

progress

1.1.0

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Chapter 1

README

1.1 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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1.4 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`.)

1.5 Build and Install Instructions

1.5.1 How to build

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

1.5.2 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
```

1.6 Citing

```
@misc{2016progress,  
  title={\texttt{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

2.1 Testing program for the progress library

2.1.1 To run the tests:

Go into the build folder and type:

```
make test
```

To run the tests in verbose mode:

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

2.1.2 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

2.1.3 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.

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Module Index

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Chapter 7

File Index

7.1 File List

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/tmp/qmd-progress/src/prg_initmatrices_mod.F90	306
/tmp/qmd-progress/src/prg_kernelparser_mod.F90	307
/tmp/qmd-progress/src/prg_modelham_mod.F90	307
/tmp/qmd-progress/src/prg_nonortho_mod.F90	308
/tmp/qmd-progress/src/prg_normalize_mod.F90	308
/tmp/qmd-progress/src/prg_openfiles_mod.F90	309
/tmp/qmd-progress/src/prg_parallel_mod.F90	309
/tmp/qmd-progress/src/prg_partition_mod.F90	310
/tmp/qmd-progress/src/prg_progress_mod.F90	312
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/tmp/qmd-progress/src/prg_pulaycomponent_mod.F90	314
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/tmp/qmd-progress/src/prg_sp2_mod.F90	318
/tmp/qmd-progress/src/prg_sp2parser_mod.F90	319
/tmp/qmd-progress/src/prg_subgraphloop_mod.F90	320
/tmp/qmd-progress/src/prg_syrotation_mod.F90	320
/tmp/qmd-progress/src/prg_system_mod.F90	321
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/tmp/qmd-progress/src/prg_xlbo_mod.F90	324
/tmp/qmd-progress/src/prg_xlkernel_mod.F90	325

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 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 prg_get_charges()

```
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 )
```

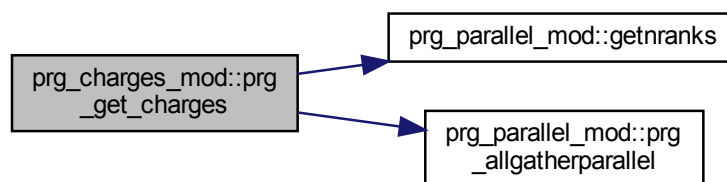
Constructs the charges from the density matrix.

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 prg_get_hscf()

```

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.

Parameters

<code>coulomb_pot↔ _r</code>	Coulombic potential (r contribution)
<code>coulomb_pot↔ _k</code>	Coulombic potential (k contribution)
<code>mdim</code>	Maximum non zeroes elements per row for every row.
<code>threshold</code>	Threshold value for matrix elements.

Definition at line 100 of file prg_charges_mod.F90.

9.1.3 Variable Documentation

9.1.3.1 dp

```
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 absmaxderivative()

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

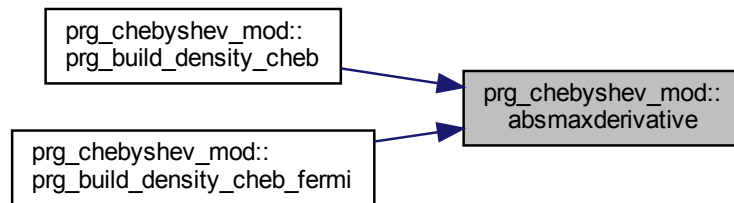
Gets the absolute maximum of the derivative of a function.

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 fermi()

```

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

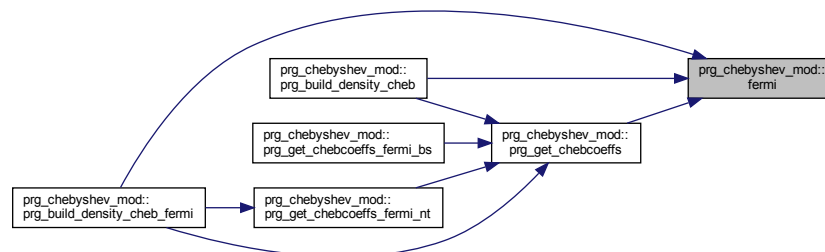
Gives the Fermi distribution value for energy *e*.

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 jackson()

```
real(dp) function prg_chebyshev_mod::jackson (
    integer, intent(in) ncoeffs,
    integer, intent(in) i,
    logical, intent(in) jon ) [private]
```

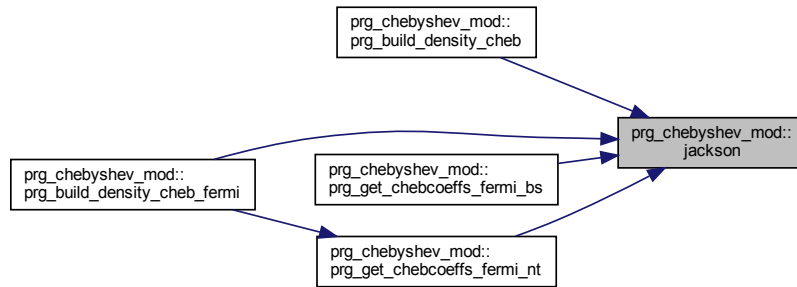
Evaluates the Jackson Kernel Coefficients.

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 prg_build_density_cheb()

```
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.

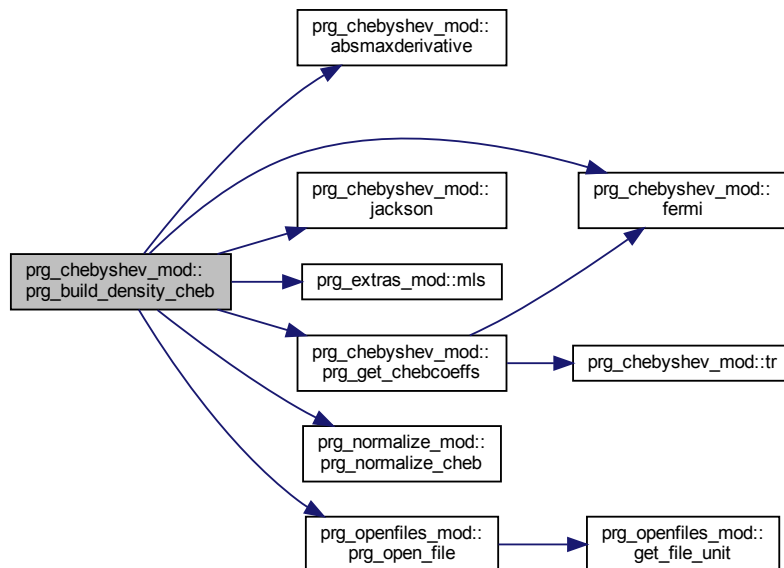
$\rho_{n+1} = b_{n+1}T_{n+1} + \rho_n$ Where, T_n is the nth Chebyshev polynomial and b_n is the nth coefficient of the expansion for the Fermi function. In the sparse version (when ellpack is used) the threshold can be varied linearly with the polynomial degree. The function is the following: $Thresh(n)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

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 prg_build_density_cheb_fermi()

```

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(out) 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.

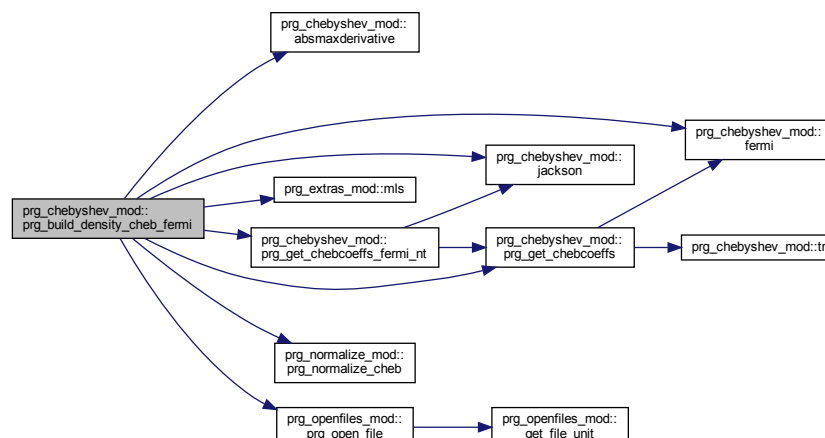
$\rho_{n+1} = b_{n+1}T_{n+1} + \rho_n$ Where, T_n is the nth Chebyshev polynomial and b_n is the nth coefficient of the expansion for the Fermi function. In the sparse version (when ellpack is used) the threshold can be varied linearly with the polynomial degree. The function is the following: $Thresh(n)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

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>npts</i>	Number of energy points to compute the coefficients
<i>verbose</i>	Verbosity level.

Definition at line 309 of file prg_chebyshev_mod.F90.

Here is the call graph for this function:



9.2.2.6 prg_get_chebcoeffs()

```

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]

```

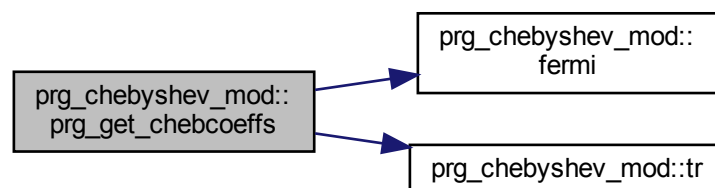
Gets the coefficients of the Chebyshev expansion.

Parameters

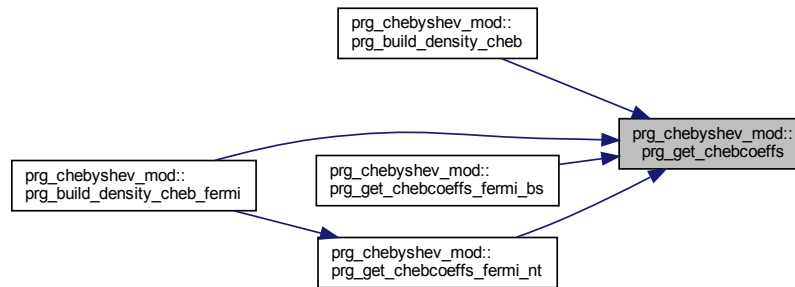
<i>npts</i>	Number of points for discretization.
<i>kbt</i>	Electronic temperature.
<i>ef</i>	Fermi level.
<i>ncoeffs</i>	Number of Chebyshev coefficients.
<i>coeffs</i>	Output vector for the Chebyshev coefficients.
<i>emin</i>	lowest boundary for the eigenvalues of H.
<i>emax</i>	highest boundary for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

```

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.

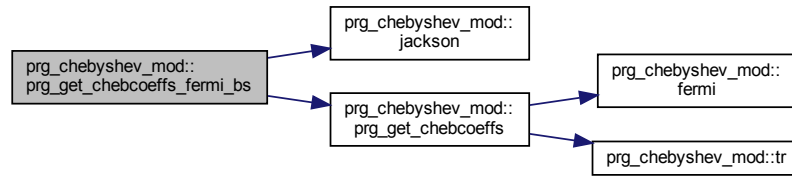
In this case we are applying the bisection method to find the root.

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 prg_get_chebcoeffs_fermi_nt()

```

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.

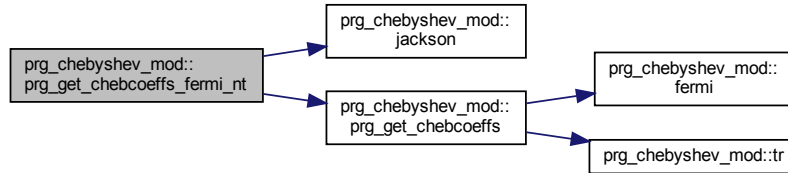
In this case the Newton-Raphson method is applied to find the root.

Parameters

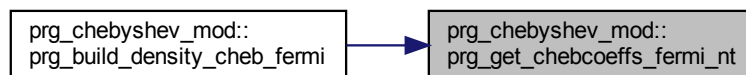
<i>npst</i>	Number of points for the discretization.
<i>kbt</i>	Electronic temperature.
<i>ef</i>	Fermi level.
<i>tracesT</i>	Input traces for matrix polynomials.
<i>ncoeffs</i>	Number of Chebyshev coefficients.
<i>coeffs</i>	Output vector for the Chebyshev coefficients.
<i>emin</i>	lowest boundary for the eigenvalues of H.
<i>emax</i>	highest boundary for the eigenvalues of H.
<i>bndfil</i>	Band filing 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 prg_parse_cheb()

```

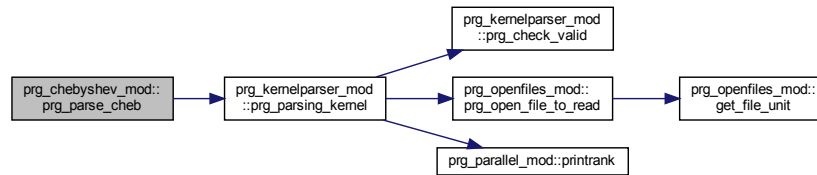
subroutine, public prg_chebyshev_mod::prg_parse_cheb (
    type(chebdata_type), intent(inout) chebdata,
    character(len=*) filename )
  
```

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 tr()

```

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

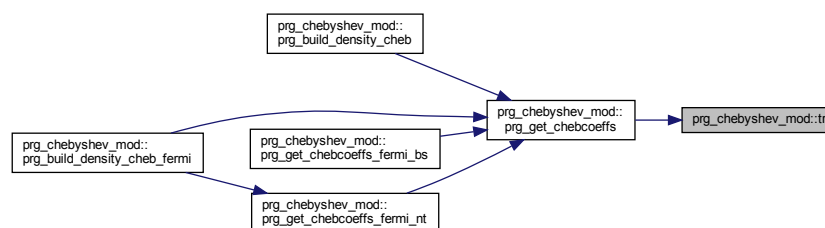
Chebyshev polynomial obtained by recursion.

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 dp

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

Definition at line 23 of file prg_chebyshev_mod.F90.

9.2.3.2 pi

```
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 orthogonalized Hamiltonian.

Functions/Subroutines

- subroutine, public [prg_build_density_t0](#) (ham_bml, rho_bml, threshold, bndfil, eigenvalues_out)
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 ϵ is the matrix eigenvalue. $\Theta()$ is the Heaviside function.
- subroutine, public [prg_build_density_t](#) (ham_bml, rho_bml, threshold, bndfil, kbt, ef, eigenvalues_out)
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 ϵ is the matrix eigenvalue. f is the Fermi function.
- subroutine, public [prg_build_density_t_fulldata](#) (ham_bml, rho_bml, threshold, bndfil, kbt, ef, eigenvalues_out, evecs_bml, fvals)
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 ϵ 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 ϵ 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_flevel_nt](#) (eigenvalues, kbt, bndfil, tol, ef, verbose)
Routine to compute the Fermi level given a set of eigenvalues and a temperature. It applies the Newton-Raphson 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 orthogonalized Hamiltonian.

9.3.2 Function/Subroutine Documentation

9.3.2.1 fermi()

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

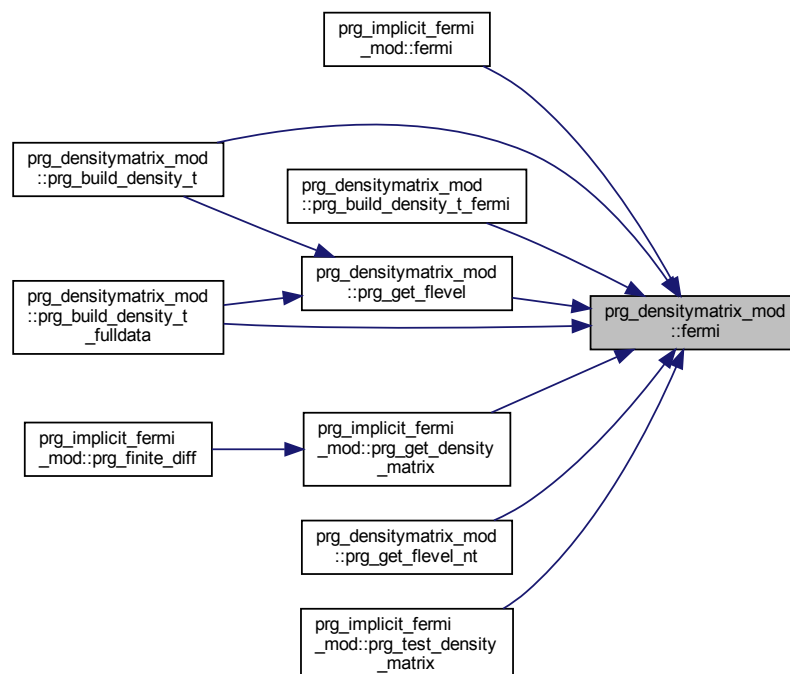
Gives the Fermi distribution value for energy *e*.

Parameters

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

Definition at line 599 of file prg_densitymatrix_mod.F90.

Here is the caller graph for this function:



9.3.2.2 prg_build_atomic_density()

```
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 320 of file prg_densitymatrix_mod.F90.

9.3.2.3 prg_build_density_t()

```
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(dp), intent(in) threshold,
    real(dp), intent(in) bndfil,
    real(dp), intent(in) kbt,
    real(dp), intent(inout) ef,
    real(dp), dimension(:), intent(out), optional, allocatable eigenvalues_out )
```

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 ϵ is the matrix eigenvalue. f is the Fermi function.

Parameters

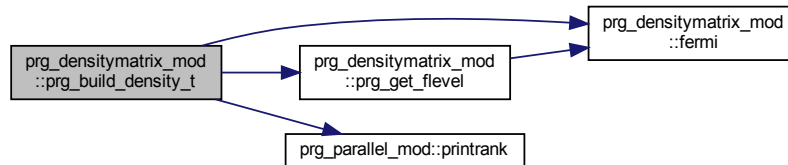
<i>ham_bml</i>	Input Orthogonalized Hamiltonian matrix.
<i>rho_bml</i>	Output density matrix,
<i>threshold</i>	Threshold for sparse matrix algebra.
<i>bndfil</i>	Filing factor.
<i>kbt</i>	Electronic temperature.
<i>ef</i>	Fermi level.
<i>eigenvalues_out</i>	Output the eigenvalues.

