p6" , "[Ne]3s" , "[Ne]3s2" , "[Ne]3s23p" , "[Ne]3s23p2" , "[Ne]3s23p3" , "[Ne]3s23p4" , "[Ne]3s23p5" , "[Ne]3s23p6" , "[Ar]4s" , "[Ar]4s2" , "[Ar]3d4s2" , "[Ar]3d24s2" , "[Ar]3d34s2" , "[Ar]3d54s" , "[Ar]3d54s2" , "[Ar]3d64s2" , "[Ar]3d74s2" , "[Ar]3d84s2" , "[Ar]3d104s" , "[Ar]3d104s2" , "[Ar]3d104s24p" , "[Ar]3d104s24p2" , "[Ar]3d104s24p3" , "[Ar]3d104s24p4" , "[Ar]3d104s24p5" , "[Ar]3d104s24p6" , "[Kr]5s" , "[Kr]5s2" , "[Kr]4d5s2" , "[Kr]4d25s2" , "[Kr]4d45s" , "[Kr]4d55s" , "[Kr]4d55s2" , "[Kr]4d75s" , "[Kr]4d85s" , "[Kr]4d10" , "[Kr]4d105s" , "[Kr]4d105s2" , "[Cd]5p" , "[Cd]5p2" , "[Cd]5p3" , "[Cd]5p4" , "[Cd]5p5" , "[Cd]5p6" , "[Xe]6s" , "[Xe]6s2" , "[Xe]5d6s2" , "[Xe]4f5d6s2" , "[Xe]4f36s2" , "[Xe]4f46s2" , "[Xe]4f56s2" , "[Xe]4f66s2" , "[Xe]4f76s2" , "[Xe]4f75d6s2" , "[Xe]4f96s2" , "[Xe]4f106s2" , "[Xe]4f116s2" , "[Xe]4f126s2" , "[Xe]4f136s2" , "[Xe]4f146s2" , "[Xe]4f145d6s2" , "[Xe]4f145d26s2" , "[Xe]4f145d36s2" , "[Xe]4f145d46s2" , "[Xe]4f145d56s2" , "[Xe]4f145d66s2" , "[Xe]4f145d76s2" , "[Xe]4f145d96s" , "[Xe]4f145d106s" , "[Xe]4f145d106s2" , "[Hg]6p" , "[Hg]6p2" , "[Hg]6p3" , "[Hg]6p4" , "[Hg]6p5" , "[Hg]6p6" , "[Rn]7s" , "[Rn]7s2" , "[Rn]6d7s2" , "[Rn]6d27s2" , "[Rn]5f26d7s2" , "[Rn]5f36d7s2" , "[Rn]5f46d7s2" , "[Rn]5f67s2" , "[Rn]5f77s2" , "[Rn]5f76d7s2" , "[Rn]5f97s2" , "[Rn]5f107s2" , "[Rn]5f117s2" , "[Rn]5f127s2" , "[Rn]5f137s2" , "[Rn]5f147s2" , "[Rn]5f147s27p" ]

*The electronic configuration.*

## 9.19.1 Detailed Description

Periodic table of elements.

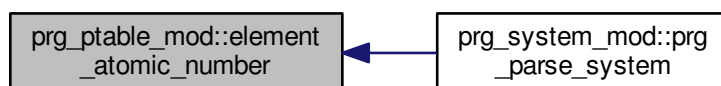
This data was prg\_generated with pybabel and openbable packages Openbabel: <http://openbabel.org/dev-api/index.shtml> Pybel: [https://openbabel.org/docs/dev/UseTheLibrary/Python\\_Pybel.html#](https://openbabel.org/docs/dev/UseTheLibrary/Python_Pybel.html#) Other sources includes NIST: [http://www.nist.gov/pml/data/ion\\_energy.cfm](http://www.nist.gov/pml/data/ion_energy.cfm)

## 9.19.2 Function/Subroutine Documentation

### 9.19.2.1 integer function, public prg\_ptable\_mod::element\_atomic\_number ( character(len=\*) *symbol* )

Definition at line 394 of file prg\_ptable\_mod.F90.

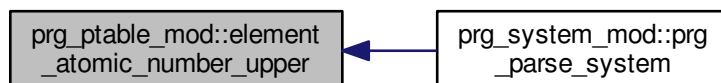
Here is the caller graph for this function:



### 9.19.2.2 integer function prg\_ptable\_mod::element\_atomic\_number\_upper ( character(len=\*) *symbol* )

Definition at line 408 of file prg\_ptable\_mod.F90.

Here is the caller graph for this function:



## 9.19.3 Variable Documentation

9.19.3.1 **real(dp), dimension(nz), parameter** prg\_ptable\_mod::atom\_en = (/ 2.2 , 0.0 , 0.98 , 1.57 , 2.04 , 2.55 , 3.04 , 3.44 , 3.98 , 0.0 , 0.93 , 1.31 , 1.61 , 1.9 , 2.19 , 2.58 , 3.16 , 0.0 , 0.82 , 1.0 , 1.36 , 1.54 , 1.63 , 1.66 , 1.55 , 1.83 , 1.88 , 1.91 , 1.9 , 1.65 , 1.81 , 2.01 , 2.18 , 2.55 , 2.96 , 3.0 , 0.82 , 0.95 , 1.22 , 1.33 , 1.6 , 2.16 , 1.9 , 2.2 , 2.28 , 2.2 , 1.93 , 1.69 , 1.78 , 1.96 , 2.05 , 2.1 , 2.66 , 2.6 , 0.79 , 0.89 , 1.1 , 1.12 , 1.13 , 1.14 , 0.0 , 1.17 , 0.0 , 1.2 , 0.0 , 1.22 , 1.23 , 1.24 , 1.25 , 0.0 , 1.27 , 1.3 , 1.5 , 2.36 , 1.9 , 2.2 , 2.2 , 2.28 , 2.54 , 2.0 , 1.62 , 2.33 , 2.02 , 2.0 , 2.2 , 0.0 , 0.7 , 0.9 , 1.1 , 1.3 , 1.5 , 1.38 , 1.36 , 1.28 , 1.3 , 1.3 , 1.3 , 1.3 , 1.3 , 1.3 , 1.3 , 0.0 /)

The Pauling electronegativity for this element.

Definition at line 266 of file prg\_ptable\_mod.F90.

### 9.19.3.2 integer, parameter, private prg\_ptable\_mod::dp = kind(1.0d0) [private]

Definition at line 13 of file prg\_ptable\_mod.F90.

9.19.3.3 real(dp), dimension(nz), parameter prg\_ptable\_mod::element\_covr = (/ 0.31 , 0.28 , 1.28 , 0.96 , 0.84 , 0.76 , 0.71 , 0.66 , 0.57 , 0.58 , 1.66 , 1.41 , 1.21 , 1.11 , 1.07 , 1.05 , 1.02 , 1.06 , 2.03 , 1.76 , 1.7 , 1.6 , 1.53 , 1.39 , 1.39 , 1.32 , 1.26 , 1.24 , 1.32 , 1.22 , 1.22 , 1.2 , 1.19 , 1.2 , 1.2 , 1.16 , 2.2 , 1.95 , 1.9 , 1.75 , 1.64 , 1.54 , 1.47 , 1.46 , 1.42 , 1.39 , 1.45 , 1.44 , 1.42 , 1.39 , 1.39 , 1.38 , 1.39 , 1.4 , 2.44 , 2.15 , 2.07 , 2.04 , 2.03 , 2.01 , 1.99 , 1.98 , 1.98 , 1.96 , 1.94 , 1.92 , 1.92 , 1.89 , 1.9 , 1.87 , 1.87 , 1.75 , 1.7 , 1.62 , 1.51 , 1.44 , 1.41 , 1.36 , 1.36 , 1.32 , 1.45 , 1.46 , 1.48 , 1.4 , 1.5 , 1.5 , 2.6 , 2.21 , 2.15 , 2.06 , 2.0 , 1.96 , 1.9 , 1.87 , 1.8 , 1.69 , 1.6 , 1.6 , 1.6 , 1.6 , 1.6 , 1.6 , 1.6 /)

Covalent radius (in Angstroms)

Definition at line 173 of file prg\_ptable\_mod.F90.

9.19.3.4 real(dp), dimension(nz), parameter prg\_ptable\_mod::element\_ea = (/ 0.75420375 , 0.0 , 0.618049 , 0.0 , 0.279723 , 1.262118 , -0.07 , 1.461112 , 3.4011887 , 0.0 , 0.547926 , 0.0 , 0.43283 , 1.389521 , 0.7465 , 2.0771029 , 3.612724 , 0.0 , 0.501459 , 0.02455 , 0.188 , 0.084 , 0.525 , 0.67584 , 0.0 , 0.151 , 0.6633 , 1.15716 , 1.23578 , 0.0 , 0.41 , 1.232712 , 0.814 , 2.02067 , 3.363588 , 0.0 , 0.485916 , 0.05206 , 0.307 , 0.426 , 0.893 , 0.7472 , 0.55 , 1.04638 , 1.14289 , 0.56214 , 1.30447 , 0.0 , 0.404 , 1.112066 , 1.047401 , 1.970875 , 3.059038 , 0.0 , 0.471626 , 0.14462 , 0.47 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.0 , 0.322 , 0.815 , 0.15 , 1.0778 , 1.56436 , 2.1251 , 2.30861 , 0.0 , 0.377 , 0.364 , 0.942363 , 1.9 , 2.8 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 , 0.0 /)

Electron affprg\_inity (in eV)

Definition at line 235 of file prg\_ptable\_mod.F90.

9.19.3.5 character(50), dimension(nz), parameter prg\_ptable\_mod::element\_econf = [character(50) :: "1s", "1s2", "1s22s", "1s22s2", "1s22s22p", "1s22s22p2", "1s22s22p3", "1s22s22p4", "1s22s22p5", "1s22s22p6", "[Ne]3s", "[Ne]3s2", "[Ne]3s23p", "[Ne]3s23p2", "[Ne]3s23p3", "[Ne]3s23p4", "[Ne]3s23p5", "[Ne]3s23p6", "[Ar]4s", "[Ar]4s2", "[Ar]3d4s2", "[Ar]3d24s2", "[Ar]3d34s2", "[Ar]3d54s", "[Ar]3d54s2", "[Ar]3d64s2", "[Ar]3d74s2", "[Ar]3d84s2", "[Ar]3d104s", "[Ar]3d104s2", "[Ar]3d104s24p", "[Ar]3d104s24p2", "[Ar]3d104s24p3", "[Ar]3d104s24p4", "[Ar]3d104s24p5", "[Ar]3d104s24p6", "[Kr]5s", "[Kr]5s2", "[Kr]4d5s2", "[Kr]4d25s2", "[Kr]4d45s", "[Kr]4d55s", "[Kr]4d55s2", "[Kr]4d75s", "[Kr]4d85s", "[Kr]4d10", "[Kr]4d105s", "[Kr]4d105s2", "[Cd]5p", "[Cd]5p2", "[Cd]5p3", "[Cd]5p4", "[Cd]5p5", "[Cd]5p6", "[Xe]6s", "[Xe]6s2", "[Xe]5d6s2", "[Xe]4f5d6s2", "[Xe]4f36s2", "[Xe]4f46s2", "[Xe]4f56s2", "[Xe]4f66s2", "[Xe]4f76s2", "[Xe]4f75d6s2", "[Xe]4f96s2", "[Xe]4f106s2", "[Xe]4f116s2", "[Xe]4f126s2", "[Xe]4f136s2", "[Xe]4f146s2", "[Xe]4f145d6s2", "[Xe]4f145d26s2", "[Xe]4f145d36s2", "[Xe]4f145d46s2", "[Xe]4f145d56s2", "[Xe]4f145d66s2", "[Xe]4f145d76s2", "[Xe]4f145d96s", "[Xe]4f145d106s", "[Xe]4f145d106s2", "[Hg]6p", "[Hg]6p2", "[Hg]6p3", "[Hg]6p4", "[Hg]6p5", "[Hg]6p6", "[Rn]7s", "[Rn]7s2", "[Rn]6d7s2", "[Rn]6d27s2", "[Rn]5f26d7s2", "[Rn]5f36d7s2", "[Rn]5f46d7s2", "[Rn]5f67s2", "[Rn]5f77s2", "[Rn]5f76d7s2", "[Rn]5f97s2", "[Rn]5f107s2", "[Rn]5f117s2", "[Rn]5f127s2", "[Rn]5f137s2", "[Rn]5f147s2", "[Rn]5f147s27p"]]

The electronic configuration.

Definition at line 360 of file prg\_ptable\_mod.F90.



9.19.3.6 `real(dp), dimension(nz), parameter prg_ptable_mod::element_ip = (/ 13.5984 , 24.5874 , 5.3917 , 9.3227 , 8.298 , 11.2603 , 14.5341 , 13.6181 , 17.4228 , 21.5645 , 5.1391 , 7.6462 , 5.9858 , 8.1517 , 10.4867 , 10.36 , 12.9676 , 15.7596 , 4.3407 , 6.1132 , 6.5615 , 6.8281 , 6.7462 , 6.7665 , 7.434 , 7.9024 , 7.881 , 7.6398 , 7.7264 , 9.3942 , 5.9993 , 7.8994 , 9.7886 , 9.7524 , 11.8138 , 13.9996 , 4.1771 , 5.6949 , 6.2173 , 6.6339 , 6.7589 , 7.0924 , 7.28 , 7.3605 , 7.4589 , 8.3369 , 7.5762 , 8.9938 , 5.7864 , 7.3439 , 8.6084 , 9.0096 , 10.4513 , 12.1298 , 3.8939 , 5.2117 , 5.5769 , 5.5387 , 5.473 , 5.525 , 5.582 , 5.6437 , 5.6704 , 6.1498 , 5.8638 , 5.9389 , 6.0215 , 6.1077 , 6.1843 , 6.2542 , 5.4259 , 6.8251 , 7.5496 , 7.864 , 7.8335 , 8.4382 , 8.967 , 8.9588 , 9.2255 , 10.4375 , 6.1082 , 7.4167 , 7.2855 , 8.414 , 0.0 , 10.7485 , 4.0727 , 5.2784 , 5.17 , 6.3067 , 5.89 , 6.1941 , 6.2657 , 6.026 , 5.9738 , 5.9914 , 6.1979 , 6.2817 , 6.42 , 6.5 , 6.58 , 6.65 , 4.9 /)`

Ionization energy (in eV)

Definition at line 204 of file `prg_ptable_mod.F90`.

9.19.3.7 `real(dp), dimension(nz), parameter prg_ptable_mod::element_mass = (/ 1.007825032 , 4.002603254 , 7.01600455 , 9.0121822 , 11.0093054 , 12.0 , 14.003074005 , 15.99491462 , 18.99840322 , 19.992440175 , 22.989769281 , 23.9850417 , 26.98153863 , 27.976926532 , 30.97376163 , 31.972071 , 34.96885268 , 39.962383123 , 38.96370668 , 39.96259098 , 44.9559119 , 47.9479463 , 50.9439595 , 51.9405075 , 54.9380451 , 55.9349375 , 58.933195 , 57.9353429 , 62.9295975 , 63.929142 , 68.925573 , 73.921177 , 74.921596 , 79.916521 , 78.918337 , 83.911507 , 84.911789 , 87.905612 , 88.905848 , 89.904704 , 92.906378 , 97.905408 , 97.907216 , 101.904349 , 102.905504 , 105.903486 , 106.905097 , 113.903358 , 114.903878 , 119.902194 , 120.903815 , 129.906224 , 126.904473 , 131.904153 , 132.905451 , 137.905247 , 138.906353 , 139.905438 , 140.907652 , 141.907723 , 144.912749 , 151.919732 , 152.92123 , 157.924103 , 158.925346 , 163.929174 , 164.930322 , 165.930293 , 168.934213 , 173.938862 , 174.940771 , 179.94655 , 180.947995 , 183.950931 , 186.955753 , 191.96148 , 192.962926 , 194.964791 , 196.966568 , 201.970643 , 204.974427 , 207.976652 , 208.980398 , 208.98243 , 209.987148 , 222.017577 , 223.019735 , 226.025409 , 227.027752 , 232.038055 , 231.035884 , 238.050788 , 237.048173 , 244.064204 , 243.061381 , 247.070354 , 247.070307 , 251.079587 , 252.08298 , 257.095105 , 258.098431 , 259.10103 , 262.10963 /)`

Element mass in atomic mass units ( $1.66 \times 10^{-27}$  kg)

Definition at line 110 of file `prg_ptable_mod.F90`.

9.19.3.8 `integer, dimension(nz), parameter prg_ptable_mod::element_maxbonds = (/ 1 , 0 , 1 , 2 , 4 , 4 , 4 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 8 , 6 , 6 , 6 , 6 , 6 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 12 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 6 /)`

The maximum expected number of bonds to this element.

Definition at line 297 of file `prg_ptable_mod.F90`.

9.19.3.9 `character(20), dimension(nz), parameter prg_ptable_mod::element_name = [character(20) :: "Hydrogen" , "Helium" , "Lithium" , "Beryllium" , "Boron" , "Carbon" , "Nitrogen" , "Oxygen" , "Fluorine" , "Neon" , "Sodium" , "Magnesium" , "Aluminium" , "Silicon" , "Phosphorus" , "Sulfur" , "Chlorine" , "Argon" , "Potassium" , "Calcium" , "Scandium" , "Titanium" , "Vanadium" , "Chromium" , "Manganese" , "Iron" , "Cobalt" , "Nickel" , "Copper" , "Zinc" , "Gallium" , "Germanium" , "Arsenic" , "Selenium" , "Bromine" , "Krypton" , "Rubidium" , "Strontium" , "Yttrium" , "Zirconium" , "Niobium" , "Molybdenum" , "Technetium" , "Ruthenium" , "Rhodium" , "Palladium" , "Silver" , "Cadmium" , "Indium" , "Tin" , "Antimony" , "Tellurium" , "Iodine" , "Xenon" , "Caesium" , "Barium" , "Lanthanum" , "Cerium" , "Praseodymium" , "Neodymium" , "Promethium" , "Samarium" , "Europium" , "Gadolinium" , "Terbium" , "Dysprosium" , "Holmium" , "Erbium" , "Thulium" , "Ytterbium" , "Lutetium" , "Hafnium" , "Tantalum" , "Tungsten" , "Rhenium" , "Osmium" , "Iridium" , "Platinum" , "Gold" , "Mercury" , "Thallium" , "Lead" , "Bismuth" , "Polonium" , "Astatine" , "Radon" , "Francium" , "Radium" , "Actinium" , "Thorium" , "Protactinium" , "Uranium" , "Neptunium" , "Plutonium" , "Americium" , "Curium" , "Berkelium" , "Californium" , "Einsteinium" , "Fermium" , "Mendelevium" , "Nobelium" , "Lawrencium" ]`

Element name.

Definition at line 79 of file `prg_ptable_mod.F90`.

9.19.3.10 integer, dimension(nz), parameter prg\_ptable\_mod::element\_numel = (/ 1, 2, 1, 2, 3, 4, 5, 6, 7, 8, 1, 2, 3, 4, 5, 6, 7, 8, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17 /)

Last shell number of electrons.

Definition at line 329 of file prg\_ptable\_mod.F90.

9.19.3.11 character(2), dimension(nz), parameter prg\_ptable\_mod::element\_symbol = [character(2) :: "H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne", "Na", "Mg", "Al", "Si", "P", "S", "Cl", "Ar", "K", "Ca", "Sc", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn", "Ga", "Ge", "As", "Se", "Br", "Kr", "Rb", "Sr", "Y", "Zr", "Nb", "Mo", "Tc", "Ru", "Rh", "Pd", "Ag", "Cd", "In", "Sn", "Sb", "Te", "I", "Xe", "Cs", "Ba", "La", "Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb", "Lu", "Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg", "Tl", "Pb", "Bi", "Po", "At", "Rn", "Fr", "Ra", "Ac", "Th", "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk", "Cf", "Es", "Fm", "Md", "No", "Lr"]

Element symbol.

Definition at line 17 of file prg\_ptable\_mod.F90.

9.19.3.12 character(2), dimension(nz), parameter prg\_ptable\_mod::element\_symbol\_upper = [character(2) :: "H", "HE", "LI", "BE", "B", "C", "N", "O", "F", "NE", "NA", "MG", "AL", "SI", "P", "S", "CL", "AR", "K", "CA", "SC", "TI", "V", "CR", "MN", "FE", "CO", "NI", "CU", "ZN", "GA", "GE", "AS", "SE", "BR", "KR", "RB", "SR", "Y", "ZR", "NB", "MO", "TC", "RU", "RH", "PD", "AG", "CD", "IN", "SN", "SB", "TE", "I", "XE", "CS", "BA", "LA", "CE", "PR", "ND", "PM", "SM", "EU", "GD", "TB", "DY", "HO", "ER", "TM", "YB", "LU", "HF", "TA", "W", "RE", "OS", "IR", "PT", "AU", "HG", "TL", "PB", "BI", "PO", "AT", "RN", "FR", "RA", "AC", "TH", "PA", "U", "NP", "PU", "AM", "CM", "BK", "CF", "ES", "FM", "MD", "NO", "LR"]

Element symbol upper.

Definition at line 48 of file prg\_ptable\_mod.F90.

9.19.3.13 real(dp), dimension(nz), parameter prg\_ptable\_mod::element\_vdwr = (/ 1.1, 1.4, 1.81, 1.53, 1.92, 1.7, 1.55, 1.52, 1.47, 1.54, 2.27, 1.73, 1.84, 2.1, 1.8, 1.8, 1.75, 1.88, 2.75, 2.31, 2.3, 2.15, 2.05, 2.05, 2.05, 2.05, 2.0, 2.0, 2.0, 2.1, 1.87, 2.11, 1.85, 1.9, 1.83, 2.02, 3.03, 2.49, 2.4, 2.3, 2.15, 2.1, 2.05, 2.05, 2.0, 2.05, 2.1, 2.2, 2.2, 1.93, 2.17, 2.06, 1.98, 2.16, 3.43, 2.68, 2.5, 2.48, 2.47, 2.45, 2.43, 2.42, 2.4, 2.38, 2.37, 2.35, 2.33, 2.32, 2.3, 2.28, 2.27, 2.25, 2.2, 2.1, 2.05, 2.0, 2.0, 2.05, 2.1, 2.05, 1.96, 2.02, 2.07, 1.97, 2.02, 2.2, 3.48, 2.83, 2.0, 2.4, 2.0, 2.3, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0, 2.0 /)

van der Waals radius (in Angstroms)

Definition at line 141 of file prg\_ptable\_mod.F90.

9.19.3.14 integer, parameter prg\_ptable\_mod::nz = 103

Definition at line 12 of file prg\_ptable\_mod.F90.

## 9.20 prg\_pulaycomponent\_mod Module Reference

Produces a matrix to get the Pulay Component of the forces.

### Functions/Subroutines

- subroutine, public [prg\\_pulaycomponent0](#) (rho\_bml, ham\_bml, pcm\_bml, threshold, M, bml\_type, verbose)  
 $At T = 0K, P = \rho H \rho.$
- subroutine, public [prg\\_pulaycomponentt](#) (rho\_bml, ham\_bml, zmat\_bml, pcm\_bml, threshold, M, bml\_type, verbose)  
 $At T > 0K, P = \rho H S^{-1} + S^{-1} H \rho.$
- subroutine, public [prg\\_get\\_pulayforce](#) (nats, zmat\_bml, ham\_bml, rho\_bml, dSx\_bml, dSy\_bml, dSz\_bml, hindex, FPUL, threshold)  
*Pulay Force FPUL from  $2Tr[ZZ'HD\frac{dS}{dR}]$ .*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.20.1 Detailed Description

Produces a matrix to get the Pulay Component of the forces.

For a further explanation please see Niklasson 2008 [\[3\]](#)

#### 9.20.2 Function/Subroutine Documentation

- 9.20.2.1 subroutine, public prg\_pulaycomponent\_mod::prg\_get\_pulayforce ( integer, intent(in) *nats*, type(bml\_matrix\_t), intent(in) *zmat\_bml*, type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(in) *rho\_bml*, type(bml\_matrix\_t), intent(in) *dSx\_bml*, type(bml\_matrix\_t), intent(in) *dSy\_bml*, type(bml\_matrix\_t), intent(in) *dSz\_bml*, integer, dimension(:, :), intent(in) *hindex*, real(dp), dimension(:, :), intent(inout), allocatable *FPUL*, real(dp), intent(in) *threshold* )

Pulay Force FPUL from  $2Tr[ZZ'HD\frac{dS}{dR}]$ .

##### Parameters

|                 |   |
|-----------------|---|
| <i>nats</i>     | Number of atoms.  |
| <i>zmat_bml</i> | Congruence transform in bml format.                               |
| <i>rho_bml</i>  | Density matrix.   |
| <i>dSx_bml</i>  | x derivative of S.  |
| <i>dSy_bml</i>  | y derivative of S.  |
| <i>dSz_bml</i>  | z derivative of S.  |
| <i>hindex</i>   | Contains the Hamiltonian indices for every atom (see get_hindex). |

Definition at line 152 of file prg\_pulaycomponent\_mod.F90.

9.20.2.2 subroutine, public prg\_pulaycomponent\_mod::prg\_pulaycomponent0 ( type(bml\_matrix\_t), intent(in) *rho\_bml*, type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(inout) *pcm\_bml*, real(dp), intent(in) *threshold*, integer, intent(in) *M*, character(20), intent(in) *bml\_type*, integer *verbose* )

At  $T = 0K$ ,  $P = \rho H \rho$ .

#### Parameters

|                  |                                    |
|------------------|------------------------------------|
| <i>rho_bml</i>   | Density matrix in bml format.      |
| <i>ham_bml</i>   | Hamiltonian matrix in bml format.  |
| <i>pcm_bml</i>   | Pulay matix output in bml format.  |
| <i>threshold</i> | Threshold for the matrix elements. |
| <i>M</i>         | Maximum nonzero values per row.    |
| <i>bml_type</i>  | Bml format type.                   |
| <i>verbose</i>   | Verbosity level.                   |

**Todo** M and bml\_type will have to be removed from the input parameter.

Definition at line 32 of file prg\_pulaycomponent\_mod.F90.

9.20.2.3 subroutine, public prg\_pulaycomponent\_mod::prg\_pulaycomponentt ( type(bml\_matrix\_t), intent(in) *rho\_bml*, type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(in) *zmat\_bml*, type(bml\_matrix\_t), intent(inout) *pcm\_bml*, real(dp), intent(in) *threshold*, integer, intent(in) *M*, character(20), intent(in) *bml\_type*, integer *verbose* )

At  $T > 0K$ ,  $P = \rho H S^{-1} + S^{-1} H \rho$ .

#### Parameters

|                  |                                     |
|------------------|-------------------------------------|
| <i>rho_bml</i>   | Density matrix in bml format.       |
| <i>ham_bml</i>   | Hamiltonian matrix in bml format.   |
| <i>Z_bml</i>     | Congruence transform in bml format. |
| <i>pcm_bml</i>   | Pulay matrix output in bml format.  |
| <i>threshold</i> | Threshold for the matrix elements.  |
| <i>M</i>         | Maximum nonzero values per row.     |
| <i>bml_type</i>  | Bml format type.                    |
| <i>verbose</i>   | Verbosity level.                    |

**Todo** M and bml\_type will have to be removed from the input parameter.

Definition at line 83 of file prg\_pulaycomponent\_mod.F90.

## 9.20.3 Variable Documentation

9.20.3.1 integer, parameter prg\_pulaycomponent\_mod::dp = kind(1.0d0) [private]

Definition at line 13 of file prg\_pulaycomponent\_mod.F90.

## 9.21 prg\_pulaymixer\_mod Module Reference

Pulay mixer mode.

### Data Types

- type [mx\\_type](#)

### Functions/Subroutines

- subroutine, public [prg\\_parse\\_mixer](#) (input, filename)  
*The parser for the mixer routines.*
- subroutine, public [prg\\_qmixer](#) (charges, oldcharges, dqin, dqout, scferror, piter, pulaycoef, mpulay, verbose)  
*Mixing the charges to accelerate scf convergence.*
- subroutine, public [prg\\_linearmixer](#) (charges, oldcharges, scferror, linmixcoef, verbose)  
*Routine to perform linear mixing.*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.21.1 Detailed Description

Pulay mixer mode.

Gets the best coefficient for mixing the charges during scf.

**Todo** add the density matrix mixer.

#### 9.21.2 Function/Subroutine Documentation

**9.21.2.1** subroutine, public prg\_pulaymixer\_mod::prg\_linearmixer ( real([dp](#)), dimension(:), intent(inout), allocatable *charges*, real([dp](#)), dimension(:), intent(inout), allocatable *oldcharges*, real([dp](#)), intent(inout) *scferror*, real([dp](#)), intent(in) *linmixcoef*, integer, intent(in) *verbose* )

Routine to perform linear mixing.

##### Parameters

|                   |                               |
|-------------------|-------------------------------|
| <i>charges</i>    | Actual charges of the system. |
| <i>oldcharges</i> | Previous scf charges.         |
| <i>scferror</i>   | SCF error.                    |
| <i>linmixcoef</i> | Mixing coefficient.           |
| <i>verbose</i>    | Verbosity level.              |

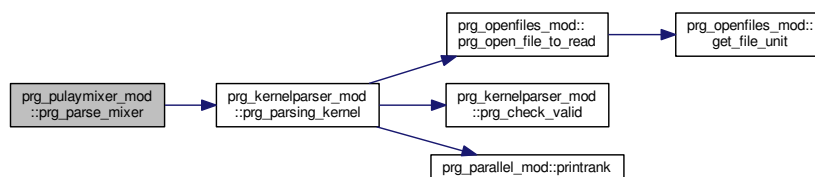
Definition at line 237 of file prg\_pulaymixer\_mod.F90.

9.21.2.2 subroutine, public prg\_pulaymixer\_mod::prg\_parse\_mixer ( type(mx\_type), intent(inout) *input*, character(len=\*) *filename* )

The parser for the mixer routines.

Definition at line 42 of file prg\_pulaymixer\_mod.F90.

Here is the call graph for this function:



9.21.2.3 subroutine, public prg\_pulaymixer\_mod::prg\_qmixer ( real(dp), dimension(:), intent(inout) *charges*, real(dp), dimension(:), intent(inout), allocatable *oldcharges*, real(dp), dimension(:,:), intent(inout), allocatable *dqin*, real(dp), dimension(:,:), intent(inout), allocatable *dqout*, real(dp), intent(inout) *scferror*, integer *piter*, real(dp), intent(in) *pulaycoef*, integer, intent(in) *mpulay*, integer, intent(in) *verbose* )

Mixing the charges to accelerate scf convergence.

#### Parameters

|                   |  |
|-------------------|--|
| <i>charges</i>    | System charges.  |
| <i>oldcharges</i> | Old charges of the system.                                     |
| <i>dqin</i>       | Matrix for charges history in.                                 |
| <i>dqout</i>      | Matrix for charges history out.                                |
| <i>scferror</i>   | SCF error.   |
| <i>piter</i>      | scf iteration number.  |
| <i>pulaycoef</i>  | Coefficient for pulay mixing (generally between 0.01 and 0.1). |
| <i>mpulay</i>     | Number of matrices stored (generally 3-5).                     |
| <i>verbose</i>    | Different levels of verbosity.                                 |

Definition at line 103 of file prg\_pulaymixer\_mod.F90.

### 9.21.3 Variable Documentation

9.21.3.1 integer, parameter prg\_pulaymixer\_mod::dp = kind(1.0d0) [private]

Definition at line 14 of file prg\_pulaymixer\_mod.F90.

## 9.22 prg\_quantumdynamics\_mod Module Reference

A module to add in common quantum dynamical operations.

### Functions/Subroutines

- subroutine, public [prg\\_kick\\_density](#) (kick\_dirac, kick\_mag, dens, norbs, mdim, S, SINV, which\_atom, r, bml\_type, thresh)  
*Provides perturbation to initial density matrix in the form of an electric field kick. This routine does:  $\rho_{kick} = \exp \frac{-i}{\hbar} \hat{V} \hat{\rho} \hat{S} \exp \frac{i}{\hbar} \hat{V} \hat{S}^{-1}$  where  $\hat{V}$  is the field disturbance.*
- subroutine, public [prg\\_get\\_sparsity\\_cplxmat](#) (matrix\_type, element\_type, thresh, a\_dense)  
*This computes the sparsity of a complex matrix given a threshold value This routine does:  $f = \frac{N_0}{N_{tot}}$  where  $f$  is the sparsity,  $N_0$  is the number of values less than the threshold, and  $N_{tot}$  is the total number of values. The sparsity and threshold are printed to the screen.*
- subroutine, public [prg\\_get\\_sparsity\\_realmat](#) (matrix\_type, element\_type, thresh, a\_dense)  
*This computes the sparsity of a real matrix given a threshold value This routine does:  $f = \frac{N_0}{N_{tot}}$  where  $f$  is the sparsity,  $N_0$  is the number of values less than the threshold, and  $N_{tot}$  is the total number of values. The sparsity and threshold are printed to the screen.*
- subroutine, public [prg\\_kick\\_density\\_bml](#) (kick\_dirac, kick\_mag, rho\_bml, s\_bml, sinv\_bml, mdim, which\_atom, r, matrix\_type, thresh)  
*Provides perturbation to initial density matrix in the form of an electric field kick given input matrices in BML format. This routine does:  $\rho_{kick} = \exp \frac{-i}{\hbar} \hat{V} \hat{\rho} \hat{S} \exp \frac{i}{\hbar} \hat{V} \hat{S}^{-1}$  where  $\hat{V}$  is the field disturbance.*
- subroutine, public [prg\\_lvni\\_bml](#) (h1\_bml, sinv\_bml, dt, hbar, rhoold\_bml, rho\_bml, aux\_bml, matrix\_type, mdim, thresh)  
*Performs Liouville-von Neumann integration using leap-frog method. This routine does:  $\hat{\rho}(t + \Delta t) = \hat{\rho}(t - \Delta t) + 2\Delta t \frac{\partial \hat{\rho}(t)}{\partial t}$  where the time derivative of the density matrix is defined as follows:  $\frac{\partial \hat{\rho}(t)}{\partial t} = \frac{-i}{\hbar} (S^{-1} \hat{H}(t) \hat{\rho}(t) - \hat{\rho}(t) \hat{H}(t) S^{-1})$ .*
- subroutine, public [prg\\_getcharge](#) (rho\_bml, s\_bml, charges, aux\_bml, z, spindex, N, nats, thresh)  
*Constructs the charges from the density matrix.*
- subroutine, public [prg\\_getdipole](#) (charges, r, mu)  
*This routine computes the dipole moment of the system with units determined by the units of the coordinate matrix and charges given.*
- subroutine, public [prg\\_excitation](#) (fill\_mat, orbit\_orig, orbit\_exc)  
*Produce an excitation in the initially calculated density matrix to.*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.22.1 Detailed Description

A module to add in common quantum dynamical operations.

This module contains routines that perform the following tasks: apply a apply an excitation or perturbation to the initial density matrix, compute the comutator of two two matrices, calculate the sparsity of a real or complex matrix, and time evolve a density matrix using Liouville-von Neumann equation with the leap-frog method of integration.

### Author

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## 9.22.2 Function/Subroutine Documentation

9.22.2.1 subroutine, public prg\_quantumdynamics\_mod::prg\_excitation ( integer, dimension(:), intent(inout) *fill\_mat*, integer, intent(in) *orbit\_orig*, integer, intent(in) *orbit\_exci* )

Produce an excitation in the initially calculated density matrix to.

Definition at line 312 of file prg\_quantumdynamics\_mod.F90.

9.22.2.2 subroutine, public prg\_quantumdynamics\_mod::prg\_get\_sparsity\_cplxmat ( character(len=\*) , intent(in) *matrix\_type*, character(len=\*) , intent(in) *element\_type*, real(dp), intent(in) *thresh*, complex(dp), dimension(:, :), intent(in) *a\_dense* )

This computes the sparsity of a complex matrix given a threshold value This routine does:  $f = \frac{N_0}{N_{tot}}$  where  $f$  is the sparsity,  $N_0$  is the number of values less than the threshold, and  $N_{tot}$  is the total number of values. The sparsity and threshold are printed to the screen.

### Parameters

|                     |   |
|---------------------|---|
| <i>matrix_type</i>  | the BML matrix type                                   |
| <i>element_type</i> | the BML element type                                  |
| <i>thresh</i>       | the threshold for sparsity evaluation                 |
| <i>a_dense</i>      | the dense complex matrix to be evaluated for sparsity |

Definition at line 103 of file prg\_quantumdynamics\_mod.F90.

9.22.2.3 subroutine, public prg\_quantumdynamics\_mod::prg\_get\_sparsity\_realmat ( character(len=\*) , intent(in) *matrix\_type*, character(len=\*) , intent(in) *element\_type*, real(dp), intent(in) *thresh*, real(dp), dimension(:, :), intent(in) *a\_dense* )

This computes the sparsity of a real matrix given a threshold value This routine does:  $f = \frac{N_0}{N_{tot}}$  where  $f$  is the sparsity,  $N_0$  is the number of values less than the threshold, and  $N_{tot}$  is the total number of values. The sparsity and threshold are printed to the screen.

### Parameters

|                     |  |
|---------------------|--|
| <i>matrix_type</i>  | the BML matrix type                                |
| <i>element_type</i> | the BML element type                               |
| <i>thresh</i>       | the threshold for sparsity evaluation              |
| <i>a_dense</i>      | the dense real matrix to be evaluated for sparsity |

Definition at line 127 of file prg\_quantumdynamics\_mod.F90.

9.22.2.4 subroutine, public prg\_quantumdynamics\_mod::prg\_getcharge ( type(bml\_matrix\_t), intent(in) *rho\_bml*, type(bml\_matrix\_t), intent(in) *s\_bml*, real(dp), dimension(:), allocatable *charges*, type(bml\_matrix\_t) *aux\_bml*, real(dp), dimension(:), intent(in) *z*, integer, dimension(:), intent(in), allocatable *spindex*, integer, dimension(:), intent(in), allocatable *N*, integer *nats*, real(dp), intent(in) *thresh* )

Constructs the charges from the density matrix.



## Parameters

|                 |   |
|-----------------|---|
| <i>rho_bml</i>  | Density matrix in BML format.                     |
| <i>over_bml</i> | Overlap matrix in BML format.                     |
| <i>charges</i>  | the array of charges.                             |
| <i>aux_bml</i>  | the auxiliary matrix in BML format.               |
| <i>spindex</i>  | Start and end index for every atom in the system. |
| <i>z</i>        |   |
| <i>nats</i>     | the number of atoms                               |
| <i>N</i>        |   |
| <i>thresh</i>   | threshold for the BML matrix                      |

Definition at line 252 of file prg\_quantumdynamics\_mod.F90.

9.22.2.5 subroutine, public prg\_quantumdynamics\_mod::prg\_getdipole ( real(dp), dimension(:), intent(in) *charges*, real(dp), dimension(:, :), intent(in) *r*, real(dp), dimension(3), intent(inout) *mu* )

This routine computes the dipole moment of the system with units determined by the units of the coordinate matrix and charges given.

## Parameters

|                |                                 |
|----------------|---------------------------------|
| <i>charges</i> | Charge on each atom.            |
| <i>r</i>       | Coordinate matrix of the atoms. |
| <i>p</i>       | Dipole moment vector.           |

Definition at line 287 of file prg\_quantumdynamics\_mod.F90.

9.22.2.6 subroutine, public prg\_quantumdynamics\_mod::prg\_kick\_density ( integer, intent(in) *kick\_dirac*, real(dp) *kick\_mag*, complex(dp), dimension(:, :), intent(inout), allocatable *dens*, integer, intent(in) *norbs*, integer, intent(in) *mdim*, complex(dp), dimension(:, :), allocatable *S*, complex(dp), dimension(:, :), allocatable *SINV*, integer, dimension(:), intent(in), allocatable *which\_atom*, real(dp), dimension(:, :), allocatable *r*, character(len=\*) , intent(in) *bmltype*, real(dp) *thresh* )

Provides perturbation to initial density matrix in the form of an electric field kick. This routine does:  $\rho_{kick} = \exp \frac{i}{\hbar} \hat{V} \hat{\rho} \hat{S} \exp \frac{i}{\hbar} \hat{V} \hat{S}^{-1}$  where  $\hat{V}$  is the field disturbance.

## Parameters

|                   |   |
|-------------------|---|
| <i>kick_dirac</i> | the direction of the kick in the electric field               |
| <i>kick_mag</i>   | the magnitude of the kick in the electric field               |
| <i>dens</i>       | the initial density matrix to be kicked.                      |
| <i>norbs</i>      | the number of orbitals in the density matrix                  |
| <i>S</i>          | the overlap matrix  |
| <i>SINV</i>       | the inverse of the overlap matrix                             |
| <i>which_atom</i> | vector containing atom identification                         |
| <i>r</i>          | direction vector for kick based on atom and <i>kick_dirac</i> |
| <i>bmltype</i>    | type of BML matrix desired for faster computation             |
| <i>thresh</i>     | threshold for BML matrix conversion                           |

Definition at line 48 of file prg\_quantumdynamics\_mod.F90.

9.22.2.7 subroutine, public prg\_quantumdynamics\_mod::prg\_kick\_density\_bml ( integer, intent(in) *kick\_dirac*, real(dp) *kick\_mag*, type(bml\_matrix\_t) *rho\_bml*, type(bml\_matrix\_t) *s\_bml*, type(bml\_matrix\_t) *sinv\_bml*, integer *mdim*, integer, dimension(:), intent(in), allocatable *which\_atom*, real(dp), dimension(:, :), allocatable *r*, character(len=\*) , intent(in) *matrix\_type*, real(dp) *thresh* )

Provides perturbation to initial density matrix in the form of an electric field kick given input matrices in BML format. This routine does:  $\rho_{kick} = \exp \frac{-i}{\hbar} \hat{V} \hat{\rho} \hat{S} \exp \frac{i}{\hbar} \hat{V} \hat{S}^{-1}$  where  $\hat{V}$  is the field disturbance.

#### Parameters

|                    |  |
|--------------------|--|
| <i>kick_dirac</i>  | the direction of the kick in the electric field        |
| <i>kick_mag</i>    | the magnitude of the kick in the electric field        |
| <i>rho_bml</i>     | the initial density matrix to be kicked in BML format. |
| <i>s_bml</i>       | the overlap matrix                                     |
| <i>sinv_bml</i>    | the inverse of the overlap matrix                      |
| <i>mdim</i>        | maximum number of nonzero values per row in BML matrix |
| <i>which_atom</i>  | vector containing atom identification                  |
| <i>r</i>           | position vector for kicked atom                        |
| <i>matrix_type</i> | the type of BML format                                 |
| <i>thresh</i>      | the threshold for the BML matrix                       |

Definition at line 159 of file prg\_quantumdynamics\_mod.F90.

9.22.2.8 subroutine, public prg\_quantumdynamics\_mod::prg\_lvni\_bml ( type(bml\_matrix\_t) *h1\_bml*, type(bml\_matrix\_t) *sinv\_bml*, real(dp) *dt*, real(dp) *hbar*, type(bml\_matrix\_t) *rhoold\_bml*, type(bml\_matrix\_t) *rho\_bml*, type(bml\_matrix\_t) *aux\_bml*, character(len=\*) , intent(in) *matrix\_type*, integer *mdim*, real(dp), intent(in) *thresh* )

Performs Liouville-von Neumann integration using leap-frog method. This routine does:  $\hat{\rho}(t + \Delta t) = \hat{\rho}(t - \Delta t) + 2\Delta t \frac{\partial \hat{\rho}(t)}{\partial t}$  where the time derivative of the density matrix is defined as follows:  $\frac{\partial \hat{\rho}(t)}{\partial t} = \frac{-i}{\hbar} \left( S^{-1} \hat{H}(t) \hat{\rho}(t) - \hat{\rho}(t) \hat{H}(t) S^{-1} \right)$ .

#### Parameters

|                    |  |
|--------------------|--|
| <i>H</i>           | the Hamiltonian matrix at time t                                 |
| <i>sinv_bml</i>    | the inverse overlap matrix                                       |
| <i>dt</i>          | the timestep for integration                                     |
| <i>hbar</i>        | the Dirac constant (generally taken to be 1 in simulation units) |
| <i>rho_old</i>     | the density matrix at previous time-step                         |
| <i>rho_bml</i>     | the density matrix at current time-step                          |
| <i>aux_bml</i>     | the temp matrix used for value storage during computation        |
| <i>matrix_type</i> | the type of BML matrix   |
| <i>thresh</i>      | the threshold for the BML matrix                                 |

Definition at line 216 of file prg\_quantumdynamics\_mod.F90.

### 9.22.3 Variable Documentation

#### 9.22.3.1 integer, parameter prg\_quantumdynamics\_mod::dp = kind(1.0d0) [private]

Definition at line 19 of file prg\_quantumdynamics\_mod.F90.

## 9.23 prg\_response\_mod Module Reference

Module to compute the density matrix response and related quantities.

### Data Types

- type [respdata\\_type](#)

### Functions/Subroutines

- subroutine, public [prg\\_parse\\_response](#) (RespData, filename)  
*The parser for the calculation of the DM response.*
- subroutine, public [prg\\_compute\\_dipole](#) (charges, coordinate, dipoleMoment, factor, verbose)  
*To compute the dipole moment of the system. The units of the dipole moment are determined by the units of the coordinates and charges that are given.*
- subroutine, public [prg\\_write\\_dipole\\_tcl](#) (dipoleMoment, file, factor, verbose)  
*To visualize a dipole moment using VMD. This will prg\_generate a .tcl script that could be run using VMD To visualize with VMD: \$ vmd -e dipole.tcl.*
- subroutine, public [prg\\_compute\\_polarizability](#) (rsp\_bml, prt\_bml, polarizability, factor, verbose)  
*To compute the polarizability of the system. The units of the directional polarizability are determined by the units of the perturbation and Hamiltonian. This equation can be found in [5] equation 4a. Note that in equation 4a of the reference there is a 2 that account for the double occupancy which is not present in this case cause the density matrix construction is done by taking the occupancy into account.*
- subroutine, public [prg\\_pert\\_from\\_file](#) (prt\_bml, norb)  
*Read perturbation from file.*
- subroutine, public [prg\\_compute\\_response\\_rs](#) (ham\_bml, prt\_bml, rsp\_bml, lambda, bndfil, threshold, verbose)  
*Computes the first order response density matrix using Rayleigh Schrodinger Perturbation theory The transformation hereby performed are:*
- subroutine, public [prg\\_compute\\_response\\_fd](#) (ham\_bml, prt\_bml, rsp\_bml, prg\_delta, bndfil, threshold, verbose)  
*Computes the first order response density matrix using finite differences. The transformation hereby performed are:*
- subroutine, public [prg\\_pert\\_constant\\_field](#) (field, intensity, coordinate, lambda, prt\_bml, threshold, spindex, norbi, verbose, over\_bml)  
*Apply a constant field perturbation through the dipole moment operator ( $\hat{\mu} = e\hat{r}$ ). In the matrix representation, this is:  $H^{(1)} = \lambda \frac{1}{2} (S e \mathbf{r} \cdot \mathbf{E} + e \mathbf{r} \cdot \mathbf{E} S)$ . The symmetrization is done in order to preserve the Hermiticity of  $H$ . In this case the whole system will be affected by the field. In a latter version we will add the possibility of applying this field to a region of the system. In this implementation  $e = 1$  and units can be transformed by using the parameter  $\lambda$ .*
- subroutine, public [prg\\_pert\\_sin\\_pot](#) (direction, lx, coordinate, lambda, prt\_bml, threshold, spindex, norbi, verbose, over\_bml)  
*Apply a sinusoidal length dependent potential ( $\sin(\tilde{\mathbf{r}}_x)$ ) where  $\mathbf{r}_x$  is the x coordinate. The Hamiltonian gets modified as follows:  $H^{(1)} = \frac{1}{2} \lambda (S \sin(\tilde{\mathbf{r}}_x) + \sin(\tilde{\mathbf{r}}_x) S)$ .  $\tilde{\mathbf{r}}_x = 2\pi(\mathbf{r}/l_x) - \pi$ . The symmetrization is done in order to preserve the Hermiticity of  $H$ . Units can be transformed by using the parameter  $\lambda$ .*

- subroutine, public `prg_pert_cos_pot` (direction, lx, coordinate, lambda, prt\_bml, threshold, spindex, norbi, verbose, over\_bml)  
*Apply a cosine length dependent potential ( $\cos(\tilde{r}_x)$ ) where  $\tilde{r}_x$  is the x coordinate. The Hamiltonian gets modified as follows:  $H^{(1)} = \frac{1}{2}\lambda(S\sin(\tilde{r}_x) + \sin(\tilde{r}_x)S)$ .  $\tilde{r}_x = 2\pi(\mathbf{r}/l_x) - \pi$ . The symmetrization is done in order to preserve the Hermiticity of  $H$ . Units can be transformed by using the parameter  $\lambda$ .*
- subroutine, public `prg_compute_response_sp2` (ham\_bml, prt\_bml, rsp\_bml, rho\_bml, lambda, bndfil, minsp2iter, maxsp2iter, sp2conv, idemt看, threshold, verbose)  
*Finds the first order response matrix from a Hamiltonian matrix.*
- subroutine, public `prg_project_response` (rsp\_bml, over\_bml, spindex, norbi, coordinates, rspfunc, verbose)  
*Project the response onto atomic positions. First order response to the perturbation ( $\rho^{(1)}$ ) projected onto the atomic position. Basically:  $rsp(i) = \sum_{\alpha \in i} \rho_{\alpha\alpha}^{(1)}$ , where orbital  $\alpha$  belong to atom  $i$ .*

## Variables

- integer, parameter `dp` = kind(1.0d0)
- real(`dp`), parameter `pi` = 3.14159265358979323846264338327950\_dp

### 9.23.1 Detailed Description

Module to compute the density matrix response and related quantities.

**Todo** Add the response scf

Change name response\_SP2 to dm\_prt\_response

Change name response\_rs to rs\_prt\_response

More information about the theory can be found at [4] and Niklasson2015

### 9.23.2 Function/Subroutine Documentation

**9.23.2.1** subroutine, public `prg_response_mod::prg_compute_dipole` ( real(`dp`), dimension(:), intent(in) *charges*, real(`dp`), dimension(:,:), intent(in) *coordinate*, real(`dp`), dimension(3), intent(inout) *dipoleMoment*, real(`dp`), intent(in) *factor*, integer *verbose* )

To compute the dipole moment of the system. The units of the dipole moment are determined by the units of the coordinates and charges that are given.

#### Parameters

|                     |   |
|---------------------|---|
| <i>charges</i>      | Charges on each atomic position.  |
| <i>coordinate</i>   | Coordinates of the atoms.   |
| <i>nats</i>         | Number of atoms.  |
| <i>dipoleMoment</i> | Dipole moment vector.   |
| <i>factor</i>       | Unit conversion factor (use 1.0 if no conversion is required).  |
| <i>verbose</i>      | To give different verbosity levels. If coordinates are in Å and charges are in fractions of electron, then transformation ea2debye from LATTE lib can be used to change units to Debye. |

Definition at line 120 of file `prg_response_mod.F90`.

9.23.2.2 subroutine, public prg\_response\_mod::prg\_compute\_polarizability ( type(bml\_matrix\_t), intent(in) *rsp\_bml*, type(bml\_matrix\_t), intent(in) *prt\_bml*, real(dp), intent(inout) *polarizability*, real(dp), intent(in) *factor*, integer *verbose* )

To compute the polarizability of the system. The units of the directional polarizability are determined by the units of the perturbation and Hamiltonian. This equation can be found in [5] equation 4a. Note that in equation 4a of the reference there is a 2 that account for the double occupancy which is not present in this case cause the density matrix construction is done by taking the occupancy into account.

#### Parameters

|                     |   |
|---------------------|---|
| <i>charges</i>      | Charges on each atomic position.  |
| <i>coordinate</i>   | Coordinates of the atoms.   |
| <i>nats</i>         | Number of atoms.  |
| <i>dipoleMoment</i> | Dipole moment vector.   |
| <i>factor</i>       | Unit conversion factor (use 1.0 is no conversion is required).  |
| <i>verbose</i>      | To give different verbosity levels. If coordinates are in Å and charges are in fractions of electron, then transformation ea2debye from LATTE lib can be used to change units to Debye. |

Definition at line 198 of file prg\_response\_mod.F90.

9.23.2.3 subroutine, public prg\_response\_mod::prg\_compute\_response\_fd ( type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(in) *prt\_bml*, type(bml\_matrix\_t), intent(inout) *rsp\_bml*, real(dp) *prg\_delta*, real(dp), intent(in) *bndfil*, real(dp), intent(in) *threshold*, integer *verbose* )

Computes the first order response density matrix using finite differences. The transformation hereby performed are:

- $H^+ = H^{(0)} + \delta H^{(1)}$
- $H^- = H^{(0)} - \delta H^{(1)}$
- $\rho^+ = f(H^+)$
- $\rho^- = f(H^-)$
- $\rho^{(1)} = (\rho^+ - \rho^-)/(2\delta)$ . Where f denotes the Fermi function (construction of the density matrix)

#### Parameters

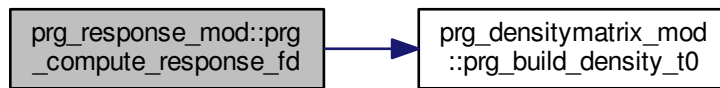
|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Hamiltonian in bml format ( $H^{(0)}$ ).                   |
| <i>prt_bml</i>   | Perturbation in bml format ( $H^{(1)}$ ).                  |
| <i>rsp_bml</i>   | First order response to the perturbation ( $\rho^{(1)}$ ). |
| <i>bndfil</i>    | Filing factor.   |
| <i>threshold</i> | Threshold value for matrix elements.                       |
| <i>verbose</i>   | Different levels of verbosity.                             |

#### Warning

This works only for the prg\_orthogonalized form of ham\_bml.  
The response must be in the prg\_orthogonalized form.

Definition at line 379 of file prg\_response\_mod.F90.

Here is the call graph for this function:



9.23.2.4 subroutine, public prg\_response\_mod::prg\_compute\_response\_rs ( type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(in) *prt\_bml*, type(bml\_matrix\_t), intent(inout) *rsp\_bml*, real(dp) *lambda*, real(dp), intent(in) *bndfil*, real(dp), intent(in) *threshold*, integer *verbose* )

Computes the first order response density matrix using Rayleigh Schrodinger Perturbation theory The transformation hereby performed are:

- $V = C^\dagger H^{(1)} C$
- $\tilde{V}_{ij} = \frac{V_{ij}}{\epsilon_j - \epsilon_i}$ , with  $\tilde{V}_{ii} = 0 \forall i$ .
- $C^{(1)} = C \tilde{V}$
- And finally:  $\rho^{(1)} = C f(C^{(1)})^\dagger + C^{(1)} f C^\dagger$

#### Parameters

|                  |  |
|------------------|--|
| <i>ham_bml</i>   | Hamiltonian in bml format ( $H^{(0)}$ ).                   |
| <i>prt_bml</i>   | Perturbation in bml format ( $H^{(1)}$ ).                  |
| <i>rsp_bml</i>   | First order response to the perturbation ( $\rho^{(1)}$ ). |
| <i>bndfil</i>    | Filing factor.   |
| <i>threshold</i> | Threshold value for matrix elements.                       |
| <i>verbose</i>   | Different levels of verbosity.                             |

#### Warning

This works only for the prg\_orthogonalized form of ham\_bml.  
The response must be in the prg\_orthogonalized form.

Definition at line 249 of file prg\_response\_mod.F90.

9.23.2.5 subroutine, public prg\_response\_mod::prg\_compute\_response\_sp2 ( type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(in) *prt\_bml*, type(bml\_matrix\_t), intent(inout) *rsp\_bml*, type(bml\_matrix\_t), intent(inout) *rho\_bml*, real(dp) *lambda*, real(dp), intent(in) *bndfil*, integer, intent(in) *minsp2iter*, integer, intent(in) *maxsp2iter*, character(len=\*) , intent(in) *sp2conv*, real(dp), intent(in) *idemtol*, real(dp), intent(in) *threshold*, integer *verbose* )

Finds the first order response matrix from a Hamiltonian matrix.

Definition at line 652 of file prg\_response\_mod.F90.

9.23.2.6 subroutine, public prg\_response\_mod::prg\_parse\_response ( type(respdata\_type) *RespData*, character(len=\*) *filename* )

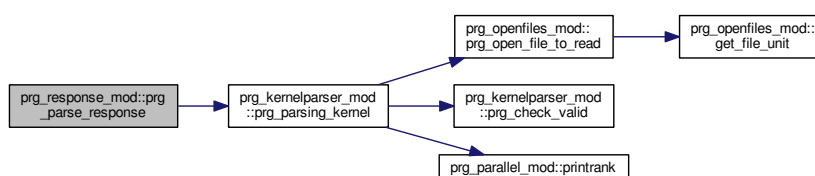
The parser for the calculation of the DM response.

#### Parameters

|                 |                            |
|-----------------|----------------------------|
| <i>RespData</i> | Response data type.        |
| <i>filename</i> | Name of the file to parse. |

Definition at line 45 of file prg\_response\_mod.F90.

Here is the call graph for this function:



9.23.2.7 subroutine, public prg\_response\_mod::prg\_pert\_constant\_field ( real(dp), dimension(3), intent(in) *field*, real(dp) *intensity*, real(dp), dimension(:,:), intent(in) *coordinate*, real(dp) *lambda*, type(bml\_matrix\_t), intent(inout) *prt\_bml*, real(dp) *threshold*, integer, dimension(:), intent(in) *spindex*, integer, dimension(:), intent(in) *norbi*, integer, intent(in) *verbose*, type(bml\_matrix\_t), intent(in), optional *over\_bml* )

Apply a constant field perturbation through the dipole moment operator ( $\hat{\mu} = e\hat{\mathbf{r}}$ ). In the matrix representation, this is:  $H^{(1)} = \lambda \frac{1}{2} (S \mathbf{e} \mathbf{r} \cdot \mathbf{E} + \mathbf{e} \mathbf{r} \cdot \mathbf{E} S)$ . The symmetrization is done in order to preserve the Hermiticity of H. In this case the whole system will be affected by the field. In a latter version we will add the possibility of applying this field to a region of the system. In this implementation  $e = 1$  and units can be transformed by using the parameter  $\lambda$ .

#### Note

If the Hamiltonian is already in the prg\_orthogonalized form, then parameter *over\_bml* can be omitted.

#### Parameters

|                   |  |
|-------------------|--|
| <i>field</i>      | Direction of the applied field ( $\hat{\mathbf{E}}$ ).           |
| <i>intensity</i>  | Intensity of the field ( $  \mathbf{E}  $ ).                     |
| <i>coordinate</i> | Coordinates of the system ( $\mathbf{r}$ ).                      |
| <i>lambda</i>     | Constant to premultiply the perturbation ( $\lambda$ ).          |
| <i>prt_bml</i>    | Perturbation in bml format ( $H^{(1)}$ ).                        |
| <i>threshold</i>  | Threshold value for bml format matrices.                         |
| <i>spindex</i>    | Species index. It gives the species index of a particular atom.  |
| <i>norbi</i>      | Number of orbitals for each atomic site.                         |
| <i>verbose</i>    | Different levels of verbosity.                                   |
| <i>over_bml</i>   | It has to be present for a nonorthogonal representation ( $S$ ). |

Definition at line 446 of file prg\_response\_mod.F90.

9.23.2.8 subroutine, public prg\_response\_mod::prg\_pert\_cos\_pot ( character *direction*, real(dp) *lx*, real(dp), dimension(:,:), intent(in) *coordinate*, real(dp) *lambda*, type(bml\_matrix\_t), intent(inout) *prt\_bml*, real(dp) *threshold*, integer, dimension(:), intent(in) *spindex*, integer, dimension(:), intent(in) *norbi*, integer, intent(in) *verbose*, type(bml\_matrix\_t), intent(in), optional *over\_bml* )

Apply a cosine length dependent potential (  $\cos(\tilde{\mathbf{r}}_x)$  ) where  $\mathbf{r}_x$  is the x coordinate. The Hamiltonian gets modified as follows:  $H^{(1)} = \frac{1}{2}\lambda(S \sin(\tilde{\mathbf{r}}_x) + \sin(\tilde{\mathbf{r}}_x)S)$ .  $\tilde{\mathbf{r}}_x = 2\pi(\mathbf{r}/l_x) - \pi$ . The symmetrization is done in order to preserve the Hermiticity of H. Units can be transformed by using the parameter  $\lambda$ .

#### Note

If the Hamiltonian is already in the prg\_orthogonalized form, then parameter over\_bml can be omitted.

#### Parameters

|                   |  |
|-------------------|--|
| <i>direction</i>  | Direction of the potential gradient (x,y or z).                  |
| <i>lx</i>         | Lenght of the box in x direction.                                |
| <i>coordinate</i> | Coordinates of the system ( $\mathbf{r}$ ).                      |
| <i>lambda</i>     | Constant to premultiply the perturbation ( $\lambda$ ).          |
| <i>prt_bml</i>    | Perturbation in bml format ( $H^{(1)}$ ).                        |
| <i>threshold</i>  | Threshold value for bml format matrices.                         |
| <i>norbi</i>      | Number of orbitals for each atomic site.                         |
| <i>verbose</i>    | Different levels of verbosity.                                   |
| <i>over_bml</i>   | It has to be present for a nonorthogonal representation ( $S$ ). |

Definition at line 591 of file prg\_response\_mod.F90.

9.23.2.9 subroutine, public prg\_response\_mod::prg\_pert\_from\_file ( type(bml\_matrix\_t), intent(inout) *prt\_bml*, integer *norb* )

Read perturbation from file.

**Todo** Add read perturbation from file

Definition at line 223 of file prg\_response\_mod.F90.

9.23.2.10 subroutine, public prg\_response\_mod::prg\_pert\_sin\_pot ( character *direction*, real(dp) *lx*, real(dp), dimension(:,:), intent(in) *coordinate*, real(dp) *lambda*, type(bml\_matrix\_t), intent(inout) *prt\_bml*, real(dp) *threshold*, integer, dimension(:), intent(in) *spindex*, integer, dimension(:), intent(in) *norbi*, integer, intent(in) *verbose*, type(bml\_matrix\_t), intent(in), optional *over\_bml* )

Apply a sinusoidal length dependent potential (  $\sin(\tilde{\mathbf{r}}_x)$  ) where  $\mathbf{r}_x$  is the x coordinate. The Hamiltonian gets modified as follows:  $H^{(1)} = \frac{1}{2}\lambda(S \sin(\tilde{\mathbf{r}}_x) + \sin(\tilde{\mathbf{r}}_x)S)$ .  $\tilde{\mathbf{r}}_x = 2\pi(\mathbf{r}/l_x) - \pi$ . The symmetrization is done in order to preserve the Hermiticity of H. Units can be transformed by using the parameter  $\lambda$ .

#### Note

If the Hamiltonian is already in the prg\_orthogonalized form, then parameter over\_bml can be omitted.



## Parameters

|                   |   |
|-------------------|---|
| <i>direction</i>  | Direction of the potential gradient (x,y or z).                       |
| <i>lx</i>         | Length of the box in x direction.                                     |
| <i>coordinate</i> | Coordinates of the system ( <i>r</i> ).                               |
| <i>lambda</i>     | Constant to premultiply the perturbation ( $\lambda$ ).               |
| <i>pvt_bml</i>    | Perturbation in bml format ( $H^{(1)}$ ).                             |
| <i>threshold</i>  | Threshold value for bml format matrices.                              |
| <i>norbi</i>      | Number of orbitals for each atomic site.                              |
| <i>verbose</i>    | Different levels of verbosity.  |
| <i>over_bml</i>   | It has to be present for a nonorthogonal representation ( <i>S</i> ). |

Definition at line 523 of file prg\_response\_mod.F90.

9.23.2.11 subroutine, public prg\_response\_mod::prg\_project\_response ( type(bml\_matrix\_t), intent(inout) *rsp\_bml*, type(bml\_matrix\_t), intent(in) *over\_bml*, integer, dimension(:), intent(in) *spindex*, integer, dimension(:), intent(in) *norbi*, real(dp), dimension(:,:), intent(in) *coordinates*, real(dp), dimension(:), intent(inout), allocatable *rspfunc*, integer, intent(in) *verbose* )

Project the response onto atomic positions. First order response to the perturbation (  $\rho^{(1)}$  ) projected onto the atomic position. Basically:  $rsp(i) = \sum_{\alpha \in i} \rho_{\alpha\alpha}^{(1)}$ , where orbital  $\alpha$  belong to atom  $i$ .

## Parameters

|                    |  |
|--------------------|--|
| <i>rsp_bml</i>     | First order response density matrix.             |
| <i>spindex</i>     | It gives the species index of a particular atom. |
| <i>norbi</i>       | Number of orbitals of species i.                 |
| <i>coordinates</i> | Atomic coordinates.                              |
| <i>rspfunc</i>     | Response function at atomic positions.           |
| <i>verbose</i>     | Different levels of verbosity.                   |

Definition at line 795 of file prg\_response\_mod.F90.

9.23.2.12 subroutine, public prg\_response\_mod::prg\_write\_dipole\_tcl ( real(dp), dimension(3), intent(in) *dipoleMoment*, character(\*), intent(in) *file*, real(dp), intent(in) *factor*, integer *verbose* )

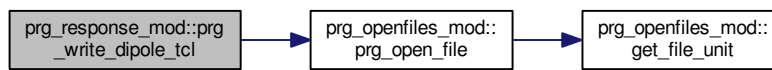
To visualize a dipole moment using VMD. This will prg\_generate a .tcl script that could be run using VMD To visualize with VMD: \$ vmd -e dipole.tcl.

## Parameters

|                     |   |
|---------------------|---|
| <i>dipoleMoment</i> | Dipole moment vector.                   |
| <i>file</i>         | PDB/XYZ file to load for visualization. |
| <i>factor</i>       | Arbitrary scale for visualization.      |
| <i>verbose</i>      | To give different verbosity levels.     |

Definition at line 158 of file prg\_response\_mod.F90.

Here is the call graph for this function:



### 9.23.3 Variable Documentation

9.23.3.1 integer, parameter `prg_response_mod::dp = kind(1.0d0)` `[private]`

Definition at line 18 of file `prg_response_mod.F90`.

9.23.3.2 `real(dp)`, parameter `prg_response_mod::pi = 3.14159265358979323846264338327950_dp` `[private]`

Definition at line 19 of file `prg_response_mod.F90`.

## 9.24 prg\_sp2\_fermi\_mod Module Reference

The SP2 Fermi module.

### Functions/Subroutines

- subroutine, public [prg\\_sp2\\_fermi\\_init](#) (`h_bml`, `nsteps`, `nocc`, `tscale`, `threshold`, `occErrLimit`, `traceLimit`, `x_bml`, `mu`, `beta`, `h1`, `hN`, `sgnlist`)  
*Truncated SP2 prg\_initialization.*
- subroutine, public [prg\\_sp2\\_fermi\\_init\\_norecs](#) (`h_bml`, `nsteps`, `nocc`, `tscale`, `threshold`, `occErrLimit`, `traceLimit`, `x_bml`, `mu`, `beta`, `h1`, `hN`, `sgnlist`, `verbose`)  
*Truncated SP2 prg\_initialization. This routine also gives back the Number of SP2 recursive steps that gets a Pseudo-Fermi distribution with a temperature close to the target temperature which is entered using parameter  $\beta = (1/KbT)$ .*
- subroutine, public [prg\\_sp2\\_fermi](#) (`h_bml`, `osteps`, `nsteps`, `nocc`, `mu`, `beta`, `h1`, `hN`, `sgnlist`, `threshold`, `eps`, `traceLimit`, `x_bml`)  
*Calculate Truncated SP2.*
- subroutine, public [prg\\_sp2\\_entropy\\_function](#) (`mu`, `h1`, `hN`, `nsteps`, `sgnlist`, `GG`, `ee`)  
*Calculate SP2 entropy function using gaussian quadrature. Note that GG and ee are allocated and returned from this routine.*
- `real(dp)` function, public [sp2\\_entropy\\_ts](#) (`D0_bml`, `GG`, `ee`)  
*Test SP2 entropy. Get the entropy contribution TS to the total free energy.*
- `real(dp)` function, public [sp2\\_inverse](#) (`f`, `mu`, `h1`, `hN`, `nsteps`, `sgnlist`)  
*Calculate the SP2 inverse.*
- `real(dp)` function [absmaxderivative](#) (`func`, `de`)  
*Gets the absolute maximum of the derivative of a function.*

## Variables

- integer, parameter `dp = kind(1.0d0)`

### 9.24.1 Detailed Description

The SP2 Fermi module.

### 9.24.2 Function/Subroutine Documentation

**9.24.2.1** `real(dp) function prg_sp2_fermi_mod::absmaxderivative ( real(dp), dimension(:), intent(in) func, real(dp), intent(in) de ) [private]`

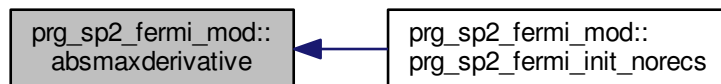
Gets the absolute maximum of the derivative of a function.

#### Parameters

|              |              |
|--------------|--------------|
| <i>func.</i> |              |
| <i>de</i>    | Energy step. |

Definition at line 615 of file `prg_sp2_fermi_mod.F90`.

Here is the caller graph for this function:



**9.24.2.2** `subroutine, public prg_sp2_fermi_mod::prg_sp2_entropy_function ( real(dp), intent(in) mu, real(dp), intent(in) h1, real(dp), intent(in) hN, integer, intent(in) nsteps, integer, dimension(:), intent(in) sgnlist, real(dp), dimension(:), intent(inout), allocatable GG, real(dp), dimension(:), intent(inout), allocatable ee )`

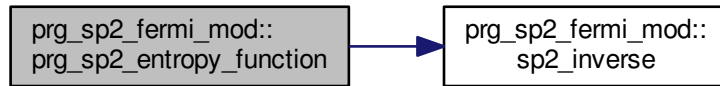
Calculate SP2 entropy function using gaussian quadrature. Note that *GG* and *ee* are allocated and returned from this routine.

#### Parameters

|                |                                 |
|----------------|---------------------------------|
| <i>mu</i>      | Shifted chemical potential      |
| <i>h1</i>      | Minimum scaled Gershgorin bound |
| <i>hN</i>      | Maximum scaled Gershgorin bound |
| <i>nsteps</i>  | Number of SP2 steps             |
| <i>sgnlist</i> | SP2 sequence                    |
| <i>GG</i>      | Entropy function                |
| <i>ee</i>      | 1D mesh                         |

Definition at line 480 of file prg\_sp2\_fermi\_mod.F90.

Here is the call graph for this function:



9.24.2.3 subroutine, public prg\_sp2\_fermi\_mod::prg\_sp2\_fermi ( type(bml\_matrix\_t), intent(in) *h\_bml*, integer, intent(in) *osteps*, integer, intent(in) *nsteps*, real(dp), intent(in) *nocc*, real(dp), intent(inout) *mu*, real(dp), intent(inout) *beta*, real(dp), intent(inout) *h1*, real(dp), intent(inout) *hN*, integer, dimension(:), intent(in) *sgnlist*, real(dp), intent(in) *threshold*, real(dp), intent(in) *eps*, real(dp), intent(in) *traceLimit*, type(bml\_matrix\_t), intent(inout) *x\_bml* )

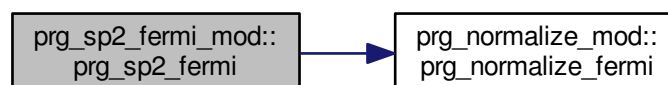
Calculate Truncated SP2.

#### Parameters

|                   |                                  |
|-------------------|----------------------------------|
| <i>h_bml</i>      | Hamiltonian matrix               |
| <i>osteps</i>     | Outer loop steps                 |
| <i>nsteps</i>     | Number of sequence branches      |
| <i>nocc</i>       | Number of occupation states      |
| <i>mu</i>         | Shifted chemical potential       |
| <i>beta</i>       | Inverse temperature              |
| <i>h1</i>         | Minimum scaled Gershgorin bound. |
| <i>hN</i>         | Maximum scaled Gershgorin bound. |
| <i>sgnlist</i>    | SP2 sequence                     |
| <i>threshold</i>  | Threshold for multiplies         |
| <i>eps</i>        | Occupation error limit           |
| <i>traceLimit</i> | Trace limit                      |
| <i>x_bml</i>      | Output density matrix            |

Definition at line 387 of file prg\_sp2\_fermi\_mod.F90.

Here is the call graph for this function:



9.24.2.4 subroutine, public prg\_sp2\_fermi\_mod::prg\_sp2\_fermi\_init ( type(bml\_matrix\_t), intent(in) *h\_bml*, integer, intent(in) *nsteps*, real(dp), intent(in) *nocc*, real(dp), intent(in) *tscale*, real(dp), intent(in) *threshold*, real(dp), intent(in) *occErrLimit*, real(dp), intent(in) *traceLimit*, type(bml\_matrix\_t), intent(inout) *x\_bml*, real(dp), intent(inout) *mu*, real(dp), intent(inout) *beta*, real(dp), intent(inout) *h1*, real(dp), intent(inout) *hN*, integer, dimension(:), intent(inout) *sgnlist* )

Truncated SP2 prg\_initialization.

#### Parameters

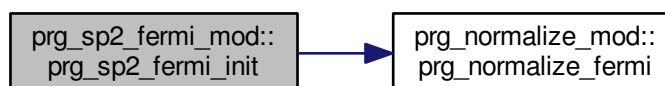
|                    |   |
|--------------------|---|
| <i>h_bml</i>       | Input Hamiltonian matrix.                           |
| <i>nsteps</i>      | Number of sp2 iterations.                           |
| <i>nocc</i>        | Number of occupied states.                          |
| <i>tscale</i>      | Temperature rescaling factor.                       |
| <i>threshold</i>   | Threshold for multiplication.                       |
| <i>occErrLimit</i> | Occupation error limit.                             |
| <i>traceLimit</i>  | Trace limit.  |
| <i>x_bml</i>       | Output prg_initial matrix.                          |
| <i>mu</i>          | Shifted chemical potential                          |
| <i>beta</i>        | Output inverse temperature.                         |
| <i>h1</i>          | Output temperature-scaled minimum gershgorin bound. |
| <i>hN</i>          | Output temperature-scaled maximum gershgorin bound. |
| <i>sgnlist</i>     | SP2 sequence  |

Calculate Gershgorin bounds and rescale

Determine sequence branching first time through

Definition at line 46 of file prg\_sp2\_fermi\_mod.F90.