Warning

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

Definition at line 111 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:

**9.3.2.4 prg_build_density_t0()**

```

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,
    real(dp), dimension(:), intent(out), optional, allocatable eigenvalues_out )
  
```

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 ϵ is the matrix eigenvalue. $\Theta()$ is the Heaviside function.

Parameters

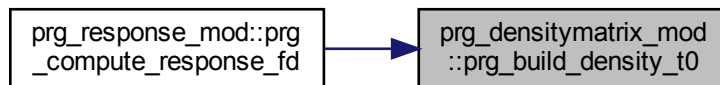
<i>ham_bml</i>	Input Orthogonalized Hamiltonian matrix.
<i>rho_bml</i>	Output density matrix.
<i>threshold</i>	Threshold for sparse matrix algebra.
<i>bndfil</i>	Filing factor.
<i>eigenvalues_out</i>	Output the eigenvalues.

Warning

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

Definition at line 35 of file prg_densitymatrix_mod.F90.

Here is the caller graph for this function:



9.3.2.5 prg_build_density_t_fermi()

```

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(dp), intent(in) threshold,
    real(dp), intent(in) kbt,
    real(dp), 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 ϵ is the matrix eigenvalue. f is the Fermi function. In this routine the Fermi level is passed as an argument.

Parameters

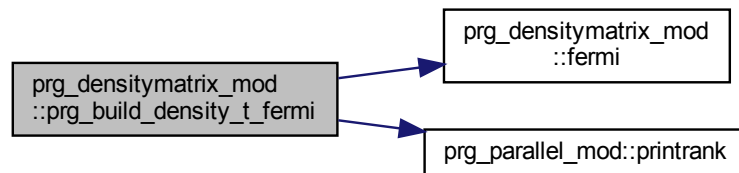
<i>ham_bml</i>	Input Orthogonalized Hamiltonian matrix.
<i>rho_bml</i>	Output density matrix,
<i>threshold</i>	Threshold for sparse matrix algebra.

Warning

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

Definition at line 258 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:



9.3.2.6 prg_build_density_t_fulldata()

```

subroutine, public prg_densitymatrix_mod::prg_build_density_t_fulldata (
    type(bml_matrix_t), intent(in) ham_bml,
    type(bml_matrix_t), intent(inout) rho_bml,
    real(dp), intent(in) threshold,
    real(dp), intent(in) bndfil,
    real(dp), intent(in) kbt,
    real(dp), intent(inout) ef,
    real(dp), dimension(:), intent(inout), allocatable eigenvalues_out,
    type(bml_matrix_t), intent(inout) evects_bml,
    real(dp), dimension(:), intent(inout), allocatable fvals )
  
```

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 ϵ is the matrix eigenvalue. f is the Fermi function.

Parameters

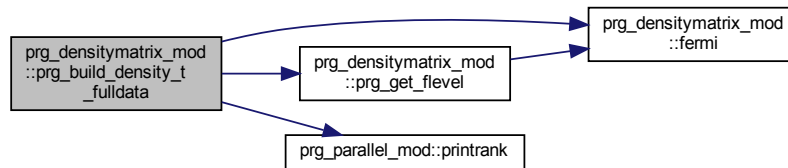
<i>ham_bml</i>	Input Orthogonalized Hamiltonian matrix.
<i>rho_bml</i>	Output density matrix,
<i>threshold</i>	Threshold for sparse matrix algebra.
<i>bndfil</i>	Filing factor.
<i>kbt</i>	Electronic temperature.
<i>ef</i>	Fermi level.
<i>eigenvalues_out</i>	Output the eigenvalues.
<i>evects_bml</i>	Output the eigenvectors.
<i>fvals</i>	Output the occupancies.

Warning

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

Definition at line 188 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:



9.3.2.7 prg_check_idempotency()

```

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 575 of file prg_densitymatrix_mod.F90.

9.3.2.8 prg_get_eigenvalues()

```

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 530 of file prg_densitymatrix_mod.F90.

9.3.2.9 prg_get_flevel()

```

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

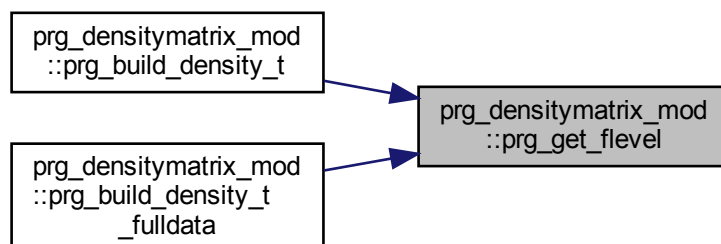
<i>eigenvalues</i>	Eigenvalues of the system ($\{\epsilon_k\}$).
<i>kbt</i>	Temperature times the Boltzmann's constant ($k_b T$).
<i>bndfil</i>	Filing factor ($N_{el}/(2 * N_{orbs})$).
<i>tol</i>	Tolerance for the bisection method.
<i>Ef</i>	Fermi level (μ).

Definition at line 384 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.3.2.10 prg_get_flevel_nt()

```
subroutine, public prg_densitymatrix_mod::prg_get_flevel_nt (
    real(dp), dimension(:), intent(in) eigenvalues,
    real(dp), intent(in) kbt,
    real(dp), intent(in) bndfil,
    real(dp), intent(in) tol,
    real(dp), intent(inout) ef,
    integer, intent(in), optional verbose )
```

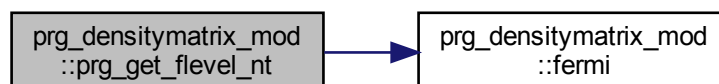
Routine to compute the Fermi level given a set of eigenvalues and a temperature. It applies the Newton-Raphson method over the function: $g(\mu) = \sum_k 2f(\epsilon_k - \mu) - N = 0$ Where $f(\epsilon_k - \mu) = \frac{1}{1 + \exp((\epsilon_k - \mu)/(k_b T))}$.

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 (μ).

Definition at line 452 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:



9.3.3 Variable Documentation

9.3.3.1 dp

```
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 lorentz()

```
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.

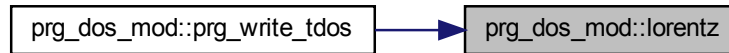
Computes: $L(\epsilon) = \sum_k \frac{\omega(k)\Gamma}{2\pi} \frac{1}{(\epsilon - \epsilon_k)^2 + (\Gamma/2)^2}$

Parameters

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

Definition at line 77 of file prg_dos_mod.F90.

Here is the caller graph for this function:



9.4.2.2 prg_write_tdos()

```

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

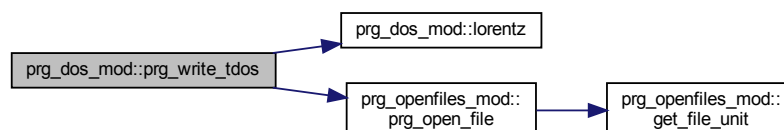
DOS is NOT shifted respect to Ef.

Parameters

<i>eigenvals</i>	Eigenvalues of the system. \para 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 35 of file prg_dos_mod.F90.

Here is the call graph for this function:



9.4.3 Variable Documentation

9.4.3.1 dp

```
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 $\|X^tSX - I\|$.
- subroutine, public [prg_get_mem](#) (procname, tag)
Get proc memory.
- subroutine [prg_twonorm](#) (a, nn, norm2)
Gets the norm2 of a square matrix.
- real(dp) function, public [prg_norm2](#) (a)
Gets the norm2 of a vector.

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 routine.

9.5.2 Function/Subroutine Documentation

9.5.2.1 mls()

```
real(dp) function, public prg_extras_mod::mls
```

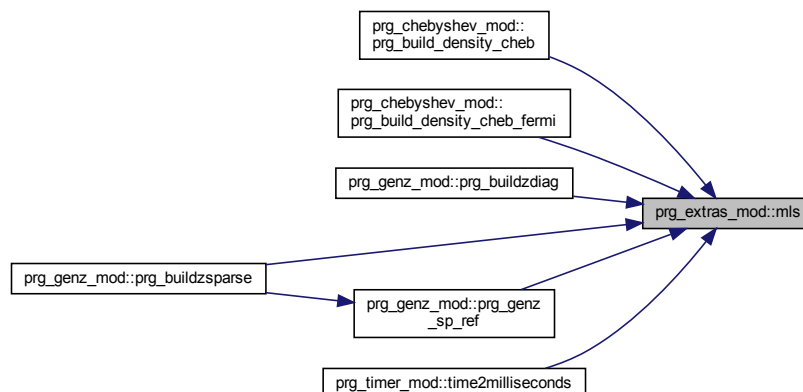
To get the actual time in milliseconds.

Parameters

<i>mls</i>	Output value with the machine time in milliseconds.
------------	---

Definition at line 140 of file prg_extras_mod.F90.

Here is the caller graph for this function:



9.5.2.2 prg_delta()

```
subroutine, public prg_extras_mod::prg_delta (
    real(dp), dimension(nn,nn) x,
```

```

real(dp), dimension(nn,nn) s,
integer nn,
real(dp) dta )

```

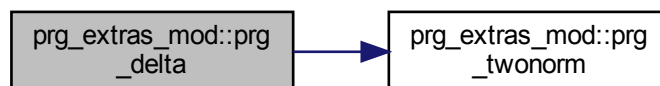
Delta function $\|X^t S X - I\|$.

Parameters

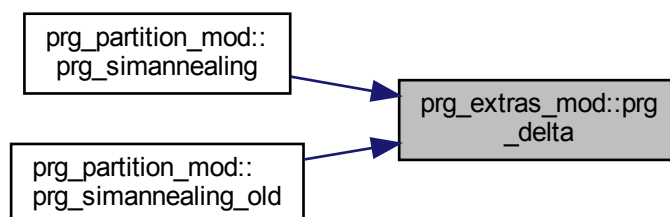
<i>x</i>	input matrix.
<i>s</i>	overlap matrix.
<i>dta</i>	Delta output value.

Definition at line 156 of file prg_extras_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.5.2.3 prg_get_mem()

```

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 192 of file prg_extras_mod.F90.

9.5.2.4 prg_norm2()

```
real(dp) function, public prg_extras_mod::prg_norm2 (
    real(dp), dimension(:), intent(in) a )
```

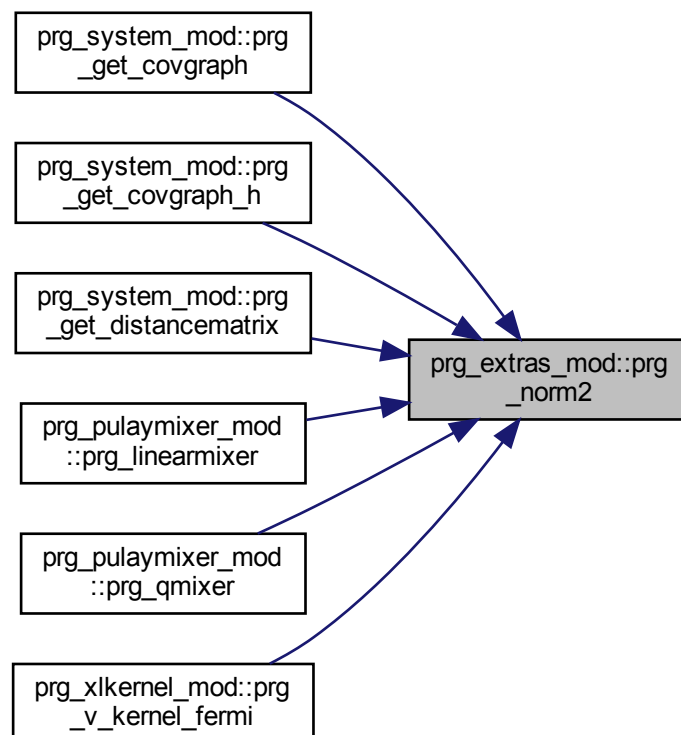
Gets the norm2 of a vector.

Parameters

<i>a</i>	Vector.
----------	---------

Definition at line 241 of file prg_extras_mod.F90.

Here is the caller graph for this function:



9.5.2.5 prg_print_matrix()

```
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 101 of file prg_extras_mod.F90.

9.5.2.6 prg_twonorm()

```
subroutine prg_extras_mod::prg_twonorm (
    real(dp), dimension(nn,nn) a,
    integer nn,
    real(dp) norm2 ) [private]
```

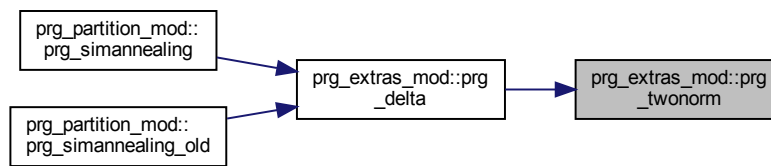
Gets the norm2 of a square matrix.

Parameters

<i>a</i>	Square matrix.
<i>nn</i>	Matrix size.
<i>norm2</i>	Two-norm of matrix a.

Definition at line 216 of file prg_extras_mod.F90.

Here is the caller graph for this function:



9.5.2.7 to_string_double()

```
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 81 of file prg_extras_mod.F90.

9.5.2.8 to_string_integer()

```
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 47 of file prg_extras_mod.F90.

9.5.2.9 to_string_long_long()

```
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 63 of file prg_extras_mod.F90.

9.5.3 Variable Documentation

9.5.3.1 dp

```
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 [genzspinp](#)

Input for the genz driver. This type controls all the variables that are needed by genz.

Functions/Subroutines

- subroutine, public [prg_parse_zsp](#) (input, filename)
The parser for genz solver.
- subroutine, public [prg_init_zspmat](#) (igenz, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, norb, bml_type, bml_element_type)
Initiates the matrices for the XI integration of Z.
- subroutine, public [prg_buildzdiag](#) (smat_bml, zmat_bml, threshold, mdimin, bml_type, 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.
- 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)
Initial estimation of Z.
- subroutine, public [prg_genz_sp_initial_zmat](#) (smat_bml, zmat_bml, norb, mdim, bml_type_f, threshold)
Initial estimation of Z.
- subroutine [prg_genz_sp_int](#) (zmat_bml, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, igenz, norb, bml_type, threshold)
Inverse factorization using Niklasson's algorithm.
- subroutine, public [prg_genz_sp_ref](#) (smat_bml, zmat_bml, nref, norb, bml_type, threshold)
Iterative refinement.

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 prg_buildzdiag()

```
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=*), intent(in) bml_type,
    integer, intent(in), optional verbose )
```

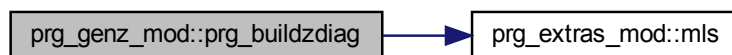
Usual subroutine involving diagonalization. $Z = U\sqrt{s}U^\dagger$, where U = eigenvectors and s = eigenvalues. The purpose of this subroutine is to have an exact way of computing z for comparing with the sparse approach.

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 175 of file prg_genz_mod.F90.

Here is the call graph for this function:



9.6.2.2 prg_buildzsparse()

```

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

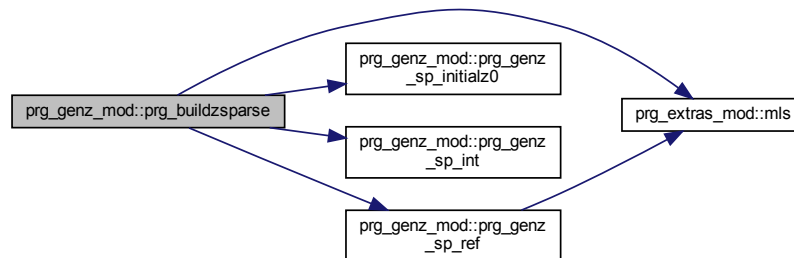
<i>smat_bml</i>	overlap matrix
<i>zmat_bml</i>	congruence transform to be updated or computed. (bml format)
<i>igenz</i>	counter to keep track of the calls to this subroutine.

Parameters

<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 319 of file prg_genz_mod.F90.

Here is the call graph for this function:



9.6.2.3 prg_genz_sp_initial_zmat()

```

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 )

```

Initial estimation of Z.

Note

Most of the operations are done in pure dense format. 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>norb</i>	Congruence transform in bml format.
<i>mdim</i>	Congruence transform in bml format.
<i>bml_type_f</i>	The bml final type of zmat_bml.
<i>threshold</i>	Threshold value to use, in this case, only in the backtransformation to ellpack format.

Definition at line 522 of file prg_genz_mod.F90.

9.6.2.4 prg_genz_sp_initialz0()

```
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 )
```

Initial estimation of Z.

Note

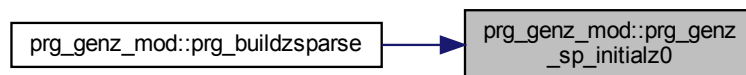
Most of the operations are done in pure dense format. The purpose of this subroutine is to have an exact way of computing z for comparing with the sparse approach.

Parameters

<i>smat_bml</i>	Overlap matrix in bml format.
<i>zmat_bml</i>	Congruence transform in bml format.
<i>norb</i>	Congruence transform in bml format.
<i>mdim</i>	Congruence transform in bml format.
<i>bml_↔ type_f</i>	The bml final type of zmat_bml.
<i>threshold</i>	Threshold value to use, in this case, only in the backtransformation to ellpack format.

Definition at line 382 of file prg_genz_mod.F90.

Here is the caller graph for this function:



9.6.2.5 prg_genz_sp_int()

```
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]

```

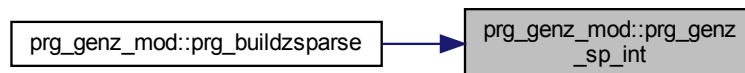
Inverse factorization using Niklasson's algorithm.

Parameters

<i>smat_bml</i>	overlap matrix
<i>zmat_bml</i>	congruence transform to be updated or computed. (bml format)
<i>mdim</i>	dimension of the maxnonzero per row.
<i>zk1_bml-zk6_bml</i>	history of the past congruence transforms.
<i>igenz</i>	counter to keep track of the calls to this subroutine.
<i>norb</i>	Congruence transform in bml format.
<i>bml_type_f</i>	The bml final type of <i>zmat_bml</i> .
<i>threshold</i>	Threshold value to use.

Definition at line 679 of file prg_genz_mod.F90.

Here is the caller graph for this function:



9.6.2.6 prg_genz_sp_ref()