Here is the call graph for this function:



9.24.2.5 subroutine, public prg\_sp2\_fermi\_mod::prg\_sp2\_fermi\_init\_norecs ( type(bml\_matrix\_t), intent(in) *h\_bml*, integer, intent(inout) *nsteps*, real(dp), intent(in) *nocc*, real(dp), intent(in) *tscale*, real(dp), intent(in) *threshold*, real(dp), intent(in) *occErrLimit*, real(dp), intent(in) *traceLimit*, type(bml\_matrix\_t), intent(inout) *x\_bml*, real(dp), intent(inout) *mu*, real(dp), intent(inout) *beta*, real(dp), intent(inout) *h1*, real(dp), intent(inout) *hN*, integer, dimension(:), intent(inout) *sgnlist*, integer, optional *verbose* )

Truncated SP2 prg\_initialization. This routine also gives back the Number of SP2 recursive steps that gets a Pseudo-Fermi distribution with a temperature close to the target temperature which is entered using parameter *beta* = (1/KbT).

## Parameters

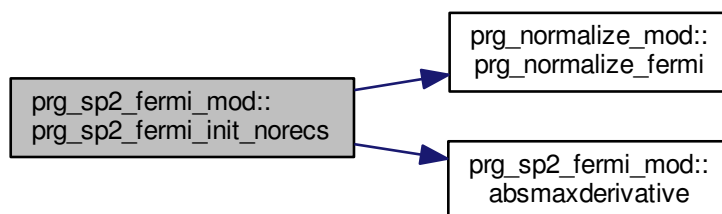
|                    |   |
|--------------------|---|
| <i>h_bml</i>       | Input Hamiltonian matrix.                           |
| <i>nsteps</i>      | Output number of sp2 iterations.                    |
| <i>nocc</i>        | Number of occupied states.                          |
| <i>tscale</i>      | Temperature rescaling factor.                       |
| <i>threshold</i>   | Threshold for multiplication.                       |
| <i>occErrLimit</i> | Occupation error limit.                             |
| <i>traceLimit</i>  | Trace limit.  |
| <i>x_bml</i>       | Output prg_initial matrix.                          |
| <i>mu</i>          | Shifted chemical potential                          |
| <i>beta</i>        | Input guess and output inverse temperature.         |
| <i>h1</i>          | Output temperature-scaled minimum gershgorin bound. |
| <i>hN</i>          | Output temperature-scaled maximum gershgorin bound. |
| <i>sgnlist</i>     | SP2 sequence  |
| <i>verbose</i>     | Optional parameter for verbosity.                   |

Calculate Gershgorin bounds and rescale

Determine sequence branching first time through

Definition at line 201 of file prg\_sp2\_fermi\_mod.F90.

Here is the call graph for this function:



9.24.2.6 `real(dp) function, public prg_sp2_fermi_mod::sp2_entropy_ts ( type(bml_matrix_t), intent(in) D0_bml, real(dp), dimension(*), intent(in) GG, real(dp), dimension(*), intent(in) ee )`

Test SP2 entropy. Get the entropy contribution TS to the total free energy.

## Parameters

|               |                     |
|---------------|---------------------|
| <i>D0_bml</i> | BML matrix          |
| <i>GG</i>     | Entropy function    |
| <i>ee</i>     | 1D mesh             |
| <i>TS</i>     | Energy contribution |

Definition at line 538 of file prg\_sp2\_fermi\_mod.F90.

9.24.2.7 `real(dp)` function, public `prg_sp2_fermi_mod::sp2_inverse ( real(dp), intent(in) f, real(dp), intent(in) mu, real(dp), intent(in) h1, real(dp), intent(in) hN, integer, intent(in) nsteps, integer, dimension(:), intent(in) sgnlist )`

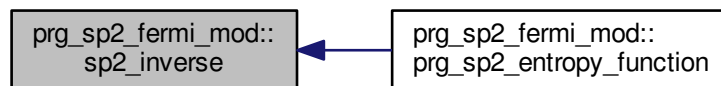
Calculate the SP2 inverse.

#### Parameters

|                |                                 |
|----------------|---------------------------------|
| <i>f</i>       | Occupation factor               |
| <i>mu</i>      | Shifted chemical potential      |
| <i>h1</i>      | Minimum scaled Gershgorin bound |
| <i>hN</i>      | Maximum scaled Gershgorin bound |
| <i>nsteps</i>  | Numbers of SP2 iterations       |
| <i>sgnlist</i> | SP2 sequence                    |
| <i>ee</i>      | Energy value                    |

Definition at line 590 of file prg\_sp2\_fermi\_mod.F90.

Here is the caller graph for this function:



### 9.24.3 Variable Documentation

9.24.3.1 integer, parameter `prg_sp2_fermi_mod::dp = kind(1.0d0)` [`private`]

Definition at line 19 of file prg\_sp2\_fermi\_mod.F90.

## 9.25 prg\_sp2\_mod Module Reference

The SP2 module.

## Functions/Subroutines

- subroutine, public [prg\\_sp2\\_basic](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)  
*Calculates the density matrix from a Hamiltonian matrix by purification. The method implemented here is the very first version of the SP2 method.*
- subroutine, public [prg\\_sp2\\_alg2](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)
- subroutine, public [prg\\_sp2\\_alg2\\_genseq](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, pp, icount, vv, verbose)
- subroutine, public [prg\\_sp2\\_alg2\\_seq](#) (h\_bml, rho\_bml, threshold, pp, icount, vv, verbose)
- subroutine, public [prg\\_prg\\_sp2\\_alg2\\_seq\\_inplace](#) (rho\_bml, threshold, pp, icount, vv, mineval, maxeval, verbose)
- subroutine, public [prg\\_sp2\\_alg1](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)
- subroutine, public [prg\\_sp2\\_alg1\\_genseq](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, pp, icount, vv)
- subroutine, public [prg\\_sp2\\_alg1\\_seq](#) (h\_bml, rho\_bml, threshold, pp, icount, vv)
- subroutine, public [prg\\_prg\\_sp2\\_alg1\\_seq\\_inplace](#) (rho\_bml, threshold, pp, icount, vv, mineval, maxeval)
- subroutine, public [prg\\_sp2\\_submatrix](#) (ham\_bml, rho\_bml, threshold, pp, icount, vv, mineval, maxeval, core\_↵\_size)  
*Perform SP2 algorithm using sequence and calculate norm for a submatrix.*
- subroutine, public [prg\\_sp2\\_submatrix\\_inplace](#) (rho\_bml, threshold, pp, icount, vv, mineval, maxeval, core\_↵\_size)

## Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.25.1 Detailed Description

The SP2 module.

#### Author

S. Mniszewski ([smn@lanl.gov](mailto:smn@lanl.gov))

This subroutine implements Niklasson's SP2 density matrix purification algorithm.

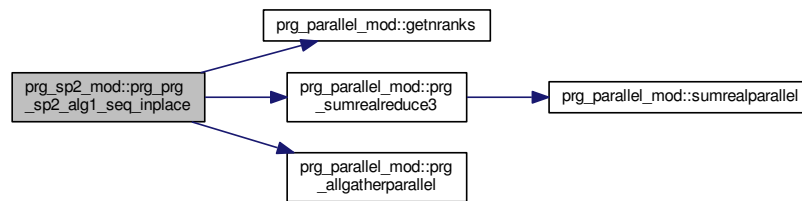
### 9.25.2 Function/Subroutine Documentation

- 9.25.2.1 subroutine, public prg\_sp2\_mod::prg\_prg\_sp2\_alg1\_seq\_inplace ( type(bml\_matrix\_t), intent(inout) rho\_bml, real(dp), intent(in) threshold, integer, dimension(:), intent(inout) pp, integer, intent(inout) icount, real(dp), dimension(:), intent(inout) vv, real(dp), intent(in) mineval, real(dp), intent(in) maxeval )

Definition at line 971 of file prg\_sp2\_mod.F90.



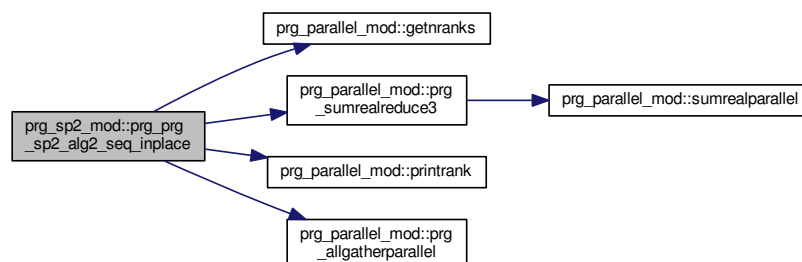
Here is the call graph for this function:



9.25.2.2 subroutine, public `prg_sp2_mod::prg_prg_sp2_alg2_seq_inplace` ( `type(bml_matrix_t)`, `intent(inout) rho_bml`, `real(dp)`, `intent(in) threshold`, `integer, dimension(:)`, `intent(inout) pp`, `integer, intent(inout) icount`, `real(dp)`, `dimension(:)`, `intent(inout) vv`, `real(dp)`, `intent(in)`, optional `mineval`, `real(dp)`, `intent(in)`, optional `maxeval`, `integer, intent(in)`, optional `verbose` )

Definition at line 528 of file `prg_sp2_mod.F90`.

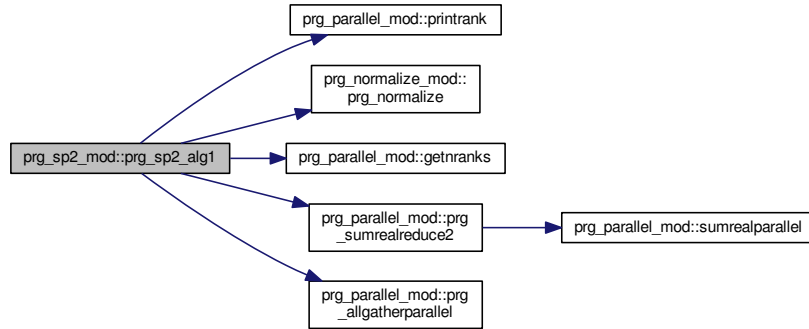
Here is the call graph for this function:



9.25.2.3 subroutine, public `prg_sp2_mod::prg_sp2_alg1` ( `type(bml_matrix_t)`, `intent(in) h_bml`, `type(bml_matrix_t)`, `intent(inout) rho_bml`, `real(dp)`, `intent(in) threshold`, `real(dp)`, `intent(in) bndfil`, `integer, intent(in) minsp2iter`, `integer, intent(in) maxsp2iter`, `character(len=*)`, `intent(in) sp2conv`, `real(dp)`, `intent(in) idemtol`, `integer, intent(in)`, optional `verbose` )

Definition at line 624 of file `prg_sp2_mod.F90`.

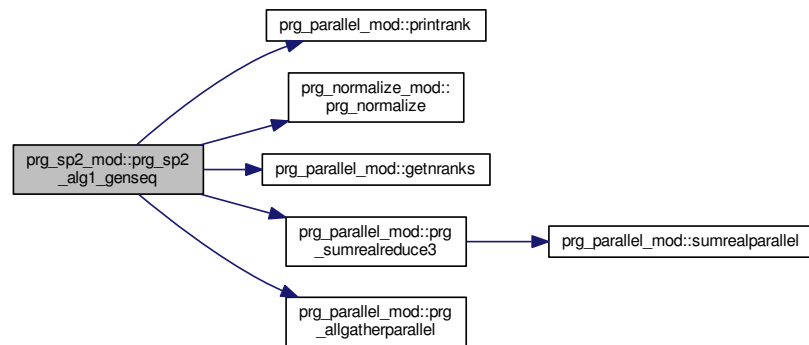
Here is the call graph for this function:



9.25.2.4 subroutine, public `prg_sp2_mod::prg_sp2_alg1_genseq` ( `type(bml_matrix_t)`, `intent(in) h_bml`, `type(bml_matrix_t)`, `intent(inout) rho_bml`, `real(dp)`, `intent(in) threshold`, `real(dp)`, `intent(in) bndfil`, `integer`, `intent(in) minsp2iter`, `integer`, `intent(in) maxsp2iter`, `character(len=*)`, `intent(in) sp2conv`, `real(dp)`, `intent(in) idemtol`, `integer`, `dimension(:)`, `intent(inout) pp`, `integer`, `intent(inout) icount`, `real(dp)`, `dimension(:)`, `intent(inout) vv` )

Definition at line 751 of file `prg_sp2_mod.F90`.

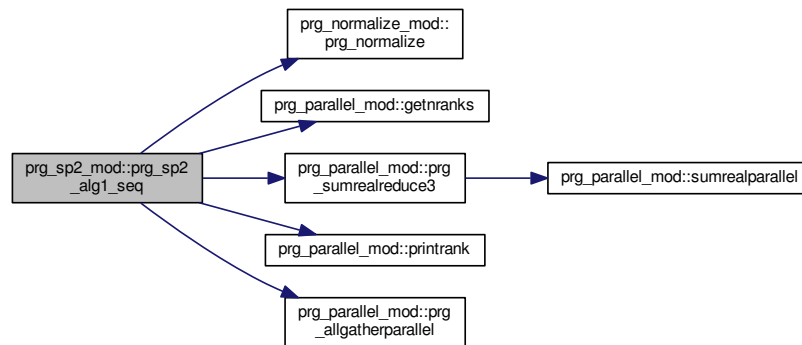
Here is the call graph for this function:



9.25.2.5 subroutine, public `prg_sp2_mod::prg_sp2_alg1_seq` ( `type(bml_matrix_t)`, `intent(in) h_bml`, `type(bml_matrix_t)`, `intent(inout) rho_bml`, `real(dp)`, `intent(in) threshold`, `integer`, `dimension(:)`, `intent(inout) pp`, `integer`, `intent(inout) icount`, `real(dp)`, `dimension(:)`, `intent(inout) vv` )

Definition at line 880 of file `prg_sp2_mod.F90`.

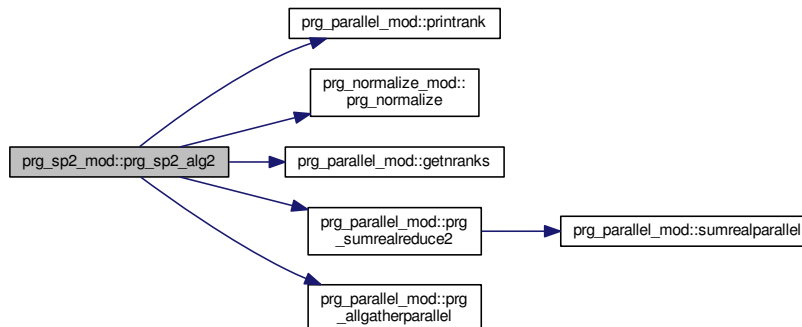
Here is the call graph for this function:



9.25.2.6 subroutine, public `prg_sp2_mod::prg_sp2_alg2` ( `type(bml_matrix_t)`, intent(in) `h_bml`, `type(bml_matrix_t)`, intent(inout) `rho_bml`, `real(dp)`, intent(in) `threshold`, `real(dp)`, intent(in) `bndfil`, integer, intent(in) `minsp2iter`, integer, intent(in) `maxsp2iter`, character(len=\*), intent(in) `sp2conv`, `real(dp)`, intent(in) `idemtol`, integer, intent(in), optional `verbose` )

Definition at line 153 of file `prg_sp2_mod.F90`.

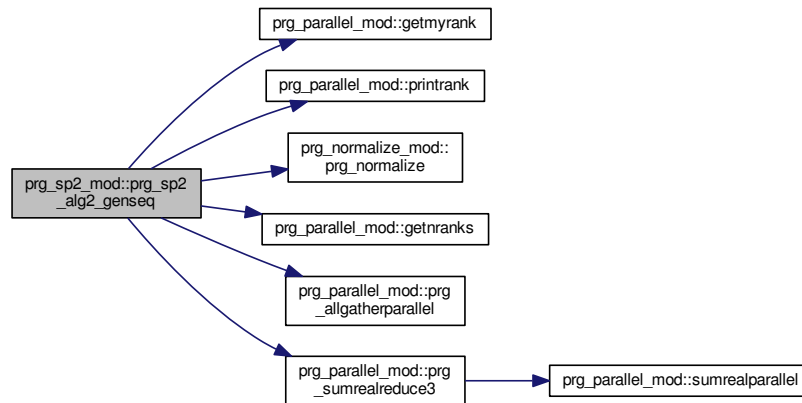
Here is the call graph for this function:



9.25.2.7 subroutine, public `prg_sp2_mod::prg_sp2_alg2_genseq` ( `type(bml_matrix_t)`, intent(in) `h_bml`, `type(bml_matrix_t)`, intent(inout) `rho_bml`, `real(dp)`, intent(in) `threshold`, `real(dp)`, intent(in) `bndfil`, integer, intent(in) `minsp2iter`, integer, intent(in) `maxsp2iter`, character(len=\*), intent(in) `sp2conv`, `real(dp)`, intent(in) `idemtol`, integer, dimension(:), intent(inout) `pp`, integer, intent(inout) `icount`, `real(dp)`, dimension(:), intent(inout) `vv`, integer, intent(in), optional `verbose` )

Definition at line 285 of file `prg_sp2_mod.F90`.

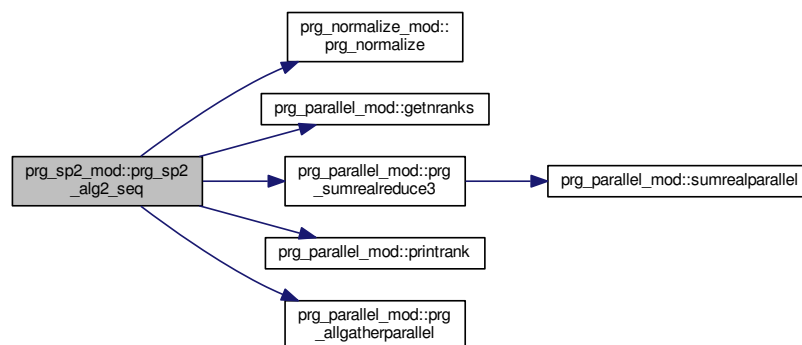
Here is the call graph for this function:



9.25.2.8 subroutine, public `prg_sp2_mod::prg_sp2_alg2_seq` ( `type(bml_matrix_t)`, `intent(in) h_bml`, `type(bml_matrix_t)`, `intent(inout) rho_bml`, `real(dp)`, `intent(in) threshold`, `integer`, `dimension(:)`, `intent(inout) pp`, `integer`, `intent(inout) icount`, `real(dp)`, `dimension(:)`, `intent(inout) vv`, `integer`, `intent(in)`, optional `verbose` )

Definition at line 432 of file `prg_sp2_mod.F90`.

Here is the call graph for this function:



9.25.2.9 subroutine, public `prg_sp2_mod::prg_sp2_basic` ( `type(bml_matrix_t)`, `intent(in) h_bml`, `type(bml_matrix_t)`, `intent(inout) rho_bml`, `real(dp) threshold`, `real(dp) bndfil`, `integer minsp2iter`, `integer maxsp2iter`, `character(len=*)`, `intent(in) sp2conv`, `real(dp) idemt看`, `integer verbose` )

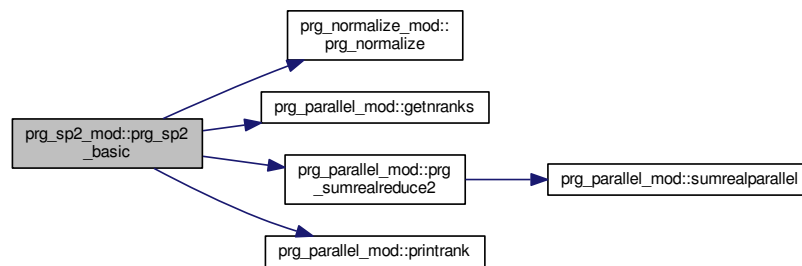
Calculates the density matrix from a Hamiltonian matrix by purification. The method implemented here is the very first version of the SP2 method.

## Parameters

|                   |                                     |
|-------------------|-------------------------------------|
| <i>h_bml</i>      | Input Hamiltonian matrix            |
| <i>rho_bml</i>    | Output density matrix               |
| <i>threshold</i>  | Threshold for sparse matrix algebra |
| <i>bndfil</i>     | Bond                                |
| <i>minsp2iter</i> | Minimum sp2 iterations              |
| <i>maxsp2iter</i> | Maximum SP2 iterations              |
| <i>sp2conv</i>    | Convergence type                    |
| <i>idemtol</i>    | Idempotency tolerance               |
| <i>verbose</i>    | A verbosity level                   |

Definition at line 52 of file prg\_sp2\_mod.F90.

Here is the call graph for this function:



**9.25.2.10** subroutine, public prg\_sp2\_mod::prg\_sp2\_submatrix ( type(bml\_matrix\_t), intent(in) *ham\_bml*, type(bml\_matrix\_t), intent(inout) *rho\_bml*, real(dp), intent(in) *threshold*, integer, dimension(:), intent(in) *pp*, integer, intent(in) *icount*, real(dp), dimension(:), intent(inout) *vv*, real(dp), intent(in) *mineval*, real(dp), intent(in) *maxeval*, integer, intent(in) *core\_size* )

Perform SP2 algorithm using sequence and calculate norm for a submatrix.

## Parameters

|                  |   |
|------------------|---|
| <i>rho_bml</i>   | Input Hamiltonian/Output density matrix     |
| <i>threshold</i> | Threshold for sparse matrix algebra         |
| <i>pp</i>        | Vector containing sequence of 0s and 1s     |
| <i>icount</i>    | Sequence count                              |
| <i>vv</i>        | Vector of sum of squares per iteration      |
| <i>mineval</i>   | Min value used for normalization (optional) |
| <i>maxeval</i>   | Max value used for normalization (optional) |
| <i>core_size</i> | Number of core rows                         |

Definition at line 1061 of file prg\_sp2\_mod.F90.

9.25.2.11 subroutine, public prg\_sp2\_mod::prg\_sp2\_submatrix\_inplace ( type(bml\_matrix\_t), intent(inout) rho\_bml, real(dp), intent(in) threshold, integer, dimension(:), intent(inout) pp, integer, intent(inout) icount, real(dp), dimension(:), intent(inout) vv, real(dp), intent(in) mineval, real(dp), intent(in) maxeval, integer, intent(in) core\_size )

Definition at line 1130 of file prg\_sp2\_mod.F90.

Here is the caller graph for this function:



### 9.25.3 Variable Documentation

9.25.3.1 integer, parameter prg\_sp2\_mod::dp = kind(1.0d0) [private]

Definition at line 21 of file prg\_sp2\_mod.F90.

## 9.26 prg\_sp2parser\_mod Module Reference

SP2 parser.

### Data Types

- type [sp2data\\_type](#)  
*General SP2 solver type.*

### Functions/Subroutines

- subroutine, public [prg\\_parse\\_sp2](#) (sp2data, filename)  
*The parser for SP2 solver.*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.26.1 Detailed Description

SP2 parser.

This module is used to parse all the input variables for the SP2 method electronic structure solver. Adding a new input keyword to the parser:

- If the variable is real, we have to increase nkey\_re.
- Add the keyword (character type) in the keyvector\_re vector.
- Add a default value (real type) in the valvector\_re.
- Define a new variable and pass the value through valvector\_re(num) where num is the position of the new keyword in the vector.

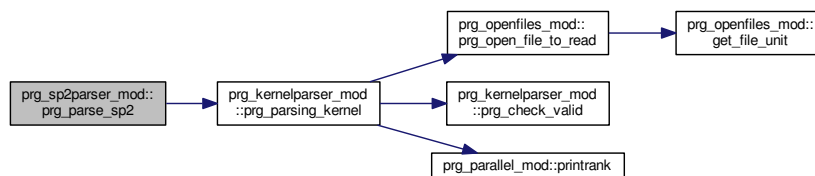
### 9.26.2 Function/Subroutine Documentation

9.26.2.1 subroutine, public prg\_sp2parser\_mod::prg\_parse\_sp2 ( type(sp2data\_type), intent(inout) sp2data, character(len=\*) filename )

The parser for SP2 solver.

Definition at line 50 of file prg\_sp2parser\_mod.F90.

Here is the call graph for this function:



### 9.26.3 Variable Documentation

9.26.3.1 integer, parameter prg\_sp2parser\_mod::dp = kind(1.0d0) [private]

Definition at line 22 of file prg\_sp2parser\_mod.F90.

## 9.27 prg\_subgraphloop\_mod Module Reference

The subgraphloop module.

## Functions/Subroutines

- subroutine, public [prg\\_subgraphsp2loop](#) (h\_bml, g\_bml, rho\_bml, gp, threshold)
- subroutine, public [prg\\_collectmatrixfromparts](#) (gp, rho\_bml)  
*Collect distributed parts into same matrix.*
- subroutine, public [prg\\_balanceparts](#) (gp)
- subroutine, public [prg\\_partordering](#) (gp)  
*Set row ordering bases on parts.*
- subroutine, public [prg\\_getgrouppartitionhalosfromgraph](#) (gp, g\_bml, hnode, djflag)  
*Get core+halo indeces for all partitions only using the graph.*
- subroutine, public [prg\\_getpartitionhalosfromgraph](#) (gp, g\_bml, djflag)  
*Get core+halo indeces for all partitions only using the graph.*

## Variables

- integer, parameter [dp](#) = kind(1.0d0)

### 9.27.1 Detailed Description

The subgraphloop module.

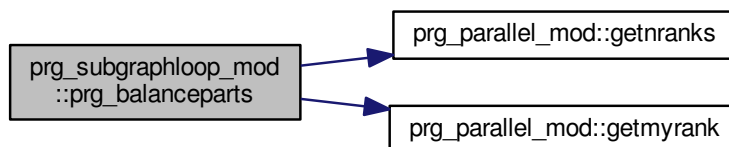
### 9.27.2 Function/Subroutine Documentation

9.27.2.1 subroutine, public `prg_subgraphloop_mod::prg_balanceparts` ( type (graph\_partitioning\_t), intent(inout) *gp* )

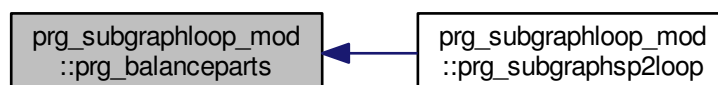
Renumber parts Handle unbalanced numbers of parts.

Definition at line 165 of file `prg_subgraphloop_mod.F90`.

Here is the call graph for this function:



Here is the caller graph for this function:





9.27.2.2 subroutine, public prg\_subgraphloop\_mod::prg\_collectmatrixfromparts ( type (graph\_partitioning\_t), intent(inout) *gp*, type (bml\_matrix\_t), intent(inout) *rho\_bml* )

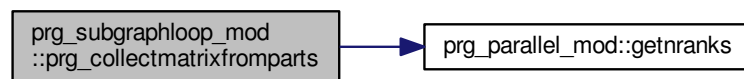
Collect distributed parts into same matrix.

#### Parameters

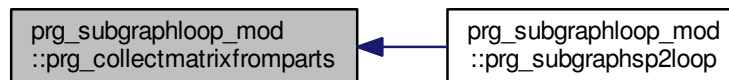
|                |                             |
|----------------|-----------------------------|
| <i>gp</i>      | Graph partitioning          |
| <i>rho_bml</i> | Matrix to be collected into |

Definition at line 133 of file prg\_subgraphloop\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.27.2.3 subroutine, public prg\_subgraphloop\_mod::prg\_getgrouppartitionhalosfromgraph ( type (graph\_partitioning\_t), intent(inout) *gp*, type (bml\_matrix\_t), intent(in) *g\_bml*, integer, dimension(\*), intent(in) *hnode*, logical, intent(in) *djflag* )

Get core+halo indeces for all partitions only using the graph.

#### Parameters

|              |                               |
|--------------|-------------------------------|
| <i>gp</i>    | Graph partitioning            |
| <i>g_bml</i> | Graph                         |
| <i>hnode</i> | Group start indeces           |
| <i>djflg</i> | Double jump flag (true/false) |

Determine halo elements for each subgraph

Definition at line 292 of file prg\_subgraphloop\_mod.F90.

9.27.2.4 subroutine, public prg\_subgraphloop\_mod::prg\_getpartitionhalosfromgraph ( type (graph\_partitioning\_t),  
intent(inout) *gp*, type (bml\_matrix\_t), intent(in) *g\_bml*, logical, intent(in) *djflag* )

Get core+halo indeces for all partitions only using the graph.

#### Parameters

|              |                               |
|--------------|-------------------------------|
| <i>gp</i>    | Graph partitioning            |
| <i>g_bml</i> | Graph                         |
| <i>djflg</i> | Double jump flag (true/false) |

Determine halo elements for each subgraph

Definition at line 337 of file prg\_subgraphloop\_mod.F90.

9.27.2.5 subroutine, public prg\_subgraphloop\_mod::prg\_partordering ( type (graph\_partitioning\_t), intent(inout) *gp* )

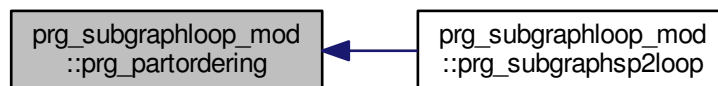
Set row ordering bases on parts.

#### Parameters

|           |                    |
|-----------|--------------------|
| <i>gp</i> | Graph partitioning |
|-----------|--------------------|

Definition at line 263 of file prg\_subgraphloop\_mod.F90.

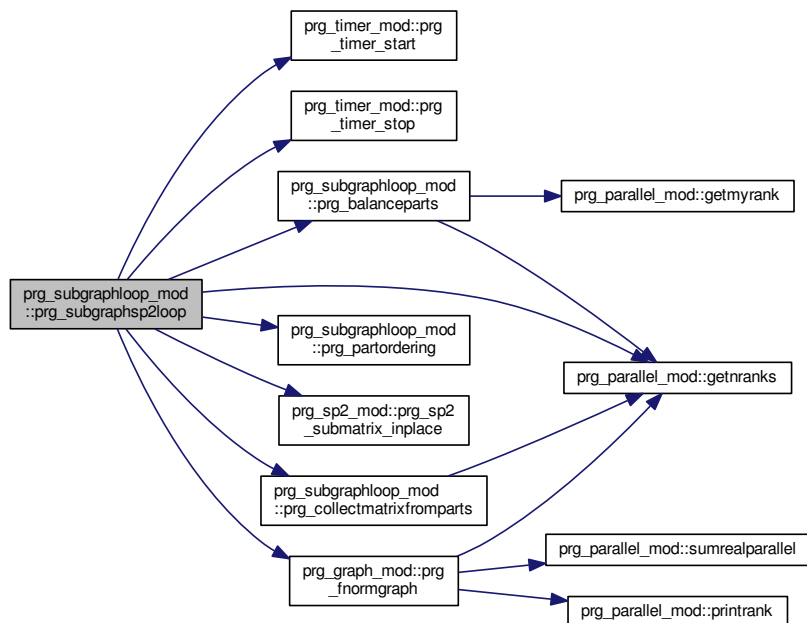
Here is the caller graph for this function:



9.27.2.6 subroutine, public prg\_subgraphloop\_mod::prg\_subgraphsp2loop ( type (bml\_matrix\_t), intent(in) *h\_bml*, type (bml\_matrix\_t), intent(in) *g\_bml*, type (bml\_matrix\_t), intent(inout) *rho\_bml*, type (graph\_partitioning\_t),  
intent(inout) *gp*, real(dp), intent(in) *threshold* )

Definition at line 37 of file prg\_subgraphloop\_mod.F90.

Here is the call graph for this function:



### 9.27.3 Variable Documentation

9.27.3.1 integer, parameter `prg_subgraphloop_mod::dp = kind(1.0d0)` [private]

Definition at line 18 of file `prg_subgraphloop_mod.F90`.

## 9.28 prg\_syrotation\_mod Module Reference

A module to rotate the coordinates of a sybsystem in chemical systems.

### Data Types

- type `rotation_type`  
*Rotation type.*

### Functions/Subroutines

- subroutine, public `prg_parse_rotation` (rot, filename)  
*The parser for rotation.*
- subroutine, public `prg_rotate` (rot, r, verbose)  
*Rotation routine.*

## Variables

- integer, parameter `dp = kind(1.0d0)`

### 9.28.1 Detailed Description

A module to rotate the coordinates of a sybssystem in chemical systems.

It works by specifying two orientations and a rotation point.

#### Author

C. F. A. Negre ([cnegre@lanl.gov](mailto:cnegre@lanl.gov))

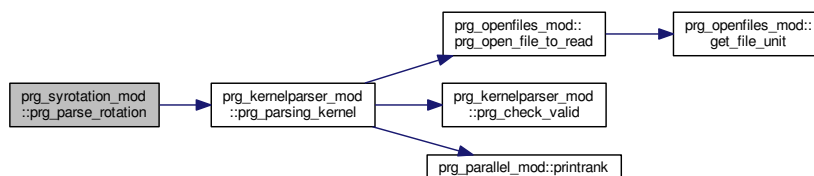
### 9.28.2 Function/Subroutine Documentation

**9.28.2.1** subroutine, public `prg_syrotation_mod::prg_parse_rotation ( type(rotation_type), intent(inout) rot, character(len=*) filename )`

The parser for rotation.

Definition at line 49 of file `prg_syrotation_mod.F90`.

Here is the call graph for this function:



**9.28.2.2** subroutine, public `prg_syrotation_mod::prg_rotate ( type(rotation_type), intent(in) rot, real(dp), dimension(:,:), intent(inout) r, integer, intent(in) verbose )`

Rotation routine.

It works by indicating the orientations ( $v1$  and  $v1$ ) and a rotation center. The orientation can be passed either directly by setting  $v1$  and  $v2$  or by indicating two points  $pQ1$  and  $pQ2$ . Orientation can also be specified with an atom position if  $patom1$  and  $patom2$  indices are not zero this atoms are used to determine the initial and final orientation.

#### Parameters

|                |                           |
|----------------|---------------------------|
| <i>rot</i>     | Rotation type             |
| <i>r</i>       | Coordinates to be rotated |
| <i>verbose</i> | Verbosity level           |

Example:

```
rot%patom1 = 4
rot%patom2 = 0
rot%catom2 = 6
rot%v2 = 0.0 ; rot%v2(1) = 1
call prg_rotate(rot,r)
```

The latter will orient the system such that atom 4 points to the (1,0,0) direction.

Definition at line 142 of file prg\_syrotation\_mod.F90.

### 9.28.3 Variable Documentation

9.28.3.1 integer, parameter prg\_syrotation\_mod::dp = kind(1.0d0) [private]

Definition at line 14 of file prg\_syrotation\_mod.F90.

## 9.29 prg\_system\_mod Module Reference

A module to read and handle chemical systems.

### Data Types

- type [estruct\\_type](#)  
*Electronic structure type.*
- type [system\\_type](#)  
*System type.*

### Functions/Subroutines

- subroutine, public [prg\\_get\\_nameandext](#) (fullfilename, filename, ext)  
*Get the name and extension of a file.*
- subroutine, public [prg\\_parse\\_system](#) (system, filename, extin)  
*The parser for the chemical system.*
- subroutine, public [prg\\_write\\_system](#) (system, filename, extension)  
*Write system in .xyz, .dat or pdb file.*
- subroutine, public [prg\\_write\\_trajectory](#) (system, iter, each, prg\_deltat, filename, extension)  
*Write trajectory in .xyz, .dat or pdb file.*
- subroutine, public [prg\\_write\\_trajectoryandproperty](#) (system, iter, each, prg\_deltat, scalarprop, filename, extension)  
*Write trajectory and atomic properties. Only pdb file.*
- subroutine, public [prg\\_make\\_random\\_system](#) (system, nats, seed, lx, ly, lz)  
*Make random Xx system.*
- subroutine [prg\\_parameters\\_to\\_vectors](#) (abc\_angles, lattice\_vector)  
*Transforms the lattice parameters into lattice vectors.*
- subroutine [prg\\_vectors\\_to\\_parameters](#) (lattice\_vector, abc\_angles)

- Transforms the lattice vectors into lattice parameters.*
- subroutine, public [prg\\_get\\_origin](#) (coords, origin)
  - Get the origin of the coordinates.*
- subroutine, public [prg\\_get\\_distancematrix](#) (coords, dmat)
  - Get the distance matrix.*
- subroutine, public [prg\\_translateandfoldtobox](#) (coords, lattice\_vectors, origin, verbose)
  - Translate and fold to box.*
- subroutine, public [prg\\_centeratbox](#) (coords, lattice\_vectors, verbose)
  - Translate geometric center to the center of the box.*
- subroutine, public [prg\\_wraparound](#) (coords, lattice\_vectors, index, verbose)
  - Wrap around atom i using pbc.*
- subroutine, public [prg\\_translatetogeomcandfoldtobox](#) (coords, lattice\_vectors, origin)
  - Translate to geometric center.*
- subroutine, public [prg\\_replicate](#) (coords, symbols, lattice\_vectors, nx, ny, nz)
  - Extend/replicate system along lattice vectors.*
- subroutine, public [prg\\_get\\_recip\\_vects](#) (lattice\_vectors, recip\_vectors, volr, volk)
  - Get the volume of the cell and the reciprocal vectors: This subroutine computes:*
- subroutine, public [prg\\_get\\_dihedral](#) (coords, id1, id2, id3, id4, dihedral)
  - Get the dihedral angle given four atomic positions.*
- subroutine, public [prg\\_get\\_covgraph](#) (sy, nnStructMindist, nnStruct, nrrnnstruct, bml\_type, factor, gcov\_bml, mdimin, verbose)
  - Get the covalency graph in bml format.*
- subroutine [prg\\_get\\_covgraph\\_int](#) (sy, nnStructMindist, nnStruct, nrrnnstruct, bml\_type, factor, gcov\_bml, mdimin, verbose)
  - Get the covanlency graph.*
- subroutine, public [prg\\_get\\_subsystem](#) (sy, lsize, indices, sbsy, verbose)
  - Get a subsystem out of the total system.*
- subroutine, public [prg\\_destroy\\_subsystems](#) (sbsy, verbose)
  - Destroy allocated subsystem.*
- subroutine, public [prg\\_molpartition](#) (sy, npart, nnStructMindist, nnStruct, nrrnnstruct, hetatm, gp, verbose)
  - Partition by molecule.*
- subroutine, public [prg\\_get\\_partial\\_atomgraph](#) (rho\_bml, hindex, gch\_bml, threshold, verbose)
  - Get partial subgraph based on the Density matrix.*
- subroutine, public [prg\\_collect\\_graph\\_p](#) (rho\_bml, nc, nats, hindex, chindex, graph\_p, threshold, mdimin, verbose)
  - Collect the small graph to build the full graph.*
- subroutine, public [prg\\_merge\\_graph](#) (graph\_p, graph\_h)
  - Get partial subgraph based on the Density matrix.*
- subroutine, public [prg\\_merge\\_graph\\_adj](#) (graph\_p, graph\_h, xadj, adjncy)
  - Get partial subgraph based on the Density matrix.*
- subroutine, public [prg\\_adj2bml](#) (xadj, adjncy, bml\_type, g\_bml)
  - prg\_adj2bml*
- subroutine, public [prg\\_graph2bml](#) (graph, bml\_type, g\_bml)
  - Graph2bml.*
- subroutine, public [prg\\_graph2vector](#) (graph, vector, maxnz)
  - Vectorize graph.*
- subroutine, public [prg\\_vector2graph](#) (vector, graph, maxnz)
  - Back to graph.*
- subroutine, public [prg\\_sortadj](#) (xadj, adjncy)
  - Sort adj NOTE: this might not be needed anymore since the bml\_get\_adj routine is sorting the values.*

## Variables

- integer, parameter `dp` = kind(1.0d0)

### 9.29.1 Detailed Description

A module to read and handle chemical systems.

This module will be used to build and handle a molecular system.

#### Author

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### 9.29.2 Function/Subroutine Documentation

9.29.2.1 subroutine, public `prg_system_mod::prg_adj2bml` ( integer, dimension(:), intent(in) *xadj*, integer, dimension(:), intent(in) *adjncy*, character(20), intent(in) *bml\_type*, type(bml\_matrix\_t), intent(inout) *g\_bml* )

`prg_adj2bml`

#### Parameters

|                 |  |
|-----------------|--|
| <i>xadj</i>     | CSR start values for the adjacency matrix. |
| <i>adjncy</i>   | CSR positions of adjacency matrix.         |
| <i>bml_type</i> | bml format.                                |
| <i>g_bml</i>    | graph in bml format.                       |

Definition at line 2299 of file `prg_system_mod.F90`.

9.29.2.2 subroutine, public `prg_system_mod::prg_centeratbox` ( real(dp), dimension(:,:), intent(inout), allocatable *coords*, real(dp), dimension(:,:), intent(in) *lattice\_vectors*, integer, intent(in), optional *verbose* )

Translate geometric center to the center of the box.

#### Parameters

|                        |   |
|------------------------|---|
| <i>coords</i>          | Coordinates of the system (see <a href="#">system_type</a> ). |
| <i>lattice_vectors</i> | System lattice vectors.                                       |
| <i>verbose</i>         | Verbosity level.  |

Definition at line 1293 of file `prg_system_mod.F90`.

9.29.2.3 subroutine, public prg\_system\_mod::prg\_collect\_graph\_p ( type(bml\_matrix\_t), intent(in) rho\_bml, integer, intent(in) nc, integer, intent(in) nats, integer, dimension(:,:), intent(in) hindex, integer, dimension(:), intent(in) chindex, integer, dimension(:,:), intent(inout), allocatable graph\_p, real(dp), intent(in) threshold, integer, intent(in) mdimin, integer, intent(in), optional verbose )

Collect the small graph to build the full graph.

#### Parameters

|           |   |
|-----------|---|
| rho_bml   | Density matix in bml format.                              |
| nc        | Number of core atoms.                                     |
| nats      | Number of atoms.  |
| hindex    | Hindex for the small part (see haindex)                   |
| chindex   | Core-hallo index for the small part.                      |
| graph_p   | Graph in an "ellpack" format.                             |
| threshold | Threshold to buil the density based atom projected graph. |
| verbose   | Verbosity level.  |

Definition at line 2082 of file prg\_system\_mod.F90.

9.29.2.4 subroutine, public prg\_system\_mod::prg\_destroy\_subsystems ( type(system\_type), intent(inout) sbsy, integer, intent(in), optional verbose )

Destroy allocated subsystem.

This routine will deallocate all the arrays of the structures.

#### Parameters

|    |  |
|----|--|
| sy | System to de deallocated (see <a href="#">system_type</a> ). |
|----|--|

Definition at line 1867 of file prg\_system\_mod.F90.

9.29.2.5 subroutine, public prg\_system\_mod::prg\_get\_covgraph ( type(system\_type), intent(in) sy, real(dp), dimension(:,:), intent(in) nnStructMindist, integer, dimension(:,:), intent(in) nnStruct, integer, dimension(:), intent(in) nrnnstruct, character(20), intent(in) bml\_type, real(dp) factor, type(bml\_matrix\_t), intent(inout) gcov\_bml, integer, intent(in) mdimin, integer, intent(in), optional verbose )

Get the covalency graph in bml format.

This is the graph composed by the covalent bonds (edges) that are determined with the VDW radius.

#### Parameters

|                 |   |
|-----------------|---|
| sy              | System structure (see <a href="#">system_type</a> ).              |
| nnStructMindist | Minimun distance between atoms.                                   |
| nnStruct        | The neighbors J to I within Rcut that are all within the box.     |
| nrnnstruct      | Number of neighbors to I within Rcut that are all within the box. |
| bml_type        | The bml type for constructing the graph.                          |
| gconv_bml       | Covanlency graph in bml format.                                   |
| verbose         | Verbosity level.  |



Definition at line 1582 of file prg\_system\_mod.F90.

9.29.2.6 subroutine, public prg\_system\_mod::prg\_get\_covgraph\_h ( type(system\_type), intent(in) sy, real(dp), dimension(:, :), intent(in) nnStructMindist, integer, dimension(:, :), intent(in) nnStruct, integer, dimension(:, :), intent(in) nnnstruct, real(dp), intent(in) rcut, integer, dimension(:, :), intent(inout), allocatable graph\_h, integer, intent(in) mdimin, integer, intent(in), optional verbose )

Get the covanlency graph.

This is the graph composed by the covalent bonds (edges) that are determined with the VDW radius.

#### Parameters

|                 |   |
|-----------------|---|
| sy              | System structure (see <a href="#">system_type</a> ).              |
| nnStructMindist | Minimun distance between atoms.                                   |
| nnStruct        | The neighbors J to I within Rcut that are all within the box.     |
| nnnstruct       | Number of neighbors to I within Rcut that are all within the box. |
| bml_type        | The bml type for constructing the graph.                          |
| gconv_bml       | Covanlency graph in bml format.                                   |
| verbose         | Verbosity level.  |

Definition at line 1715 of file prg\_system\_mod.F90.

9.29.2.7 subroutine prg\_system\_mod::prg\_get\_covgraph\_int ( type(system\_type), intent(in) sy, real(dp), dimension(:, :), intent(in) nnStructMindist, integer, dimension(:, :), intent(in) nnStruct, integer, dimension(:, :), intent(in) nnnstruct, character(20), intent(in) bml\_type, real(dp) factor, type(bml\_matrix\_t), intent(inout) gcov\_bml, integer, intent(in) mdimin, integer, intent(in), optional verbose ) [private]

Definition at line 1656 of file prg\_system\_mod.F90.

9.29.2.8 subroutine, public prg\_system\_mod::prg\_get\_dihedral ( real(dp), dimension(:, :), intent(in) coords, integer, intent(in) id1, integer, intent(in) id2, integer, intent(in) id3, integer, intent(in) id4, real(dp), intent(out) dihedral )

Get the dihedral angle given four atomic positions.

#### Parameters

|          |                       |
|----------|-----------------------|
| sy       | System structure      |
| id1      | Atom index 1          |
| id2      | Atom index 1          |
| id3      | Atom index 1          |
| id4      | Atom index 1          |
| dihedral | Output dihedral angle |

Definition at line 1526 of file prg\_system\_mod.F90.

9.29.2.9 subroutine, public prg\_system\_mod::prg\_get\_distancematrix ( real(dp), dimension(:,,:), intent(in) *coords*, real(dp), dimension(:,,:), intent(out), allocatable *dmat* )

Get the distance matrix.

#### Parameters

|               |   |
|---------------|---|
| <i>coords</i> | Coordinates of the system (see <a href="#">system_type</a> ). |
| <i>dmat</i>   | Distance matrix (nats x nats).                                |

Definition at line 1219 of file prg\_system\_mod.F90.

9.29.2.10 subroutine, public prg\_system\_mod::prg\_get\_nameandext ( character(30), intent(in) *fullfilename*, character(30), intent(inout) *filename*, character(3), intent(inout) *ext* )

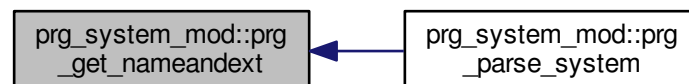
Get the name and extension of a file.

#### Parameters

|                     |                         |
|---------------------|-------------------------|
| <i>fullfilename</i> | Full filename.          |
| <i>filename</i>     | Filename of the system. |
| <i>extension</i>    | Extension of the file.  |

Definition at line 206 of file prg\_system\_mod.F90.

Here is the caller graph for this function:



9.29.2.11 subroutine, public prg\_system\_mod::prg\_get\_origin ( real(dp), dimension(:,,:), intent(in) *coords*, real(dp), dimension(:,,:), intent(inout), allocatable *origin* )

Get the origin of the coordinates.

#### Parameters

|               |   |
|---------------|---|
| <i>coords</i> | Coordinates of the system (see <a href="#">system_type</a> ). |
| <i>origin</i> | (min(x),min(y),min(z)) set as the origin of the system.       |

Definition at line 1183 of file prg\_system\_mod.F90.

**9.29.2.12** subroutine, public prg\_system\_mod::prg\_get\_partial\_atomgraph ( type(bml\_matrix\_t), intent(in) rho\_bml, integer, dimension(:,:), intent(in) hindex, type(bml\_matrix\_t), intent(inout) gch\_bml, real(dp), intent(in) threshold, integer, intent(in), optional verbose )

Get partial subgraph based on the Density matrix.

#### Parameters

|                  |   |
|------------------|---|
| <i>rho_bml</i>   | Density matrix in bml format.                     |
| <i>hindex</i>    | Start and end index for every atom in the system. |
| <i>gch_bml</i>   | Atom based graph in bml format.                   |
| <i>threshold</i> | Threshold value for constructing the graph.       |
| <i>verbose</i>   | Verbosity levels.                                 |

Definition at line 2016 of file prg\_system\_mod.F90.

**9.29.2.13** subroutine, public prg\_system\_mod::prg\_get\_recip\_vects ( real(dp), dimension(:,:), intent(in) lattice\_vectors, real(dp), dimension(:,:), intent(inout), allocatable recip\_vectors, real(dp), intent(inout) volr, real(dp), intent(inout) volk )

Get the volume of the cell and the reciprocal vectors: This subroutine computes:

- $b_1 = \frac{1}{V_c} a_1 \times a_2$
- $b_2 = \frac{1}{V_c} a_2 \times a_3$
- $b_3 = \frac{1}{V_c} a_3 \times a_1$
- $V_c = ||a_1 \cdot (a_2 \times a_3)||$
- $V_{BZ} = ||b_1 \cdot (b_2 \times b_3)||$

#### Parameters

|                        |                                   |
|------------------------|-----------------------------------|
| <i>lattice_vectors</i> | Lattice vectors for the system.   |
| <i>recip_vectors</i>   | Reciprocal vectors of the system. |
| <i>volr</i>            | Volume of the cell.               |
| <i>volk</i>            | Volume of the reciprocal cell.    |

Definition at line 1477 of file prg\_system\_mod.F90.

**9.29.2.14** subroutine, public prg\_system\_mod::prg\_get\_subsystem ( type(system\_type), intent(in) sy, integer, intent(in) lsize, integer, dimension(:), intent(in) indices, type(system\_type), intent(inout) sbsy, integer, intent(in), optional verbose )

Get a subsystem out of the total system.

This will get a subsystem from the total system guided by a partition.

## Parameters

|                |  |
|----------------|--|
| <i>sy</i>      | System structure (see <a href="#">system_type</a> ). |
| <i>lsize</i>   | Core+Halo subsystem size.                            |
| <i>indices</i> | Partition indices.                                   |
| <i>sbsy</i>    | Subsystem to be extracted.                           |

Definition at line 1780 of file prg\_system\_mod.F90.

9.29.2.15 subroutine, public prg\_system\_mod::prg\_graph2bml ( integer, dimension(:, :), intent(inout), allocatable *graph*, character(20), intent(in) *bml\_type*, type(bml\_matrix\_t), intent(inout) *g\_bml* )

Graph2bml.

## Parameters

|                 |  |
|-----------------|--|
| <i>graph</i>    | Atom based graph in "ellpack" like format.   |
| <i>bml_type</i> | Bml type (usually ellpack for graph storage) |
| <i>g_bml</i>    | Graph in bml format.                         |

Definition at line 2333 of file prg\_system\_mod.F90.

9.29.2.16 subroutine, public prg\_system\_mod::prg\_graph2vector ( integer, dimension(:, :), intent(inout) *graph*, integer, dimension(:), allocatable *vector*, integer *maxnz* )

Vectorize graph.

## Parameters

|               |                            |
|---------------|----------------------------|
| <i>graph</i>  | Ellpack graph.             |
| <i>vector</i> | Vector to store the graph. |

Definition at line 2376 of file prg\_system\_mod.F90.

9.29.2.17 subroutine, public prg\_system\_mod::prg\_make\_random\_system ( type(system\_type), intent(out) *system*, integer *nats*, integer *seed*, real(dp) *lx*, real(dp) *ly*, real(dp) *lz* )

Make random Xx system.

## Parameters

|               |   |
|---------------|---|
| <i>system</i> | System to be constructed.               |
| <i>nats</i>   | Number of atoms.                        |
| <i>lx</i>     | length of the box for the x coordinate. |
| <i>ly</i>     | length of the box for the y coordinate. |
| <i>lz</i>     | length of the box for the z coordinate. |

Definition at line 1059 of file prg\_system\_mod.F90.

9.29.2.18 subroutine, public prg\_system\_mod::prg\_merge\_graph ( integer, dimension(:,,:), intent(inout) *graph\_p*, integer, dimension(:,,:), intent(inout) *graph\_h* )

Get partial subgraph based on the Density matrix.

#### Parameters

|   |   |
|---|---|
| <i>graph</i> <sub>←→</sub><br><i>_p</i> | Density matrix based graph in bml format.     |
| <i>graph</i> <sub>←→</sub><br><i>_h</i> | Hamiltonian matrix based graph in bml format. |

Definition at line 2174 of file prg\_system\_mod.F90.

9.29.2.19 subroutine, public prg\_system\_mod::prg\_merge\_graph\_adj ( integer, dimension(:,,:), intent(inout), allocatable *graph\_p*, integer, dimension(:,,:), intent(inout), allocatable *graph\_h*, integer, dimension(:), intent(inout), allocatable *xadj*, integer, dimension(:), intent(inout), allocatable *adjncy* )

Get partial subgraph based on the Density matrix.

#### Parameters

|   |  |
|---|--|
| <i>graph</i> <sub>←→</sub><br><i>_p</i> | Density matrix based graph in "ellpack type format".     |
| <i>graph</i> <sub>←→</sub><br><i>_h</i> | Hamiltonian matrix based graph in "ellpack type format". |
| <i>xadj</i>                             | CSR start values for the adjacency matrix.               |
| <i>adjncy</i>                           | CSR positions of adjacency matrix.                       |

Definition at line 2225 of file prg\_system\_mod.F90.

9.29.2.20 subroutine, public prg\_system\_mod::prg\_molpartition ( type(system\_type), intent(in) *sy*, integer, intent(inout) *npart*, real(dp), dimension(:,,:), intent(in) *nnStructMindist*, integer, dimension(:,,:), intent(in) *nnStruct*, integer, dimension(:), intent(in) *nrnnstruct*, character(2), intent(in) *hetatm*, type(graph\_partitioning\_t), intent(inout) *gp*, integer, intent(inout), optional *verbose* )

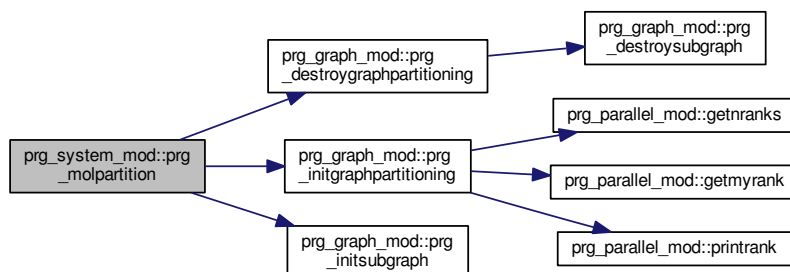
Partition by molecule.

#### Parameters

|                        |   |
|------------------------|---|
| <i>sy</i>              | System structure.   |
| <i>npart</i>           | Number of parts.  |
| <i>nnStructMindist</i> | Minimum distance between neighbors.                               |
| <i>nnStruct</i>        | The neighbors J to I within Rcut that are all within the box.     |
| <i>nrnnstruct</i>      | Number of neighbors to I within Rcut that are all within the box. |
| <i>hetatm</i>          | Atom to be taken as the "center" of the by molecule partition.    |
| <i>gp</i>              | Graph partition structure.  |
| <i>verbose</i>         | Verbosity level.  |

Definition at line 1929 of file prg\_system\_mod.F90.

Here is the call graph for this function:



9.29.2.21 subroutine `prg_system_mod::prg_parameters_to_vectors` ( `real(dp)`, `dimension(2,3)`, `intent(in)` `abc_angles`, `real(dp)`, `dimension(3,3)`, `intent(out)` `lattice_vector` ) [`private`]

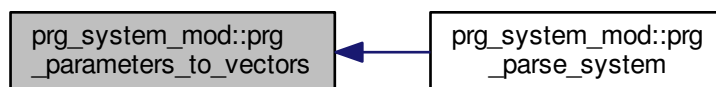
Transforms the lattice parameters into lattice vectors.

#### Parameters

|                       |   |
|-----------------------|---|
| <i>abc_angles</i>     | 2x3 array containing the lattice parameters. <code>abc_angles(1,1) = a</code> , <code>abc_angles(1,2) = b</code> , and <code>abc_angles(1,3) = c</code> <code>abc_angles(2,1) = <math>\alpha</math></code> , <code>abc_angles(2,2) = <math>\beta</math></code> and <code>abc_angles(2,3) = <math>\gamma</math></code> |
| <i>lattice_vector</i> | 3x3 array containing the lattice vectors. <code>lattice_vector(1,:) = <math>\vec{a}</math></code>   |

Definition at line 1105 of file prg\_system\_mod.F90.

Here is the caller graph for this function:



9.29.2.22 subroutine, public `prg_system_mod::prg_parse_system` ( `type(system_type)`, `intent(out)` `system`, `character(len=*)` `filename`, `character(3)`, `intent(in)`, optional `extin` )

The parser for the chemical system.

## Parameters

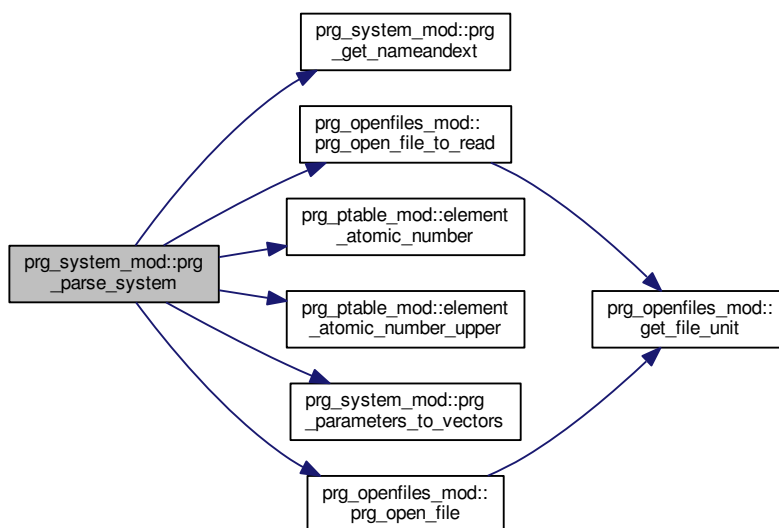
|                 |                           |
|-----------------|---------------------------|
| <i>system</i>   | System to be constructed. |
| <i>filename</i> | Filename of the system.   |
| <i>extin</i>    | Extension of the file.    |

Assignment of species index for every atom.

**Todo** Integrate this loop in the loop for building the splist.

Definition at line 229 of file prg\_system\_mod.F90.

Here is the call graph for this function:



**9.29.2.23** subroutine, public `prg_system_mod::prg_replicate ( real(dp), dimension(:,:), intent(inout), allocatable coords, character(2), dimension(:), intent(inout), allocatable symbols, real(dp), dimension(:,:), intent(inout) lattice_vectors, integer, intent(in) nx, integer, intent(in) ny, integer, intent(in) nz )`

Extend/replicate system along lattice vectors.

## Parameters

|                        |   |
|------------------------|---|
| <i>coords</i>          | Coordinates of the system (see <a href="#">system_type</a> ). |
| <i>symbols</i>         | Symbols for elements.   |
| <i>lattice_vectors</i> | System lattice vectors.                                       |
| <i>nx</i>              | Number of lattice points in the v1 direction.                 |
| <i>ny</i>              | Number of lattice points in the v2 direction.                 |
| <i>nz</i>              | Number of lattice points in the v2 direction.                 |

Definition at line 1417 of file prg\_system\_mod.F90.

9.29.2.24 subroutine, public prg\_system\_mod::prg\_sortadj ( integer, dimension(:), intent(inout) *xadj*, integer, dimension(:), intent(inout), allocatable *adjncy* )

Sort adj NOTE: this might not be needed anymore since the bml\_get\_adj routine is sorting the values.

Definition at line 2433 of file prg\_system\_mod.F90.

9.29.2.25 subroutine, public prg\_system\_mod::prg\_translateandfoldtobox ( real(dp), dimension(:, :), intent(inout), allocatable *coords*, real(dp), dimension(:, :), intent(in) *lattice\_vectors*, real(dp), dimension(:), intent(inout), allocatable *origin*, integer, intent(in), optional *verbose* )

Translate and fold to box.

#### Parameters

|                        |   |
|------------------------|---|
| <i>coords</i>          | Coordinates of the system (see <a href="#">system_type</a> ). |
| <i>lattice_vectors</i> | System lattice vectors.                                       |
| <i>origin</i>          | (min(x),min(y),min(z)) set as the origin of the system.       |

Definition at line 1243 of file prg\_system\_mod.F90.

9.29.2.26 subroutine, public prg\_system\_mod::prg\_translategeomcandfoldtobox ( real(dp), dimension(:, :), intent(inout), allocatable *coords*, real(dp), dimension(:, :), intent(in) *lattice\_vectors*, real(dp), dimension(:), intent(inout), allocatable *origin* )

Translate to geometric center.

#### Parameters

|                        |   |
|------------------------|---|
| <i>coords</i>          | Coordinates of the system (see <a href="#">system_type</a> ). |
| <i>lattice_vectors</i> | System lattice vectors.                                       |
| <i>origin</i>          | (min(x),min(y),min(z)) set as the origin of the system.       |

Definition at line 1376 of file prg\_system\_mod.F90.

9.29.2.27 subroutine, public prg\_system\_mod::prg\_vector2graph ( integer, dimension(:), intent(inout), allocatable *vector*, integer, dimension(:, :), intent(inout) *graph*, integer *maxnz* )

Back to graph.

#### Parameters

|               |                            |
|---------------|----------------------------|
| <i>vector</i> | Vector to store the graph. |
| <i>graph</i>  | Ellpack graph.             |



Definition at line 2405 of file prg\_system\_mod.F90.

**9.29.2.28** subroutine prg\_system\_mod::prg\_vectors\_to\_parameters ( real(dp), dimension(3,3), intent(in) *lattice\_vector*, real(dp), dimension(2,3), intent(out) *abc\_angles* ) [private]

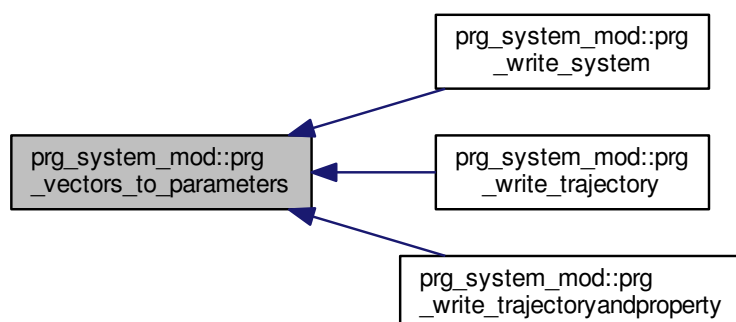
Transforms the lattice vectors into lattice parameters.

#### Parameters

|                       |  |
|-----------------------|--|
| <i>lattice_vector</i> | 3x3 array containing the lattice vectors. $\text{lattice\_vector}(1,:) = \vec{a}$  |
| <i>abc_angles</i>     | 2x3 array containing the lattice parameters. $\text{abc\_angles}(1,1) = a$ , $\text{abc\_angles}(1,2) = b$ and $\text{abc\_angles}(1,3) = c$ $\text{abc\_angles}(2,1) = \alpha$ , $\text{abc\_angles}(2,2) = \beta$ , and $\text{abc\_angles}(2,3) = \gamma$ . |

Definition at line 1147 of file prg\_system\_mod.F90.

Here is the caller graph for this function:



**9.29.2.29** subroutine, public prg\_system\_mod::prg\_wraparound ( real(dp), dimension(:,,:), intent(inout), allocatable *coords*, real(dp), dimension(:,,:), intent(in) *lattice\_vectors*, integer, intent(in) *index*, integer, intent(in), optional *verbose* )

Wrap around atom i using pbc.

#### Parameters

|                        |   |
|------------------------|---|
| <i>coords</i>          | Coordinates of the system (see <a href="#">system_type</a> ). |
| <i>lattice_vectors</i> | System lattice vectors.                                       |
| <i>index</i>           | Index atom to wrap around                                     |

Definition at line 1333 of file prg\_system\_mod.F90.

9.29.2.30 subroutine, public prg\_system\_mod::prg\_write\_system ( type(system\_type), intent(in) system, character(\*) filename, character(3) extension )

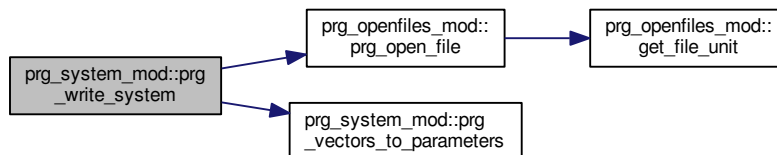
Write system in .xyz, .dat or pdb file.

#### Parameters

|                  |                           |
|------------------|---------------------------|
| <i>system</i>    | System to be constructed. |
| <i>filename</i>  | File name.                |
| <i>extension</i> | Extension of the file.    |

Definition at line 638 of file prg\_system\_mod.F90.

Here is the call graph for this function:



9.29.2.31 subroutine, public prg\_system\_mod::prg\_write\_trajectory ( type(system\_type), intent(in) system, integer, intent(in) iter, integer, intent(in) each, real(dp), intent(in) prg\_deltat, character(\*) filename, character(3) extension )

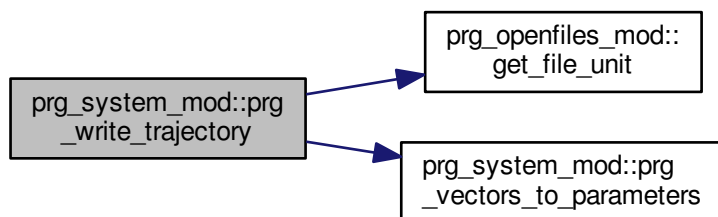
Write trajectory in .xyz, .dat or pdb file.

#### Parameters

|                  |   |
|------------------|---|
| <i>system</i>    | System to be appended to the trajectory file. |
| <i>iter</i>      | Simulation step.                              |
| <i>each</i>      | Writing frequency.                            |
| <i>filename</i>  | File name for the trajectory.                 |
| <i>extension</i> | Extension of the file.                        |

Definition at line 826 of file prg\_system\_mod.F90.

Here is the call graph for this function:



9.29.2.32 subroutine, public `prg_system_mod::prg_write_trajectoryandproperty` ( `type(system_type)`, `intent(in) system`, `integer`, `intent(in) iter`, `integer`, `intent(in) each`, `real(dp)`, `intent(in) prg_deltat`, `real(dp)`, `dimension(:)`, `intent(in) scalarprop`, `character(*) filename`, `character(3) extension` )

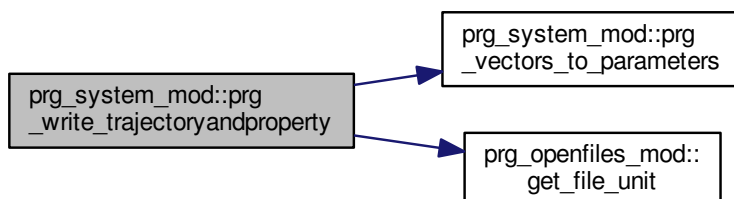
Write trajectory and atomic properties. Only pdb file.

#### Parameters

|                   |   |
|-------------------|---|
| <i>system</i>     | System to be appended to the trajectory file. |
| <i>iter</i>       | Simulation step.                              |
| <i>each</i>       | Writing frequency.                            |
| <i>prg_deltat</i> | Integration step.                             |
| <i>scalarprop</i> | Scalar property to plot on atoms.             |
| <i>filename</i>   | File name for the trajectory.                 |
| <i>extension</i>  | Extension of the file.                        |

Definition at line 949 of file `prg_system_mod.F90`.

Here is the call graph for this function:



### 9.29.3 Variable Documentation

#### 9.29.3.1 integer, parameter `prg_system_mod::dp = kind(1.0d0)` [private]

Definition at line 19 of file `prg_system_mod.F90`.

## 9.30 `prg_timer_mod` Module Reference

The timer module.

### Data Types

- type `timer_status_t`  
*Timer status type.*

### Functions/Subroutines

- subroutine, public `timer_prg_init` ()  
*Initialize timers.*
- subroutine `prg_timer_getid` ()  
*Get timer id.*
- subroutine, public `prg_timer_shutdown` ()  
*Done with timers.*
- subroutine, public `prg_timer_start` (itimer, tag)  
*Start Timing.*
- subroutine, public `prg_timer_stop` (itimer, verbose)  
*Stop timing.*
- subroutine, public `prg_timer_collect` ()
- subroutine, public `prg_timer_results` ()
- real(8) function, public `time2milliseconds` ()
- subroutine, public `prg_print_date_and_time` (tag)
- character(2) function, private `int2char` (ival)

### Variables

- integer, parameter `dp = kind(1.0d0)`
- integer, public `loop_timer`
- integer, public `sp2_timer`
- integer, public `genx_timer`
- integer, public `part_timer`
- integer, public `subgraph_timer`
- integer, public `deortho_timer`
- integer, public `ortho_timer`
- integer, public `zdiag_timer`
- integer, public `graphsp2_timer`
- integer, public `subind_timer`
- integer, public `subext_timer`
- integer, public `subsp2_timer`

- integer, public [suball\\_timer](#)
- integer, public [bmult\\_timer](#)
- integer, public [badd\\_timer](#)
- integer, public [dyn\\_timer](#)
- integer, public [mdloop\\_timer](#)
- integer, public [buildz\\_timer](#)
- integer, public [realcoul\\_timer](#)
- integer, public [recipcoul\\_timer](#)
- integer, public [pairpot\\_timer](#)
- integer, public [halfverlet\\_timer](#)
- integer, public [pos\\_timer](#)
- integer, public [nlist\\_timer](#)
- integer [tstart\\_clock](#)
- integer [tstop\\_clock](#)
- integer [tclock\\_rate](#)
- integer [tclock\\_max](#)
- integer [num\\_timers](#)
- type([timer\\_status\\_t](#)), dimension(:), allocatable [ptimer](#)

### 9.30.1 Detailed Description

The timer module.

Sets up timers that can be used to time other routines.

Example use of dynamic timing:

call [timer\\_prg\\_init\(\)](#)

call [prg\\_timer\\_start](#)(dyn\_timer,"timer\_tag")

.... code lines ...

call [prg\\_timer\\_stop](#)(dyn\_timer,1)

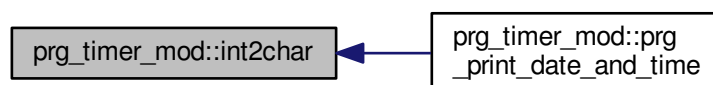
This will write the time it takes to execute "code lines" and it will name it "timer\_tag"

### 9.30.2 Function/Subroutine Documentation

9.30.2.1 [character\(2\) function, private `prg\_timer\_mod::int2char` \( integer, intent\(in\) \*ival\* \)](#) `[private]`

Definition at line 394 of file `prg_timer_mod.F90`.

Here is the caller graph for this function:



### 9.30.2.2 subroutine, public prg\_timer\_mod::prg\_print\_date\_and\_time ( character(len=\*), intent(in) tag )

Definition at line 371 of file prg\_timer\_mod.F90.

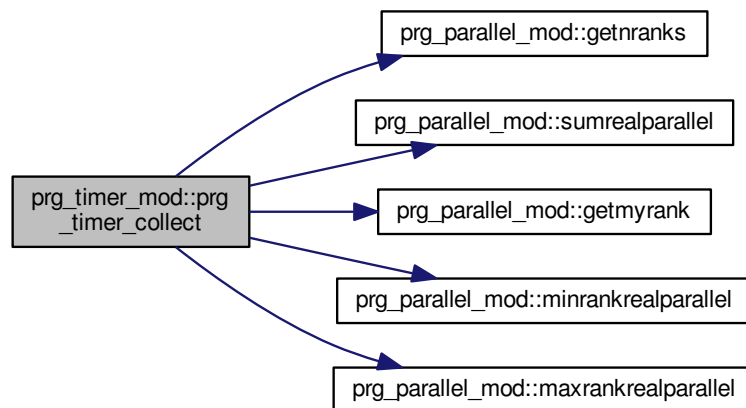
Here is the call graph for this function:



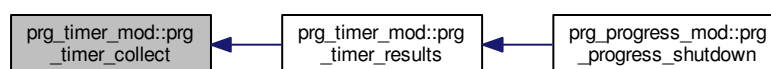
### 9.30.2.3 subroutine, public prg\_timer\_mod::prg\_timer\_collect ( )

Definition at line 253 of file prg\_timer\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



#### 9.30.2.4 subroutine prg\_timer\_mod::prg\_timer\_getid ( ) [private]

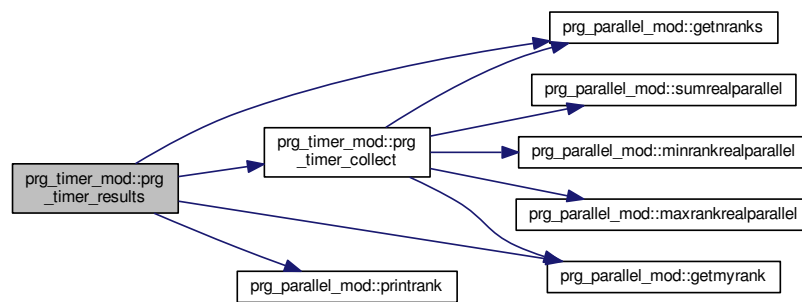
Get timer id.

Definition at line 200 of file prg\_timer\_mod.F90.

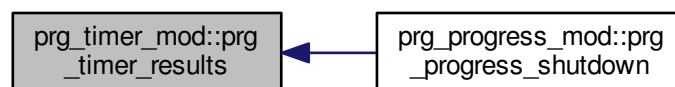
#### 9.30.2.5 subroutine, public prg\_timer\_mod::prg\_timer\_results ( )

Definition at line 317 of file prg\_timer\_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:

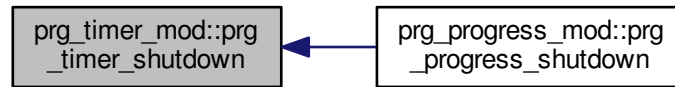


#### 9.30.2.6 subroutine, public prg\_timer\_mod::prg\_timer\_shutdown ( )

Done with timers.