```

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 )

```

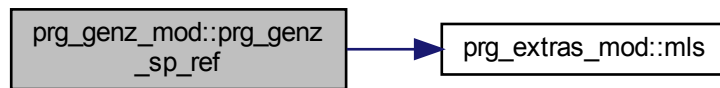
Iterative refinement.

Parameters

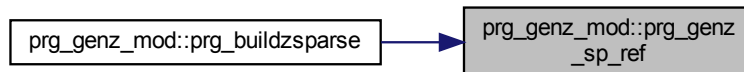
<i>smat_bml</i>	overlap matrix
<i>zmat_bml</i>	congruence transform to be updated or computed. (bml format)
<i>nref</i>	Number of refinement iterations.
<i>bml_↔ type_f</i>	The bml final type of zmat_bml.
<i>threshold</i>	Threshold value to use.
<i>verbose</i>	to print extra information.

Definition at line 763 of file prg_genz_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.6.2.7 prg_init_zspmat()

```

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,
    character(20), optional bml_element_type )
  
```

Initiates 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 135 of file prg_genz_mod.F90.

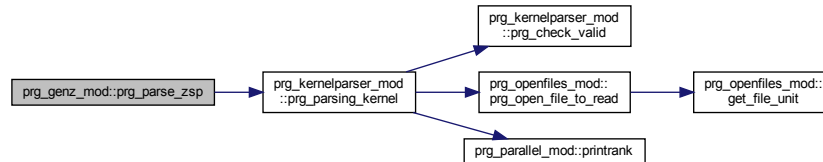
9.6.2.8 prg_parse_zsp()

```
subroutine, public prg_genz_mod::prg_parse_zsp (
    type(genzspinp), intent(inout) input,
    character(len=*) filename )
```

The parser for genz solver.

Definition at line 68 of file prg_genz_mod.F90.

Here is the call graph for this function:



9.6.3 Variable Documentation

9.6.3.1 dp

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

Definition at line 18 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 prg_destroygraphpartitioning()

```
subroutine, public prg_graph_mod::prg_destroygraphpartitioning (
    type (graph_partitioning_t), intent(inout) gp )
```

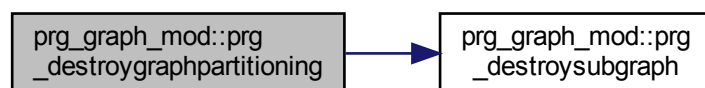
Destroy graph partitioning.

Parameters

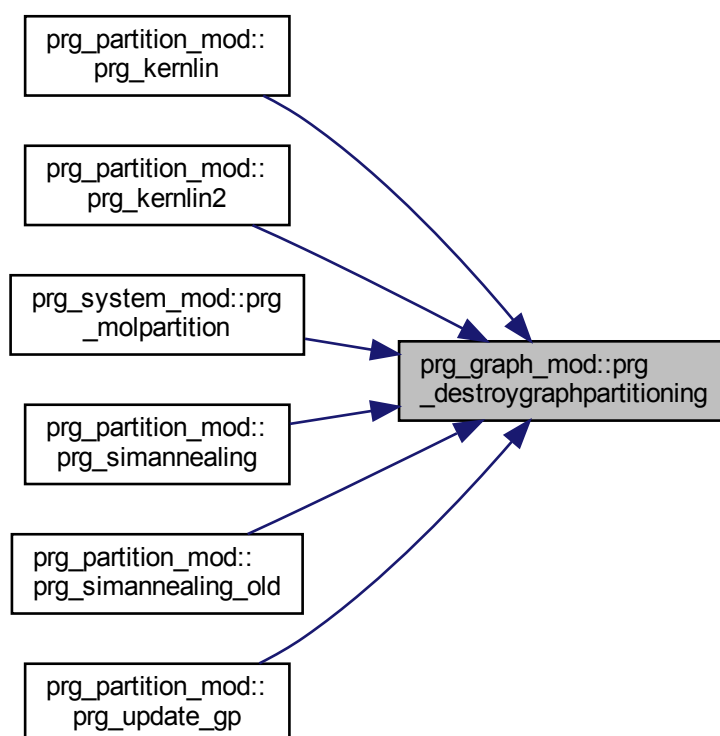
<code>sg</code>	Subgraph
-----------------	----------

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 prg_destroysubgraph()

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

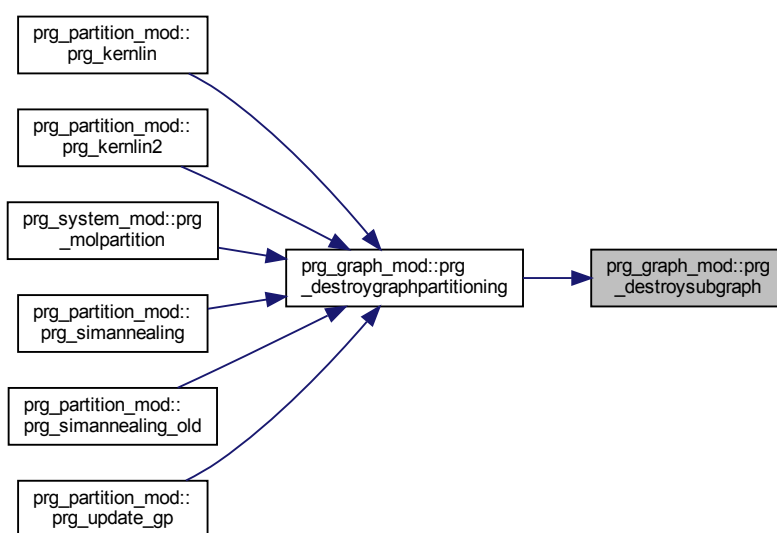
Destroy subgraph.

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 prg_equalgrouppartition()

```
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

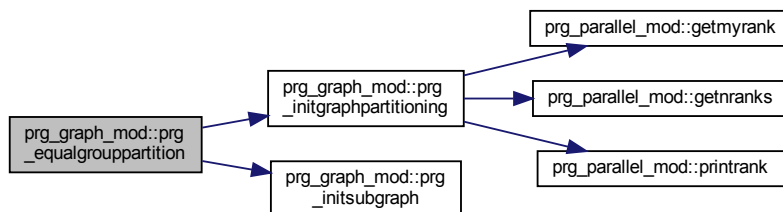
<i>gp</i>	Graph partitioning
-----------	--------------------

Parameters

<i>hindex</i>	Node indices 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 prg_equalpartition()

```

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

```

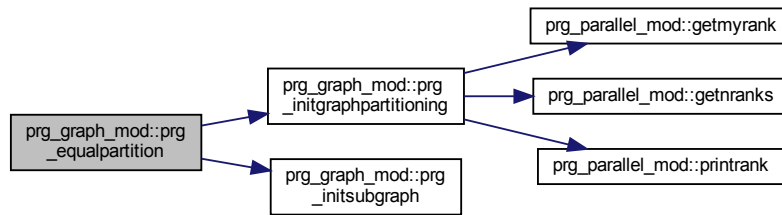
Create equal graph partitions, based on number of rows/orbitals.

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 prg_filepartition()

```

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

```

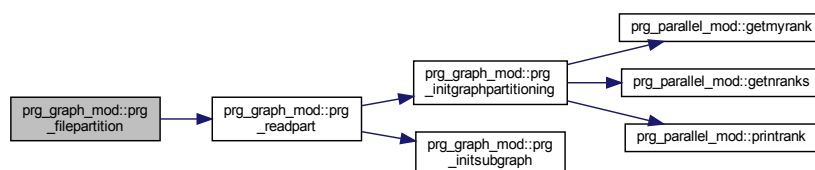
Read graph partitions from a file, based on number of rows/orbitals.

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 prg_fnormgraph()

```

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

```

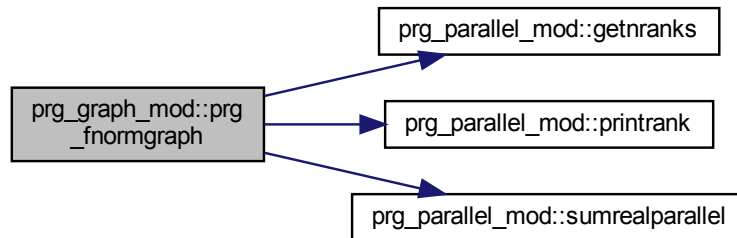
Accumulate trace norm across all subgraphs.

Parameters

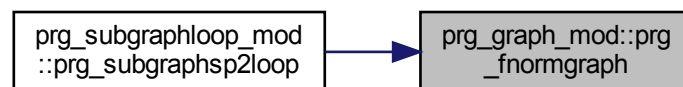
<i>gp</i>	Graph partitioning
-----------	--------------------

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 prg_initgraphpartitioning()

```

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 )
  
```

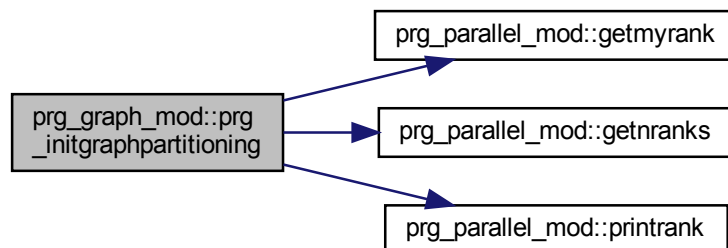
Initialize graph partitioning.

Parameters

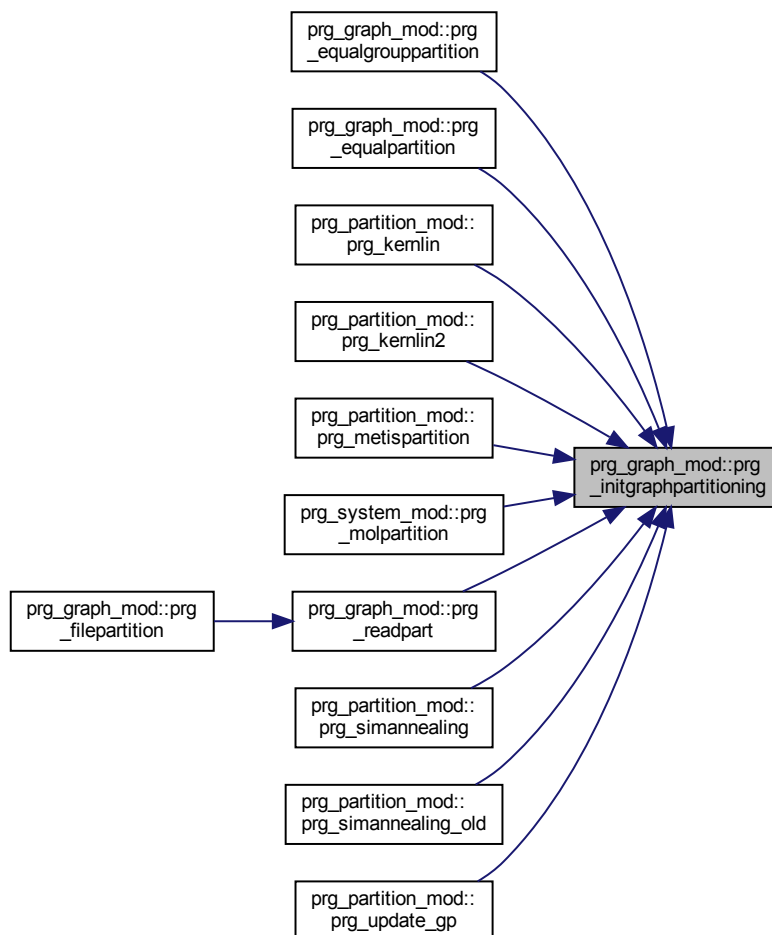
<i>gp</i>	Graph partitioning
<i>pname</i>	Partitioning name
<i>np</i>	Number of partitions
<i>nnodes</i>	Number of groups/nodes
<i>nnodes2</i>	Number of nodes

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 prg_initsubgraph()

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

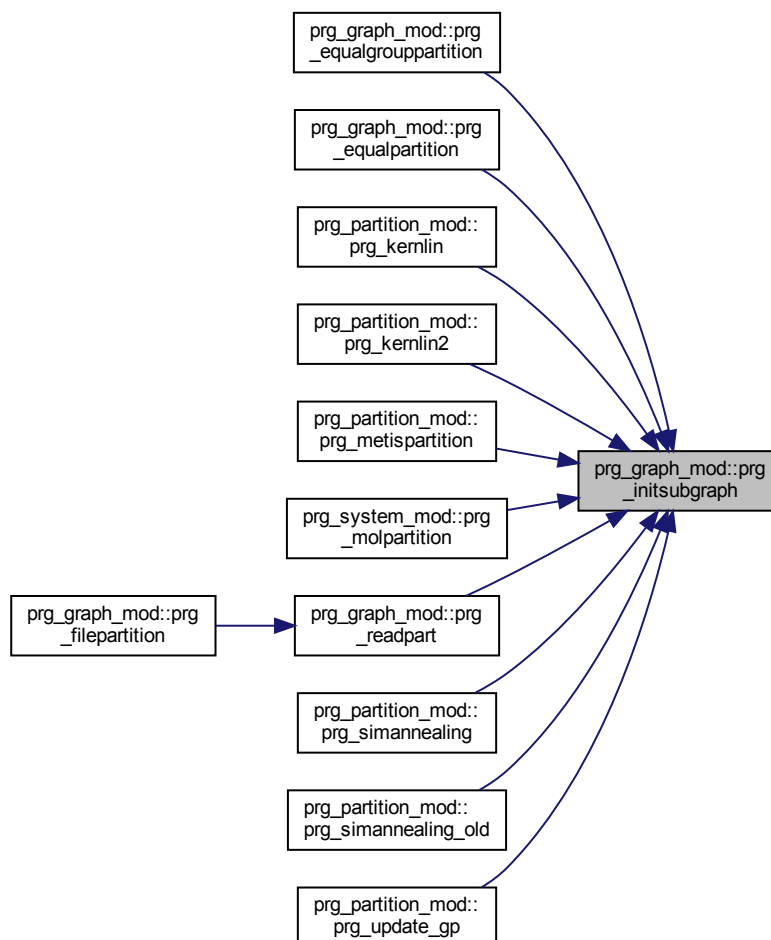
Initialize subgraph.

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 prg_printgraphpartitioning()

```
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 prg_readpart()

```
subroutine prg_graph_mod::prg_readpart (
    type (graph_partitioning_t), intent(inout) gp,
    character(len=*), intent(in) partFile ) [private]
```

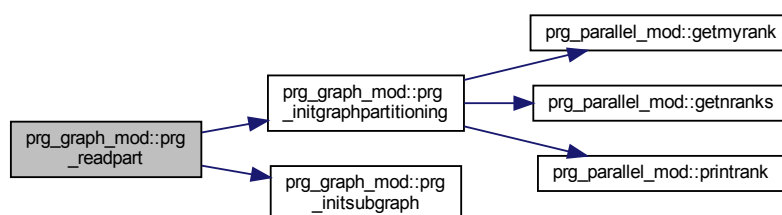
Read parts (core) from part file.

Parameters

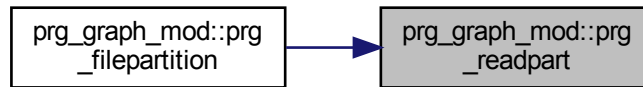
<i>gp</i>	Graph partitioning
<i>partFile</i>	Partition file

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 dp

```
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

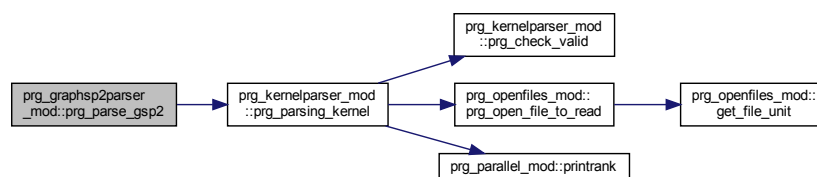
9.8.2.1 prg_parse_gsp2()

```
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 dp

```
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 prg_homolumogap()

```
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 prg_sp2sequence()

```
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 98 of file prg_homolumo_mod.F90.

9.9.3 Variable Documentation

9.9.3.1 dp

```
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, p_bml, nsteps, k, nocc, mu, beta, method, osteps, occErrLimit, threshold, tol)
Recursive Implicit Fermi Dirac for finite temperature.
- subroutine, public [prg_implicit_fermi_zero](#) (h_bml, p_bml, nsteps, mu, method, threshold, tol)
Recursive Implicit Fermi Dirac for zero temperature.
- subroutine, public [prg_implicit_fermi_response](#) (H0_bml, H1_bml, H2_bml, H3_bml, P0_bml, P1_bml, P2_bml, P3_bml, nsteps, mu0, mu, beta, nocc, occ_tol, lin_tol, order, threshold)
Calculate density matrix response to perturbations using Implicit Fermi Dirac.
- subroutine, public [prg_finite_diff](#) (H0_bml, H_list, mu0, mu_list, beta, order, lambda, h, threshold)
Calculate density matrix response from perturbations in the Hamiltonian.
- subroutine [prg_setup_linsys](#) (p_bml, A_bml, b_bml, p2_bml, y_bml, aux_bml, aux1_bml, k, threshold)
Set up linear system for Implicit Fermi Dirac.
- subroutine [prg_newtonschulz](#) (a_bml, ai_bml, r_bml, tmp_bml, tol, threshold)
Find the inverse of the matrix A with Newton-Schulz iteration.
- subroutine [prg_pcg](#) (A_bml, p_bml, p2_bml, d_bml, wtmp_bml, cg_tol, threshold)
Solve the system $AX = B$ with conjugate gradient.
- subroutine [prg_conjgrad](#) (A_bml, p_bml, p2_bml, d_bml, w_bml, cg_tol, threshold)
Solve the system $AX = B$ with conjugate gradient.
- subroutine [prg_get_density_matrix](#) (ham_bml, p_bml, beta, mu, threshold)
Calculate the density matrix with diagonalization.
- subroutine, public [prg_test_density_matrix](#) (ham_bml, p_bml, beta, mu, nocc, osteps, occErrLimit, threshold)
Calculate the density matrix with diagonalization and converge chemical.
- real(dp) function [fermi](#) (e, mu, beta)
Gives the Fermi distribution value for energy e.

Variables

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

9.10.1 Function/Subroutine Documentation

9.10.1.1 `fermi()`

```
real(dp) function prg_implicit_fermi_mod::fermi (  
    real(dp), intent(in) e,  
    real(dp), intent(in) mu,  
    real(dp), intent(in) beta ) [private]
```

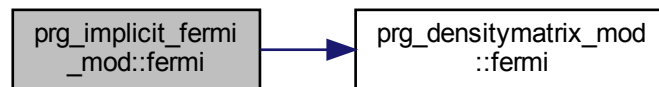
Gives the Fermi distribution value for energy `e`.

Parameters

<i>e</i>	Energy.
<i>mu</i>	Fermi energy.
<i>beta</i>	Inverse temperature

Definition at line 905 of file prg_implicit_fermi_mod.F90.

Here is the call graph for this function:



9.10.1.2 prg_conjgrad()

```

subroutine prg_implicit_fermi_mod::prg_conjgrad (
    type(bml_matrix_t), intent(in) A_bml,
    type(bml_matrix_t), intent(inout) p_bml,
    type(bml_matrix_t), intent(inout) p2_bml,
    type(bml_matrix_t), intent(inout) d_bml,
    type(bml_matrix_t), intent(inout) w_bml,
    real(dp), intent(in) cg_tol,
    real(dp), intent(in) threshold ) [private]
  
```

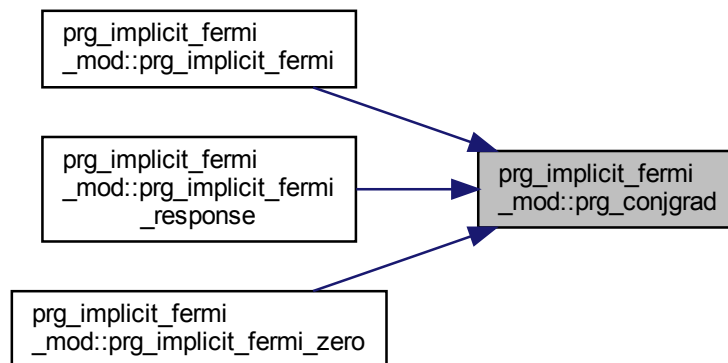
Solve the system $AX = B$ with conjugate gradient.

Parameters

<i>A_bml</i>	Coefficient matrix A
<i>p_bml</i>	Output solution X
<i>p2_bml</i>	Right side matrix B
<i>d_bml</i>	Auxillary matrix
<i>w_bml</i>	Auxillary matrix
<i>cg_tol</i>	Convergence condition (OBS squared Frobenius norm of residual matrix)
<i>threshold</i>	Threshold for matrix algebra

Definition at line 721 of file prg_implicit_fermi_mod.F90.

Here is the caller graph for this function:



9.10.1.3 prg_finite_diff()

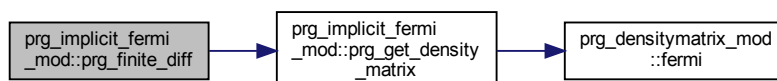
```

subroutine, public prg_implicit_fermi_mod::prg_finite_diff (
    type(bml_matrix_t), intent(in) H0_bml,
    type(bml_matrix_t), dimension(:), intent(in), allocatable H_list,
    real(dp), intent(in) mu0,
    real(dp), dimension(:), intent(in), allocatable mu_list,
    real(dp), intent(in) beta,
    integer, intent(in) order,
    real(dp), intent(in) lambda,
    real(dp), intent(in) h,
    real(dp), intent(in) threshold )
  
```

Calculate density matrix response from perturbations in the Hamiltonian.

Definition at line 450 of file `prg_implicit_fermi_mod.F90`.

Here is the call graph for this function:



9.10.1.4 prg_get_density_matrix()

```

subroutine prg_implicit_fermi_mod::prg_get_density_matrix (
    type(bml_matrix_t), intent(in) ham_bml,
    type(bml_matrix_t), intent(inout) p_bml,
    real(dp), intent(in) beta,
    real(dp), intent(in) mu,
    real(dp), intent(in) threshold ) [private]

```

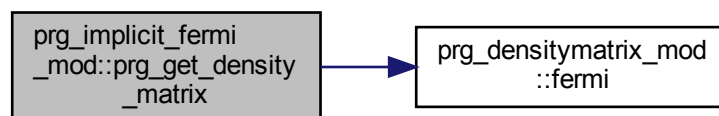
Calculate the density matrix with diagonalization.

Parameters

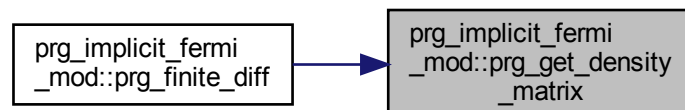
<i>ham_bml</i>	Input hamiltonian
<i>p_bml</i>	Output density matrix
<i>beta</i>	Inverse temperature
<i>mu</i>	Chemical potential
<i>threshold</i>	Threshold for matrix algebra

Definition at line 771 of file prg_implicit_fermi_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.10.1.5 prg_implicit_fermi()

```

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

```

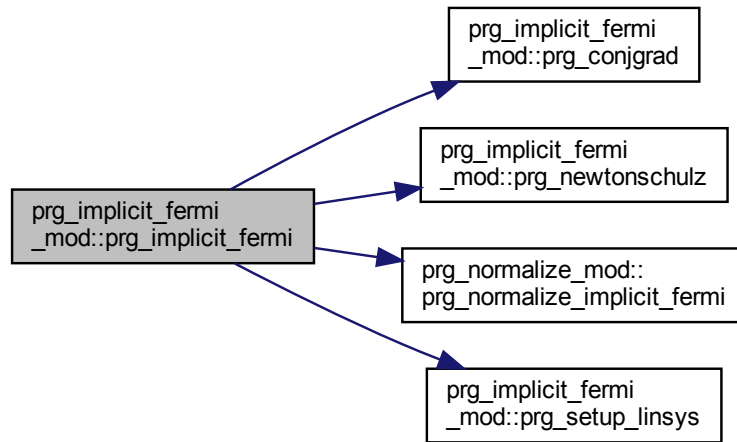
Recursive Implicit Fermi Dirac for finite temperature.

Parameters

<i>h_bml</i>	Input Hamiltonian matrix.
<i>p_bml</i>	Output density matrix.
<i>nsteps</i>	Number of recursion steps.
<i>k</i>	Expansion order
<i>nocc</i>	Number of occupied states.
<i>mu</i>	Shifted chemical potential
<i>beta</i>	Input inverse temperature.
<i>method</i>	0 - conjugate gradient, 1 - newton-schultz
<i>osteps</i>	Outer loop steps to converge chemical potential
<i>occErrLimit</i>	Occupation error limit.
<i>threshold</i>	Threshold for multiplication.
<i>tol</i>	Tolerance for linear system solver See

Definition at line 44 of file prg_implicit_fermi_mod.F90.

Here is the call graph for this function:



9.10.1.6 prg_implicit_fermi_response()

```

subroutine, public prg_implicit_fermi_mod::prg_implicit_fermi_response (
    type(bml_matrix_t), intent(in) H0_bml,
    type(bml_matrix_t), intent(in) H1_bml,
    type(bml_matrix_t), intent(in) H2_bml,
    type(bml_matrix_t), intent(in) H3_bml,
    type(bml_matrix_t), intent(inout) P0_bml,
    type(bml_matrix_t), intent(inout) P1_bml,
    type(bml_matrix_t), intent(inout) P2_bml,
    type(bml_matrix_t), intent(inout) P3_bml,
    integer, intent(in) nsteps,
    real(dp), intent(inout) mu0,
    real(dp), dimension(:), intent(inout), allocatable mu,
    real(dp), intent(in) beta,
    real(dp), intent(in) nocc,
    real(dp), intent(in) occ_tol,
    real(dp), intent(in) lin_tol,
    integer order,
    real(dp) threshold )
  
```

Calculate density matrix response to perturbations using Implicit Fermi Dirac.

Parameters

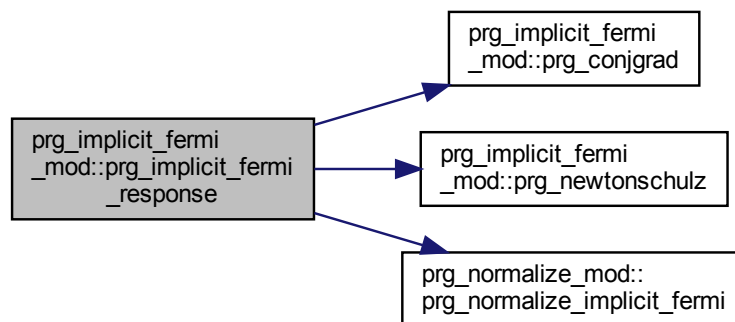
<i>H0_bml</i>	Input Hamiltonian matrix.
<i>H1_bml,H2_bml,H3_bml</i>	Input First to third order perturbations of H0.
<i>P0_bml</i>	Output density matrix.
<i>P1_bml,P2_bml,P3_bml</i>	Output First to third order density matrix response.

Parameters

<i>nsteps</i>	Number of recursion steps.
<i>mu0</i>	Shifted chemical potential.
<i>mu</i>	Pre-allocated array of length order.
<i>beta</i>	Input inverse temperature.
<i>nocc</i>	Number of occupied states.
<i>occ_tol</i>	Occupation error tolerance.
<i>lin_tol</i>	Linear solver tolerance.
<i>order</i>	Calculate response up to this order.
<i>threshold</i>	Threshold for matrix algebra. See

Definition at line 273 of file `prg_implicit_fermi_mod.F90`.

Here is the call graph for this function:



9.10.1.7 prg_implicit_fermi_zero()

```

subroutine, public prg_implicit_fermi_mod::prg_implicit_fermi_zero (
    type(bml_matrix_t), intent(in) h_bml,
    type(bml_matrix_t), intent(inout) p_bml,
    integer, intent(in) nsteps,
    real(dp), intent(in) mu,
    integer, intent(in) method,
    real(dp), intent(in) threshold,
    real(dp), intent(inout), optional tol )

```

Recursive Implicit Fermi Dirac for zero temperature.

Parameters

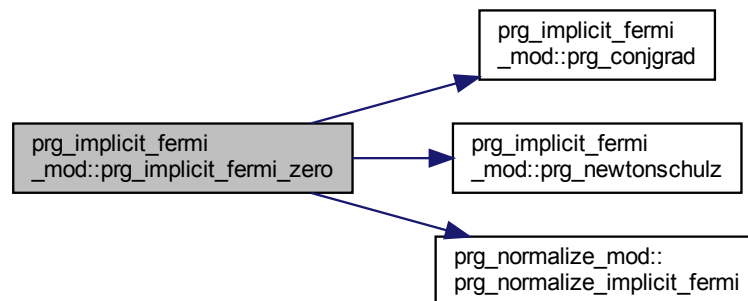
<i>h_bml</i>	Input Hamiltonian matrix.
<i>p_bml</i>	Output density matrix.

Parameters

<i>nsteps</i>	Number of recursion steps.
<i>mu</i>	Shifted chemical potential
<i>beta</i>	Input inverse temperature.
<i>method</i>	0 - conjugate gradient, 1 - newton-schultz
<i>threshold</i>	Threshold for multiplication.
<i>tol</i>	Tolerance for linear system solver

Definition at line 179 of file prg_implicit_fermi_mod.F90.

Here is the call graph for this function:



9.10.1.8 prg_newtonschulz()

```

subroutine prg_implicit_fermi_mod::prg_newtonschulz (
    type(bml_matrix_t), intent(in) a_bml,
    type(bml_matrix_t), intent(inout) ai_bml,
    type(bml_matrix_t), intent(inout) r_bml,
    type(bml_matrix_t), intent(inout) tmp_bml,
    real(dp), intent(in) tol,
    real(dp), intent(in) threshold ) [private]
  
```

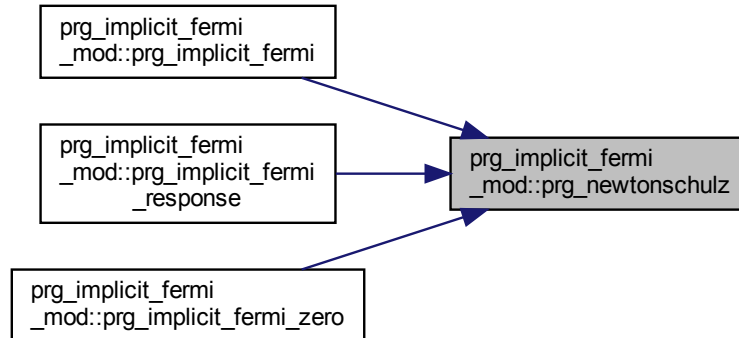
Find the inverse of the matrix A with Newton-Schulz iteration.

Parameters

<i>a_bml</i>	Input matrix A
<i>ai_bml</i>	Input starting guess and output inverse
<i>r_bml</i>	Auxillary matrix
<i>tmp_bml</i>	Auxillary matrix
<i>tol</i>	Convergence criterion (Frobenius norm of residual matrix)
<i>threshold</i>	Threshold for matrix algebra

Definition at line 612 of file prg_implicit_fermi_mod.F90.

Here is the caller graph for this function:



9.10.1.9 prg_pcg()

```

subroutine prg_implicit_fermi_mod::prg_pcg (
    type(bml_matrix_t), intent(in) A_bml,
    type(bml_matrix_t), intent(inout) p_bml,
    type(bml_matrix_t), intent(inout) p2_bml,
    type(bml_matrix_t), intent(inout) d_bml,
    type(bml_matrix_t), intent(inout) wtmp_bml,
    real(dp), intent(in) cg_tol,
    real(dp), intent(in) threshold ) [private]
  
```

Solve the system $AX = B$ with conjugate gradient.

Parameters

<i>A_bml</i>	Coefficient matrix A
<i>p_bml</i>	Output solution X
<i>p2_bml</i>	Right side matrix B
<i>d_bml</i>	Auxillary matrix
<i>w_bml</i>	Auxillary matrix
<i>cg_tol</i>	Convergence condition (OBS squared Frobenius norm of residual matrix)
<i>threshold</i>	Threshold for matrix algebra

Definition at line 649 of file prg_implicit_fermi_mod.F90.

9.10.1.10 prg_setup_linsys()

```

subroutine prg_implicit_fermi_mod::prg_setup_linsys (
    type(bml_matrix_t), intent(in)  p_bml,
    type(bml_matrix_t), intent(inout) A_bml,
    type(bml_matrix_t), intent(inout) b_bml,
    type(bml_matrix_t), intent(inout) p2_bml,
    type(bml_matrix_t), intent(inout) y_bml,
    type(bml_matrix_t), intent(inout) aux_bml,
    type(bml_matrix_t), intent(inout) aux1_bml,
    integer, intent(in) k,
    real(dp), intent(in) threshold ) [private]

```

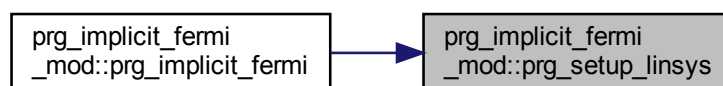
Set up linear system for Implicit Fermi Dirac.

Parameters

<i>p_bml</i>	Input X_i matrix.
<i>p2_bml</i>	Output X_i^k matrix.
<i>A_bml</i>	Output $[X_i^k + (I - X_i)^k]$ matrix.
<i>y_bml</i>	Auxillary matrix.
<i>aux_bml</i>	Auxillary matrix
<i>aux1_bml</i>	Auxillary matrix.
<i>k</i>	Expansion order (an even number)
<i>threshold</i>	Threshold for multiplication. OBS this routine can be numerically unstable for $k > 4$

Definition at line 568 of file prg_implicit_fermi_mod.F90.

Here is the caller graph for this function:



9.10.1.11 prg_test_density_matrix()

```

subroutine, public prg_implicit_fermi_mod::prg_test_density_matrix (
    type(bml_matrix_t), intent(in)  ham_bml,
    type(bml_matrix_t), intent(inout) p_bml,
    real(dp), intent(in) beta,
    real(dp), intent(inout) mu,
    real(dp), intent(in) nocc,
    integer, intent(in) osteps,

```

```

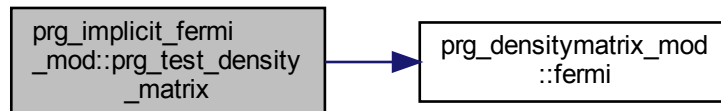
real(dp), intent(in) occErrLimit,
real(dp), intent(in) threshold )

```

Calculate the density matrix with diagonalization and converge chemical.

Definition at line 827 of file prg_implicit_fermi_mod.F90.

Here is the call graph for this function:



9.10.2 Variable Documentation

9.10.2.1 dp

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

Definition at line 18 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 initialize several matrices that will be used in the code.

9.11.2 Function/Subroutine Documentation

9.11.2.1 prg_init_hsmat()

```
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 29 of file prg_initmatrices_mod.F90.

9.11.2.2 prg_init_ortho()

```
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 73 of file prg_initmatrices_mod.F90.

9.11.2.3 prg_init_pzmat()

```
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 51 of file prg_initmatrices_mod.F90.