Definition at line 205 of file prg\_timer\_mod.F90.

Here is the caller graph for this function:



9.30.2.7 subroutine, public `prg_timer_mod::prg_timer_start ( integer, intent(in) itimer, character(len=*), intent(in), optional tag )`

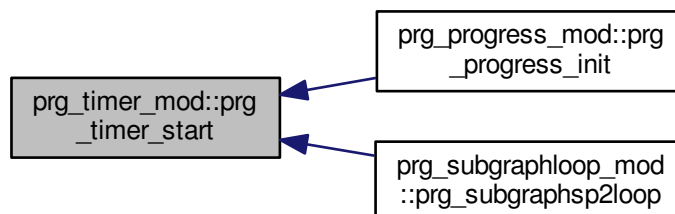
Start Timing.

#### Parameters

|               |   |
|---------------|---|
| <i>itimer</i> | The index of the timer to start.                  |
| <i>tag</i>    | Optional parameter to retag the timer on the fly. |

Definition at line 215 of file `prg_timer_mod.F90`.

Here is the caller graph for this function:



9.30.2.8 subroutine, public `prg_timer_mod::prg_timer_stop ( integer, intent(in) itimer, integer, intent(in), optional verbose )`

Stop timing.

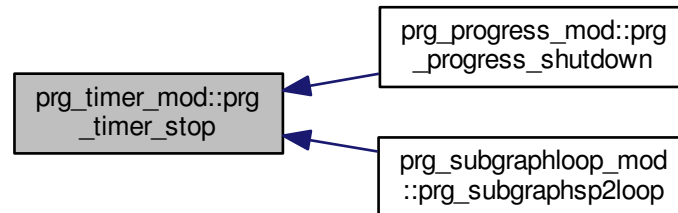
#### Parameters

|                |   |
|----------------|---|
| <i>itimer</i>  | The index of the timer to stop.             |
| <i>verbose</i> | Optional parameters to print partial times. |



Definition at line 233 of file prg\_timer\_mod.F90.

Here is the caller graph for this function:



#### 9.30.2.9 real(8) function, public prg\_timer\_mod::time2milliseconds ( )

Definition at line 360 of file prg\_timer\_mod.F90.

#### 9.30.2.10 subroutine, public prg\_timer\_mod::timer\_prg\_init ( )

Initialize timers.

Definition at line 132 of file prg\_timer\_mod.F90.

Here is the caller graph for this function:



### 9.30.3 Variable Documentation

#### 9.30.3.1 integer, public prg\_timer\_mod::badd\_timer

Definition at line 48 of file prg\_timer\_mod.F90.

9.30.3.2 integer, public prg\_timer\_mod::bmult\_timer

Definition at line 48 of file prg\_timer\_mod.F90.

9.30.3.3 integer, public prg\_timer\_mod::buildz\_timer

Definition at line 49 of file prg\_timer\_mod.F90.

9.30.3.4 integer, public prg\_timer\_mod::deortho\_timer

Definition at line 45 of file prg\_timer\_mod.F90.

9.30.3.5 integer, parameter prg\_timer\_mod::dp = kind(1.0d0) [private]

Definition at line 32 of file prg\_timer\_mod.F90.

9.30.3.6 integer, public prg\_timer\_mod::dyn\_timer

Definition at line 49 of file prg\_timer\_mod.F90.

9.30.3.7 integer, public prg\_timer\_mod::genx\_timer

Definition at line 44 of file prg\_timer\_mod.F90.

9.30.3.8 integer, public prg\_timer\_mod::graphsp2\_timer

Definition at line 46 of file prg\_timer\_mod.F90.

9.30.3.9 integer, public prg\_timer\_mod::halfverlet\_timer

Definition at line 51 of file prg\_timer\_mod.F90.

9.30.3.10 integer, public prg\_timer\_mod::loop\_timer

Definition at line 44 of file prg\_timer\_mod.F90.

9.30.3.11 integer, public prg\_timer\_mod::mdloop\_timer

Definition at line 49 of file prg\_timer\_mod.F90.

9.30.3.12 integer, public prg\_timer\_mod::nlist\_timer

Definition at line 51 of file prg\_timer\_mod.F90.

9.30.3.13 integer prg\_timer\_mod::num\_timers [private]

Definition at line 122 of file prg\_timer\_mod.F90.

9.30.3.14 integer, public prg\_timer\_mod::ortho\_timer

Definition at line 46 of file prg\_timer\_mod.F90.

9.30.3.15 integer, public prg\_timer\_mod::pairpot\_timer

Definition at line 50 of file prg\_timer\_mod.F90.

9.30.3.16 integer, public prg\_timer\_mod::part\_timer

Definition at line 45 of file prg\_timer\_mod.F90.

9.30.3.17 integer, public prg\_timer\_mod::pos\_timer

Definition at line 51 of file prg\_timer\_mod.F90.

9.30.3.18 type (timer\_status\_t), dimension(:), allocatable prg\_timer\_mod::ptimer [private]

Definition at line 124 of file prg\_timer\_mod.F90.

9.30.3.19 integer, public prg\_timer\_mod::realcoul\_timer

Definition at line 50 of file prg\_timer\_mod.F90.

9.30.3.20 integer, public prg\_timer\_mod::recipcoul\_timer

Definition at line 50 of file prg\_timer\_mod.F90.

9.30.3.21 integer, public prg\_timer\_mod::sp2\_timer

Definition at line 44 of file prg\_timer\_mod.F90.

9.30.3.22 integer, public prg\_timer\_mod::suball\_timer

Definition at line 48 of file prg\_timer\_mod.F90.

9.30.3.23 integer, public prg\_timer\_mod::subext\_timer

Definition at line 47 of file prg\_timer\_mod.F90.

9.30.3.24 integer, public prg\_timer\_mod::subgraph\_timer

Definition at line 45 of file prg\_timer\_mod.F90.

9.30.3.25 integer, public prg\_timer\_mod::subind\_timer

Definition at line 47 of file prg\_timer\_mod.F90.

9.30.3.26 integer, public prg\_timer\_mod::subsp2\_timer

Definition at line 47 of file prg\_timer\_mod.F90.

9.30.3.27 integer prg\_timer\_mod::tclock\_max [private]

Definition at line 121 of file prg\_timer\_mod.F90.

9.30.3.28 integer prg\_timer\_mod::tclock\_rate [private]

Definition at line 121 of file prg\_timer\_mod.F90.

9.30.3.29 integer prg\_timer\_mod::tstart\_clock [private]

Definition at line 121 of file prg\_timer\_mod.F90.

9.30.3.30 integer prg\_timer\_mod::tstop\_clock [private]

Definition at line 121 of file prg\_timer\_mod.F90.

9.30.3.31 integer, public prg\_timer\_mod::zdiag\_timer

Definition at line 46 of file prg\_timer\_mod.F90.

## 9.31 prg\_xlbo\_mod Module Reference

A module to perform XLBO integration.

### Data Types

- type `xlbo_type`

*General xlbo solver type.*

### Functions/Subroutines

- subroutine, public `prg_parse_xlbo` (xlbo, filename)  
*The parser for XLBO parser.*
- subroutine, public `prg_xlbo_nint` (charges, n, n\_0, n\_1, n\_2, n\_3, n\_4, n\_5, mdstep, xl)  
*This routine integrates the dynamical variable "n".*
- subroutine, public `prg_xlbo_fcoulupdate` (fcoul, charges, n)  
*Adjust forces for the linearized XLBOMD functional.*

### Variables

- integer, parameter `dp` = kind(1.0d0)
- real(`dp`), parameter `c0` = -6.0\_dp  
*Coefficients for modified Verlet integration.*
- real(`dp`), parameter `c1` = 14.0\_dp
- real(`dp`), parameter `c2` = -8.0\_dp
- real(`dp`), parameter `c3` = -3.0\_dp
- real(`dp`), parameter `c4` = 4.0\_dp
- real(`dp`), parameter `c5` = -1.0\_dp
- real(`dp`), parameter `kappa` = 1.82\_dp  
*Coefficients for modified Verlet integration.*
- real(`dp`), parameter `alpha` = 0.018\_dp
- real(`dp`), parameter `cc` = 0.9\_dp

#### 9.31.1 Detailed Description

A module to perform XLBO integration.

This module will be used to compute integrate the dynamical variable "n" in xlbo.

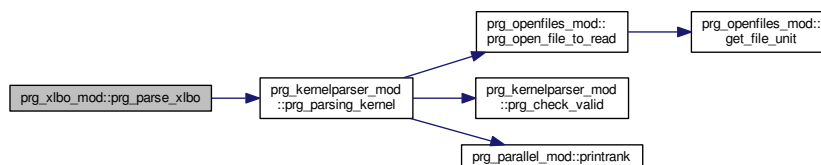
### 9.31.2 Function/Subroutine Documentation

9.31.2.1 subroutine, public prg\_xlbo\_mod::prg\_parse\_xlbo ( type(xlbo\_type), intent(inout) *xlbo*, character(len=\*) *filename* )

The parser for XLBO parser.

Definition at line 62 of file prg\_xlbo\_mod.F90.

Here is the call graph for this function:



9.31.2.2 subroutine, public prg\_xlbo\_mod::prg\_xlbo\_fcoulupdate ( real(dp), dimension(:, :), intent(inout) *fcoul*, real(dp), dimension(:), intent(inout) *charges*, real(dp), dimension(:), intent(inout) *n* )

Adjust forces for the linearized XLBOMD functional.

Parameters

|                |  |
|----------------|--|
| <i>charges</i> |  |
|----------------|--|

Definition at line 158 of file prg\_xlbo\_mod.F90.

9.31.2.3 subroutine, public prg\_xlbo\_mod::prg\_xlbo\_nint ( real(dp), dimension(:), intent(in), allocatable *charges*, real(dp), dimension(:), intent(inout), allocatable *n*, real(dp), dimension(:), intent(inout), allocatable *n\_0*, real(dp), dimension(:), intent(inout), allocatable *n\_1*, real(dp), dimension(:), intent(inout), allocatable *n\_2*, real(dp), dimension(:), intent(inout), allocatable *n\_3*, real(dp), dimension(:), intent(inout), allocatable *n\_4*, real(dp), dimension(:), intent(inout), allocatable *n\_5*, integer, intent(in) *mdstep*, type(xlbo\_type), intent(in) *xl* )

This routine integrates the dynamical variable "n".

Parameters

|                |  |
|----------------|--|
| <i>charges</i> |  |
|----------------|--|

Definition at line 118 of file prg\_xlbo\_mod.F90.

### 9.31.3 Variable Documentation

9.31.3.1 `real(dp), parameter prg_xlbo_mod::alpha = 0.018_dp` `[private]`

Definition at line 28 of file prg\_xlbo\_mod.F90.

9.31.3.2 `real(dp), parameter prg_xlbo_mod::c0 = -6.0_dp` `[private]`

Coefficients for modified Verlet integration.

Definition at line 19 of file prg\_xlbo\_mod.F90.

9.31.3.3 `real(dp), parameter prg_xlbo_mod::c1 = 14.0_dp` `[private]`

Definition at line 20 of file prg\_xlbo\_mod.F90.

9.31.3.4 `real(dp), parameter prg_xlbo_mod::c2 = -8.0_dp` `[private]`

Definition at line 21 of file prg\_xlbo\_mod.F90.

9.31.3.5 `real(dp), parameter prg_xlbo_mod::c3 = -3.0_dp` `[private]`

Definition at line 22 of file prg\_xlbo\_mod.F90.

9.31.3.6 `real(dp), parameter prg_xlbo_mod::c4 = 4.0_dp` `[private]`

Definition at line 23 of file prg\_xlbo\_mod.F90.

9.31.3.7 `real(dp), parameter prg_xlbo_mod::c5 = -1.0_dp` `[private]`

Definition at line 24 of file prg\_xlbo\_mod.F90.

9.31.3.8 `real(dp), parameter prg_xlbo_mod::cc = 0.9_dp` `[private]`

Definition at line 29 of file prg\_xlbo\_mod.F90.

9.31.3.9 `integer, parameter prg_xlbo_mod::dp = kind(1.0d0)` `[private]`

Definition at line 16 of file prg\_xlbo\_mod.F90.

9.31.3.10 `real(dp), parameter prg_xlbo_mod::kappa = 1.82_dp` `[private]`

Coefficients for modified Verlet integration.

Definition at line 27 of file prg\_xlbo\_mod.F90.

## 9.32 prg\_xlkernel\_mod Module Reference

Add name.

### Data Types

- type [xlk\\_type](#)

### Functions/Subroutines

- subroutine, public [prg\\_parse\\_xlkernel](#) (input, filename)  
*The parser for the mixer routines.*
- subroutine, public [prg\\_fermi](#) (D0, QQ, ee, gap, Fe\_vec, mu0, H, Z, Nocc, T, OccErrLim, MaxIt, HDIM)
- subroutine, public [prg\\_kernel\\_fermi\\_full](#) (KK, JJ, D0, mu0, mu1, T, RX, RY, RZ, LBox, Hubbard\_U, Element↵\_Type, Nr\_atoms, MaxIt, eps, m, HDIM, Max\_Nr\_Neigh, Coulomb\_acc, TIMERATIO, nnRx, nnRy, nnRz, nrnnlist, nnType, H\_INDEX\_START, H\_INDEX\_END, H, S, Z, Nocc, Znuc, QQ, ee, Fe\_vec)
- subroutine, public [prg\\_v\\_kernel\\_fermi](#) (D0, dq\_dv, v, mu0, mu1, T, RX, RY, RZ, LBox, Hubbard\_U, Element↵\_Type, Nr\_atoms, MaxIt, eps, m, HDIM, Max\_Nr\_Neigh, Coulomb\_acc, TIMERATIO, nnRx, nnRy, nnRz, nrnnlist, nnType, H\_INDEX\_START, H\_INDEX\_END, H, S, Z, Nocc, Znuc, QQ, ee, Fe\_vec)
- subroutine, private [prg\\_get\\_deriv\\_finite\\_temp](#) (P1, H0, H1, Nocc, T, Q, ev, fe, mu0, eps, HDIM)
- subroutine, private [prg\\_mmult](#) (alpha, A, B, beta, C, TA, TB, HDIM)
- subroutine, private [prg\\_eig](#) (A, Q, ee, type, HDIM)
- subroutine, private [prg\\_inv](#) (X, XI, HDIM)
- subroutine, public [prg\\_rank1](#) (verbose)  
*Rank1 kernel ....*

### Variables

- integer, parameter [dp](#) = kind(1.0d0)

#### 9.32.1 Detailed Description

Add name.

XL kernel (To be integrated)

#### Note

This module is still not functional

#### 9.32.2 Function/Subroutine Documentation

- 9.32.2.1 subroutine, private [prg\\_xlkernel\\_mod::prg\\_eig](#) ( real(prec), dimension(hdim,hdim), intent(in) A, real(prec), dimension(hdim,hdim), intent(out) Q, real(prec), dimension(hdim), intent(out) ee, character(1), intent(in) type, integer(prec), intent(in) HDIM ) [private]

Definition at line 384 of file prg\_xlkernel\_mod.F90.



9.32.2.2 subroutine, public prg\_xlkernel\_mod::prg\_fermi ( real(prec), dimension(hdim,hdim), intent(out) *D0*, real(prec), dimension(hdim,hdim), intent(out) *QQ*, real(prec), dimension(hdim), intent(out) *ee*, real(prec), intent(out) *gap*, real(prec), dimension(hdim), intent(out) *Fe\_vec*, real(prec), intent(inout) *mu0*, real(prec), dimension(hdim,hdim), intent(in) *H*, real(prec), dimension(hdim,hdim), intent(in) *Z*, integer(prec), intent(in) *Nocc*, real(prec), intent(in) *T*, real(prec), intent(in) *OccErrLim*, integer(prec), intent(in) *MaxIt*, integer(prec), intent(in) *HDIM* )

Definition at line 88 of file prg\_xlkernel\_mod.F90.

9.32.2.3 subroutine, private prg\_xlkernel\_mod::prg\_get\_deriv\_finite\_temp ( real(prec), dimension(hdim,hdim), intent(out) *P1*, real(prec), dimension(hdim,hdim), intent(in) *H0*, real(prec), dimension(hdim,hdim), intent(in) *H1*, integer(prec), intent(in) *Nocc*, real(prec), intent(in) *T*, real(prec), dimension(hdim,hdim), intent(in) *Q*, real(prec), dimension(hdim), intent(in) *ev*, real(prec), dimension(hdim), intent(in) *fe*, real(prec), intent(inout) *mu0*, real(prec), intent(in) *eps*, integer(prec), intent(in) *HDIM* ) [private]

Definition at line 306 of file prg\_xlkernel\_mod.F90.

9.32.2.4 subroutine, private prg\_xlkernel\_mod::prg\_inv ( real(prec), dimension(hdim,hdim), intent(in) *X*, real(prec), dimension(hdim,hdim), intent(out) *XI*, integer(prec), intent(in) *HDIM* ) [private]

Definition at line 411 of file prg\_xlkernel\_mod.F90.

9.32.2.5 subroutine, public prg\_xlkernel\_mod::prg\_kernel\_fermi\_full ( real(prec), dimension(nr\_atoms,nr\_atoms), intent(out) *KK*, real(prec), dimension(nr\_atoms,nr\_atoms), intent(out) *JJ*, real(prec), dimension(hdim,hdim), intent(inout) *D0*, real(prec), intent(inout) *mu0*, real(prec), intent(inout) *mu1*, real(prec), intent(in) *T*, real(prec), dimension(nr\_atoms), intent(in) *RX*, real(prec), dimension(nr\_atoms), intent(in) *RY*, real(prec), dimension(nr\_atoms), intent(in) *RZ*, real(prec), dimension(3), intent(in) *LBox*, real(prec), dimension(nr\_atoms), intent(in) *Hubbard\_U*, character(10), dimension(nr\_atoms), intent(in) *Element\_Type*, integer(prec), intent(in) *Nr\_atoms*, integer(prec), intent(in) *MaxIt*, real(prec), intent(in) *eps*, integer(prec), intent(in) *m*, integer(prec), intent(in) *HDIM*, integer(prec), intent(in) *Max\_Nr\_Neigh*, real(prec), intent(in) *Coulomb\_acc*, real(prec), intent(in) *TIMERATIO*, real(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnRx*, real(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnRy*, real(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnRz*, integer(prec), dimension(nr\_atoms), intent(in) *nnnlist*, integer(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnType*, integer(prec), dimension(nr\_atoms), intent(in) *H\_INDEX\_START*, integer(prec), dimension(nr\_atoms), intent(in) *H\_INDEX\_END*, real(prec), dimension(hdim,hdim), intent(in) *H*, real(prec), dimension(hdim,hdim), intent(in) *S*, real(prec), dimension(hdim,hdim), intent(in) *Z*, integer(prec), intent(in) *Nocc*, real(prec), dimension(nr\_atoms), intent(in) *Znuc*, real(prec), dimension(hdim,hdim), intent(in) *QQ*, real(prec), dimension(hdim), intent(in) *ee*, real(prec), dimension(hdim), intent(in) *Fe\_vec* )

Definition at line 144 of file prg\_xlkernel\_mod.F90.

9.32.2.6 subroutine, private prg\_xlkernel\_mod::prg\_mmult ( real(prec), intent(in) *alpha*, real(prec), dimension(hdim,hdim), intent(in) *A*, real(prec), dimension(hdim,hdim), intent(in) *B*, real(prec), intent(in) *beta*, real(prec), dimension(hdim,hdim), intent(inout) *C*, character(1), intent(in) *TA*, character(1), intent(in) *TB*, integer(prec), intent(in) *HDIM* ) [private]

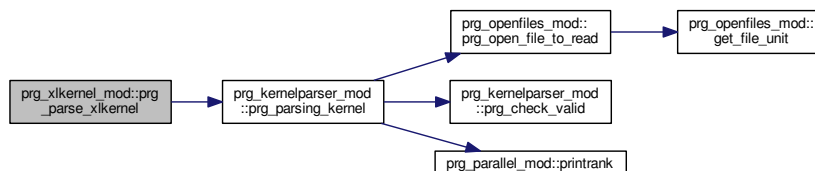
Definition at line 366 of file prg\_xlkernel\_mod.F90.

9.32.2.7 subroutine, public prg\_xlkernel\_mod::prg\_parse\_xlkernel ( type(xlk\_type), intent(inout) *input*, character(len=\*) *filename* )

The parser for the mixer routines.

Definition at line 39 of file prg\_xlkernel\_mod.F90.

Here is the call graph for this function:



9.32.2.8 subroutine, public prg\_xlkernel\_mod::prg\_rank1 ( integer, intent(in) *verbose* )

Rank1 kernel ....

Parameters

|                |                                |
|----------------|--------------------------------|
| <i>param1</i>  | ..                             |
| <i>verbose</i> | Different levels of verbosity. |

Definition at line 439 of file prg\_xlkernel\_mod.F90.

9.32.2.9 subroutine, public prg\_xlkernel\_mod::prg\_v\_kernel\_fermi ( real(prec), dimension(hdim,hdim), intent(inout) *D0*, real(prec), dimension(nr\_atoms), intent(out) *dq\_dv*, real(prec), dimension(nr\_atoms), intent(in) *v*, real(prec), intent(inout) *mu0*, real(prec), intent(inout) *mu1*, real(prec), intent(in) *T*, real(prec), dimension(nr\_atoms), intent(in) *RX*, real(prec), dimension(nr\_atoms), intent(in) *RY*, real(prec), dimension(nr\_atoms), intent(in) *RZ*, real(prec), dimension(3), intent(in) *LBox*, real(prec), dimension(nr\_atoms), intent(in) *Hubbard\_U*, character(10), dimension(nr\_atoms), intent(in) *Element\_Type*, integer(prec), intent(in) *Nr\_atoms*, integer(prec), intent(in) *MaxIt*, real(prec), intent(in) *eps*, integer(prec), intent(in) *m*, integer(prec), intent(in) *HDIM*, integer(prec), intent(in) *Max\_Nr\_Neigh*, real(prec), intent(in) *Coulomb\_acc*, real(prec), intent(in) *TIMERATIO*, real(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnRx*, real(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnRy*, real(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnRz*, integer(prec), dimension(nr\_atoms), intent(in) *nnnlist*, integer(prec), dimension(nr\_atoms,max\_nr\_neigh), intent(in) *nnType*, integer(prec), dimension(nr\_atoms), intent(in) *H\_INDEX\_START*, integer(prec), dimension(nr\_atoms), intent(in) *H\_INDEX\_END*, real(prec), dimension(hdim,hdim), intent(in) *H*, real(prec), dimension(hdim,hdim), intent(in) *S*, real(prec), dimension(hdim,hdim), intent(in) *Z*, integer(prec), intent(in) *Nocc*, real(prec), dimension(nr\_atoms), intent(in) *Znuc*, real(prec), dimension(hdim,hdim), intent(in) *QQ*, real(prec), dimension(hdim), intent(in) *ee*, real(prec), dimension(hdim), intent(in) *Fe\_vec* )

Definition at line 235 of file prg\_xlkernel\_mod.F90.

### 9.32.3 Variable Documentation

9.32.3.1 integer, parameter prg\_xlkernel\_mod::dp = kind(1.0d0) [private]

Definition at line 15 of file prg\_xlkernel\_mod.F90.



## Chapter 10

# Data Type Documentation

### 10.1 prg\_chebyshev\_mod::chebdata\_type Type Reference

General Cheb solver type.

#### Public Attributes

- character(100) [flavor](#)
- character(100) [bml\\_type](#)
- character(100) [jobname](#)
- integer [mdim](#)
- integer [ncoeffs](#)
- integer [ndim](#)
- integer [verbose](#)
- integer [npts](#)
- real(dp) [atr](#)
- real(dp) [bndfil](#)
- real(dp) [ef](#)
- real(dp) [estep](#)
- real(dp) [fermitol](#)
- real(dp) [kbt](#)
- real(dp) [threshold](#)
- logical [getef](#)
- logical [jon](#)
- logical [trkfunc](#)

#### 10.1.1 Detailed Description

General Cheb solver type.

Definition at line 28 of file prg\_chebyshev\_mod.F90.

## 10.1.2 Member Data Documentation

### 10.1.2.1 `real(dp) prg_chebyshev_mod::chebdata_type::atr`

Definition at line 33 of file `prg_chebyshev_mod.F90`.

### 10.1.2.2 `character(100) prg_chebyshev_mod::chebdata_type::bml_type`

Definition at line 30 of file `prg_chebyshev_mod.F90`.

### 10.1.2.3 `real(dp) prg_chebyshev_mod::chebdata_type::bndfil`

Definition at line 33 of file `prg_chebyshev_mod.F90`.

### 10.1.2.4 `real(dp) prg_chebyshev_mod::chebdata_type::ef`

Definition at line 33 of file `prg_chebyshev_mod.F90`.

### 10.1.2.5 `real(dp) prg_chebyshev_mod::chebdata_type::estep`

Definition at line 33 of file `prg_chebyshev_mod.F90`.

### 10.1.2.6 `real(dp) prg_chebyshev_mod::chebdata_type::fermitol`

Definition at line 34 of file `prg_chebyshev_mod.F90`.

### 10.1.2.7 `character(100) prg_chebyshev_mod::chebdata_type::flavor`

Definition at line 29 of file `prg_chebyshev_mod.F90`.

### 10.1.2.8 `logical prg_chebyshev_mod::chebdata_type::getef`

Definition at line 35 of file `prg_chebyshev_mod.F90`.

### 10.1.2.9 `character(100) prg_chebyshev_mod::chebdata_type::jobname`

Definition at line 30 of file `prg_chebyshev_mod.F90`.

### 10.1.2.10 `logical prg_chebyshev_mod::chebdata_type::jon`

Definition at line 35 of file `prg_chebyshev_mod.F90`.

10.1.2.11 `real(dp) prg_chebyshev_mod::chebdata_type::kbt`

Definition at line 34 of file `prg_chebyshev_mod.F90`.

10.1.2.12 `integer prg_chebyshev_mod::chebdata_type::mdim`

Definition at line 31 of file `prg_chebyshev_mod.F90`.

10.1.2.13 `integer prg_chebyshev_mod::chebdata_type::ncoeffs`

Definition at line 31 of file `prg_chebyshev_mod.F90`.

10.1.2.14 `integer prg_chebyshev_mod::chebdata_type::ndim`

Definition at line 31 of file `prg_chebyshev_mod.F90`.

10.1.2.15 `integer prg_chebyshev_mod::chebdata_type::npts`

Definition at line 32 of file `prg_chebyshev_mod.F90`.

10.1.2.16 `real(dp) prg_chebyshev_mod::chebdata_type::threshold`

Definition at line 34 of file `prg_chebyshev_mod.F90`.

10.1.2.17 `logical prg_chebyshev_mod::chebdata_type::trkfunc`

Definition at line 35 of file `prg_chebyshev_mod.F90`.

10.1.2.18 `integer prg_chebyshev_mod::chebdata_type::verbose`

Definition at line 31 of file `prg_chebyshev_mod.F90`.

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

- `/home/christian/qmd-progress/src/prg_chebyshev_mod.F90`

## 10.2 prg\_system\_mod::estruct\_type Type Reference

Electronic structure type.

## Public Attributes

- integer [norbs](#)  
*Number of orbitals of the system.*
- integer [nel](#)  
*Number of electrons.*
- integer, dimension(:,:), allocatable [hindex](#)  
*Hindex.*
- type(bml\_matrix\_t) [ham](#)  
*SCC-Hamiltonian of the system.*
- type(bml\_matrix\_t) [ham0](#)  
*Hamiltonian of the system.*
- type(bml\_matrix\_t) [oham](#)  
*Orthogonalized Hamiltonian.*
- type(bml\_matrix\_t) [over](#)  
*Overlap matrix of the system.*
- type(bml\_matrix\_t) [rho](#)  
*Density matrix of the system.*
- type(bml\_matrix\_t) [orho](#)  
*Orthogonalized density matrix.*
- type(bml\_matrix\_t) [zmat](#)  
*Congruence transformation.*
- real([dp](#)), dimension(:), allocatable [coul\\_pot\\_r](#)  
*Real Coulombic contribution.*
- real([dp](#)), dimension(:), allocatable [coul\\_pot\\_k](#)  
*Reciprocal Coulombic contribution.*
- real([dp](#)), dimension(:,:), allocatable [skforce](#)  
*Slater Koster force.*
- real([dp](#)), dimension(:,:), allocatable [fpul](#)  
*Pulay force.*
- real([dp](#)), dimension(:,:), allocatable [fscoul](#)  
*Nonorthogonal Coulombic force.*
- real([dp](#)) [eband](#)  
*Band energy.*

### 10.2.1 Detailed Description

Electronic structure type.

The electronic structure type.

Definition at line 22 of file prg\_system\_mod.F90.

### 10.2.2 Member Data Documentation

#### 10.2.2.1 `real(dp), dimension(:), allocatable prg_system_mod::estruct_type::coul_pot_k`

Reciprocal Coulombic contribution.

Definition at line 58 of file prg\_system\_mod.F90.



**10.2.2.2 real(dp), dimension(:), allocatable prg\_system\_mod::estruct\_type::coul\_pot\_r**

Real Coulombic contribution.

Definition at line 55 of file prg\_system\_mod.F90.

**10.2.2.3 real(dp) prg\_system\_mod::estruct\_type::eband**

Band energy.

Definition at line 70 of file prg\_system\_mod.F90.

**10.2.2.4 real(dp), dimension(:,,:), allocatable prg\_system\_mod::estruct\_type::fpul**

Pulay force.

Definition at line 64 of file prg\_system\_mod.F90.

**10.2.2.5 real(dp), dimension(:,,:), allocatable prg\_system\_mod::estruct\_type::fscoul**

Nonorthogonal Coulombic force.

Definition at line 67 of file prg\_system\_mod.F90.

**10.2.2.6 type(bml\_matrix\_t) prg\_system\_mod::estruct\_type::ham**

SCC-Hamiltonian of the system.

Definition at line 34 of file prg\_system\_mod.F90.

**10.2.2.7 type(bml\_matrix\_t) prg\_system\_mod::estruct\_type::ham0**

Hamiltonian of the system.

Definition at line 37 of file prg\_system\_mod.F90.

**10.2.2.8 integer, dimension(:,,:), allocatable prg\_system\_mod::estruct\_type::hindex**

Hindex.

Definition at line 31 of file prg\_system\_mod.F90.

**10.2.2.9 integer prg\_system\_mod::estruct\_type::nel**

Number of electrons.

Definition at line 28 of file prg\_system\_mod.F90.

#### 10.2.2.10 integer prg\_system\_mod::estruct\_type::norbs

Number of orbitals of the system.

Definition at line 25 of file prg\_system\_mod.F90.

#### 10.2.2.11 type(bml\_matrix\_t) prg\_system\_mod::estruct\_type::oham

Orthogonalized Hamiltonian.

Definition at line 40 of file prg\_system\_mod.F90.

#### 10.2.2.12 type(bml\_matrix\_t) prg\_system\_mod::estruct\_type::orho

Orthogonalized density matrix.

Definition at line 49 of file prg\_system\_mod.F90.

#### 10.2.2.13 type(bml\_matrix\_t) prg\_system\_mod::estruct\_type::over

Overlap matrix of the system.

Definition at line 43 of file prg\_system\_mod.F90.

#### 10.2.2.14 type(bml\_matrix\_t) prg\_system\_mod::estruct\_type::rho

Density matrix of the system.

Definition at line 46 of file prg\_system\_mod.F90.

#### 10.2.2.15 real(dp), dimension(:, :), allocatable prg\_system\_mod::estruct\_type::skforce

Slater Koster force.

Definition at line 61 of file prg\_system\_mod.F90.

#### 10.2.2.16 type(bml\_matrix\_t) prg\_system\_mod::estruct\_type::zmat

Congruence transformation.

Definition at line 52 of file prg\_system\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_system\\_mod.F90](#)

## 10.3 prg\_genz\_mod::genzspdata Type Reference

contains the data for the genZ driver.

### Public Member Functions

- procedure [prg\\_init](#)
- procedure [prg\\_generate](#)
- procedure [prg\\_allocatezspmat](#)

### Public Attributes

- integer [verbose](#)
- integer [nfirst](#)
- integer [nrefi](#)
- integer [nreff](#)
- real(dp) [numthresi](#)
- real(dp) [numthresf](#)
- logical [integration](#)

#### 10.3.1 Detailed Description

contains the data for the genZ driver.

Definition at line 67 of file prg\_genz\_mod.F90.

#### 10.3.2 Member Function/Subroutine Documentation

##### 10.3.2.1 procedure prg\_genz\_mod::genzspdata::prg\_allocatezspmat ( )

Definition at line 79 of file prg\_genz\_mod.F90.

##### 10.3.2.2 procedure prg\_genz\_mod::genzspdata::prg\_generate ( )

Definition at line 78 of file prg\_genz\_mod.F90.

##### 10.3.2.3 procedure prg\_genz\_mod::genzspdata::prg\_init ( )

Definition at line 77 of file prg\_genz\_mod.F90.

#### 10.3.3 Member Data Documentation

##### 10.3.3.1 logical prg\_genz\_mod::genzspdata::integration

Definition at line 75 of file prg\_genz\_mod.F90.

#### 10.3.3.2 integer prg\_genz\_mod::genzspdata::nfirst

Definition at line 70 of file prg\_genz\_mod.F90.

#### 10.3.3.3 integer prg\_genz\_mod::genzspdata::nreff

Definition at line 72 of file prg\_genz\_mod.F90.

#### 10.3.3.4 integer prg\_genz\_mod::genzspdata::nrefi

Definition at line 71 of file prg\_genz\_mod.F90.

#### 10.3.3.5 real(dp) prg\_genz\_mod::genzspdata::numthresf

Definition at line 74 of file prg\_genz\_mod.F90.

#### 10.3.3.6 real(dp) prg\_genz\_mod::genzspdata::numthresi

Definition at line 73 of file prg\_genz\_mod.F90.

#### 10.3.3.7 integer prg\_genz\_mod::genzspdata::verbose

Definition at line 69 of file prg\_genz\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_genz\\_mod.F90](#)

## 10.4 prg\_genz\_mod::genzspinp Type Reference

Input for the genz driver.

## Public Attributes

- integer [verbose](#)  
*To have different levels of verbose.*
- integer [nfirst](#)  
*!Lentgth of the "firsts iteration period".*
- integer [nrefi](#)  
*!Initial number of recursive refinements.*
- integer [nreff](#)  
*!Initial number of recursive refinements.*
- real(dp) [numthresi](#)  
*Initial threshold value.*
- real(dp) [numthresf](#)  
*Final threshold value.*
- logical [integration](#)  
*If we want to do XL integration scheme for Z.*
- integer [igenz](#)  
*To keep track of the genz iterations.*
- logical [zsp](#)  
*Logical variable to compute in sparse or dense mode.*
- integer [mdim](#)  
*Max nonzero elements per row for every row see [1] .*
- character(20) [bml\\_type](#)  
*Matrix format (Dense or Ellpack).*

### 10.4.1 Detailed Description

Input for the genz driver.

This type controls all the variables that are needed by genz

Definition at line 28 of file prg\_genz\_mod.F90.

### 10.4.2 Member Data Documentation

#### 10.4.2.1 character(20) prg\_genz\_mod::genzspin::bml\_type

Matrix format (Dense or Ellpack).

Definition at line 61 of file prg\_genz\_mod.F90.

#### 10.4.2.2 integer prg\_genz\_mod::genzspin::igenz

To keep track of the genz iterations.

Definition at line 52 of file prg\_genz\_mod.F90.

#### 10.4.2.3 logical prg\_genz\_mod::genzspinp::integration

If we want to do XL integration scheme for Z.

Definition at line 49 of file prg\_genz\_mod.F90.

#### 10.4.2.4 integer prg\_genz\_mod::genzspinp::mdim

Max nonzero elements per row for every row see [1] .

Definition at line 58 of file prg\_genz\_mod.F90.

#### 10.4.2.5 integer prg\_genz\_mod::genzspinp::nfirst

!Lentgth of the "firsts iteration period".

Definition at line 34 of file prg\_genz\_mod.F90.

#### 10.4.2.6 integer prg\_genz\_mod::genzspinp::nreff

!Initial number of recursive refinements.

Definition at line 40 of file prg\_genz\_mod.F90.

#### 10.4.2.7 integer prg\_genz\_mod::genzspinp::nrefi

!Initial number of recursive refinements.

Definition at line 37 of file prg\_genz\_mod.F90.

#### 10.4.2.8 real(dp) prg\_genz\_mod::genzspinp::numthresf

Final threshold value.

Definition at line 46 of file prg\_genz\_mod.F90.

#### 10.4.2.9 real(dp) prg\_genz\_mod::genzspinp::numthresi

Initial threshold value.

Definition at line 43 of file prg\_genz\_mod.F90.

#### 10.4.2.10 integer prg\_genz\_mod::genzspinp::verbose

To have different levels of verbose.

Definition at line 31 of file prg\_genz\_mod.F90.

## 10.4.2.11 logical prg\_genz\_mod::genzspinp::zsp

Logical variable to compute in sparse or dense mode.

Definition at line 55 of file prg\_genz\_mod.F90.

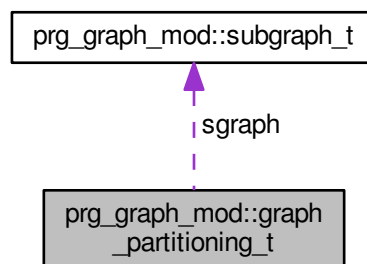
The documentation for this type was generated from the following file:

- [/home/christian/qmd-progress/src/prg\\_genz\\_mod.F90](#)

## 10.5 prg\_graph\_mod::graph\_partitioning\_t Type Reference

Trace per iteration.

Collaboration diagram for prg\_graph\_mod::graph\_partitioning\_t:



## Private Attributes

- character(len=100) [pname](#)  
*Partition name.*
- integer [myrank](#)  
*Local processor.*
- integer [totalprocs](#)  
*Number of processors.*
- integer [totalparts](#)  
*Total number of global partitions.*
- integer [totalnodes](#)  
*Total number of global groups, nodes (or matrix rows)*
- integer [totalnodes2](#)  
*Total number of global nodes (or matrix rows)*
- integer [globalpartmin](#)  
*Minimum global part number.*
- integer [globalpartmax](#)  
*Maximum global part number.*

- integer [globalpartextent](#)  
*Total global parts.*
- integer, dimension(:), allocatable [localpartmin](#)  
*Minimum part per processor.*
- integer, dimension(:), allocatable [localpartmax](#)  
*Maximum part per processor.*
- integer, dimension(:), allocatable [localpartextent](#)  
*Number of parts per processor.*
- integer, dimension(:), allocatable [order](#)  
*Original ordering if required.*
- integer, dimension(:), allocatable [reorder](#)  
*Reordering if required.*
- integer [nparts](#)  
*Total number of local partitions.*
- integer, dimension(:), allocatable [nnodesinpart](#)  
*Number of nodes in each local partition.*
- integer, dimension(:), allocatable [nnodesinpartall](#)  
*Number of nodes in each partition.*
- integer, dimension(100) [pp](#)  
*Sequence for SP2.*
- integer [maxiter](#)  
*Number of SP2 iterations.*
- real(dp) [ehomo](#)  
*Homo value.*
- real(dp) [elummo](#)  
*Lumo value.*
- real(dp) [mineval](#)  
*Min eval for prg\_normalize.*
- real(dp) [maxeval](#)  
*Max eval for prg\_normalize.*
- real(dp), dimension(100) [vv](#)  
*Trace per iteration.*
- type([subgraph\\_t](#)), dimension(:), allocatable [sgraph](#)  
*Subgraph details.*

### 10.5.1 Detailed Description

Trace per iteration.

Graph partitioning type

Definition at line 57 of file prg\_graph\_mod.F90.

### 10.5.2 Member Data Documentation

#### 10.5.2.1 `real(dp) prg_graph_mod::graph_partitioning_t::ehomo` [private]

Homo value.

Definition at line 117 of file prg\_graph\_mod.F90.



**10.5.2.2** `real(dp) prg_graph_mod::graph_partitioning_t::elumo` `[private]`

Lumo value.

Definition at line 120 of file prg\_graph\_mod.F90.

**10.5.2.3** `integer prg_graph_mod::graph_partitioning_t::globalpartextent` `[private]`

Total global parts.

Definition at line 84 of file prg\_graph\_mod.F90.

**10.5.2.4** `integer prg_graph_mod::graph_partitioning_t::globalpartmax` `[private]`

Maximum global part number.

Definition at line 81 of file prg\_graph\_mod.F90.

**10.5.2.5** `integer prg_graph_mod::graph_partitioning_t::globalpartmin` `[private]`

Minimum global part number.

Definition at line 78 of file prg\_graph\_mod.F90.

**10.5.2.6** `integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::localpartextent` `[private]`

Number of parts per processor.

Definition at line 93 of file prg\_graph\_mod.F90.

**10.5.2.7** `integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::localpartmax` `[private]`

Maximum part per processor.

Definition at line 90 of file prg\_graph\_mod.F90.

**10.5.2.8** `integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::localpartmin` `[private]`

Minimum part per processor.

Definition at line 87 of file prg\_graph\_mod.F90.

**10.5.2.9** `real(dp) prg_graph_mod::graph_partitioning_t::maxeval` `[private]`

Max eval for prg\_normalize.

Definition at line 126 of file prg\_graph\_mod.F90.

10.5.2.10 `integer prg_graph_mod::graph_partitioning_t::maxiter` `[private]`

Number of SP2 iterations.

Definition at line 114 of file `prg_graph_mod.F90`.

10.5.2.11 `real(dp) prg_graph_mod::graph_partitioning_t::mineval` `[private]`

Min eval for `prg_normalize`.

Definition at line 123 of file `prg_graph_mod.F90`.

10.5.2.12 `integer prg_graph_mod::graph_partitioning_t::myrank` `[private]`

Local processor.

Definition at line 63 of file `prg_graph_mod.F90`.

10.5.2.13 `integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::nnodesinpart` `[private]`

Number of nodes in each local partition.

Definition at line 105 of file `prg_graph_mod.F90`.

10.5.2.14 `integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::nnodesinpartall` `[private]`

Number of nodes in each partition.

Definition at line 108 of file `prg_graph_mod.F90`.

10.5.2.15 `integer prg_graph_mod::graph_partitioning_t::nparts` `[private]`

Total number of local partitions.

Definition at line 102 of file `prg_graph_mod.F90`.

10.5.2.16 `integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::order` `[private]`

Original ordering if required.

Definition at line 96 of file `prg_graph_mod.F90`.

10.5.2.17 `character(len=100) prg_graph_mod::graph_partitioning_t::pname` `[private]`

Partition name.

Definition at line 60 of file `prg_graph_mod.F90`.

10.5.2.18 integer, dimension(100) prg\_graph\_mod::graph\_partitioning\_t::pp [private]

Sequence for SP2.

Definition at line 111 of file prg\_graph\_mod.F90.

10.5.2.19 integer, dimension(:), allocatable prg\_graph\_mod::graph\_partitioning\_t::reorder [private]

Reordering if required.

Definition at line 99 of file prg\_graph\_mod.F90.

10.5.2.20 type (subgraph\_t), dimension(:), allocatable prg\_graph\_mod::graph\_partitioning\_t::sgraph [private]

Subgraph details.

Definition at line 132 of file prg\_graph\_mod.F90.

10.5.2.21 integer prg\_graph\_mod::graph\_partitioning\_t::totalnodes [private]

Total number of global groups, nodes (or matrix rows)

Definition at line 72 of file prg\_graph\_mod.F90.

10.5.2.22 integer prg\_graph\_mod::graph\_partitioning\_t::totalnodes2 [private]

Total number of global nodes (or matrix rows)

Definition at line 75 of file prg\_graph\_mod.F90.

10.5.2.23 integer prg\_graph\_mod::graph\_partitioning\_t::totalparts [private]

Total number of global partitions.

Definition at line 69 of file prg\_graph\_mod.F90.

10.5.2.24 integer prg\_graph\_mod::graph\_partitioning\_t::totalprocs [private]

Number of processors.

Definition at line 66 of file prg\_graph\_mod.F90.

10.5.2.25 `real(dp), dimension(100) prg_graph_mod::graph_partitioning_t::vv` `[private]`

Trace per iteration.

Definition at line 129 of file `prg_graph_mod.F90`.

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

- [/home/christian/qmd-progress/src/prg\\_graph\\_mod.F90](#)

## 10.6 prg\_graphsp2parser\_mod::gsp2data\_type Type Reference

General SP2 solver type.

### Public Attributes

- `character(20)` [jobname](#)
- `character(50)` [hamfile](#)
- `integer` [verbose](#)
- `integer` [minsp2iter](#)
- `integer` [maxsp2iter](#)
- `integer` [nodesperpart](#)
- `integer` [natoms](#)
- `integer` [partition\\_count](#)
- `real(dp)` [sp2tol](#)
- `real(dp)` [threshold](#)
- `real(dp)` [bndfil](#)
- `real(dp)` [gthreshold](#)
- `real(dp)` [errlimit](#)
- `integer` [mdim](#)
- `integer` [ndim](#)
- `character, dimension(3)` [sdim](#)
- `real(dp), dimension(3)` [pdim](#)
- `character(20)` [bml\\_type](#)
- `character(10)` [sp2conv](#)
- `character(10)` [graph\\_element](#)
- `character(10)` [partition\\_type](#)
- `character(10)` [partition\\_refinement](#)
- `logical` [double\\_jump](#)
- `real(dp)` [covgfact](#)
- `real(dp)` [nlgcut](#)
- `integer` [parteach](#)

### 10.6.1 Detailed Description

General SP2 solver type.

Definition at line 26 of file `prg_graphsp2parser_mod.F90`.

## 10.6.2 Member Data Documentation

### 10.6.2.1 character(20) prg\_graphsp2parser\_mod::gsp2data\_type::bml\_type

Definition at line 44 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.2 real(dp) prg\_graphsp2parser\_mod::gsp2data\_type::bndfil

Definition at line 37 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.3 real(dp) prg\_graphsp2parser\_mod::gsp2data\_type::covgfact

Definition at line 50 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.4 logical prg\_graphsp2parser\_mod::gsp2data\_type::double\_jump

Definition at line 49 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.5 real(dp) prg\_graphsp2parser\_mod::gsp2data\_type::errlimit

Definition at line 39 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.6 character(10) prg\_graphsp2parser\_mod::gsp2data\_type::graph\_element

Definition at line 46 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.7 real(dp) prg\_graphsp2parser\_mod::gsp2data\_type::gthreshold

Definition at line 38 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.8 character(50) prg\_graphsp2parser\_mod::gsp2data\_type::hamfile

Definition at line 28 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.9 character(20) prg\_graphsp2parser\_mod::gsp2data\_type::jobname

Definition at line 27 of file prg\_graphsp2parser\_mod.F90.

### 10.6.2.10 integer prg\_graphsp2parser\_mod::gsp2data\_type::maxsp2iter

Definition at line 31 of file prg\_graphsp2parser\_mod.F90.

10.6.2.11 integer prg\_graphsp2parser\_mod::gsp2data\_type::mdim

Definition at line 40 of file prg\_graphsp2parser\_mod.F90.

10.6.2.12 integer prg\_graphsp2parser\_mod::gsp2data\_type::minsp2iter

Definition at line 30 of file prg\_graphsp2parser\_mod.F90.

10.6.2.13 integer prg\_graphsp2parser\_mod::gsp2data\_type::natoms

Definition at line 33 of file prg\_graphsp2parser\_mod.F90.

10.6.2.14 integer prg\_graphsp2parser\_mod::gsp2data\_type::ndim

Definition at line 41 of file prg\_graphsp2parser\_mod.F90.

10.6.2.15 real(dp) prg\_graphsp2parser\_mod::gsp2data\_type::nlgcut

Definition at line 51 of file prg\_graphsp2parser\_mod.F90.

10.6.2.16 integer prg\_graphsp2parser\_mod::gsp2data\_type::nodesperpart

Definition at line 32 of file prg\_graphsp2parser\_mod.F90.

10.6.2.17 integer prg\_graphsp2parser\_mod::gsp2data\_type::parteach

Definition at line 52 of file prg\_graphsp2parser\_mod.F90.

10.6.2.18 integer prg\_graphsp2parser\_mod::gsp2data\_type::partition\_count

Definition at line 34 of file prg\_graphsp2parser\_mod.F90.

10.6.2.19 character(10) prg\_graphsp2parser\_mod::gsp2data\_type::partition\_refinement

Definition at line 48 of file prg\_graphsp2parser\_mod.F90.

10.6.2.20 character(10) prg\_graphsp2parser\_mod::gsp2data\_type::partition\_type

Definition at line 47 of file prg\_graphsp2parser\_mod.F90.

10.6.2.21 `real(dp), dimension(3) prg_graphsp2parser_mod::gsp2data_type::pdim`

Definition at line 43 of file `prg_graphsp2parser_mod.F90`.

10.6.2.22 `character, dimension(3) prg_graphsp2parser_mod::gsp2data_type::sdim`

Definition at line 42 of file `prg_graphsp2parser_mod.F90`.

10.6.2.23 `character(10) prg_graphsp2parser_mod::gsp2data_type::sp2conv`

Definition at line 45 of file `prg_graphsp2parser_mod.F90`.

10.6.2.24 `real(dp) prg_graphsp2parser_mod::gsp2data_type::sp2tol`

Definition at line 35 of file `prg_graphsp2parser_mod.F90`.

10.6.2.25 `real(dp) prg_graphsp2parser_mod::gsp2data_type::threshold`

Definition at line 36 of file `prg_graphsp2parser_mod.F90`.

10.6.2.26 `integer prg_graphsp2parser_mod::gsp2data_type::verbose`

Definition at line 29 of file `prg_graphsp2parser_mod.F90`.

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

- [/home/christian/qmd-progress/src/prg\\_graphsp2parser\\_mod.F90](#)

## 10.7 prg\_pulaymixer\_mod::mx\_type Type Reference

### Public Attributes

- `character(20) mixertype`  
*Type or mixing scheme to be used (Linear or Pulay)*
- `integer verbose`  
*Verbosity level.*
- `integer mpulay`  
*Pulay dimension for matrix.*
- `real(dp) mixcoeff`  
*Coefficient for mixing.*
- `logical mixeron`  
*Mixer on or off (Not implemented)*

### 10.7.1 Detailed Description

Definition at line 16 of file prg\_pulaymixer\_mod.F90.

### 10.7.2 Member Data Documentation

#### 10.7.2.1 `real(dp) prg_pulaymixer_mod::mx_type::mixcoeff`

Coefficient for mixing.

Definition at line 28 of file prg\_pulaymixer\_mod.F90.

#### 10.7.2.2 `logical prg_pulaymixer_mod::mx_type::mixeron`

Mixer on or off (Not implemented)

Definition at line 31 of file prg\_pulaymixer\_mod.F90.

#### 10.7.2.3 `character(20) prg_pulaymixer_mod::mx_type::mixertype`

Type or mixing scheme to be used (Linear or Pulay)

Definition at line 19 of file prg\_pulaymixer\_mod.F90.

#### 10.7.2.4 `integer prg_pulaymixer_mod::mx_type::mpulay`

Pulay dimension for matrix.

Definition at line 25 of file prg\_pulaymixer\_mod.F90.

#### 10.7.2.5 `integer prg_pulaymixer_mod::mx_type::verbose`

Verbosity level.

Definition at line 22 of file prg\_pulaymixer\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_pulaymixer\\_mod.F90](#)

## 10.8 `prg_extras_mod::prg_memory_consumption` Interface Reference

### Private Member Functions

- subroutine [prg\\_memory\\_consumption](#) (vm\_peak, vm\_size, pid, ppid)



### 10.8.1 Detailed Description

Definition at line 15 of file prg\_extras\_mod.F90.

### 10.8.2 Constructor & Destructor Documentation

10.8.2.1 subroutine prg\_extras\_mod::prg\_memory\_consumption::prg\_memory\_consumption ( integer(c\_long\_long), intent(inout) *vm\_peak*, integer(c\_long\_long), intent(inout) *vm\_size*, integer(c\_long\_long), intent(inout) *pid*, integer(c\_long\_long), intent(inout) *ppid* ) [private]

Definition at line 17 of file prg\_extras\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_extras\\_mod.F90](#)

## 10.9 prg\_parallel\_mod::rankreducedata\_t Type Reference

Data structure for rection over MPI ranks.

### Private Attributes

- real(dp) *val*  
*Data value.*
- integer *rank*  
*MPI rank.*

### 10.9.1 Detailed Description

Data structure for rection over MPI ranks.

Definition at line 72 of file prg\_parallel\_mod.F90.

### 10.9.2 Member Data Documentation

10.9.2.1 integer prg\_parallel\_mod::rankreducedata\_t::rank [private]

MPI rank.

Definition at line 78 of file prg\_parallel\_mod.F90.

### 10.9.2.2 `real(dp) prg_parallel_mod::rankreducedata_t::val` `[private]`

Data value.

Definition at line 75 of file `prg_parallel_mod.F90`.

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

- [/home/christian/qmd-progress/src/prg\\_parallel\\_mod.F90](#)

## 10.10 `prg_response_mod::respdata_type` Type Reference

### Public Attributes

- character(20) [respmode](#)
- character(20) [typeofpert](#)
- character(20) [bmltype](#)
- integer [mdim](#)
- real(dp) [numthresh](#)
- logical [computedipole](#)
- logical [getresponse](#)
- real(dp) [fieldintensity](#)
- real(dp), dimension(3) [field](#)

### 10.10.1 Detailed Description

Definition at line 21 of file `prg_response_mod.F90`.

### 10.10.2 Member Data Documentation

#### 10.10.2.1 `character(20) prg_response_mod::respdata_type::bmltype`

Definition at line 24 of file `prg_response_mod.F90`.

#### 10.10.2.2 `logical prg_response_mod::respdata_type::computedipole`

Definition at line 27 of file `prg_response_mod.F90`.

#### 10.10.2.3 `real(dp), dimension(3) prg_response_mod::respdata_type::field`

Definition at line 30 of file `prg_response_mod.F90`.

#### 10.10.2.4 `real(dp) prg_response_mod::respdata_type::fieldintensity`

Definition at line 29 of file `prg_response_mod.F90`.

## 10.10.2.5 logical prg\_response\_mod::respdata\_type::getresponse

Definition at line 28 of file prg\_response\_mod.F90.

## 10.10.2.6 integer prg\_response\_mod::respdata\_type::mdim

Definition at line 25 of file prg\_response\_mod.F90.

## 10.10.2.7 real(dp) prg\_response\_mod::respdata\_type::numthresh

Definition at line 26 of file prg\_response\_mod.F90.

## 10.10.2.8 character(20) prg\_response\_mod::respdata\_type::respmode

Definition at line 22 of file prg\_response\_mod.F90.

## 10.10.2.9 character(20) prg\_response\_mod::respdata\_type::typeofpert

Definition at line 23 of file prg\_response\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_response\\_mod.F90](#)

## 10.11 prg\_syrotation\_mod::rotation\_type Type Reference

Rotation type.

### Public Attributes

- character(20) [jobname](#)
- character(50) [typeofrot](#)
- integer [patom1](#)  
*Atomic point to determine the initial orientation.*
- integer [patom2](#)  
*Atomic point to determine initial orientation.*
- integer [catom](#)  
*Atomic point to determine the rotation center.*
- integer [catom2](#)  
*Atomic point to determine a second rotation center.*
- real(dp), dimension(3) [pq1](#)  
*Point to determine initial orientation.*
- real(dp), dimension(3) [pq2](#)  
*Point to determine final orientation.*
- real(dp), dimension(3) [v1](#)  
*Initial orientation.*
- real(dp), dimension(3) [v2](#)  
*Final orientation.*
- real(dp), dimension(3) [vq](#)  
*Center of rotation.*
- integer, dimension(2) [rotate\\_atoms](#)  
*First and last rotated atom in the list.*

### 10.11.1 Detailed Description

Rotation type.

Definition at line 17 of file prg\_syrotation\_mod.F90.

### 10.11.2 Member Data Documentation

#### 10.11.2.1 integer prg\_syrotation\_mod::rotation\_type::catom

Atomic point to determine the rotation center.

Definition at line 25 of file prg\_syrotation\_mod.F90.

#### 10.11.2.2 integer prg\_syrotation\_mod::rotation\_type::catom2

Atomic point to determine a second rotation center.

Definition at line 27 of file prg\_syrotation\_mod.F90.

#### 10.11.2.3 character(20) prg\_syrotation\_mod::rotation\_type::jobname

Definition at line 18 of file prg\_syrotation\_mod.F90.

#### 10.11.2.4 integer prg\_syrotation\_mod::rotation\_type::patom1

Atomic point to determine the initial orientation.

Definition at line 21 of file prg\_syrotation\_mod.F90.

#### 10.11.2.5 integer prg\_syrotation\_mod::rotation\_type::patom2

Atomic point to determine initial orientation.

Definition at line 23 of file prg\_syrotation\_mod.F90.

#### 10.11.2.6 real(dp), dimension(3) prg\_syrotation\_mod::rotation\_type::pq1

Point to determine initial orientation.

Definition at line 29 of file prg\_syrotation\_mod.F90.

**10.11.2.7 real(dp), dimension(3) prg\_syrotation\_mod::rotation\_type::pq2**

Point to determine final orientation.

Definition at line 31 of file prg\_syrotation\_mod.F90.

**10.11.2.8 integer, dimension(2) prg\_syrotation\_mod::rotation\_type::rotate\_atoms**

First and last rotated atom in the list.

Definition at line 39 of file prg\_syrotation\_mod.F90.

**10.11.2.9 character(50) prg\_syrotation\_mod::rotation\_type::typeofrot**

Definition at line 19 of file prg\_syrotation\_mod.F90.

**10.11.2.10 real(dp), dimension(3) prg\_syrotation\_mod::rotation\_type::v1**

Initial orientation.

Definition at line 33 of file prg\_syrotation\_mod.F90.

**10.11.2.11 real(dp), dimension(3) prg\_syrotation\_mod::rotation\_type::v2**

Final orientation.

Definition at line 35 of file prg\_syrotation\_mod.F90.

**10.11.2.12 real(dp), dimension(3) prg\_syrotation\_mod::rotation\_type::vq**

Center of rotation.

Definition at line 37 of file prg\_syrotation\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_syrotation\\_mod.F90](#)

**10.12 prg\_sp2parser\_mod::sp2data\_type Type Reference**

General SP2 solver type.

## Public Attributes

- character(20) [jobname](#)
- integer [verbose](#)
- integer [minsp2iter](#)
- integer [maxsp2iter](#)
- real(dp) [sp2tol](#)
- real(dp) [threshold](#)
- real(dp) [bndfil](#)
- integer [mdim](#)
- integer [ndim](#)
- character, dimension(3) [sdim](#)
- real(dp), dimension(3) [pdim](#)
- character(20) [bml\\_type](#)
- character(10) [sp2conv](#)
- character(10) [flavor](#)

### 10.12.1 Detailed Description

General SP2 solver type.

Definition at line 26 of file `prg_sp2parser_mod.F90`.

### 10.12.2 Member Data Documentation

#### 10.12.2.1 character(20) `prg_sp2parser_mod::sp2data_type::bml_type`

Definition at line 38 of file `prg_sp2parser_mod.F90`.

#### 10.12.2.2 real(dp) `prg_sp2parser_mod::sp2data_type::bndfil`

Definition at line 33 of file `prg_sp2parser_mod.F90`.

#### 10.12.2.3 character(10) `prg_sp2parser_mod::sp2data_type::flavor`

Definition at line 40 of file `prg_sp2parser_mod.F90`.

#### 10.12.2.4 character(20) `prg_sp2parser_mod::sp2data_type::jobname`

Definition at line 27 of file `prg_sp2parser_mod.F90`.

#### 10.12.2.5 integer `prg_sp2parser_mod::sp2data_type::maxsp2iter`

Definition at line 30 of file `prg_sp2parser_mod.F90`.

10.12.2.6 integer prg\_sp2parser\_mod::sp2data\_type::mdim

Definition at line 34 of file prg\_sp2parser\_mod.F90.

10.12.2.7 integer prg\_sp2parser\_mod::sp2data\_type::minsp2iter

Definition at line 29 of file prg\_sp2parser\_mod.F90.

10.12.2.8 integer prg\_sp2parser\_mod::sp2data\_type::ndim

Definition at line 35 of file prg\_sp2parser\_mod.F90.

10.12.2.9 real(dp), dimension(3) prg\_sp2parser\_mod::sp2data\_type::pdim

Definition at line 37 of file prg\_sp2parser\_mod.F90.

10.12.2.10 character, dimension(3) prg\_sp2parser\_mod::sp2data\_type::sdim

Definition at line 36 of file prg\_sp2parser\_mod.F90.

10.12.2.11 character(10) prg\_sp2parser\_mod::sp2data\_type::sp2conv

Definition at line 39 of file prg\_sp2parser\_mod.F90.

10.12.2.12 real(dp) prg\_sp2parser\_mod::sp2data\_type::sp2tol

Definition at line 31 of file prg\_sp2parser\_mod.F90.

10.12.2.13 real(dp) prg\_sp2parser\_mod::sp2data\_type::threshold

Definition at line 32 of file prg\_sp2parser\_mod.F90.

10.12.2.14 integer prg\_sp2parser\_mod::sp2data\_type::verbose

Definition at line 28 of file prg\_sp2parser\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_sp2parser\\_mod.F90](#)

## 10.13 prg\_graph\_mod::subgraph\_t Type Reference

Subgraph type.

### Private Attributes

- integer [part](#)  
*Partition number.*
- integer [hsize](#)  
*Size of original matrix (h x h)*
- integer [lsize](#)  
*Size of full subgraph (l x l)*
- integer [llsize](#)  
*Size of core subgraph.*
- integer, dimension(:), allocatable [core\\_halo\\_index](#)  
*Indeces from original matrix for subgraph core+halo extraction.*
- integer, dimension(:), allocatable [nodeinpart](#)  
*Nodes in this partition.*

### 10.13.1 Detailed Description

Subgraph type.

Definition at line 31 of file prg\_graph\_mod.F90.

### 10.13.2 Member Data Documentation

**10.13.2.1** integer, dimension(:), allocatable `prg_graph_mod::subgraph_t::core_halo_index` `[private]`

Indeces from original matrix for subgraph core+halo extraction.

Definition at line 46 of file prg\_graph\_mod.F90.

**10.13.2.2** integer `prg_graph_mod::subgraph_t::hsize` `[private]`

Size of original matrix (h x h)

Definition at line 37 of file prg\_graph\_mod.F90.

**10.13.2.3** integer `prg_graph_mod::subgraph_t::llsize` `[private]`

Size of core subgraph.

Definition at line 43 of file prg\_graph\_mod.F90.



10.13.2.4 integer prg\_graph\_mod::subgraph\_t::lsize [private]

Size of full subgraph (l x l)

Definition at line 40 of file prg\_graph\_mod.F90.

10.13.2.5 integer, dimension(:), allocatable prg\_graph\_mod::subgraph\_t::nodeinpart [private]

Nodes in this partition.

Definition at line 49 of file prg\_graph\_mod.F90.

10.13.2.6 integer prg\_graph\_mod::subgraph\_t::part [private]

Partition number.

Definition at line 34 of file prg\_graph\_mod.F90.

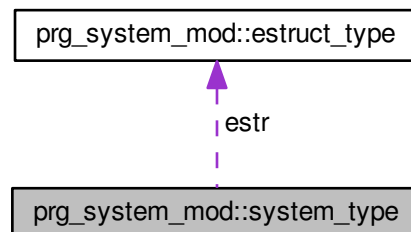
The documentation for this type was generated from the following file:

- [/home/christian/qmd-progress/src/prg\\_graph\\_mod.F90](#)

## 10.14 prg\_system\_mod::system\_type Type Reference

System type.

Collaboration diagram for prg\_system\_mod::system\_type:



## Public Attributes

- integer **nats**  
*Number of atoms of the system.*
- character(2), dimension(:), allocatable **symbol**  
*Chemical Symbols for every atom of the system. Symbol can be recovered using ptable module and calling the following routine:*
- integer, dimension(:), allocatable **atomic\_number**  
*Atomic number for every atom in the system.*
- real(**dp**), dimension(:, :), allocatable **coordinate**  
*Coordinates of every atom in the system. Allocation:*
- real(**dp**), dimension(:, :), allocatable **velocity**  
*Velocities for every atom in the system. Allocation:*
- real(**dp**), dimension(:, :), allocatable **force**  
*Forces acting on every atom in the system. Allocation:*
- real(**dp**), dimension(:), allocatable **net\_charge**  
*Charges of every atom in the system. Allocation:*
- real(**dp**), dimension(:), allocatable **mass**  
*Mass of every atom in the system. These can be automatically loaded by using the structures of the ptable mod:*
- real(**dp**), dimension(:, :), allocatable **lattice\_vector**  
*Lattice vectors of the system. Use the prg\_vectors\_to\_parameters and parameters\_to\_vector to transform from lattice vector to lattice parameters. Allocation:*
- real(**dp**), dimension(:, :), allocatable **recip\_vector**  
*Reciprocal vectors of the system. Allocation:*
- real(**dp**) **volr**  
*Volume of the system (direct space).*
- real(**dp**) **volk**  
*Volume of the system (direct space).*
- integer **nsp**  
*Number of different species. Number of species or number of different atom types (symbols) in the system. This integer is always less or equal than the total number of atoms (nsp <= nats). This information can also be found in tparams structure and the following equality holds:*
- integer, dimension(:), allocatable **spindex**  
*Species index. It gives the species index of a particular atom. Allocation:*
- character(2), dimension(:), allocatable **splist**  
*Species symbol list. A list with the different species e.g. H, C, N, etc with the order corresponding to the appearance in systemsymbol. Allocation:*
- integer, dimension(:), allocatable **spatnum**  
*Species atomic number list. A list with the atomic numbers for every species Allocation:*
- real(**dp**), dimension(:), allocatable **spmass**  
*Species mass list. A list with the atomic mass for every species Allocation:*
- real(**dp**), dimension(:), allocatable **userdef**  
*User define field.*
- integer, dimension(:), allocatable **resindex**  
*Residue index.*
- type(**estruct\_type**) **estr**  
*Electronic structure.*

### 10.14.1 Detailed Description

System type.

The molecular system type.

Definition at line 75 of file prg\_system\_mod.F90.

## 10.14.2 Member Data Documentation

### 10.14.2.1 integer, dimension(:), allocatable prg\_system\_mod::system\_type::atomic\_number

Atomic number for every atom in the system.

Definition at line 89 of file prg\_system\_mod.F90.

### 10.14.2.2 real(dp), dimension(:, :), allocatable prg\_system\_mod::system\_type::coordinate

Coordinates of every atom in the system. Allocation:

```
coordinate(3,nats)
```

Definition at line 94 of file prg\_system\_mod.F90.

### 10.14.2.3 type(estruct\_type) prg\_system\_mod::system\_type::estr

Electronic structure.

Definition at line 187 of file prg\_system\_mod.F90.

### 10.14.2.4 real(dp), dimension(:, :), allocatable prg\_system\_mod::system\_type::force

Forces acting on every atom in the system. Allocation:

```
force(3,nats)
```

Definition at line 104 of file prg\_system\_mod.F90.

### 10.14.2.5 real(dp), dimension(:, :), allocatable prg\_system\_mod::system\_type::lattice\_vector

Lattice vectors of the system. Use the prg\_vectors\_to\_parameters and parameters\_to\_vector to transform from lattice vector to lattice parameters. Allocation:

```
lattice_vector(3,3)
```

```
v1 = lattice_vector(1,:)
```

```
v2 = lattice_vector(2,:)
```

```
v3 = lattice_vector(3,:)
```

Definition at line 126 of file prg\_system\_mod.F90.

**10.14.2.6 real(dp), dimension(:), allocatable prg\_system\_mod::system\_type::mass**

Mass of every atom in the system. These can be automatically loaded by using the structures of the ptable mod:

```
system%mass(i) = mass(mystem%atomic_number(i))
```

Allocation:

```
mass(nats)
```

Definition at line 116 of file prg\_system\_mod.F90.

**10.14.2.7 integer prg\_system\_mod::system\_type::nats**

Number of atoms of the system.

Definition at line 78 of file prg\_system\_mod.F90.

**10.14.2.8 real(dp), dimension(:), allocatable prg\_system\_mod::system\_type::net\_charge**

Charges of every atom in the system. Allocation:

```
net_charge(nats)
```

Definition at line 109 of file prg\_system\_mod.F90.

**10.14.2.9 integer prg\_system\_mod::system\_type::nsp**

Number of different species. Number of species or number of different atom types (symbols) in the system. This integer is always less or equal than the total number of atoms ( $nsp \leq nats$ ). This information can also be found in tbparams structure and the following equality holds:

```
system%nsp = tbparams%nsp
```

Definition at line 149 of file prg\_system\_mod.F90.

**10.14.2.10 real(dp), dimension(:, :), allocatable prg\_system\_mod::system\_type::recip\_vector**

Reciprocal vectors of the system. Allocation:

```
recip_vector(3,3)
```

```
v1 = recip_vector(1,:)
```

```
v2 = recip_vector(2,:)
```

```
v3 = recip_vector(3,:)
```

Definition at line 134 of file prg\_system\_mod.F90.

**10.14.2.11 integer, dimension(:), allocatable prg\_system\_mod::system\_type::resindex**

Residue index.

Definition at line 184 of file prg\_system\_mod.F90.

**10.14.2.12 integer, dimension(:), allocatable prg\_system\_mod::system\_type::spatnum**

Species atomic number list. A list with the atomic numbers for every species Allocation:

```
spatnum(nsp)
```

Definition at line 172 of file prg\_system\_mod.F90.

**10.14.2.13 integer, dimension(:), allocatable prg\_system\_mod::system\_type::spindex**

Species index. It gives the species index of a particular atom. Allocation:

```
spindex(nats)
```

If we need the index of atom 30 then:

```
system%spindex(30)
```

Definition at line 157 of file prg\_system\_mod.F90.

**10.14.2.14 character(2), dimension(:), allocatable prg\_system\_mod::system\_type::splist**

Species symbol list. A list with the different species e.g. H, C, N, etc with the order corresponding to the appearance in systemsymbol. Allocation:

```
splist(nsp)
```

Definition at line 165 of file prg\_system\_mod.F90.

**10.14.2.15 real(dp), dimension(:), allocatable prg\_system\_mod::system\_type::spmass**

Species mass list. A list with the atomic mass for every species Allocation:

```
spmass(nsp)
```

Definition at line 178 of file prg\_system\_mod.F90.

**10.14.2.16** `character(2), dimension(:), allocatable prg_system_mod::system_type::symbol`

Chemical Symbols for every atom of the system. Symbol can be recovered using ptable module and calling the following routine:

```
system%symbol(i) = element_symbol(system%atomic_number(i))
```

Allocation:

```
symbol(nats)
```

Definition at line 86 of file prg\_system\_mod.F90.

**10.14.2.17** `real(dp), dimension(:), allocatable prg_system_mod::system_type::userdef`

User define field.

Definition at line 181 of file prg\_system\_mod.F90.

**10.14.2.18** `real(dp), dimension(:, :), allocatable prg_system_mod::system_type::velocity`

Velocities for every atom in the system. Allocation:

```
velocity(3, nats)
```

Definition at line 99 of file prg\_system\_mod.F90.

**10.14.2.19** `real(dp) prg_system_mod::system_type::volk`

Volume of the system (direct space).

**Note**

use prg\_get\_recip\_vects in coulomb\_latte\_mod to compute this.

Definition at line 142 of file prg\_system\_mod.F90.

**10.14.2.20** `real(dp) prg_system_mod::system_type::volr`

Volume of the system (direct space).

**Note**

use prg\_get\_recip\_vects in coulomb\_latte\_mod to compute this.

Definition at line 138 of file prg\_system\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_system\\_mod.F90](#)

## 10.15 prg\_timer\_mod::timer\_status\_t Type Reference

Timer status type.

### Private Attributes

- character(len=20) [tname](#)  
*Timer name.*
- integer [tstart](#)  
*Start time.*
- integer [ttotal](#)  
*Current total time.*
- integer [tcount](#)  
*Current call count.*
- integer [minrank](#)  
*Rank with min value.*
- integer [maxrank](#)  
*Rank with max value.*
- real(dp) [tsum](#)  
*Sum time - total time in secs.*
- real(dp) [minvalue](#)  
*Minimum value over all ranks.*
- real(dp) [maxvalue](#)  
*Maximum value over all ranks.*
- real(dp) [tavg](#)  
*Average value over all ranks.*
- real(dp) [tstdev](#)  
*Stdev across all ranks.*
- real(dp) [tpercent](#)  
*Percent of time across all timers.*

### 10.15.1 Detailed Description

Timer status type.

Definition at line 54 of file prg\_timer\_mod.F90.

### 10.15.2 Member Data Documentation

#### 10.15.2.1 integer prg\_timer\_mod::timer\_status\_t::maxrank [private]

Rank with max value.

Definition at line 72 of file prg\_timer\_mod.F90.

**10.15.2.2** `real(dp) prg_timer_mod::timer_status_t::maxvalue` `[private]`

Maximum value over all ranks.

Definition at line 81 of file `prg_timer_mod.F90`.

**10.15.2.3** `integer prg_timer_mod::timer_status_t::minrank` `[private]`

Rank with min value.

Definition at line 69 of file `prg_timer_mod.F90`.

**10.15.2.4** `real(dp) prg_timer_mod::timer_status_t::minvalue` `[private]`

Minimum value over all ranks.

Definition at line 78 of file `prg_timer_mod.F90`.

**10.15.2.5** `real(dp) prg_timer_mod::timer_status_t::tavg` `[private]`

Average value over all ranks.

Definition at line 84 of file `prg_timer_mod.F90`.

**10.15.2.6** `integer prg_timer_mod::timer_status_t::tcount` `[private]`

Current call count.

Definition at line 66 of file `prg_timer_mod.F90`.

**10.15.2.7** `character(len=20) prg_timer_mod::timer_status_t::tname` `[private]`

Timer name.

Definition at line 57 of file `prg_timer_mod.F90`.

**10.15.2.8** `real(dp) prg_timer_mod::timer_status_t::tpercent` `[private]`

Percent of time across all timers.

Definition at line 90 of file `prg_timer_mod.F90`.