9.11.3 Variable Documentation

9.11.3.1 dp

```
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.

9.12.2 Function/Subroutine Documentation

9.12.2.1 prg_check_valid()

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

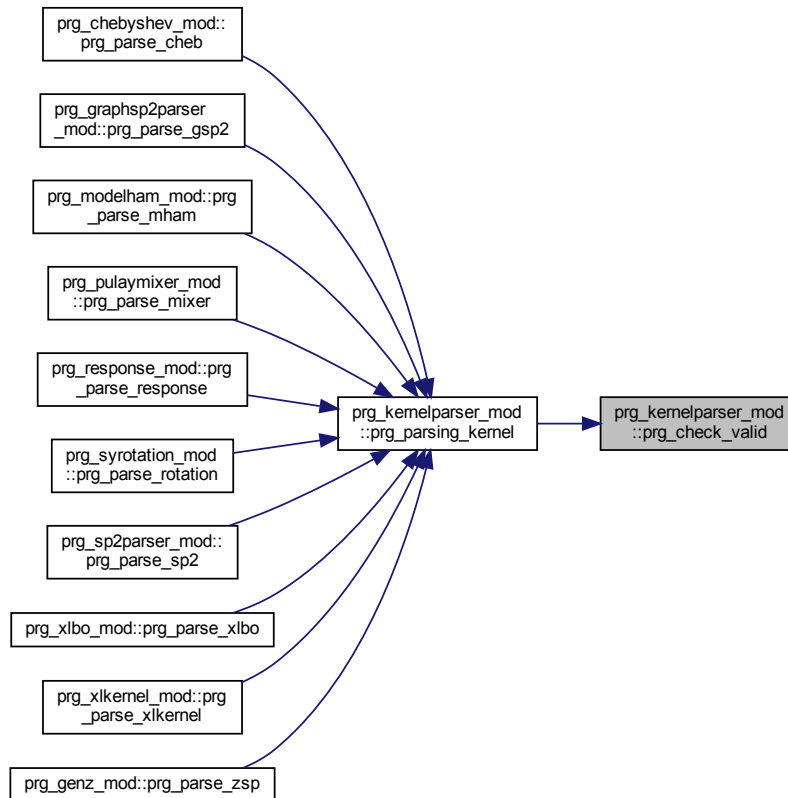
Check for valid keywords (checks for an = sign)

Parameters

<i>invalidc</i>	Keyword to check.
-----------------	-------------------

Definition at line 393 of file prg_kernelparser_mod.F90.

Here is the caller graph for this function:



9.12.2.2 prg_parsing_kernel()

```

subroutine, public prg_kemelparser_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

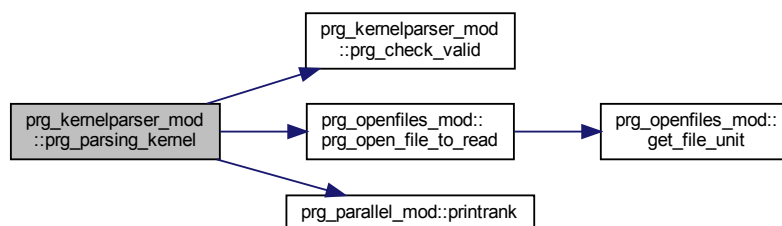
This parsing strategy can only parse a file of 500 lines by 500 words.

Warning

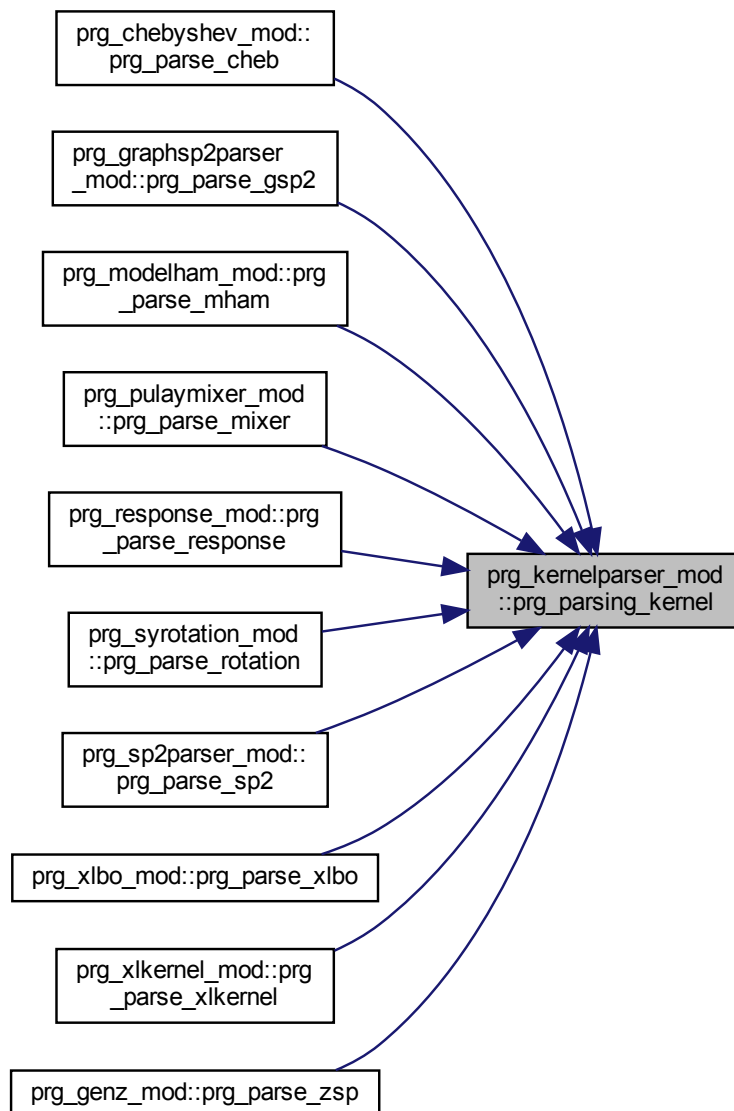
If the length of variable vect is changed, this could produce a segmentation fault.

Definition at line 30 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 dp

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

Definition at line 13 of file prg_kernelparser_mod.F90.

9.13 prg_modelham_mod Module Reference

The prg_hamiltonian module.

Data Types

- type [mham_type](#)
General ModelHam type.

Functions/Subroutines

- subroutine, public [prg_parse_mham](#) (mham, filename)
Model Ham parse.
- subroutine, public [prg_twolevel_model](#) (ea, eb, dab, daiaj, dbibj, dec, rcoeff, reshuffle, seed, h_bml, verbose)
Construct a two-level model Hamiltonian.

Variables

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

9.13.1 Detailed Description

The prg_hamiltonian module.

This module will create a model Hamiltonian for benchmarking purposes.

9.13.2 Function/Subroutine Documentation

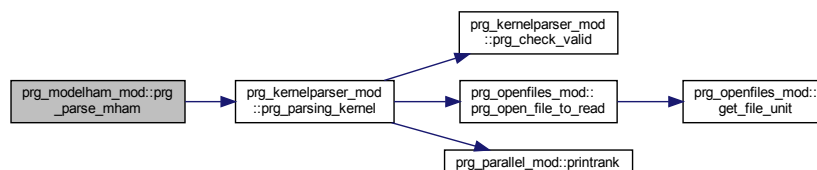
9.13.2.1 prg_parse_mham()

```
subroutine, public prg_modelham_mod::prg_parse_mham (
    type(mham\_type), intent(inout) mham,
    character(len=*) filename )
```

Model Ham parse.

Definition at line 37 of file prg_modelham_mod.F90.

Here is the call graph for this function:



9.13.2.2 prg_twolevel_model()

```
subroutine, public prg_modelham_mod::prg_twolevel_model (
    real(dp), intent(in) ea,
    real(dp), intent(in) eb,
    real(dp), intent(in) dab,
    real(dp), intent(in) daiaj,
    real(dp), intent(in) dbibj,
    real(dp) dec,
    real(dp), intent(in) rcoeff,
    logical, intent(in) reshuffle,
    integer seed,
    type(bml_matrix_t), intent(inout) h_bml,
    integer, intent(in) verbose )
```

Construct a two-level model Hamiltonian.

Parameters

<i>ea</i>	First onsite energy
<i>eb</i>	Second onsite energy
<i>dab</i>	Onsite Hamiltonian element
<i>daiaj</i>	Intersite first level Hamiltonian elements
<i>dbibj</i>	Intersite second level Hamiltonian elements
<i>dec</i>	Decay constant
<i>rcoeff</i>	Random coefficient
<i>reshuffle</i>	If rows needs to be reshuffled
<i>seed</i>	Random seed
<i>h_bml</i>	Output hamiltonian matrix
<i>verbose</i>	Verbosity level

Definition at line 116 of file prg_modelham_mod.F90.

9.13.3 Variable Documentation

9.13.3.1 dp

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

Definition at line 15 of file prg_modelham_mod.F90.

9.14 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)

9.14.1 Detailed Description

Module to prg_orthogonalize and prg_deorthogonalize any operator.

Typically the Hamiltonin 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: $\rho = Z \rho_{ortho} Z^\dagger$

9.14.2 Function/Subroutine Documentation

9.14.2.1 prg_deorthogonalize()

```
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 )
```

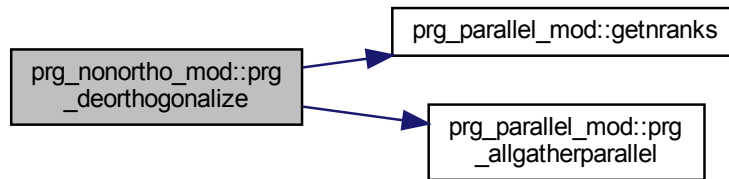
This routine performs: $A = Z A_{ortho} Z^\dagger$.

Parameters

<i>orthoA_bml</i>	Matrix to be prg_deorthogonalized.
<i>zmat_bml</i>	Congruence transform to be used.
<i>A_bml</i>	Matrix resulting from the prg_deorthogonalized in bml format.
<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 82 of file prg_nonortho_mod.F90.

Here is the call graph for this function:



9.14.2.2 prg_orthogonalize()

```

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: $A_{ortho} = Z^{\dagger}AZ$.

Parameters

<i>A_bml</i>	Matrix to be prg_orthogonalized 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`.

9.14.3 Variable Documentation

9.14.3.1 dp

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

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

9.15 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)

9.15.1 Detailed Description

The prg_normalize module.

9.15.2 Function/Subroutine Documentation

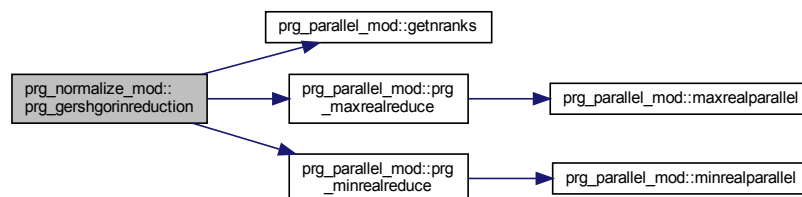
9.15.2.1 prg_gershgorinreduction()

```
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:



9.15.2.2 prg_normalize()

```
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.

$$X0 = (e_max * I - H) / (e_max - e_min)$$

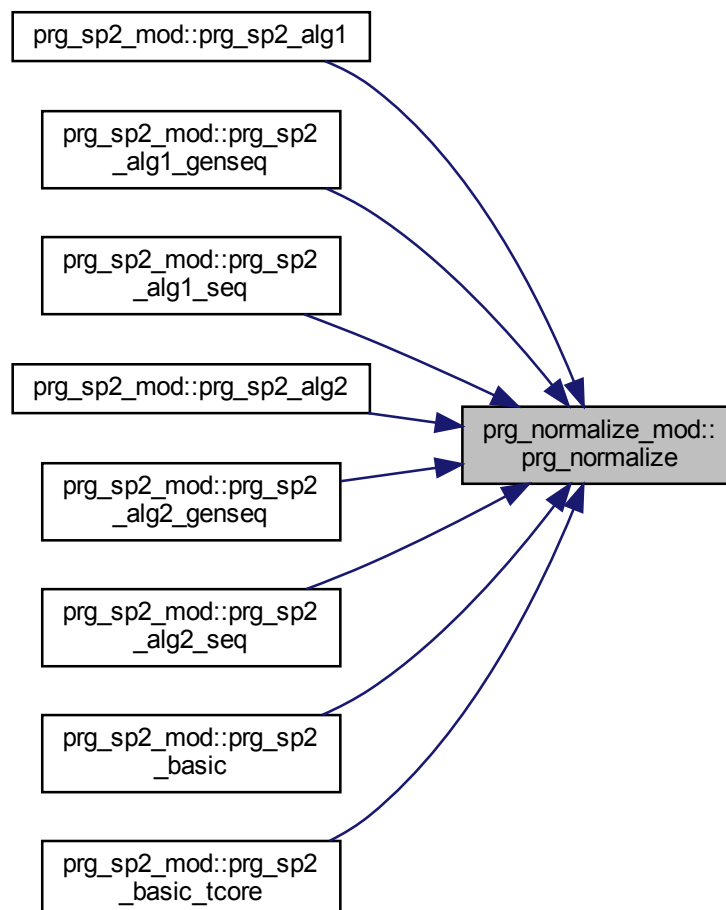
where e_max and e_min are obtained sing the Gershgorin circle theorem.

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:



9.15.2.3 prg_normalize_cheb()

```
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.

$$X0 = 2*(H - e_min*I) / (e_max - e_min) - I$$

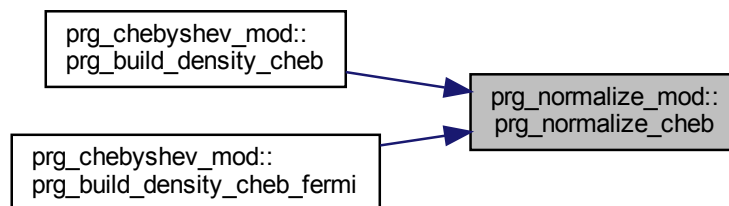
where e_max and e_min are obtained sing the Gershgorin circle theorem.

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:



9.15.2.4 prg_normalize_fermi()

```
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.

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

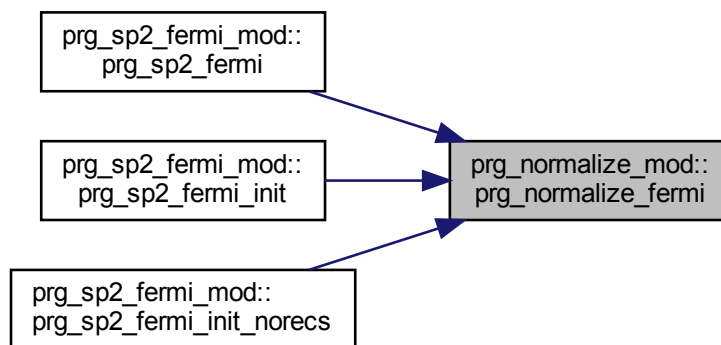
where h1 and hN are scaled Gershgorin bounds.

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:



9.15.2.5 prg_normalize_implicit_fermi()

```

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.

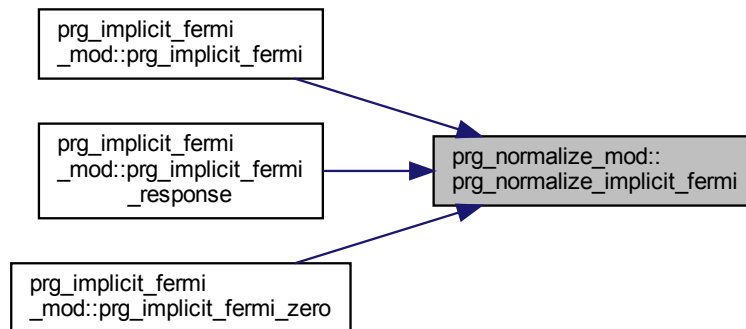
$X0 = 0.5 * II - cnst * (H0 - mu0 * II)$ or $X0 = (0.5 + cnst * mu0) * II - cnst * H0$

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:



9.15.3 Variable Documentation

9.15.3.1 dp

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

Definition at line 15 of file `prg_normalize_mod.F90`.

9.16 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.

9.16.1 Detailed Description

Module to handle input output files for the PROGRESS lib.

9.16.2 Function/Subroutine Documentation

9.16.2.1 `get_file_unit()`

```
integer function, public prg_openfiles_mod::get_file_unit (
    integer io_max )
```

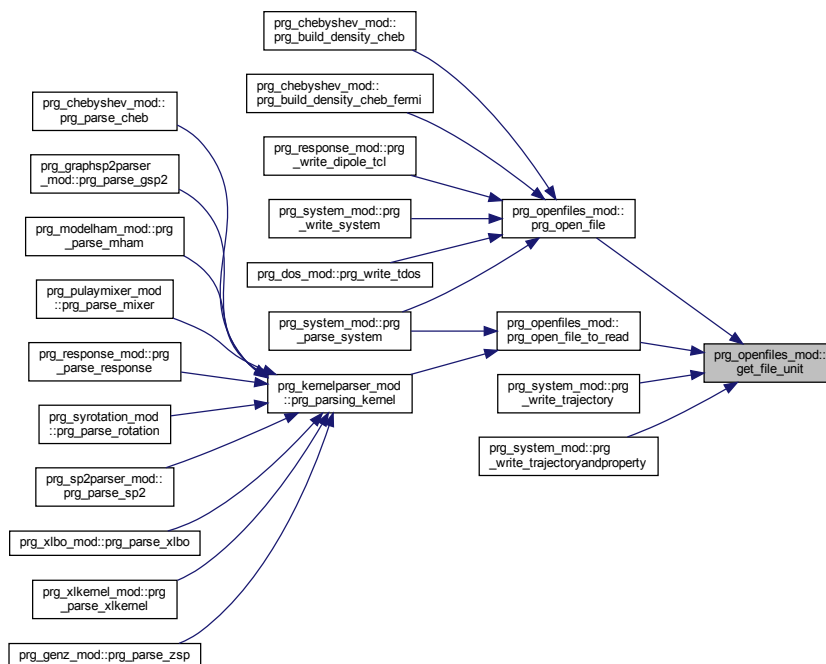
Returns a unit number that is not in use.

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:



9.16.2.2 `prg_open_file()`

```
subroutine, public prg_openfiles_mod::prg_open_file (
    integer io,
    character(len=*) name )
```

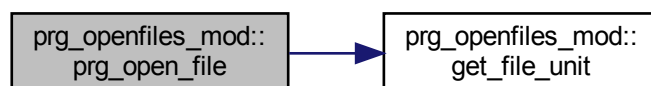
Opens a file to write.