**10.15.2.9** `integer prg_timer_mod::timer_status_t::tstart` `[private]`

Start time.

Definition at line 60 of file `prg_timer_mod.F90`.



10.15.2.10 `real(dp) prg_timer_mod::timer_status_t::tstdev` `[private]`

Stdev across all ranks.

Definition at line 87 of file `prg_timer_mod.F90`.

10.15.2.11 `real(dp) prg_timer_mod::timer_status_t::tsum` `[private]`

Sum time - total time in secs.

Definition at line 75 of file `prg_timer_mod.F90`.

10.15.2.12 `integer prg_timer_mod::timer_status_t::ttotal` `[private]`

Current total time.

Definition at line 63 of file `prg_timer_mod.F90`.

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

- [/home/christian/qmd-progress/src/prg\\_timer\\_mod.F90](#)

## 10.16 prg\_extras\_mod::to\_string Interface Reference

### Private Member Functions

- `character(len=:)` function, allocatable [to\\_string\\_integer](#) (i)  
*Convert integer to string.*
- `character(len=:)` function, allocatable [to\\_string\\_long\\_long](#) (i)  
*Convert integer to string.*
- `character(len=:)` function, allocatable [to\\_string\\_double](#) (x)  
*Convert double to string.*

### 10.16.1 Detailed Description

Definition at line 25 of file `prg_extras_mod.F90`.

### 10.16.2 Member Function/Subroutine Documentation

10.16.2.1 `character(len=:)` function, allocatable `prg_extras_mod::to_string::to_string_double` ( `double precision, intent(in) x` )  
`[private]`

Convert double to string.

**Parameters**

|          |            |
|----------|------------|
| <i>x</i> | The double |
|----------|------------|

**Returns**

The string

Definition at line 80 of file prg\_extras\_mod.F90.

**10.16.2.2** `character(len=:)` function, allocatable `prg_extras_mod::to_string::to_string_integer` ( `integer`, intent(in) *i* )  
[private]

Convert integer to string.

**Parameters**

|          |             |
|----------|-------------|
| <i>i</i> | The integer |
|----------|-------------|

**Returns**

The string

Definition at line 46 of file prg\_extras\_mod.F90.

**10.16.2.3** `character(len=:)` function, allocatable `prg_extras_mod::to_string::to_string_long_long` ( `integer(kind=c_long_long)`,  
intent(in) *i* ) [private]

Convert integer to string.

**Parameters**

|          |             |
|----------|-------------|
| <i>i</i> | The integer |
|----------|-------------|

**Returns**

The string

Definition at line 62 of file prg\_extras\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_extras\\_mod.F90](#)

## 10.17 prg\_xlbo\_mod::xlbo\_type Type Reference

General xlbo solver type.

## Public Attributes

- character(20) `jobname`
- integer `verbose`
- integer `maxscfiter`  
*Max SCF iterations at every XLBO MD step.*
- integer `maxscfinititer`  
*Max SCF iterations for the first minit steps.*
- real(dp) `threshold`
- integer `minit`  
*Use SCF the first M\_prg\_init MD steps.*
- real(dp) `cc`  
*Scaled prg\_delta Kernel.*

### 10.17.1 Detailed Description

General xlbo solver type.

Definition at line 33 of file prg\_xlbo\_mod.F90.

### 10.17.2 Member Data Documentation

#### 10.17.2.1 real(dp) prg\_xlbo\_mod::xlbo\_type::cc

Scaled prg\_delta Kernel.

Definition at line 51 of file prg\_xlbo\_mod.F90.

#### 10.17.2.2 character(20) prg\_xlbo\_mod::xlbo\_type::jobname

Definition at line 35 of file prg\_xlbo\_mod.F90.

#### 10.17.2.3 integer prg\_xlbo\_mod::xlbo\_type::maxscfinititer

Max SCF iterations for the first minit steps.

Definition at line 43 of file prg\_xlbo\_mod.F90.

#### 10.17.2.4 integer prg\_xlbo\_mod::xlbo\_type::maxscfiter

Max SCF iterations at every XLBO MD step.

Definition at line 40 of file prg\_xlbo\_mod.F90.

#### 10.17.2.5 integer prg\_xlbo\_mod::xlbo\_type::init

Use SCF the first M\_prg\_init MD steps.

Definition at line 48 of file prg\_xlbo\_mod.F90.

#### 10.17.2.6 real(dp) prg\_xlbo\_mod::xlbo\_type::threshold

Definition at line 45 of file prg\_xlbo\_mod.F90.

#### 10.17.2.7 integer prg\_xlbo\_mod::xlbo\_type::verbose

Definition at line 37 of file prg\_xlbo\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_xlbo\\_mod.F90](#)

## 10.18 prg\_xlkernel\_mod::xk\_type Type Reference

### Public Attributes

- character(20) [kerneltype](#)  
*Kernel type.*
- integer [verbose](#)  
*Verbosity level.*
- integer [nrank](#)
- real(dp) [scalecoeff](#)  
*Coefficient for mixing.*

### 10.18.1 Detailed Description

Definition at line 17 of file prg\_xlkernel\_mod.F90.

### 10.18.2 Member Data Documentation

#### 10.18.2.1 character(20) prg\_xlkernel\_mod::xk\_type::kerneltype

Kernel type.

Definition at line 20 of file prg\_xlkernel\_mod.F90.

#### 10.18.2.2 integer prg\_xlkernel\_mod::xk\_type::nrank

Definition at line 23 of file prg\_xlkernel\_mod.F90.

#### 10.18.2.3 `real(dp) prg_xlkernel_mod::xlk_type::scalecoeff`

Coefficient for mixing.

Definition at line 26 of file prg\_xlkernel\_mod.F90.

#### 10.18.2.4 `integer prg_xlkernel_mod::xlk_type::verbose`

Verbosity level.

Definition at line 23 of file prg\_xlkernel\_mod.F90.

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

- [/home/christian/qmd-progress/src/prg\\_xlkernel\\_mod.F90](#)



# Chapter 11

## File Documentation

### 11.1 /home/christian/qmd-progress/README.md File Reference

### 11.2 /home/christian/qmd-progress/tests/README.md File Reference

### 11.3 /home/christian/qmd-progress/src/prg\_charges\_mod.F90 File Reference

#### Modules

- module [prg\\_charges\\_mod](#)  
*A module to compute the Mulliken charges of a chemical system.*

#### Functions/Subroutines

- subroutine, public [prg\\_charges\\_mod::prg\\_get\\_charges](#) (rho\_bml, over\_bml, hindex, charges, numel, spindex, mdimin, threshold)  
*Constructs the charges from the density matrix.*
- subroutine, public [prg\\_charges\\_mod::prg\\_get\\_hscf](#) (ham0\_bml, over\_bml, ham\_bml, spindex, hindex, hubbard, charges, coulomb\_pot\_r, coulomb\_pot\_k, mdimin, threshold)  
*Constructs the SCF hamiltonian given H0, HubbardU and charges. This routine does:  $H = \sum_i U_i q_i + V_i$ , where  $U$  is the Hubbard parameter for every atom  $i$ .  $V$  is the coulombic potential for every atom  $i$ .*

#### Variables

- integer, parameter [prg\\_charges\\_mod::dp](#) = kind(1.0d0)

### 11.4 /home/christian/qmd-progress/src/prg\_chebyshev\_mod.F90 File Reference

#### Data Types

- type [prg\\_chebyshev\\_mod::chebdata\\_type](#)  
*General Cheb solver type.*

## Modules

- module [prg\\_chebyshev\\_mod](#)

*Module to obtain the density matrix by applying a Chebyshev polynomial expansion.*

## Functions/Subroutines

- subroutine, public [prg\\_chebyshev\\_mod::prg\\_parse\\_cheb](#) (chebdata, filename)  
*Chebyshev parser. This module is used to parse all the input variables for the cheb electronic structure solver. Adding a new input keyword to the parser:*
- subroutine, public [prg\\_chebyshev\\_mod::prg\\_build\\_density\\_cheb](#) (ham\_bml, rho\_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, jon, verbose)  
*Builds the density matrix from  $H_0$  for a Fermi function approximated with a Chebyshev polynomial expansion.*
- subroutine, public [prg\\_chebyshev\\_mod::prg\\_build\\_density\\_cheb\\_fermi](#) (ham\_bml, rho\_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, getef, fermitol, jon, npts, trkfunc, verbose)  
*Builds the density matrix from  $H_0$  for a Fermi function approximated with a Chebyshev polynomial expansion. In this case the self-consistent recursion is applied to converge to the correct number of electrons and obtain the Fermi level.*
- real(dp) function [prg\\_chebyshev\\_mod::jackson](#) (ncoeffs, i, jon)  
*Evaluates the Jackson Kernel Coefficients.*
- subroutine [prg\\_chebyshev\\_mod::prg\\_get\\_chebcoeffs](#) (npts, kbt, ef, ncoeffs, coeffs, emin, emax)  
*Gets the coefficients of the Chebyshev expansion.*
- subroutine [prg\\_chebyshev\\_mod::prg\\_get\\_chebcoeffs\\_fermi\\_bs](#) (npts, kbt, ef, tracesT, ncoeffs, coeffs, emin, emax, bndfil, norb, tol, jon, verbose)  
*Gets the coefficients of the Chebyshev expansion with  $E_f$  computation.*
- subroutine [prg\\_chebyshev\\_mod::prg\\_get\\_chebcoeffs\\_fermi\\_nt](#) (npts, kbt, ef, tracesT, ncoeffs, coeffs, emin, emax, bndfil, norb, tol, jon, verbose)  
*Gets the coefficients of the Chebyshev expansion with  $E_f$  computation.*
- real(dp) function [prg\\_chebyshev\\_mod::tr](#) (r, x)  
*Chebyshev polynomial obtained by recursion.*
- real(dp) function [prg\\_chebyshev\\_mod::fermi](#) (e, ef, kbt)  
*Gives the Fermi distribution value for energy e.*
- real(dp) function [prg\\_chebyshev\\_mod::absmaxderivative](#) (func, de)  
*Gets the absolute maximum of the derivative of a function.*

## Variables

- integer, parameter [prg\\_chebyshev\\_mod::dp](#) = kind(1.0d0)
- real(dp), parameter [prg\\_chebyshev\\_mod::pi](#) = 3.14159265358979323846264338327950\_dp

## 11.5 /home/christian/qmd-progress/src/prg\_densitymatrix\_mod.F90 File Reference

### Modules

- module [prg\\_densitymatrix\\_mod](#)

*Module to obtain the density matrix by diagonalizing an prg\_orthogonalized Hamiltonian.*



## Functions/Subroutines

- subroutine, public `prg_densitymatrix_mod::prg_build_density_t0` (ham\_bml, rho\_bml, threshold, bndfil)  
Builds the density matrix from  $H_0$  for zero electronic temperature.  $\rho = C\Theta(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $\Theta()$  is the Heaviside function.
- subroutine, public `prg_densitymatrix_mod::prg_build_density_t` (ham\_bml, rho\_bml, threshold, bndfil, kbt, ef)  
Builds the density matrix from  $H_0$  for electronic temperature  $T$ .  $\rho = Cf(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $f$  is the Fermi function.
- subroutine, public `prg_densitymatrix_mod::prg_build_density_t_fermi` (ham\_bml, rho\_bml, threshold, kbt, ef, verbose)  
Builds the density matrix from  $H_0$  for electronic temperature  $T$ .  $\rho = Cf(\mu I - \epsilon)C^\dagger$  Where,  $C$  is the matrix eigenvector and  $\epsilon$  is the matrix eigenvalue.  $f$  is the Fermi function. In this routine the Fermi level is passed as an argument.
- subroutine, public `prg_densitymatrix_mod::prg_build_atomic_density` (rhoat\_bml, numel, hindex, spindex, norb, bml\_type)  
Builds the atomic density matrix.  $\rho_{ii} = \text{mathcal{Z}}_{ii}$  Where,  $\text{mathcal{Z}}_{ii}$  is the number of electrons for orbital  $i$ .
- subroutine, public `prg_densitymatrix_mod::prg_get_flevel` (eigenvalues, kbt, bndfil, tol, Ef)  
Routine to compute the Fermi level given a set of eigenvalues and a temperature. It applies the Bisection method over the function:  $g(\mu) = \sum_k 2f(\epsilon_k - \mu) - N = 0$  Where  $f(\epsilon_k - \mu) = \frac{1}{1 + \exp((\epsilon_k - \mu)/(k_b T))}$ .
- subroutine, public `prg_densitymatrix_mod::prg_get_eigenvalues` (ham\_bml, eigenvalues, verbose)  
Gets the eigenvalues of the Orthogonalized Hamiltonian.
- subroutine, public `prg_densitymatrix_mod::prg_check_idempotency` (mat\_bml, threshold, idempotency)  
To check the idempotency error of a matrix. This is calculated as the Frobenius norm of  $(A - A^2)$ .
- real(dp) function `prg_densitymatrix_mod::fermi` (e, ef, kbt)  
Gives the Fermi distribution value for energy  $e$ .

## Variables

- integer, parameter `prg_densitymatrix_mod::dp` = kind(1.0d0)

## 11.6 /home/christian/qmd-progress/src/prg\_dos\_mod.F90 File Reference

### Modules

- module `prg_dos_mod`  
A module to compute the Density of state (DOS) and IDOS.

### Functions/Subroutines

- subroutine, public `prg_dos_mod::prg_write_tdos` (eigenvals, gamma, npts, emin, emax, filename)  
Writes the total DOS into a file.  $DOS(\epsilon) = \sum_k L(\epsilon - \epsilon_k)$  Where  $\int_{-\infty}^{\infty} DOS(\epsilon) = Nstates$ .
- real(dp) function `prg_dos_mod::lorentz` (energy, eigenvals, loads, Gamma)  
Lorentzian Function.

### Variables

- integer, parameter `prg_dos_mod::dp` = kind(1.0d0)

## 11.7 /home/christian/qmd-progress/src/prg\_doxy\_mod.F90 File Reference

## 11.8 /home/christian/qmd-progress/src/prg\_extras\_mod.F90 File Reference

### Data Types

- interface [prg\\_extras\\_mod::prg\\_memory\\_consumption](#)
- interface [prg\\_extras\\_mod::to\\_string](#)

### Modules

- module [prg\\_extras\\_mod](#)

*Extra routines:*

### Functions/Subroutines

- character(len=:) function, allocatable [prg\\_extras\\_mod::to\\_string\\_integer](#) (i)  
*Convert integer to string.*
- character(len=:) function, allocatable [prg\\_extras\\_mod::to\\_string\\_long\\_long](#) (i)  
*Convert integer to string.*
- character(len=:) function, allocatable [prg\\_extras\\_mod::to\\_string\\_double](#) (x)  
*Convert double to string.*
- subroutine, public [prg\\_extras\\_mod::prg\\_print\\_matrix](#) (matname, amat, i1, i2, j1, j2)  
*To write a dense matrix to screen.*
- real(dp) function, public [prg\\_extras\\_mod::mls](#) ()  
*To get the actual time in milliseconds.*
- subroutine, public [prg\\_extras\\_mod::prg\\_delta](#) (x, s, nn, dta)  
*Delta function  $\|X^tSX - I\|$ . CFAN, March 2015.*
- subroutine, public [prg\\_extras\\_mod::prg\\_get\\_mem](#) (procname, tag)  
*Get proc memory.*
- subroutine [prg\\_extras\\_mod::prg\\_twonorm](#) (a, nn, norm2)

### Variables

- integer, parameter [prg\\_extras\\_mod::dp](#) = kind(1.0d0)

## 11.9 /home/christian/qmd-progress/src/prg\_genz\_mod.F90 File Reference

### Data Types

- type [prg\\_genz\\_mod::genzspinp](#)  
*Input for the genz driver.*
- type [prg\\_genz\\_mod::genzspdata](#)  
*contains the data for the genZ driver.*

## Modules

- module [prg\\_genz\\_mod](#)

*To produce a matrix  $Z$  which is needed to orthogonalize  $H$ .*

## Functions/Subroutines

- subroutine, public [prg\\_genz\\_mod::prg\\_parse\\_zsp](#) (input, filename)

*The parser for genz solver.*

- subroutine [prg\\_genz\\_mod::prg\\_init](#) (self, input)

*Initializes the genz input variables.*

- subroutine [prg\\_genz\\_mod::prg\\_allocatezspmat](#) (self, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, norb, bml\_type)

*Allocates the matrices for the XI integration of  $Z$ .*

- subroutine, public [prg\\_genz\\_mod::prg\\_init\\_zspmat](#) (igenz, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, norb, bml\_type)

*Initiates the matrices for the XI integration of  $Z$ .*

- subroutine [prg\\_genz\\_mod::prg\\_generate](#) (self, over\_bml, zmat\_bml, igenz, mdim, bml\_type, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml)

*Generates the  $Z$  matrix.*

- subroutine, public [prg\\_genz\\_mod::prg\\_buildzdiag](#) (smat\_bml, zmat\_bml, threshold, mdimin, bml\_type, verbose)

*Usual subroutine involving diagonalization.*

- subroutine, public [prg\\_genz\\_mod::prg\\_buildzsparse](#) (smat\_bml, zmat\_bml, igenz, mdim, bml\_type, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, nfirst, nrefi, nreff, thresholdi, thresholdf, integration, verbose)

*Inverse factorization using niklasson's algorithm.*

- subroutine, public [prg\\_genz\\_mod::prg\\_genz\\_sp\\_initialz0](#) (smat\_bml, zmat\_bml, norb, mdim, bml\_type, f, threshold)

- subroutine, public [prg\\_genz\\_mod::prg\\_genz\\_sp\\_initial\\_zmat](#) (smat\_bml, zmat\_bml, norb, mdim, bml\_type, f, threshold)

*Estimate  $Z$  matrix.*

- subroutine [prg\\_genz\\_mod::prg\\_genz\\_sp\\_int](#) (zmat\_bml, zk1\_bml, zk2\_bml, zk3\_bml, zk4\_bml, zk5\_bml, zk6\_bml, igenz, norb, bml\_type, threshold)

- subroutine, public [prg\\_genz\\_mod::prg\\_genz\\_sp\\_ref](#) (smat\_bml, zmat\_bml, nref, norb, bml\_type, threshold)

## Variables

- integer, parameter [prg\\_genz\\_mod::dp](#) = kind(1.0d0)

## 11.10 /home/christian/qmd-progress/src/prg\_graph\_mod.F90 File Reference

### Data Types

- type [prg\\_graph\\_mod::subgraph\\_t](#)

*Subgraph type.*

- type [prg\\_graph\\_mod::graph\\_partitioning\\_t](#)

*Trace per iteration.*

## Modules

- module [prg\\_graph\\_mod](#)  
*The graph module.*

## Functions/Subroutines

- subroutine, public [prg\\_graph\\_mod::prg\\_initsubgraph](#) (sg, pnum, hsize)  
*Initialize subgraph.*
- subroutine, public [prg\\_graph\\_mod::prg\\_destroysubgraph](#) (sg)  
*Destroy subgraph.*
- subroutine, public [prg\\_graph\\_mod::prg\\_initgraphpartitioning](#) (gp, pname, np, nnodes, nnodes2)  
*Initialize graph partitioning.*
- subroutine, public [prg\\_graph\\_mod::prg\\_destroygraphpartitioning](#) (gp)  
*Destroy graph partitioning.*
- subroutine, public [prg\\_graph\\_mod::prg\\_printgraphpartitioning](#) (gp)  
*Print graph partitioning structure data.*
- subroutine, public [prg\\_graph\\_mod::prg\\_equalpartition](#) (gp, nodesPerPart, nnodes)  
*Create equal graph partitions, based on number of rows/orbitals.*
- subroutine, public [prg\\_graph\\_mod::prg\\_equalitygrouppartitioning](#) (gp, hindex, ngroup, nodesPerPart, nnodes)  
*Create equal group graph partitions, based on number of atoms/groups.*
- subroutine, public [prg\\_graph\\_mod::prg\\_filepartitioning](#) (gp, partFile)  
*Read graph partitions from a file, based on number of rows/orbitals.*
- subroutine [prg\\_graph\\_mod::prg\\_readpart](#) (gp, partFile)  
*Read parts (core) from part file.*
- subroutine, public [prg\\_graph\\_mod::prg\\_fnormgraph](#) (gp)  
*Accumulate trace norm across all subgraphs.*

## Variables

- integer, parameter [prg\\_graph\\_mod::dp](#) = kind(1.0d0)

## 11.11 /home/christian/qmd-progress/src/prg\_graphsp2parser\_mod.F90 File Reference

### Data Types

- type [prg\\_graphsp2parser\\_mod::gsp2data\\_type](#)  
*General SP2 solver type.*

## Modules

- module [prg\\_graphsp2parser\\_mod](#)  
*Graph partitioning SP2 parser.*

## Functions/Subroutines

- subroutine, public [prg\\_graphsp2parser\\_mod::prg\\_parse\\_gsp2](#) (gsp2data, filename)  
*The parser for SP2 solver.*

## Variables

- integer, parameter `prg_graphsp2parser_mod::dp` = kind(1.0d0)

## 11.12 /home/christian/qmd-progress/src/prg\_homolumo\_mod.F90 File Reference

### Modules

- module `prg_homolumo_mod`

*The homolumo module.*

### Functions/Subroutines

- subroutine, public `prg_homolumo_mod::prg_homolumogap` (vv, imax, pp, mineval, maxeval, ehomo, elumo, egap, verbose)
- subroutine, public `prg_homolumo_mod::prg_sp2sequence` (pp, imax, mineval, maxeval, ehomo, elumo, erlimit, verbose)

## Variables

- integer, parameter `prg_homolumo_mod::dp` = kind(1.0d0)

## 11.13 /home/christian/qmd-progress/src/prg\_implicit\_fermi\_mod.F90 File Reference

### Modules

- module `prg_implicit_fermi_mod`

### Functions/Subroutines

- subroutine, public `prg_implicit_fermi_mod::prg_implicit_fermi` (h\_bml, xi0\_bml, p\_bml, nsteps, nocc, mu, beta, osteps, occErrLimit, threshold)

*Recursive Implicit Fermi Dirac.*

## Variables

- integer, parameter `prg_implicit_fermi_mod::dp` = kind(1.0d0)

## 11.14 /home/christian/qmd-progress/src/prg\_initmatrices\_mod.F90 File Reference

### Modules

- module `prg_initmatrices_mod`

*Initialization module.*

## Functions/Subroutines

- subroutine, public [prg\\_initmatrices\\_mod::prg\\_init\\_hsmat](#) (ham\_bml, over\_bml, bml\_type, mdim, norb)  
*Initialize Hamiltonian and Overlap Matrix.*
- subroutine, public [prg\\_initmatrices\\_mod::prg\\_init\\_pzmat](#) (rho\_bml, zmat\_bml, bml\_type, mdim, norb)  
*Initialize Density matrix and Inverse square root Overlap.*
- subroutine, public [prg\\_initmatrices\\_mod::prg\\_init\\_ortho](#) (orthoh\_bml, orthop\_bml, bml\_type, mdim, norb)  
*Initialize The orthogonal versions of Hamiltonian and Density Matrix.*

## Variables

- integer, parameter [prg\\_initmatrices\\_mod::dp](#) = kind(1.0d0)

## 11.15 /home/christian/qmd-progress/src/prg\_kernelparser\_mod.F90 File Reference

### Modules

- module [prg\\_kernelparser\\_mod](#)  
*Some general parsing functions.*

### Functions/Subroutines

- subroutine, public [prg\\_kernelparser\\_mod::prg\\_parsing\\_kernel](#) (keyvector\_char, valvector\_char, keyvector\_↵int, valvector\_int, keyvector\_re, valvector\_re, keyvector\_log, valvector\_log, filename, startstop)  
*The general parsing function. It is used to vectorize a set of "keywords" "value" pairs as included in a general input file.*
- subroutine [prg\\_kernelparser\\_mod::prg\\_check\\_valid](#) (invalidc)  
*Check for valid keywords (checks for an = sign)*

### Variables

- integer, parameter [prg\\_kernelparser\\_mod::dp](#) = kind(1.0d0)

## 11.16 /home/christian/qmd-progress/src/prg\_nonortho\_mod.F90 File Reference

### Modules

- module [prg\\_nonortho\\_mod](#)  
*Module to prg\_orthogonalize and prg\_deorthogonalize any operator.*

### Functions/Subroutines

- subroutine, public [prg\\_nonortho\\_mod::prg\\_orthogonalize](#) (A\_bml, zmat\_bml, orthoA\_bml, threshold, bml\_↵type, verbose)  
*This routine performs:  $A_{ortho} = Z^\dagger A Z$ .*
- subroutine, public [prg\\_nonortho\\_mod::prg\\_deorthogonalize](#) (orthoA\_bml, zmat\_bml, a\_bml, threshold, bml\_↵\_type, verbose)  
*This routine performs:  $A = Z A_{ortho} Z^\dagger$ .*

## Variables

- integer, parameter `prg_nonortho_mod::dp` = kind(1.0d0)

## 11.17 /home/christian/qmd-progress/src/prg\_normalize\_mod.F90 File Reference

### Modules

- module `prg_normalize_mod`  
*The prg\_normalize module.*

### Functions/Subroutines

- subroutine, public `prg_normalize_mod::prg_normalize` (h\_bml)  
*Normalize a Hamiltonian matrix prior to running the SP2 algorithm.*
- subroutine, public `prg_normalize_mod::prg_normalize_fermi` (h\_bml, h1, hN, mu)  
*Normalize a Hamiltonian matrix prior to running the truncated SP2 algorithm.*
- subroutine, public `prg_normalize_mod::prg_normalize_implicit_fermi` (h\_bml, cnst, mu)  
*Normalize a Hamiltonian matrix prior to running the implicit fermi dirac algorithm.*
- subroutine, public `prg_normalize_mod::prg_gershgorinreduction` (gp)  
*Determine gershgorin bounds across all parts, local and distributed.*
- subroutine, public `prg_normalize_mod::prg_normalize_cheb` (h\_bml, mu, emin, emax, alpha, scaledmu)  
*Normalize a Hamiltonian matrix prior to running the Chebyshev algorithm.*

## Variables

- integer, parameter `prg_normalize_mod::dp` = kind(1.0d0)

## 11.18 /home/christian/qmd-progress/src/prg\_openfiles\_mod.F90 File Reference

### Modules

- module `prg_openfiles_mod`  
*Module to handle input output files for the PROGRESS lib.*

### Functions/Subroutines

- integer function, public `prg_openfiles_mod::get_file_unit` (io\_max)  
*Returns a unit number that is not in use.*
- subroutine, public `prg_openfiles_mod::prg_open_file` (io, name)  
*Opens a file to write.*
- subroutine, public `prg_openfiles_mod::prg_open_file_to_read` (io, name)  
*Opens a file to read.*

## 11.19 /home/christian/qmd-progress/src/prg\_parallel\_mod.F90 File Reference

### Data Types

- type [prg\\_parallel\\_mod::rankreducedata\\_t](#)  
*Data structure for rection over MPI ranks.*

### Modules

- module [prg\\_parallel\\_mod](#)  
*The parallel module.*

### Functions/Subroutines

- integer function, public [prg\\_parallel\\_mod::getnranks](#) ()
- integer function, public [prg\\_parallel\\_mod::getmyrank](#) ()
- integer function, public [prg\\_parallel\\_mod::printrank](#) ()
- subroutine, public [prg\\_parallel\\_mod::prg\\_initparallel](#) ()
- subroutine, public [prg\\_parallel\\_mod::prg\\_shutdownparallel](#) ()
- integer function [prg\\_parallel\\_mod::saverequest](#) (irequest)
- subroutine, public [prg\\_parallel\\_mod::prg\\_barrierparallel](#) ()
- subroutine, public [prg\\_parallel\\_mod::sendreceiveparallel](#) (sendBuf, sendLen, dest, recvBuf, recvLen, source, nreceived)
- subroutine, public [prg\\_parallel\\_mod::isendparallel](#) (sendBuf, sendLen, dest)
- subroutine, public [prg\\_parallel\\_mod::sendparallel](#) (sendBuf, sendLen, dest)
- subroutine, public [prg\\_parallel\\_mod::prg\\_iprg\\_recvparallel](#) (recvBuf, recvLen, rind)
- subroutine, public [prg\\_parallel\\_mod::prg\\_recvparallel](#) (recvBuf, recvLen)
- subroutine, public [prg\\_parallel\\_mod::sumintparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::sumrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::maxintparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::maxrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::minintparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::minrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::prg\\_minrealreduce](#) (rvalue)
- subroutine, public [prg\\_parallel\\_mod::prg\\_maxrealreduce](#) (rvalue)
- subroutine, public [prg\\_parallel\\_mod::prg\\_maxintreduce2](#) (value1, value2)
- subroutine, public [prg\\_parallel\\_mod::prg\\_sumintreduce2](#) (value1, value2)
- subroutine, public [prg\\_parallel\\_mod::prg\\_sumrealreduce](#) (value1)
- subroutine, public [prg\\_parallel\\_mod::prg\\_sumrealreduce2](#) (value1, value2)
- subroutine, public [prg\\_parallel\\_mod::prg\\_sumrealreduce3](#) (value1, value2, value3)
- subroutine, public [prg\\_parallel\\_mod::prg\\_sumrealreducen](#) (valueVec, N)
- subroutine, public [prg\\_parallel\\_mod::prg\\_sumintreducen](#) (valueVec, N)
- subroutine, public [prg\\_parallel\\_mod::minrankrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::maxrankrealparallel](#) (sendBuf, recvBuf, icount)
- subroutine, public [prg\\_parallel\\_mod::prg\\_bcastparallel](#) (buf, blen, root)
- subroutine, public [prg\\_parallel\\_mod::allgatherrealparallel](#) (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public [prg\\_parallel\\_mod::allgatherintparallel](#) (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public [prg\\_parallel\\_mod::allgathervrealparallel](#) (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public [prg\\_parallel\\_mod::allgathervintparallel](#) (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public [prg\\_parallel\\_mod::prg\\_allsumrealreduceparallel](#) (buf, buflen)
- subroutine, public [prg\\_parallel\\_mod::prg\\_allsumintreduceparallel](#) (buf, buflen)
- subroutine, public [prg\\_parallel\\_mod::prg\\_allgatherparallel](#) (a)
- subroutine, public [prg\\_parallel\\_mod::prg\\_wait](#) ()



## Variables

- integer, parameter `prg_parallel_mod::dp` = kind(1.0d0)
- integer `prg_parallel_mod::myrank`
- integer `prg_parallel_mod::nranks`
- integer `prg_parallel_mod::ierr`
- integer `prg_parallel_mod::reqcount`
- integer, dimension(:), allocatable `prg_parallel_mod::requestlist`
- integer, dimension(:), allocatable `prg_parallel_mod::rused`

## 11.20 /home/christian/qmd-progress/src/prg\_partition\_mod.F90 File Reference

### Modules

- module `prg_partition_mod`

*The partition module.*

### Functions/Subroutines

- subroutine, public `prg_partition_mod::prg_metispartition` (gp, ngroups, nnodes, xadj, adjncy, nparts, part, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)  
*Create graph partitions minizing number of cut edges.*
- subroutine, public `prg_partition_mod::prg_costpartition` (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)  
*Compute cost of a partition.*
- subroutine, public `prg_partition_mod::update_prg_costpartition` (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, node, new\_part)  
*Update cost of partition and the different parameters node is moves into new\_part For each neighbor of node, the following cases hold: Case 1: neighbor is in old\_part Case 2: neighbor is in new\_part Case 3: neighbor is neither in old\_ or new\_part.*
- subroutine `prg_partition_mod::prg_accept_prob` (it, prg\_delta, r)  
*Compute acceptance probability for simulated annealing.*
- subroutine `prg_partition_mod::prg_costindex` (cost, sumCubes, maxCH, smooth\_maxCH, obj\_fun)  
*Choose objective function to work with.*
- subroutine `prg_partition_mod::prg_rand_node` (gp, node, seed)  
*Pick a random node.*
- subroutine, public `prg_partition_mod::prg_simannealing` (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, niter, seed)  
*Graph partitioning based on Simulated Annealing.*
- subroutine, public `prg_partition_mod::prg_kernlin` (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, nconverg, seed)  
*Graph partitioning based on inspired by Kernighan-Lin Review METiS manual for description of k-way implementation of KL Pick a core together with its halos Place free vertices on a priority queue with (key, value) =(prg\_delta, best\_↔ part),with prg\_delta = change in obj\_value Dequeue and allow hill climbing.*
- subroutine, public `prg_partition_mod::prg_update_gp` (gp, partNumber, core\_count)
- subroutine `prg_partition_mod::prg_rand_shuffle` (array, seed)  
*Randomly shuffle array.*
- subroutine, public `prg_partition_mod::prg_check_arrays` (gp, core\_count, CH\_count, Halo\_count)  
*Error checking Checking that core\_count, CH\_count, Halo\_count match.*
- subroutine, public `prg_partition_mod::prg_kernlin_queue` (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)

*Greedy algorithm. At each step it chooses the (vertex, new\_part) pair with highest gain. Currently implementation is very slow.*

- subroutine [prg\\_partition\\_mod::prg\\_find\\_best\\_move](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, best\_node, best\_part)

*For kerlin\_queue to find (vertex, new\_part) pair with highest gain.*

- subroutine, public [prg\\_partition\\_mod::prg\\_kernlin2](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm)
- subroutine [prg\\_partition\\_mod::prg\\_get\\_largest\\_hedge\\_in\\_part](#) (gp, xadj, adjncy, partNumber, core\_count, CH\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, search\_part, largest\_Hedge)
- subroutine, public [prg\\_partition\\_mod::prg\\_simannealing\\_old](#) (gp, xadj, adjncy, partNumber, core\_count, C↔H\_count, Halo\_count, sumCubes, maxCH, smooth\_maxCH, pnorm, niter, seed)

## Variables

- integer, parameter [prg\\_partition\\_mod::dp](#) = kind(1.0d0)
- integer, parameter [prg\\_partition\\_mod::metis\\_index\\_kind](#) = METIS\_INDEX\_KIND  
*From /usr/include/metis.h.*
- integer, parameter [prg\\_partition\\_mod::metis\\_real\\_kind](#) = kind(METIS\_REAL\_KIND)  
*From /usr/include/metis.h.*

## 11.21 /home/christian/qmd-progress/src/prg\_progress\_mod.F90 File Reference

### Modules

- module [prg\\_progress\\_mod](#)  
*The progress module.*

### Functions/Subroutines

- subroutine, public [prg\\_progress\\_mod::prg\\_progress\\_init](#) ()  
*Initialize progress.*
- subroutine, public [prg\\_progress\\_mod::prg\\_progress\\_shutdown](#) ()  
*Shutdown progress.*

### Variables

- integer, parameter [prg\\_progress\\_mod::dp](#) = kind(1.0d0)

## 11.22 /home/christian/qmd-progress/src/prg\_ptable\_mod.F90 File Reference

### Modules

- module [prg\\_ptable\\_mod](#)  
*Periodic table of elements.*

## Functions/Subroutines

- integer function, public [prg\\_ptable\\_mod::element\\_atomic\\_number](#) (symbol)
- integer function [prg\\_ptable\\_mod::element\\_atomic\\_number\\_upper](#) (symbol)

## Variables

- integer, parameter [prg\\_ptable\\_mod::nz](#) = 103
- integer, parameter, private [prg\\_ptable\\_mod::dp](#) = kind(1.0d0)
- character(2), dimension(nz), parameter [prg\\_ptable\\_mod::element\\_symbol](#) = [character(2) :: "H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne", "Na", "Mg", "Al", "Si", "P", "S", "Cl", "Ar", "K", "Ca", "Sc", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn", "Ga", "Ge", "As", "Se", "Br", "Kr", "Rb", "Sr", "Y", "Zr", "Nb", "Mo", "Tc", "Ru", "Rh", "Pd", "Ag", "Cd", "In", "Sn", "Sb", "Te", "I", "Xe", "Cs", "Ba", "La", "Ce", "Pr", "Nd", "Pm", "Sm", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb", "Lu", "Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg", "Tl", "Pb", "Bi", "Po", "At", "Rn", "Fr", "Ra", "Ac", "Th", "Pa", "U", "Np", "Pu", "Am", "Cm", "Bk", "Cf", "Es", "Fm", "Md", "No", "Lr"]

*Element symbol.*

- character(2), dimension(nz), parameter [prg\\_ptable\\_mod::element\\_symbol\\_upper](#) = [character(2) :: "H", "HE", "LI", "BE", "B", "C", "N", "O", "F", "NE", "NA", "MG", "AL", "SI", "P", "S", "CL", "AR", "K", "CA", "SC", "TI", "V", "CR", "MN", "FE", "CO", "NI", "CU", "ZN", "GA", "GE", "AS", "SE", "BR", "KR", "RB", "SR", "Y", "ZR", "NB", "MO", "TC", "RU", "RH", "PD", "AG", "CD", "IN", "SN", "SB", "TE", "I", "XE", "CS", "BA", "LA", "CE", "PR", "ND", "PM", "SM", "EU", "GD", "TB", "DY", "HO", "ER", "TM", "YB", "LU", "HF", "TA", "W", "RE", "OS", "IR", "PT", "AU", "HG", "TL", "PB", "BI", "PO", "AT", "RN", "FR", "RA", "AC", "TH", "PA", "U", "NP", "PU", "AM", "CM", "BK", "CF", "ES", "FM", "MD", "NO", "LR"]

*Element symbol upper.*

- character(20), dimension(nz), parameter [prg\\_ptable\\_mod::element\\_name](#) = [character(20) :: "Hydrogen", "Helium", "Lithium", "Beryllium", "Boron", "Carbon", "Nitrogen", "Oxygen", "Fluorine", "Neon", "Sodium", "Magnesium", "Aluminium", "Silicon", "Phosphorus", "Sulfur", "Chlorine", "Argon", "Potassium", "Calcium", "Scandium", "Titanium", "Vanadium", "Chromium", "Manganese", "Iron", "Cobalt", "Nickel", "Copper", "Zinc", "Gallium", "Germanium", "Arsenic", "Selenium", "Bromine", "Krypton", "Rubidium", "Strontium", "Yttrium", "Zirconium", "Niobium", "Molybdenum", "Technetium", "Ruthenium", "Rhodium", "Palladium", "Silver", "Cadmium", "Indium", "Tin", "Antimony", "Tellurium", "Iodine", "Xenon", "Caesium", "Barium", "Lanthanum", "Cerium", "Praseodymium", "Neodymium", "Promethium", "Samarium", "Europium", "Gadolinium", "Terbium", "Dysprosium", "Holmium", "Erbium", "Thulium", "Ytterbium", "Lutetium", "Hafnium", "Tantalum", "Tungsten", "Rhenium", "Osmium", "Iridium", "Platinum", "Gold", "Mercury", "Thallium", "Lead", "Bismuth", "Polonium", "Astatine", "Radon", "Francium", "Radium", "Actinium", "Thorium", "Protactinium", "Uranium", "Neptunium", "Plutonium", "Americium", "Curium", "Berkelium", "Californium", "Einsteinium", "Fermium", "Mendelevium", "Nobelium", "Lawrencium"]

*Element name.*

- real(dp), dimension(nz), parameter [prg\\_ptable\\_mod::element\\_mass](#) = (/ 1.007825032, 4.002603254, 7.01600455, 9.0121822, 11.0093054, 12.0, 14.003074005, 15.99491462, 18.99840322, 19.992440175, 22.989769281, 23.9850417, 26.98153863, 27.976926532, 30.97376163, 31.972071, 34.96885268, 39.962383123, 38.96370668, 39.96259098, 44.9559119, 47.9479463, 50.9439595, 51.9405075, 54.9380451, 55.9349375, 58.933195, 57.9353429, 62.9295975, 63.929142, 68.925573, 73.921177, 74.921596, 79.916521, 78.918337, 83.911507, 84.911789, 87.905612, 88.905848, 89.904704, 92.906378, 97.905408, 97.907216, 101.904349, 102.905504, 105.903486, 106.905097, 113.903358, 114.903878, 119.902194, 120.903815, 129.906224, 126.904473, 131.904153, 132.905451, 137.905247, 138.906353, 139.905438, 140.907652, 141.907723, 144.912749, 151.919732, 152.92123, 157.924103, 158.925346, 163.929174, 164.930322, 165.930293, 168.934213, 173.938862, 174.940771, 179.94655, 180.947995, 183.950931, 186.955753, 191.96148, 192.962926, 194.964791, 196.966568, 201.970643, 204.974427, 207.976652, 208.980398, 208.98243, 209.987148, 222.017577, 223.019735, 226.025409, 227.027752, 232.038055, 231.035884, 238.050788, 237.048173, 244.064204, 243.061381, 247.070354, 247.070307, 251.079587, 252.08298, 257.095105, 258.098431, 259.10103, 262.10963 /)

*Element mass in atomic mass units (1.66 x 10<sup>-27</sup> kg)*



- character(50), dimension(nz), parameter `prg_ptable_mod::element_econf` = [character(50) :: "1s", "1s2", "1s22s", "1s22s2", "1s22s22p", "1s22s22p2", "1s22s22p3", "1s22s22p4", "1s22s22p5", "1s22s22p6", "[Ne]3s", "[Ne]3s2", "[Ne]3s23p", "[Ne]3s23p2", "[Ne]3s23p3", "[Ne]3s23p4", "[Ne]3s23p5", "[Ne]3s23p6", "[Ar]4s", "[Ar]4s2", "[Ar]3d4s2", "[Ar]3d24s2", "[Ar]3d34s2", "[Ar]3d54s", "[Ar]3d54s2", "[Ar]3d64s2", "[Ar]3d74s2", "[Ar]3d84s2", "[Ar]3d104s", "[Ar]3d104s2", "[Ar]3d104s24p", "[Ar]3d104s24p2", "[Ar]3d104s24p3", "[Ar]3d104s24p4", "[Ar]3d104s24p5", "[Ar]3d104s24p6", "[Kr]5s", "[Kr]5s2", "[Kr]4d5s2", "[Kr]4d25s2", "[Kr]4d45s", "[Kr]4d55s", "[Kr]4d55s2", "[Kr]4d75s", "[Kr]4d85s", "[Kr]4d10", "[Kr]4d105s", "[Kr]4d105s2", "[Cd]5p", "[Cd]5p2", "[Cd]5p3", "[Cd]5p4", "[Cd]5p5", "[Cd]5p6", "[Xe]6s", "[Xe]6s2", "[Xe]5d6s2", "[Xe]4f5d6s2", "[Xe]4f36s2", "[Xe]4f46s2", "[Xe]4f56s2", "[Xe]4f66s2", "[Xe]4f76s2", "[Xe]4f75d6s2", "[Xe]4f96s2", "[Xe]4f106s2", "[Xe]4f116s2", "[Xe]4f126s2", "[Xe]4f136s2", "[Xe]4f146s2", "[Xe]4f145d6s2", "[Xe]4f145d26s2", "[Xe]4f145d36s2", "[Xe]4f145d46s2", "[Xe]4f145d56s2", "[Xe]4f145d66s2", "[Xe]4f145d76s2", "[Xe]4f145d96s", "[Xe]4f145d106s", "[Xe]4f145d106s2", "[Hg]6p", "[Hg]6p2", "[Hg]6p3", "[Hg]6p4", "[Hg]6p5", "[Hg]6p6", "[Rn]7s", "[Rn]7s2", "[Rn]6d7s2", "[Rn]6d27s2", "[Rn]5f26d7s2", "[Rn]5f36d7s2", "[Rn]5f46d7s2", "[Rn]5f67s2", "[Rn]5f77s2", "[Rn]5f76d7s2", "[Rn]5f97s2", "[Rn]5f107s2", "[Rn]5f117s2", "[Rn]5f127s2", "[Rn]5f137s2", "[Rn]5f147s2", "[Rn]5f147s27p"]

*The electronic configuration.*

## 11.23 /home/christian/qmd-progress/src/prg\_pulaycomponent\_mod.F90 File Reference

### Modules

- module `prg_pulaycomponent_mod`  
*Produces a matrix to get the Pulay Component of the forces.*

### Functions/Subroutines

- subroutine, public `prg_pulaycomponent_mod::prg_pulaycomponent0` (rho\_bml, ham\_bml, pcm\_bml, threshold, M, bml\_type, verbose)  
 $At\ T = 0K, P = \rho H \rho.$
- subroutine, public `prg_pulaycomponent_mod::prg_pulaycomponentt` (rho\_bml, ham\_bml, zmat\_bml, pcm\_bml, threshold, M, bml\_type, verbose)  
 $At\ T > 0K, P = \rho H S^{-1} + S^{-1} H \rho.$
- subroutine, public `prg_pulaycomponent_mod::prg_get_pulayforce` (nats, zmat\_bml, ham\_bml, rho\_bml, dSx\_bml, dSy\_bml, dSz\_bml, hindex, FPUL, threshold)  
*Pulay Force FPUL from  $2Tr[Z Z' H D \frac{dS}{dR}]$ .*

### Variables

- integer, parameter `prg_pulaycomponent_mod::dp` = kind(1.0d0)

## 11.24 /home/christian/qmd-progress/src/prg\_pulaymixer\_mod.F90 File Reference

### Data Types

- type `prg_pulaymixer_mod::mx_type`

## Modules

- module [prg\\_pulaymixer\\_mod](#)

*Pulay mixer mode.*

## Functions/Subroutines

- subroutine, public [prg\\_pulaymixer\\_mod::prg\\_parse\\_mixer](#) (input, filename)  
*The parser for the mixer routines.*
- subroutine, public [prg\\_pulaymixer\\_mod::prg\\_qmixer](#) (charges, oldcharges, dqin, dqout, scferror, piter, pulay-coef, mpulay, verbose)  
*Mixing the charges to accelerate scf convergence.*
- subroutine, public [prg\\_pulaymixer\\_mod::prg\\_linearmixer](#) (charges, oldcharges, scferror, linmixcoef, verbose)  
*Routine to perform linear mixing.*

## Variables

- integer, parameter [prg\\_pulaymixer\\_mod::dp](#) = kind(1.0d0)

## 11.25 /home/christian/qmd-progress/src/prg\_quantumdynamics\_mod.F90 File Reference

## Modules

- module [prg\\_quantumdynamics\\_mod](#)

*A module to add in common quantum dynamical operations.*

## Functions/Subroutines

- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_kick\\_density](#) (kick\_dirac, kick\_mag, dens, norbs, mdim, S, SINV, which\_atom, r, bmltype, thresh)  
*Provides perturbation to initial density matrix in the form of an electric field kick. This routine does:  $\rho_{kick} = \exp \frac{-i}{\hbar} \hat{V} \hat{\rho} \hat{S} \exp \frac{i}{\hbar} \hat{V} \hat{S}^{-1}$  where  $\hat{V}$  is the field disturbance.*
- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_get\\_sparsity\\_cplxmat](#) (matrix\_type, element\_type, thresh, a\_dense)  
*This computes the sparsity of a complex matrix given a threshold value This routine does:  $f = \frac{N_0}{N_{tot}}$  where  $f$  is the sparsity,  $N_0$  is the number of values less than the threshold, and  $N_{tot}$  is the total number of values. The sparsity and threshold are printed to the screen.*
- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_get\\_sparsity\\_realmat](#) (matrix\_type, element\_type, thresh, a\_dense)  
*This computes the sparsity of a real matrix given a threshold value This routine does:  $f = \frac{N_0}{N_{tot}}$  where  $f$  is the sparsity,  $N_0$  is the number of values less than the threshold, and  $N_{tot}$  is the total number of values. The sparsity and threshold are printed to the screen.*
- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_kick\\_density\\_bml](#) (kick\_dirac, kick\_mag, rho\_bml, s\_bml, sinv\_bml, mdim, which\_atom, r, matrix\_type, thresh)  
*Provides perturbation to initial density matrix in the form of an electric field kick given input matrices in BML format. This routine does:  $\rho_{kick} = \exp \frac{-i}{\hbar} \hat{V} \hat{\rho} \hat{S} \exp \frac{i}{\hbar} \hat{V} \hat{S}^{-1}$  where  $\hat{V}$  is the field disturbance.*
- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_lvni\\_bml](#) (h1\_bml, sinv\_bml, dt, hbar, rhoold\_bml, rho\_bml, aux\_bml, matrix\_type, mdim, thresh)

Performs Liouville-von Neumann integration using leap-frog method. This routine does:  $\hat{\rho}(t + \Delta t) = \hat{\rho}(t - \Delta t) + 2\Delta t \frac{\partial \hat{\rho}(t)}{\partial t}$  where the time derivative of the density matrix is defined as follows:  $\frac{\partial \hat{\rho}(t)}{\partial t} = \frac{-i}{\hbar} \left( S^{-1} \hat{H}(t) \hat{\rho}(t) - \hat{\rho}(t) \hat{H}(t) S^{-1} \right)$ .

- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_getcharge](#) (rho\_bml, s\_bml, charges, aux\_bml, z, spin-dex, N, nats, thresh)

Constructs the charges from the density matrix.

- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_getdipole](#) (charges, r, mu)

This routine computes the dipole moment of the system with units determined by the units of the coordinate matrix and charges given.

- subroutine, public [prg\\_quantumdynamics\\_mod::prg\\_excitation](#) (fill\_mat, orbit\_orig, orbit\_exc)

Produce an excitation in the initially calculated density matrix to.

## Variables

- integer, parameter [prg\\_quantumdynamics\\_mod::dp](#) = kind(1.0d0)

## 11.26 /home/christian/qmd-progress/src/prg\_response\_mod.F90 File Reference

### Data Types

- type [prg\\_response\\_mod::respdata\\_type](#)

### Modules

- module [prg\\_response\\_mod](#)

Module to compute the density matrix response and related quantities.

### Functions/Subroutines

- subroutine, public [prg\\_response\\_mod::prg\\_parse\\_response](#) (RespData, filename)

The parser for the calculation of the DM response.

- subroutine, public [prg\\_response\\_mod::prg\\_compute\\_dipole](#) (charges, coordinate, dipoleMoment, factor, verbose)

To compute the dipole moment of the system. The units of the dipole moment are determined by the units of the coordinates and charges that are given.

- subroutine, public [prg\\_response\\_mod::prg\\_write\\_dipole\\_tcl](#) (dipoleMoment, file, factor, verbose)

To visualize a dipole moment using VMD. This will prg\_generate a .tcl script that could be run using VMD To visualize with VMD: \$ vmd -e dipole.tcl.

- subroutine, public [prg\\_response\\_mod::prg\\_compute\\_polarizability](#) (rsp\_bml, prt\_bml, polarizability, factor, verbose)

To compute the polarizability of the system. The units of the directional polarizability are determined by the units of the perturbation and Hamiltonian. This equation can be found in [5] equation 4a. Note that in equation 4a of the reference there is a 2 that account for the double occupancy which is not present in this case cause the density matrix construction is done by taking the occupancy into account.

- subroutine, public [prg\\_response\\_mod::prg\\_pert\\_from\\_file](#) (prt\_bml, norb)

Read perturbation from file.

- subroutine, public [prg\\_response\\_mod::prg\\_compute\\_response\\_rs](#) (ham\_bml, prt\_bml, rsp\_bml, lambda, bndfil, threshold, verbose)

Computes the first order response density matrix using Rayleigh Schrodinger Perturbation theory The transformation hereby performed are:

- subroutine, public `prg_response_mod::prg_compute_response_fd` (ham\_bml, prt\_bml, rsp\_bml, prg\_delta, bndfil, threshold, verbose)

Computes the first order response density matrix using finite differences. The transformation hereby performed are:

- subroutine, public `prg_response_mod::prg_pert_constant_field` (field, intensity, coordinate, lambda, prt\_bml, threshold, spindex, norbi, verbose, over\_bml)

Apply a constant field perturbation through the dipole moment operator ( $\hat{\mu} = e\hat{r}$ ). In the matrix representation, this is:  $H^{(1)} = \lambda \frac{1}{2} (S e\mathbf{r} \cdot \mathbf{E} + e\mathbf{r} \cdot \mathbf{E} S)$ . The symmetrization is done in order to preserve the Hermiticity of  $H$ . In this case the whole system will be affected by the field. In a latter version we will add the possibility of applying this field to a region of the system. In this implementation  $e = 1$  and units can be transformed by using the parameter  $\lambda$ .

- subroutine, public `prg_response_mod::prg_pert_sin_pot` (direction, lx, coordinate, lambda, prt\_bml, threshold, spindex, norbi, verbose, over\_bml)

Apply a sinusoidal length dependent potential ( $\sin(\tilde{r}_x)$ ) where  $\mathbf{r}_x$  is the x coordinate. The Hamiltonian gets modified as follows:  $H^{(1)} = \frac{1}{2}\lambda(S \sin(\tilde{r}_x) + \sin(\tilde{r}_x)S)$ .  $\tilde{r}_x = 2\pi(\mathbf{r}/l_x) - \pi$ . The symmetrization is done in order to preserve the Hermiticity of  $H$ . Units can be transformed by using the parameter  $\lambda$ .

- subroutine, public `prg_response_mod::prg_pert_cos_pot` (direction, lx, coordinate, lambda, prt\_bml, threshold, spindex, norbi, verbose, over\_bml)

Apply a cosine length dependent potential ( $\cos(\tilde{r}_x)$ ) where  $\mathbf{r}_x$  is the x coordinate. The Hamiltonian gets modified as follows:  $H^{(1)} = \frac{1}{2}\lambda(S \cos(\tilde{r}_x) + \cos(\tilde{r}_x)S)$ .  $\tilde{r}_x = 2\pi(\mathbf{r}/l_x) - \pi$ . The symmetrization is done in order to preserve the Hermiticity of  $H$ . Units can be transformed by using the parameter  $\lambda$ .

- subroutine, public `prg_response_mod::prg_compute_response_sp2` (ham\_bml, prt\_bml, rsp\_bml, rho\_bml, lambda, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtoll, threshold, verbose)

Finds the first order response matrix from a Hamiltonian matrix.

- subroutine, public `prg_response_mod::prg_project_response` (rsp\_bml, over\_bml, spindex, norbi, coordinates, rspfunc, verbose)

Project the response onto atomic positions. First order response to the perturbation ( $\rho^{(1)}$ ) projected onto the atomic position. Basically:  $rsp(i) = \sum_{\alpha \in i} \rho_{\alpha\alpha}^{(1)}$ , where orbital  $\alpha$  belong to atom  $i$ .

## Variables

- integer, parameter `prg_response_mod::dp` = kind(1.0d0)
- real(dp), parameter `prg_response_mod::pi` = 3.14159265358979323846264338327950\_dp

## 11.27 /home/christian/qmd-progress/src/prg\_sp2\_fermi\_mod.F90 File Reference

### Modules

- module `prg_sp2_fermi_mod`

The SP2 Fermi module.

### Functions/Subroutines

- subroutine, public `prg_sp2_fermi_mod::prg_sp2_fermi_init` (h\_bml, nsteps, nocc, tscale, threshold, occErrLimit, traceLimit, x\_bml, mu, beta, h1, hN, sgnlist)

Truncated SP2 prg\_initialization.

- subroutine, public `prg_sp2_fermi_mod::prg_sp2_fermi_init_norecs` (h\_bml, nsteps, nocc, tscale, threshold, occErrLimit, traceLimit, x\_bml, mu, beta, h1, hN, sgnlist, verbose)

Truncated SP2 prg\_initialization. This routine also gives back the Number of SP2 recursive steps that gets a Pseudo-Fermi distribution with a temperature close to the target temperature which is entered using parameter  $\beta = (1/KbT)$ .



- subroutine, public [prg\\_sp2\\_fermi\\_mod::prg\\_sp2\\_fermi](#) (h\_bml, osteps, nsteps, nocc, mu, beta, h1, hN, sgnlist, threshold, eps, traceLimit, x\_bml)  
*Calculate Truncated SP2.*
- subroutine, public [prg\\_sp2\\_fermi\\_mod::prg\\_sp2\\_entropy\\_function](#) (mu, h1, hN, nsteps, sgnlist, GG, ee)  
*Calculate SP2 entropy function using gaussian quadrature. Note that GG and ee are allocated and returned from this routine.*
- real(dp) function, public [prg\\_sp2\\_fermi\\_mod::sp2\\_entropy\\_ts](#) (D0\_bml, GG, ee)  
*Test SP2 entropy. Get the entropy contribution TS to the total free energy.*
- real(dp) function, public [prg\\_sp2\\_fermi\\_mod::sp2\\_inverse](#) (f, mu, h1, hN, nsteps, sgnlist)  
*Calculate the SP2 inverse.*
- real(dp) function [prg\\_sp2\\_fermi\\_mod::absmaxderivative](#) (func, de)  
*Gets the absolute maximum of the derivative of a function.*

## Variables

- integer, parameter [prg\\_sp2\\_fermi\\_mod::dp](#) = kind(1.0d0)

## 11.28 /home/christian/qmd-progress/src/prg\_sp2\_mod.F90 File Reference

### Modules

- module [prg\\_sp2\\_mod](#)  
*The SP2 module.*

### Functions/Subroutines

- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_basic](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemt看, verbose)  
*Calculates the density matrix from a Hamiltonian matrix by purification. The method implemented here is the very first verion of the SP2 method.*
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_alg2](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemt看, verbose)
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_alg2\\_genseq](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemt看, pp, icount, vv, verbose)
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_alg2\\_seq](#) (h\_bml, rho\_bml, threshold, pp, icount, vv, verbose)
- subroutine, public [prg\\_sp2\\_mod::prg\\_prg\\_sp2\\_alg2\\_seq\\_inplace](#) (rho\_bml, threshold, pp, icount, vv, mineval, maxeval, verbose)
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_alg1](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemt看, verbose)
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_alg1\\_genseq](#) (h\_bml, rho\_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemt看, pp, icount, vv)
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_alg1\\_seq](#) (h\_bml, rho\_bml, threshold, pp, icount, vv)
- subroutine, public [prg\\_sp2\\_mod::prg\\_prg\\_sp2\\_alg1\\_seq\\_inplace](#) (rho\_bml, threshold, pp, icount, vv, mineval, maxeval)
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_submatrix](#) (ham\_bml, rho\_bml, threshold, pp, icount, vv, mineval, maxeval, core\_size)  
*Perform SP2 algorithm using sequence and calculate norm for a submatrix.*
- subroutine, public [prg\\_sp2\\_mod::prg\\_sp2\\_submatrix\\_inplace](#) (rho\_bml, threshold, pp, icount, vv, mineval, maxeval, core\_size)

## Variables

- integer, parameter `prg_sp2_mod::dp` = kind(1.0d0)

## 11.29 /home/christian/qmd-progress/src/prg\_sp2parser\_mod.F90 File Reference

### Data Types

- type `prg_sp2parser_mod::sp2data_type`  
*General SP2 solver type.*

### Modules

- module `prg_sp2parser_mod`  
*SP2 parser.*

### Functions/Subroutines

- subroutine, public `prg_sp2parser_mod::prg_parse_sp2` (sp2data, filename)  
*The parser for SP2 solver.*

### Variables

- integer, parameter `prg_sp2parser_mod::dp` = kind(1.0d0)

## 11.30 /home/christian/qmd-progress/src/prg\_subgraphloop\_mod.F90 File Reference

### Modules

- module `prg_subgraphloop_mod`  
*The subgraphloop module.*

### Functions/Subroutines

- subroutine, public `prg_subgraphloop_mod::prg_subgraphsp2loop` (h\_bml, g\_bml, rho\_bml, gp, threshold)
- subroutine, public `prg_subgraphloop_mod::prg_collectmatrixfromparts` (gp, rho\_bml)  
*Collect distributed parts into same matrix.*
- subroutine, public `prg_subgraphloop_mod::prg_balanceparts` (gp)
- subroutine, public `prg_subgraphloop_mod::prg_partordering` (gp)  
*Set row ordering bases on parts.*
- subroutine, public `prg_subgraphloop_mod::prg_getgrouppartitionhalosfromgraph` (gp, g\_bml, hnode, djflag)  
*Get core+halo indeces for all partitions only using the graph.*
- subroutine, public `prg_subgraphloop_mod::prg_getpartitionhalosfromgraph` (gp, g\_bml, djflag)  
*Get core+halo indeces for all partitions only using the graph.*

## Variables

- integer, parameter `prg_subgraphloop_mod::dp` = kind(1.0d0)

## 11.31 /home/christian/qmd-progress/src/prg\_syrotation\_mod.F90 File Reference

### Data Types

- type `prg_syrotation_mod::rotation_type`  
*Rotation type.*

### Modules

- module `prg_syrotation_mod`  
*A module to rotate the coordinates of a sybsystem in chemical systems.*

### Functions/Subroutines

- subroutine, public `prg_syrotation_mod::prg_parse_rotation` (rot, filename)  
*The parser for rotation.*
- subroutine, public `prg_syrotation_mod::prg_rotate` (rot, r, verbose)  
*Rotation routine.*

## Variables

- integer, parameter `prg_syrotation_mod::dp` = kind(1.0d0)

## 11.32 /home/christian/qmd-progress/src/prg\_system\_mod.F90 File Reference

### Data Types

- type `prg_system_mod::estruct_type`  
*Electronic structure type.*
- type `prg_system_mod::system_type`  
*System type.*

### Modules

- module `prg_system_mod`  
*A module to read and handle chemical systems.*

## Functions/Subroutines

- subroutine, public [prg\\_system\\_mod::prg\\_get\\_nameandext](#) (fullfilename, filename, ext)  
*Get the name and extension of a file.*
- subroutine, public [prg\\_system\\_mod::prg\\_parse\\_system](#) (system, filename, extin)  
*The parser for the chemical system.*
- subroutine, public [prg\\_system\\_mod::prg\\_write\\_system](#) (system, filename, extension)  
*Write system in .xyz, .dat or pdb file.*
- subroutine, public [prg\\_system\\_mod::prg\\_write\\_trajectory](#) (system, iter, each, prg\_deltat, filename, extension)  
*Write trajectory in .xyz, .dat or pdb file.*
- subroutine, public [prg\\_system\\_mod::prg\\_write\\_trajectoryandproperty](#) (system, iter, each, prg\_deltat, scalarprop, filename, extension)  
*Write trajectory and atomic properties. Only pdb file.*
- subroutine, public [prg\\_system\\_mod::prg\\_make\\_random\\_system](#) (system, nats, seed, lx, ly, lz)  
*Make random Xx system.*
- subroutine [prg\\_system\\_mod::prg\\_parameters\\_to\\_vectors](#) (abc\_angles, lattice\_vector)  
*Transforms the lattice parameters into lattice vectors.*
- subroutine [prg\\_system\\_mod::prg\\_vectors\\_to\\_parameters](#) (lattice\_vector, abc\_angles)  
*Transforms the lattice vectors into lattice parameters.*
- subroutine, public [prg\\_system\\_mod::prg\\_get\\_origin](#) (coords, origin)  
*Get the origin of the coordinates.*
- subroutine, public [prg\\_system\\_mod::prg\\_get\\_distancematrix](#) (coords, dmat)  
*Get the distance matrix.*
- subroutine, public [prg\\_system\\_mod::prg\\_translateandfoldtobox](#) (coords, lattice\_vectors, origin, verbose)  
*Translate and fold to box.*
- subroutine, public [prg\\_system\\_mod::prg\\_centeratbox](#) (coords, lattice\_vectors, verbose)  
*Translate geometric center to the center of the box.*
- subroutine, public [prg\\_system\\_mod::prg\\_wraparound](#) (coords, lattice\_vectors, index, verbose)  
*Wrap around atom i using pbc.*
- subroutine, public [prg\\_system\\_mod::prg\\_translategeomcandfoldtobox](#) (coords, lattice\_vectors, origin)  
*Translate to geometric center.*
- subroutine, public [prg\\_system\\_mod::prg\\_replicate](#) (coords, symbols, lattice\_vectors, nx, ny, nz)  
*Extend/replicate system along lattice vectors.*
- subroutine, public [prg\\_system\\_mod::prg\\_get\\_recip\\_vects](#) (lattice\_vectors, recip\_vectors, volr, volk)  
*Get the volume of the cell and the reciprocal vectors: This subrountine computes:*
- subroutine, public [prg\\_system\\_mod::prg\\_get\\_dihedral](#) (coords, id1, id2, id3, id4, dihedral)  
*Get the dihedral angle given four atomic positions.*
- subroutine, public [prg\\_system\\_mod::prg\\_get\\_covgraph](#) (sy, nnStructMindist, nnStruct, nrrnnstruct, bml\_type, factor, gcov\_bml, mdimin, verbose)  
*Get the covalency graph in bml format.*
- subroutine [prg\\_system\\_mod::prg\\_get\\_covgraph\\_int](#) (sy, nnStructMindist, nnStruct, nrrnnstruct, bml\_type, factor, gcov\_bml, mdimin, verbose)
- subroutine, public [prg\\_system\\_mod::prg\\_get\\_covgraph\\_h](#) (sy, nnStructMindist, nnStruct, nrrnnstruct, rcut, graph\_h, mdimin, verbose)  
*Get the covanlency graph.*
- subroutine, public [prg\\_system\\_mod::prg\\_get\\_subsystem](#) (sy, lsize, indices, sbsy, verbose)  
*Get a subsystem out of the total system.*
- subroutine, public [prg\\_system\\_mod::prg\\_destroy\\_subsystems](#) (sbsy, verbose)  
*Destroy allocated subsystem.*
- subroutine, public [prg\\_system\\_mod::prg\\_molpartition](#) (sy, npart, nnStructMindist, nnStruct, nrrnnstruct, het-atm, gp, verbose)  
*Partition by molecule.*

- subroutine, public `prg_system_mod::prg_get_partial_atomgraph` (rho\_bml, hindex, gch\_bml, threshold, verbose)  
*Get partial subgraph based on the Density matrix.*
- subroutine, public `prg_system_mod::prg_collect_graph_p` (rho\_bml, nc, nats, hindex, chindex, graph\_p, threshold, mdimin, verbose)  
*Collect the small graph to build the full graph.*
- subroutine, public `prg_system_mod::prg_merge_graph` (graph\_p, graph\_h)  
*Get partial subgraph based on the Density matrix.*
- subroutine, public `prg_system_mod::prg_merge_graph_adj` (graph\_p, graph\_h, xadj, adjncy)  
*Get partial subgraph based on the Density matrix.*
- subroutine, public `prg_system_mod::prg_adj2bml` (xadj, adjncy, bml\_type, g\_bml)  
*prg\_adj2bml*
- subroutine, public `prg_system_mod::prg_graph2bml` (graph, bml\_type, g\_bml)  
*Graph2bml.*
- subroutine, public `prg_system_mod::prg_graph2vector` (graph, vector, maxnz)  
*Vectorize graph.*
- subroutine, public `prg_system_mod::prg_vector2graph` (vector, graph, maxnz)  
*Back to graph.*
- subroutine, public `prg_system_mod::prg_sortadj` (xadj, adjncy)  
*Sort adj NOTE: this might not be needed anymore since the bml\_get\_adj routine is sorting the values.*

## Variables

- integer, parameter `prg_system_mod::dp` = kind(1.0d0)

## 11.33 /home/christian/qmd-progress/src/prg\_timer\_mod.F90 File Reference

### Data Types

- type `prg_timer_mod::timer_status_t`  
*Timer status type.*

### Modules

- module `prg_timer_mod`  
*The timer module.*

### Functions/Subroutines

- subroutine, public `prg_timer_mod::timer_prg_init` ()  
*Initialize timers.*
- subroutine `prg_timer_mod::prg_timer_getid` ()  
*Get timer id.*
- subroutine, public `prg_timer_mod::prg_timer_shutdown` ()  
*Done with timers.*
- subroutine, public `prg_timer_mod::prg_timer_start` (itimer, tag)  
*Start Timing.*
- subroutine, public `prg_timer_mod::prg_timer_stop` (itimer, verbose)  
*Stop timing.*
- subroutine, public `prg_timer_mod::prg_timer_collect` ()
- subroutine, public `prg_timer_mod::prg_timer_results` ()
- real(8) function, public `prg_timer_mod::time2milliseconds` ()
- subroutine, public `prg_timer_mod::prg_print_date_and_time` (tag)
- character(2) function, private `prg_timer_mod::int2char` (ival)

## Variables

- integer, parameter `prg_timer_mod::dp` = kind(1.0d0)
- integer, public `prg_timer_mod::loop_timer`
- integer, public `prg_timer_mod::sp2_timer`
- integer, public `prg_timer_mod::genx_timer`
- integer, public `prg_timer_mod::part_timer`
- integer, public `prg_timer_mod::subgraph_timer`
- integer, public `prg_timer_mod::deortho_timer`
- integer, public `prg_timer_mod::ortho_timer`
- integer, public `prg_timer_mod::zdiag_timer`
- integer, public `prg_timer_mod::graphsp2_timer`
- integer, public `prg_timer_mod::subind_timer`
- integer, public `prg_timer_mod::subext_timer`
- integer, public `prg_timer_mod::subsp2_timer`
- integer, public `prg_timer_mod::suball_timer`
- integer, public `prg_timer_mod::bmult_timer`
- integer, public `prg_timer_mod::badd_timer`
- integer, public `prg_timer_mod::dyn_timer`
- integer, public `prg_timer_mod::mdloop_timer`
- integer, public `prg_timer_mod::buildz_timer`
- integer, public `prg_timer_mod::realcoul_timer`
- integer, public `prg_timer_mod::recipcoul_timer`
- integer, public `prg_timer_mod::pairpot_timer`
- integer, public `prg_timer_mod::halfverlet_timer`
- integer, public `prg_timer_mod::pos_timer`
- integer, public `prg_timer_mod::nlist_timer`
- integer `prg_timer_mod::tstart_clock`
- integer `prg_timer_mod::tstop_clock`
- integer `prg_timer_mod::tclock_rate`
- integer `prg_timer_mod::tclock_max`
- integer `prg_timer_mod::num_timers`
- type(timer\_status\_t), dimension(:), allocatable `prg_timer_mod::ptimer`

## 11.34 /home/christian/qmd-progress/src/prg\_xlbo\_mod.F90 File Reference

### Data Types

- type `prg_xlbo_mod::xlbo_type`  
*General xlbo solver type.*

### Modules

- module `prg_xlbo_mod`  
*A module to perform XLBO integration.*

## Functions/Subroutines

- subroutine, public [prg\\_xlbo\\_mod::prg\\_parse\\_xlbo](#) (xlbo, filename)  
*The parser for XLBO parser.*
- subroutine, public [prg\\_xlbo\\_mod::prg\\_xlbo\\_nint](#) (charges, n, n\_0, n\_1, n\_2, n\_3, n\_4, n\_5, mdstep, xl)  
*This routine integrates the dynamical variable "n".*
- subroutine, public [prg\\_xlbo\\_mod::prg\\_xlbo\\_fcoulupdate](#) (fcoul, charges, n)  
*Adjust forces for the linearized XLBOMD functional.*

## Variables

- integer, parameter [prg\\_xlbo\\_mod::dp](#) = kind(1.0d0)
- real(dp), parameter [prg\\_xlbo\\_mod::c0](#) = -6.0\_dp  
*Coefficients for modified Verlet integration.*
- real(dp), parameter [prg\\_xlbo\\_mod::c1](#) = 14.0\_dp
- real(dp), parameter [prg\\_xlbo\\_mod::c2](#) = -8.0\_dp
- real(dp), parameter [prg\\_xlbo\\_mod::c3](#) = -3.0\_dp
- real(dp), parameter [prg\\_xlbo\\_mod::c4](#) = 4.0\_dp
- real(dp), parameter [prg\\_xlbo\\_mod::c5](#) = -1.0\_dp
- real(dp), parameter [prg\\_xlbo\\_mod::kappa](#) = 1.82\_dp  
*Coefficients for modified Verlet integration.*
- real(dp), parameter [prg\\_xlbo\\_mod::alpha](#) = 0.018\_dp
- real(dp), parameter [prg\\_xlbo\\_mod::cc](#) = 0.9\_dp

## 11.35 /home/christian/qmd-progress/src/prg\_xlkernel\_mod.F90 File Reference

### Data Types

- type [prg\\_xlkernel\\_mod::xlk\\_type](#)

### Modules

- module [prg\\_xlkernel\\_mod](#)  
*Add name.*

## Functions/Subroutines

- subroutine, public [prg\\_xlkernel\\_mod::prg\\_parse\\_xlkernel](#) (input, filename)  
*The parser for the mixer routines.*
- subroutine, public [prg\\_xlkernel\\_mod::prg\\_fermi](#) (D0, QQ, ee, gap, Fe\_vec, mu0, H, Z, Nocc, T, OccErrLim, MaxIt, HDIM)
- subroutine, public [prg\\_xlkernel\\_mod::prg\\_kernel\\_fermi\\_full](#) (KK, JJ, D0, mu0, mu1, T, RX, RY, RZ, LBox, Hubbard\_U, Element\_Type, Nr\_atoms, MaxIt, eps, m, HDIM, Max\_Nr\_Neigh, Coulomb\_acc, TIMERAT←IO, nnRx, nnRy, nnRz, nrrnlist, nnType, H\_INDEX\_START, H\_INDEX\_END, H, S, Z, Nocc, Znuc, QQ, ee, Fe\_vec)
- subroutine, public [prg\\_xlkernel\\_mod::prg\\_v\\_kernel\\_fermi](#) (D0, dq\_dv, v, mu0, mu1, T, RX, RY, RZ, LBox, Hubbard\_U, Element\_Type, Nr\_atoms, MaxIt, eps, m, HDIM, Max\_Nr\_Neigh, Coulomb\_acc, TIMERAT←IO, nnRx, nnRy, nnRz, nrrnlist, nnType, H\_INDEX\_START, H\_INDEX\_END, H, S, Z, Nocc, Znuc, QQ, ee, Fe\_vec)
- subroutine, private [prg\\_xlkernel\\_mod::prg\\_get\\_deriv\\_finite\\_temp](#) (P1, H0, H1, Nocc, T, Q, ev, fe, mu0, eps, HDIM)
- subroutine, private [prg\\_xlkernel\\_mod::prg\\_mmult](#) (alpha, A, B, beta, C, TA, TB, HDIM)
- subroutine, private [prg\\_xlkernel\\_mod::prg\\_eig](#) (A, Q, ee, type, HDIM)
- subroutine, private [prg\\_xlkernel\\_mod::prg\\_inv](#) (X, XI, HDIM)
- subroutine, public [prg\\_xlkernel\\_mod::prg\\_rank1](#) (verbose)  
*Rank1 kernel ....*

## Variables

- integer, parameter `prg_xlkernel_mod::dp = kind(1.0d0)`



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