Parameters

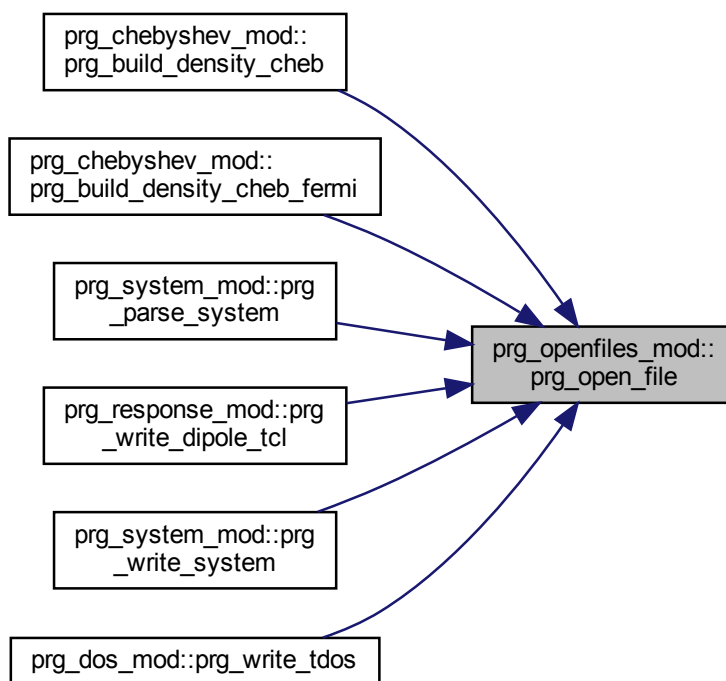
<i>io</i>	Unit for the file.
<i>name</i>	Name of the file.

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:



9.16.2.3 prg_open_file_to_read()

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

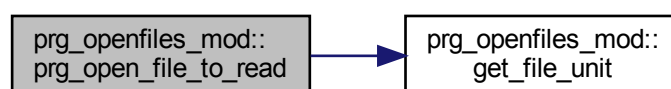
Opens a file to read.

Parameters

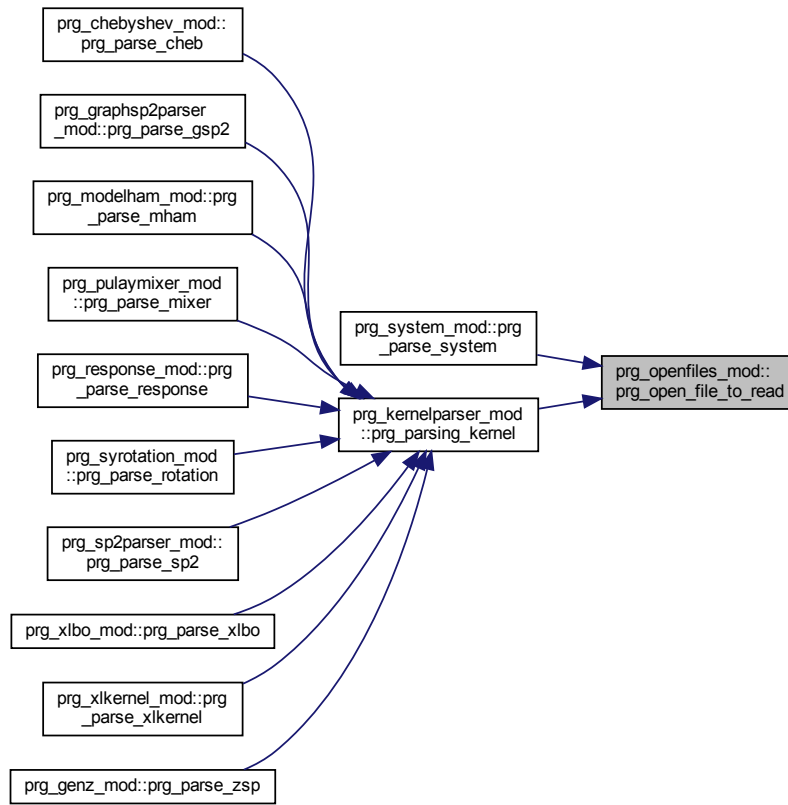
<i>io</i>	Unit for the file.
<i>name</i>	Name of the file.

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:



9.17 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_rcvparallel](#) (recvBuf, recvLen, rind)
- subroutine, public [prg_rcvparallel](#) (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](#)

9.17.1 Detailed Description

The parallel module.

9.17.2 Function/Subroutine Documentation

9.17.2.1 allgatherintparallel()

```
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.

9.17.2.2 allgatherrealparallel()

```
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.

9.17.2.3 allgathervintparallel()

```
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.

9.17.2.4 allgathervrealparallel()

```
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 )
```

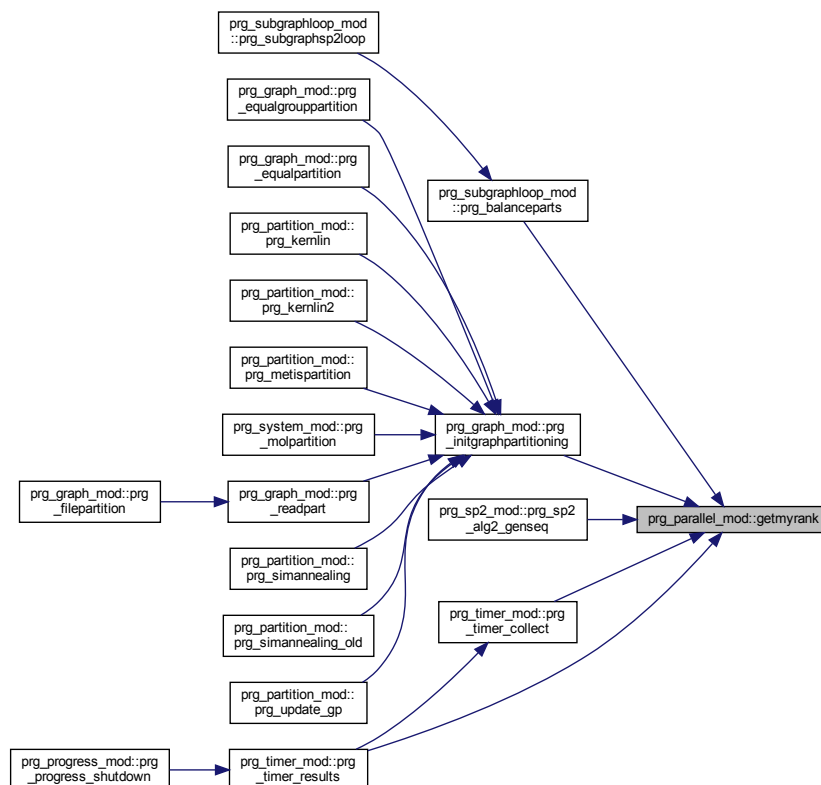
Definition at line 676 of file prg_parallel_mod.F90.

9.17.2.5 getmyrank()

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:

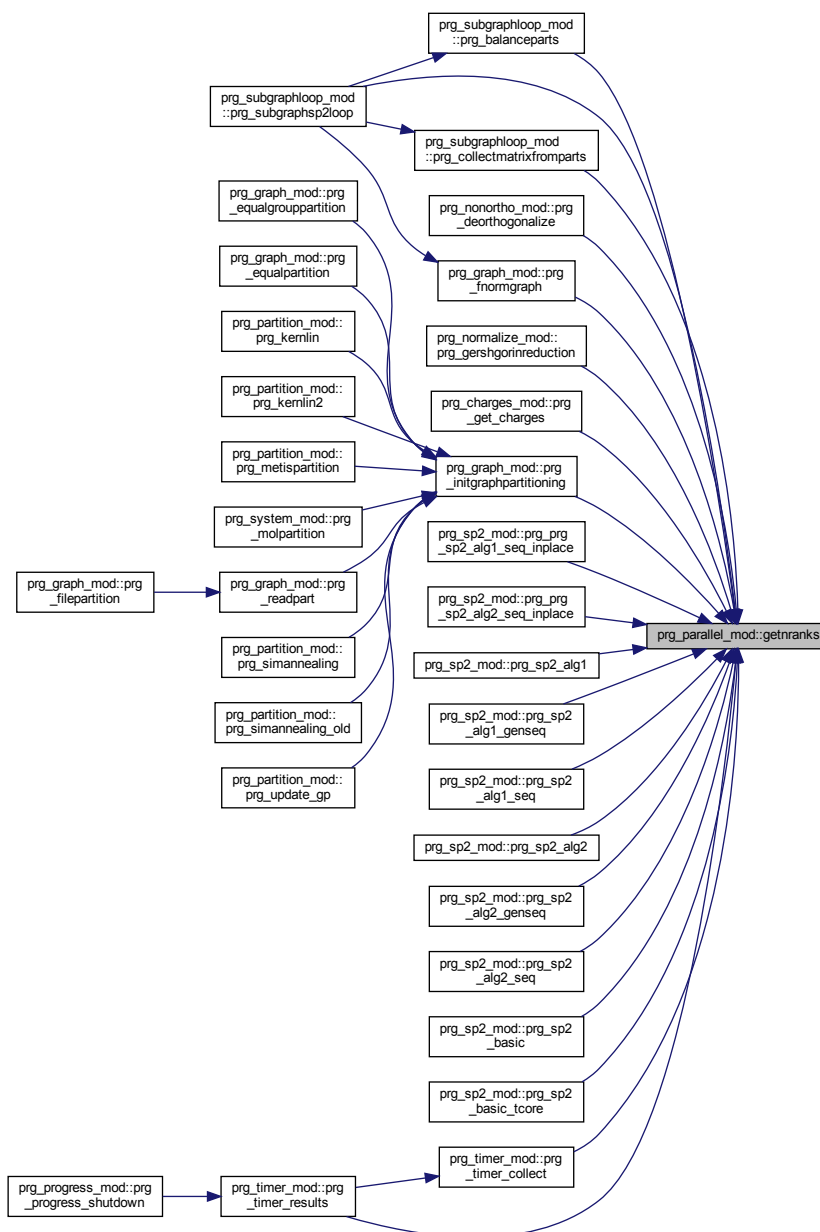


9.17.2.6 getnranks()

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:



9.17.2.7 isendparallel()

```

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

```

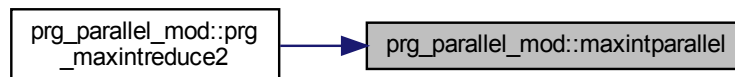
Definition at line 230 of file prg_parallel_mod.F90.

9.17.2.8 maxintparallel()

```
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:

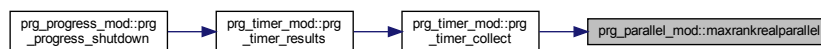


9.17.2.9 maxrankrealparallel()

```
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:

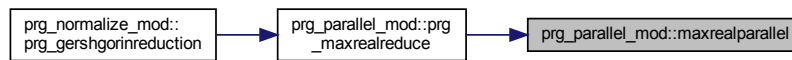


9.17.2.10 maxrealparallel()

```
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:



9.17.2.11 minintparallel()

```

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.

9.17.2.12 minrankrealparallel()

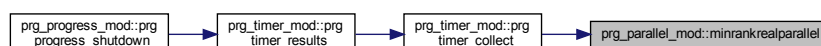
```

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:

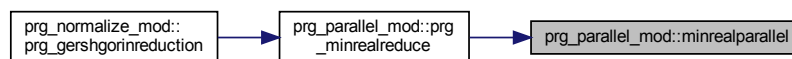


9.17.2.13 minrealparallel()

```
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:

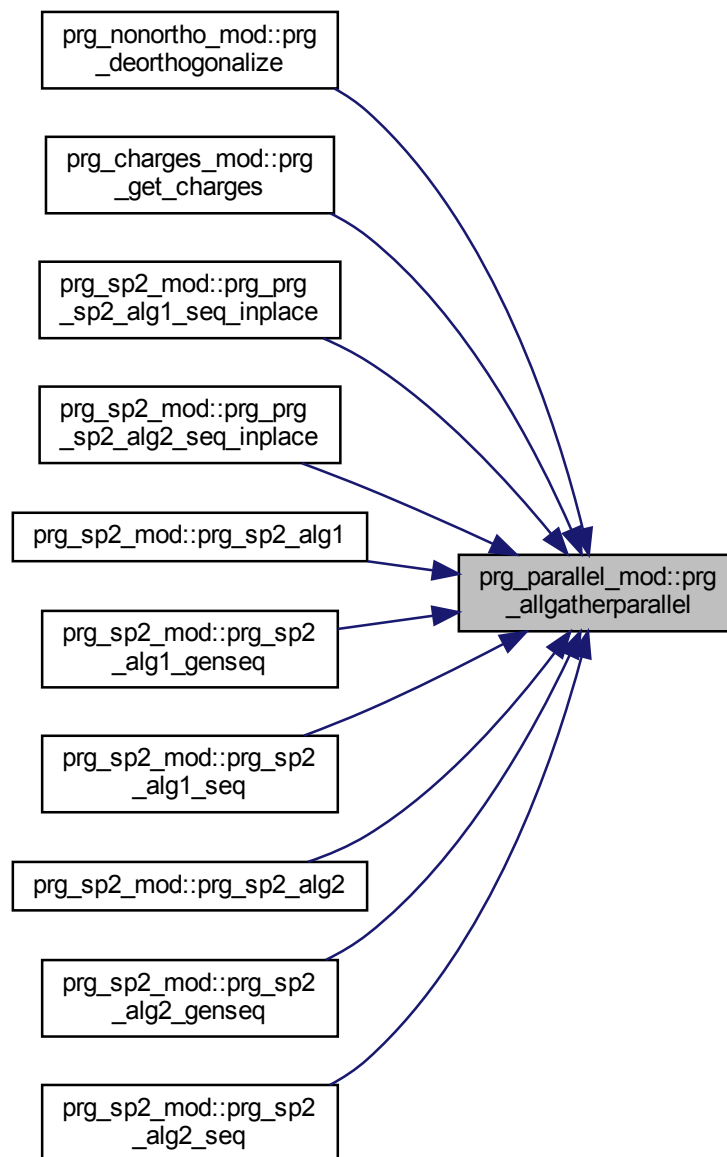


9.17.2.14 prg_allgatherparallel()

```
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:



9.17.2.15 prg_allsumintreduceparallel()

```

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`.

9.17.2.16 prg_allsumrealreduceparallel()

```
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.

9.17.2.17 prg_barrierparallel()

```
subroutine, public prg_parallel_mod::prg_barrierparallel
```

Definition at line 196 of file prg_parallel_mod.F90.

9.17.2.18 prg_bcastparallel()

```
subroutine, public prg_parallel_mod::prg_bcastparallel (
    character, dimension(*), intent(in) buf,
    integer, intent(in) blen,
    integer, intent(in) root )
```

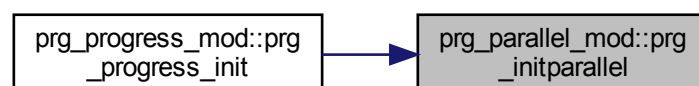
Definition at line 630 of file prg_parallel_mod.F90.

9.17.2.19 prg_initparallel()

```
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:

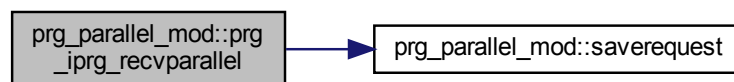


9.17.2.20 prg_iprg_recvparallel()

```
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:

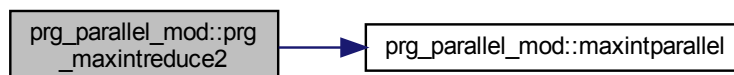


9.17.2.21 prg_maxintreduce2()

```
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:

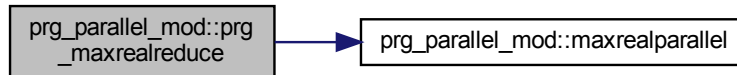


9.17.2.22 prg_maxrealreduce()

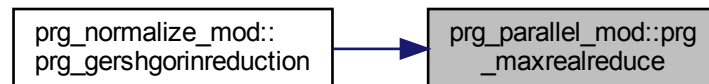
```
subroutine, public prg_parallel_mod::prg_maxrealreduce (
    real(dp), intent(inout) rvalue )
```

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:

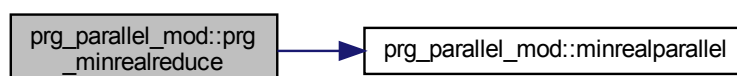


9.17.2.23 prg_minrealreduce()

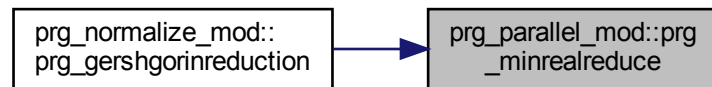
```
subroutine, public prg_parallel_mod::prg_minrealreduce (
    real(dp), intent(inout) rvalue )
```

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:



9.17.2.24 prg_recvparallel()

```
subroutine, public prg_parallel_mod::prg_recvparallel (  
    real(dp), dimension(*) recvBuf,  
    integer, intent(in) recvLen )
```

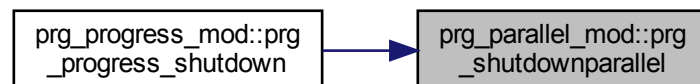
Definition at line 279 of file `prg_parallel_mod.F90`.

9.17.2.25 prg_shutdownparallel()

```
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:

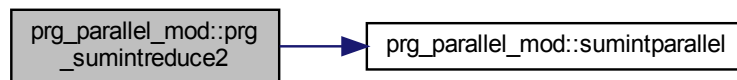


9.17.2.26 prg_sumintreduce2()

```
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:

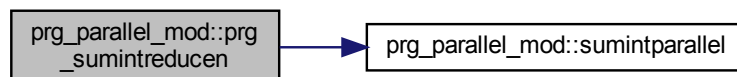


9.17.2.27 prg_sumintreducen()

```
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:

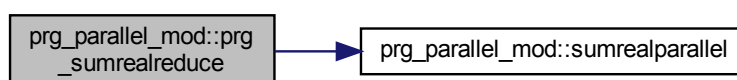


9.17.2.28 prg_sumrealreduce()

```
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:

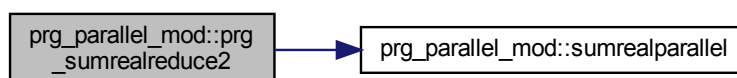


9.17.2.29 prg_sumrealreduce2()

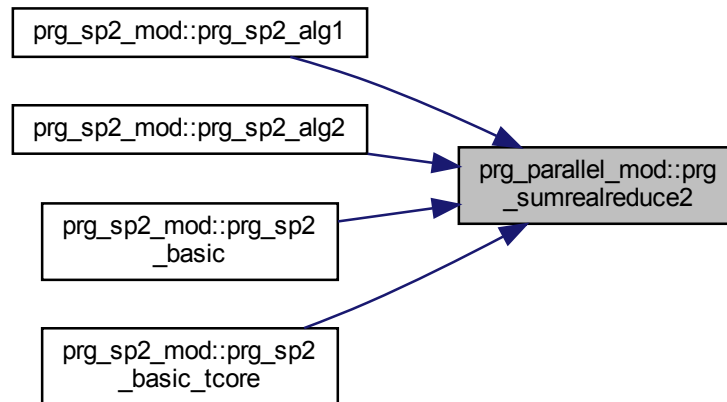
```
subroutine, public prg_parallel_mod::prg_sumrealreduce2 (
    real(dp), intent(inout) value1,
    real(dp), intent(inout) value2 )
```

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:



9.17.2.30 prg_sumrealreduce3()

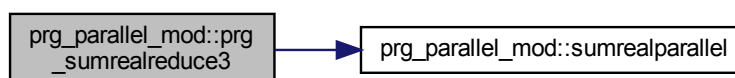
```

subroutine, public prg_parallel_mod::prg_sumrealreduce3 (
    real(dp), intent(inout) value1,
    real(dp), intent(inout) value2,
    real(dp), intent(inout) value3 )

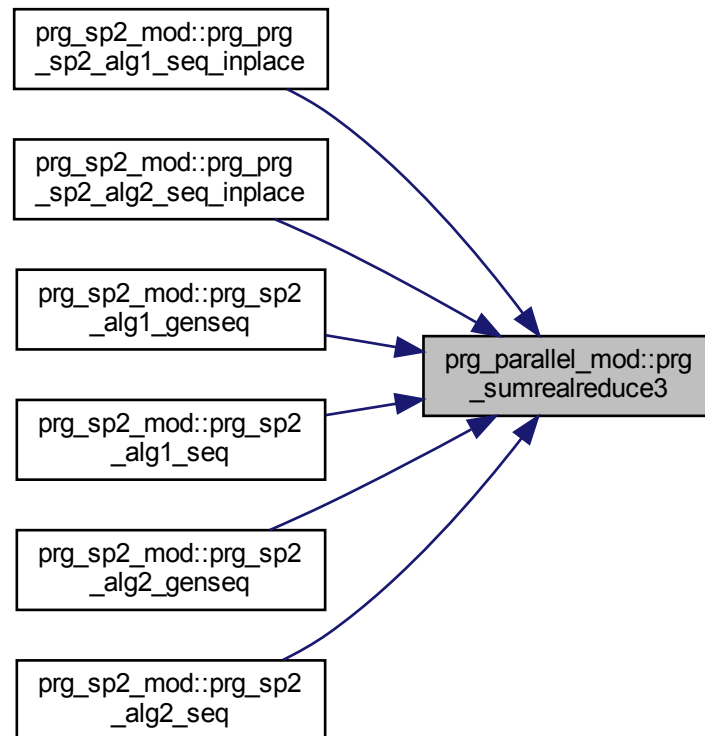
```

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:



9.17.2.31 prg_sumrealreducen()

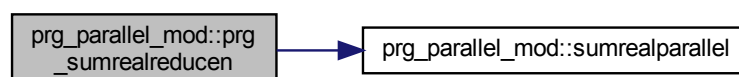
```

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:



9.17.2.32 prg_wait()

```
subroutine, public prg_parallel_mod::prg_wait
```

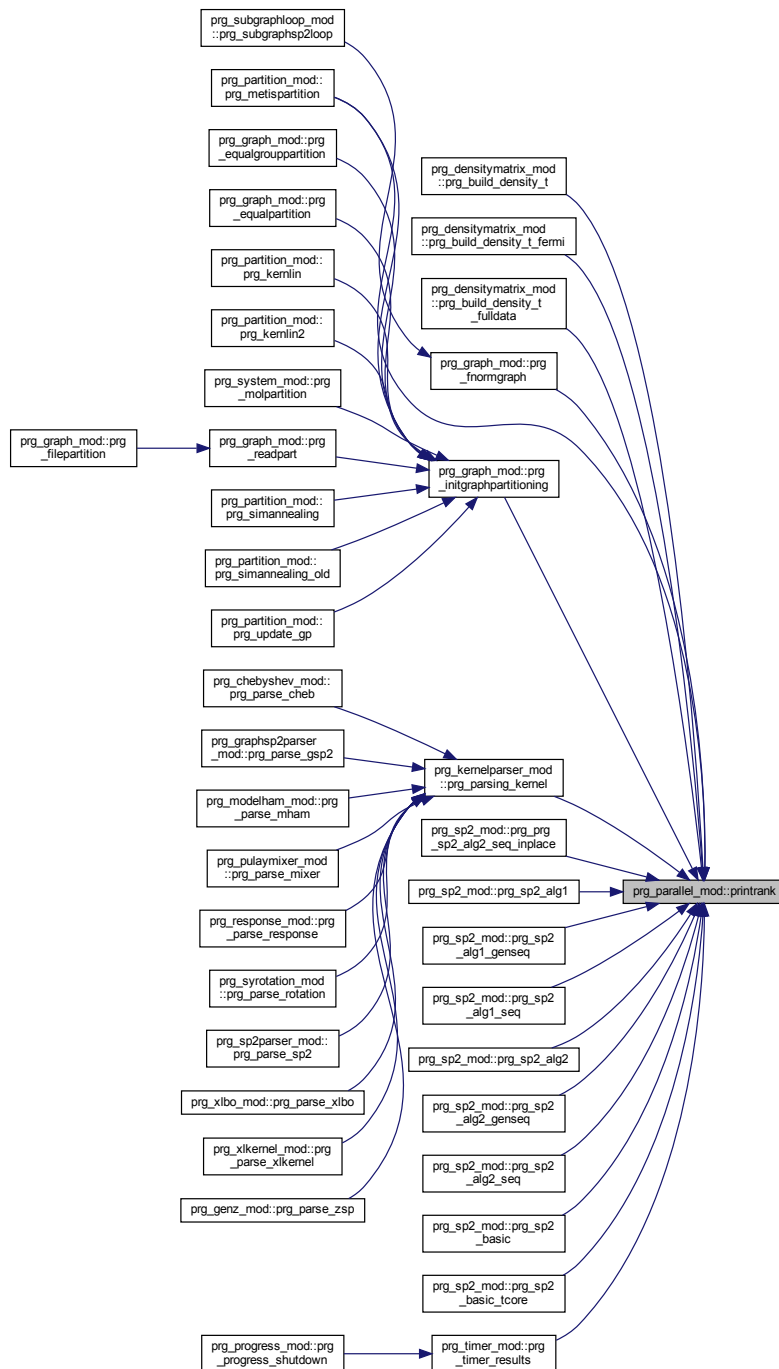
Definition at line 758 of file prg_parallel_mod.F90.

9.17.2.33 printrank()

```
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:

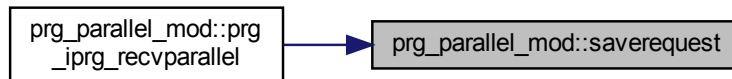


9.17.2.34 saverequest()

```
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:



9.17.2.35 sendparallel()

```

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.

9.17.2.36 sendreceiveparallel()

```

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 )
  
```

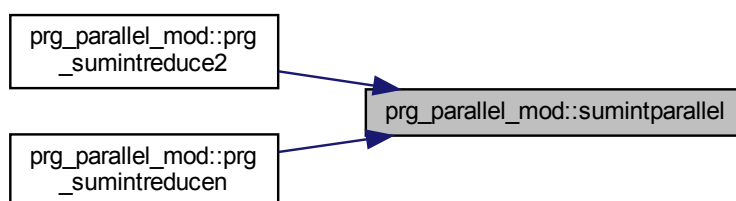
Definition at line 207 of file prg_parallel_mod.F90.

9.17.2.37 sumintparallel()

```
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:



9.17.2.38 sumrealparallel()

```
subroutine, public prg_parallel_mod::sumrealparallel (  
    real(dp), dimension(*), intent(in) sendBuf,  
    real(dp), dimension(*), intent(out) recvBuf,  
    integer, intent(in) icount )
```

Definition at line 316 of file prg_parallel_mod.F90.

9.17.3.3 myrank

```
integer prg_parallel_mod::myrank [private]
```

Definition at line 28 of file prg_parallel_mod.F90.

9.17.3.4 nrank

```
integer prg_parallel_mod::nrank [private]
```

Definition at line 28 of file prg_parallel_mod.F90.

9.17.3.5 reqcount

```
integer prg_parallel_mod::reqcount [private]
```

Definition at line 29 of file prg_parallel_mod.F90.

9.17.3.6 requestlist

```
integer, dimension(:), allocatable prg_parallel_mod::requestlist [private]
```

Definition at line 30 of file prg_parallel_mod.F90.

9.17.3.7 rused

```
integer, dimension(:), allocatable prg_parallel_mod::rused [private]
```

Definition at line 30 of file prg_parallel_mod.F90.

9.18 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 kerlin_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.

9.18.1 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.

9.18.2 Function/Subroutine Documentation

9.18.2.1 prg_accept_prob()

```
subroutine prg_partition_mod::prg_accept_prob (
    integer, intent(in) it,
    real(dp), intent(in) prg_delta,
    real, intent(inout) r ) [private]
```

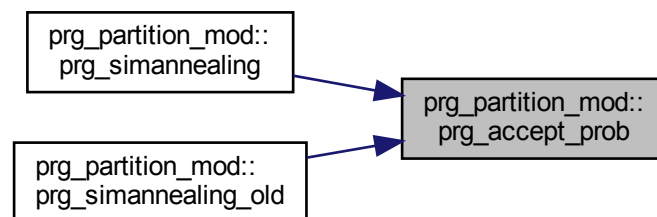
Compute acceptance probability for simulated annealing.

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:



9.18.2.2 prg_check_arrays()

```
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*.

9.18.2.3 prg_costindex()

```
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]
```

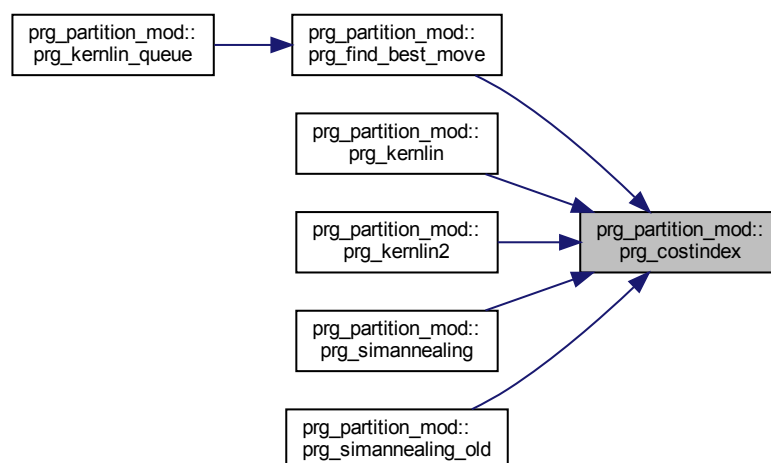
Choose objective function to work with.

Parameters

<i>cost</i>	output according to chosen <i>obj_fun</i>
<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:



9.18.2.4 prg_costpartition()

```

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.

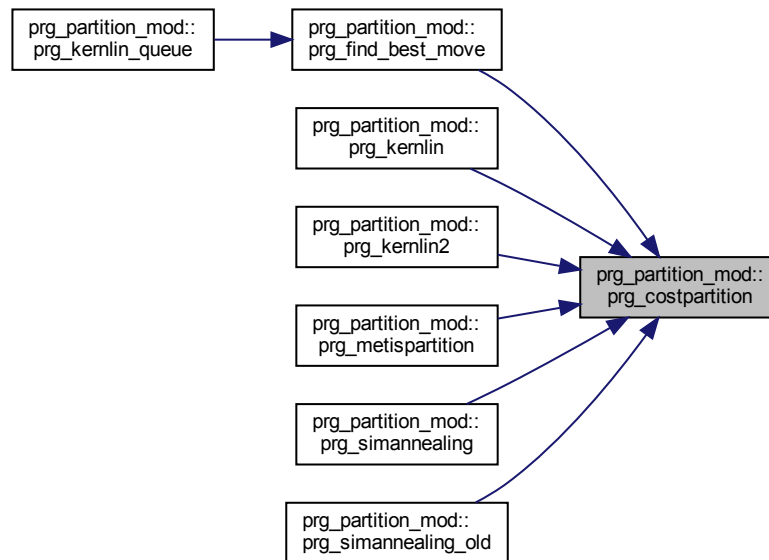
Parameters

<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:



9.18.2.5 prg_find_best_move()

```

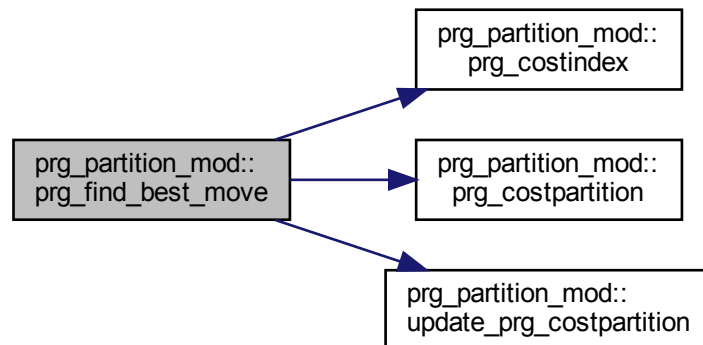
subroutine prg_partition_mod::prg_find_best_move (
    type (graph_partitioning_t), intent(inout) gp,
    integer, dimension(:), intent(inout), allocatable xadj,
    integer, dimension(:), intent(inout), allocatable adjncy,
    integer, dimension(:), intent(inout), allocatable partNumber,
    integer, 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:



9.18.2.6 prg_get_largest_hedge_in_part()

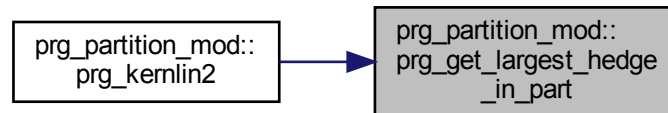
```

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 1421 of file prg_partition_mod.F90.

Here is the caller graph for this function:



9.18.2.7 prg_kernlin()

```

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

<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
<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 exit, 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

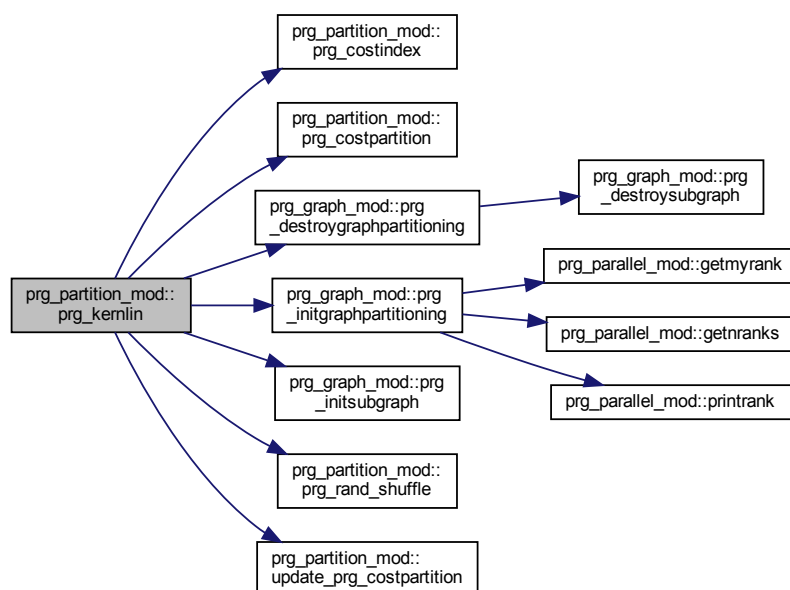
Update graph structure

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:



9.18.2.8 prg_kernlin2()

```

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 $k \leq 20$, 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

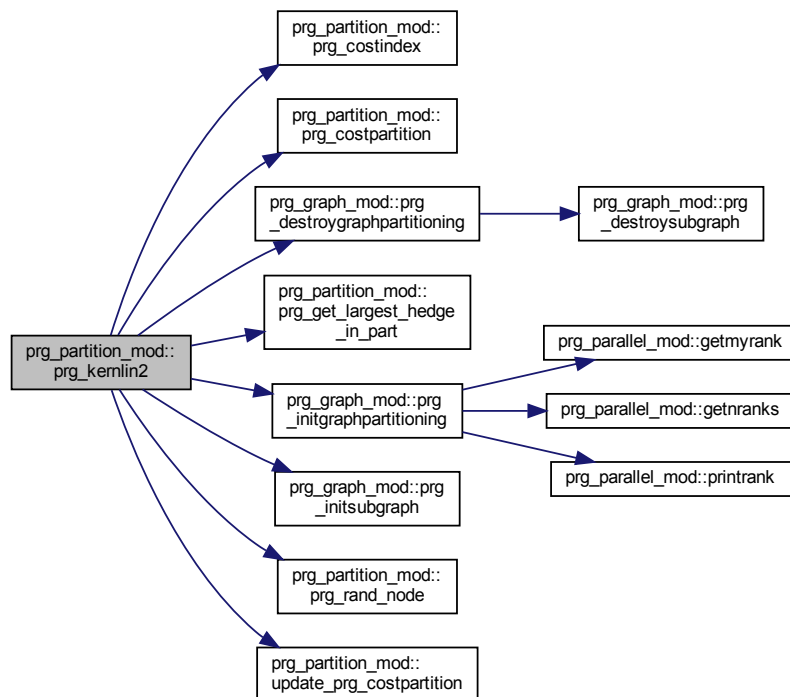
Update graph structure

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:



9.18.2.9 prg_kernlin_queue()

```

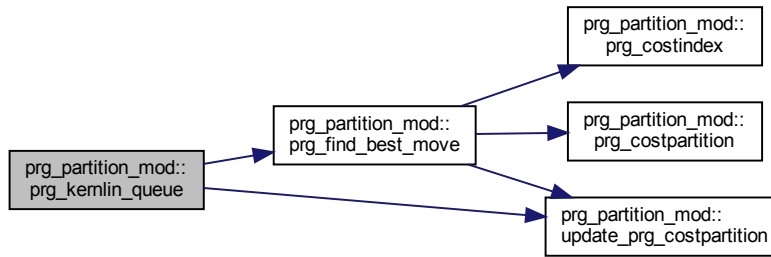
subroutine, public prg_partition_mod::prg_kernlin_queue (
  type (graph_partitioning_t), intent(inout) gp,
  integer, dimension(:), intent(inout), allocatable xadj,
  integer, dimension(:), intent(inout), allocatable adjncy,
  integer, dimension(:), intent(inout), allocatable partNumber,
  integer, dimension(:), 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:



9.18.2.10 prg_metispartition()

```

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

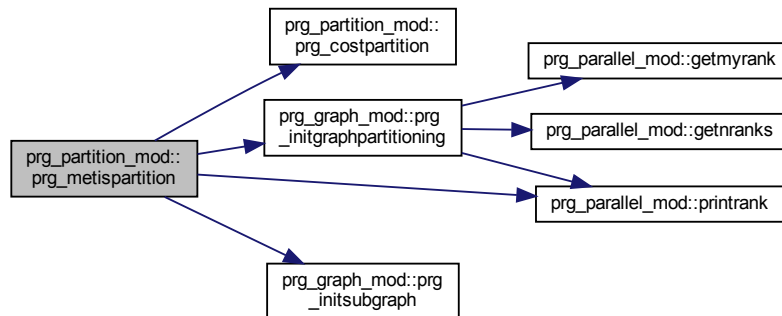
prg_initialize

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:



9.18.2.11 prg_rand_node()

```

subroutine prg_partition_mod::prg_rand_node (
    type (graph_partitioning_t), intent(inout) gp,
    integer, intent(inout) node,
    integer, intent(inout) seed ) [private]

```

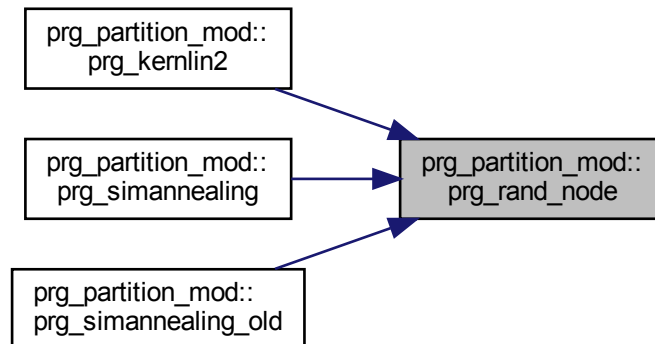
Pick a random node.

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:



9.18.2.12 prg_rand_shuffle()

```

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

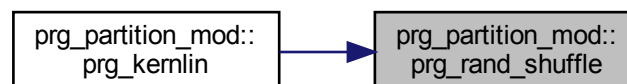
Randomly shuffle array.

Random seed

Shuffle array

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

Here is the caller graph for this function:



9.18.2.13 prg_simannealing()

```

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 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>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 smalles size (should be included in update_prg_costPartition

if part(node) == max_ch_part, try to move node and it's neighbors to min_ch_part else move neighbors to part(node)

Check empty part exist move nodes from maxpart to empty part

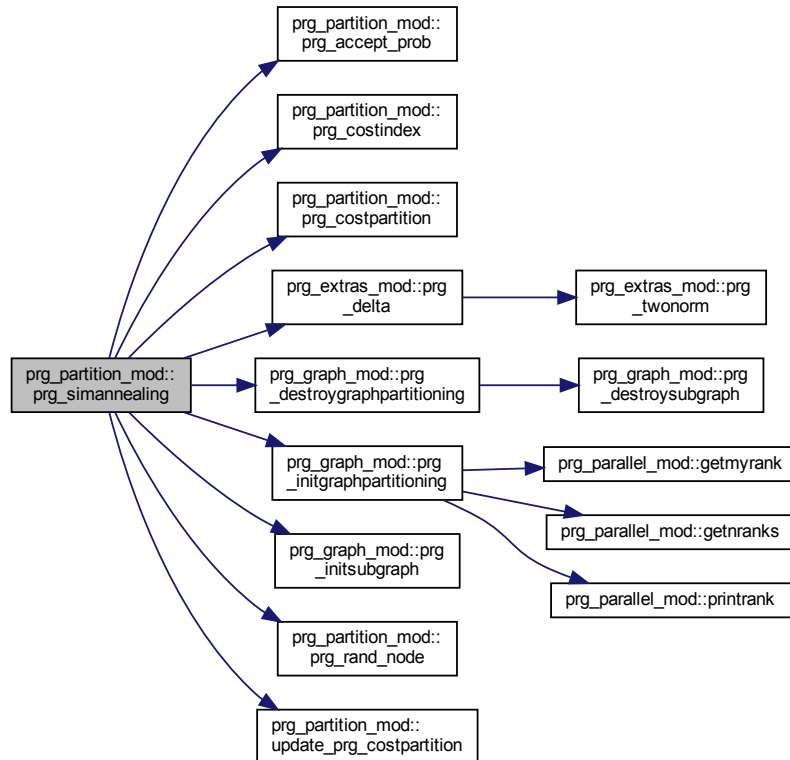
move it neighbor in the max parts to the newpart

Update graph structure

For debugging

Definition at line 552 of file prg_partition_mod.F90.

Here is the call graph for this function:



9.18.2.14 prg_simannealing_old()

```

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

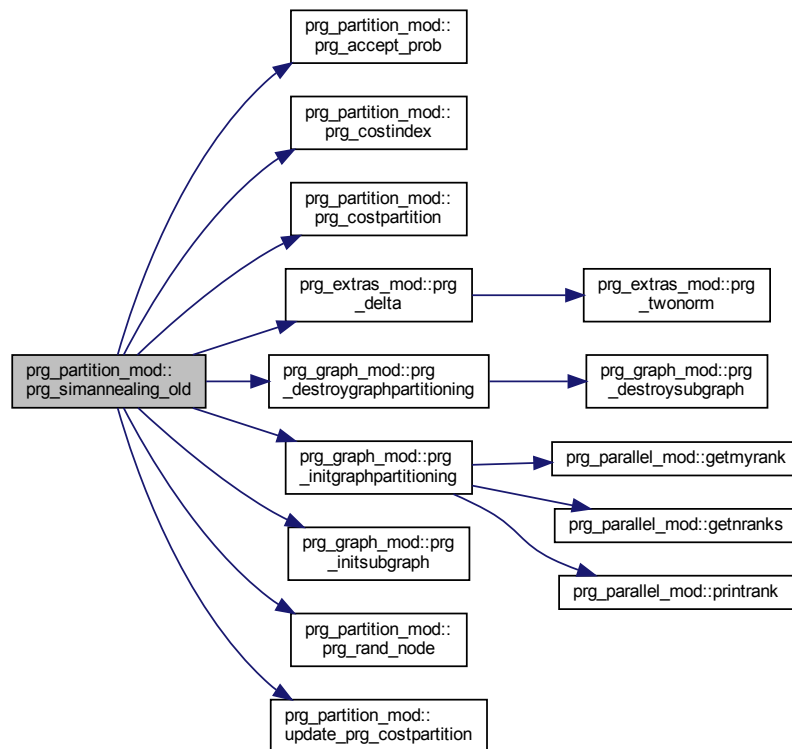
Perform SA

Update graph structure

For debugging

Definition at line 1454 of file prg_partition_mod.F90.

Here is the call graph for this function:



9.18.2.15 prg_update_gp()

```

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 )

```

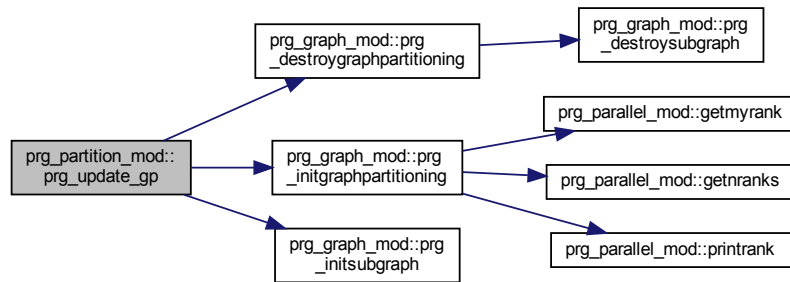
Update graph structure

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:



9.18.2.16 update_prg_costpartition()

```

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 )
  
```

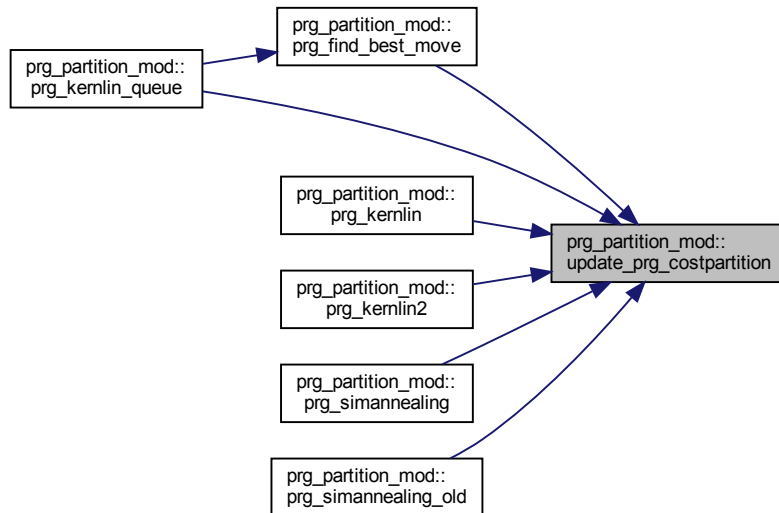
Update cost of partition and the different parameters node is moves into new_part For each neighbor of node, the following cases hold: Case 1: neighbor is in old_part Case 2: neighbor is in new_part Case 3: neighbor is neither in old_or new_part.

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:



9.18.3 Variable Documentation

9.18.3.1 dp

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

Definition at line 18 of file prg_partition_mod.F90.

9.18.3.2 metis_index_kind

```
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.

9.18.3.3 metis_real_kind

```
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.

9.19 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)

9.19.1 Detailed Description

The progress module.

9.19.2 Function/Subroutine Documentation

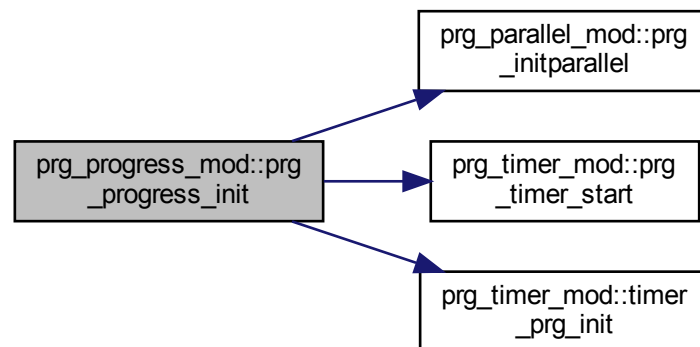
9.19.2.1 prg_progress_init()

```
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:



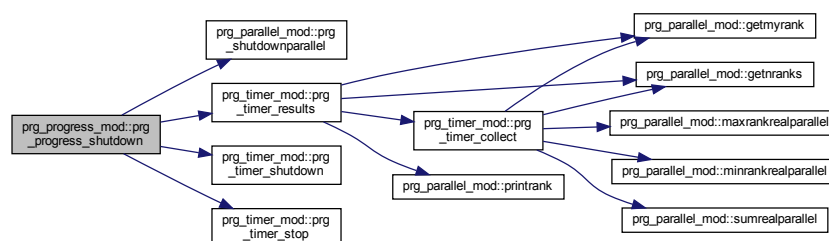
9.19.2.2 prg_progress_shutdown()

```
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:



9.19.3 Variable Documentation

9.19.3.1 dp

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

Definition at line 16 of file prg_progress_mod.F90.

9.20 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"]

- `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 /)

- 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 /)

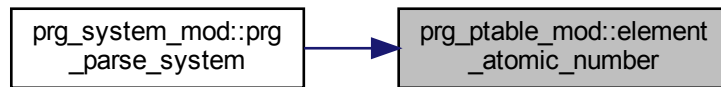
- `real(dp)`, `dimension(nz)`, `parameter element_covr = (/ 0.31, 0.28, 1.28, 0.96, 0.84, 0.76, 0.71, 0.66, 0.57, 0.58, 1.66, 1.41, 1.21, 1.11, 1.07, 1.05, 1.02, 1.06, 2.03, 1.76, 1.7, 1.6, 1.53, 1.39, 1.39, 1.32, 1.26, 1.24, 1.32, 1.22, 1.22, 1.2, 1.19, 1.2, 1.2, 1.16, 2.2, 1.95, 1.9, 1.75, 1.64, 1.54, 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 /)`

- `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 /)`

[illegible]

- `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 /)

Here is the caller graph for this function:

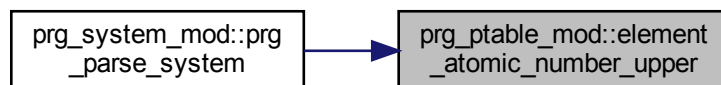


9.20.2.2 element_atomic_number_upper()

```
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:



9.20.3 Variable Documentation

9.20.3.1 atom_en

```
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 , 1.3 , 0.0 /)
```

The Pauling electronegativity for this element.

Definition at line 266 of file prg_ptable_mod.F90.

9.20.3.2 dp

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

Definition at line 13 of file prg_ptable_mod.F90.

9.20.3.3 element_covr

```
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.

9.20.3.4 element_ea

```
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.↵  
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.

9.20.3.5 element_econf

```
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.

9.20.3.6 element_ip

```
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.

9.20.3.7 element_mass

```
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 10⁻²⁷ kg)

Definition at line 110 of file prg_ptable_mod.F90.

9.20.3.8 element_maxbonds

```
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 , 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 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 ,
6 , 6 , 6 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 ,
6 , 6 , 6 /)
```

The maximum expected number of bonds to this element.

Definition at line 297 of file prg_ptable_mod.F90.

9.20.3.9 element_name

```
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.

9.20.3.10 element_numel

```
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.

9.20.3.11 element_symbol

```
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.

9.20.3.12 element_symbol_upper

```
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.

9.20.3.13 element_vdwr

```
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.

9.20.3.14 nz

```
integer, parameter prg_ptable_mod::nz = 103
```

Definition at line 12 of file prg_ptable_mod.F90.

9.21 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 $2Tr[Z Z' H D \frac{dS}{dR}]$.

Variables

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

9.21.1 Detailed Description

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

For a further explanation please see Niklasson 2008 [3]

9.21.2 Function/Subroutine Documentation

9.21.2.1 prg_get_pulayforce()

```
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.

9.21.2.2 prg_pulaycomponent0()

```
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.
----------------	-------------------------------

Parameters

<i>ham_bml</i>	Hamiltonian matrix 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 32 of file `prg_pulaycomponent_mod.F90`.

9.21.2.3 prg_pulaycomponentt()

```
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`.

9.21.3 Variable Documentation

9.21.3.1 dp

integer, parameter prg_pulaycomponent_mod::dp = kind(1.0d0) [private]

Definition at line 13 of file prg_pulaycomponent_mod.F90.

9.22 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)

9.22.1 Detailed Description

Pulay mixer mode.

Gets the best coefficient for mixing the charges during scf.

Todo add the density matrix mixer.

9.22.2 Function/Subroutine Documentation

9.22.2.1 prg_linearmixer()

```
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 )
```

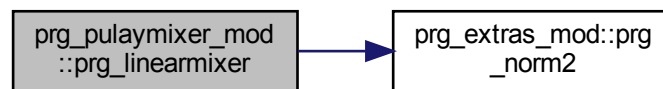
Routine to perform linear mixing.

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 238 of file prg_pulaymixer_mod.F90.

Here is the call graph for this function:



9.22.2.2 prg_parse_mixer()

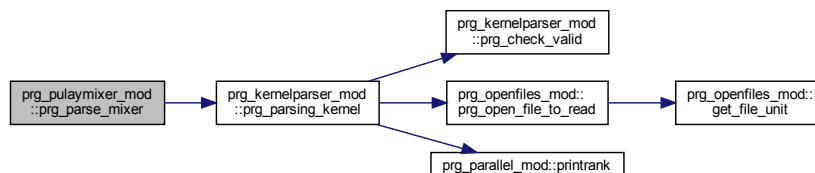
```

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 43 of file prg_pulaymixer_mod.F90.

Here is the call graph for this function:



9.22.2.3 prg_qmixer()

```
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 )
```

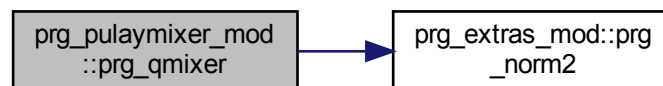
Mixing the charges to accelerate scf convergence.

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 104 of file prg_pulaymixer_mod.F90.

Here is the call graph for this function:



9.22.3 Variable Documentation

9.22.3.1 dp

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

Definition at line 15 of file prg_pulaymixer_mod.F90.

9.23 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)

9.23.1 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.

9.23.2 Function/Subroutine Documentation

9.23.2.1 prg_excitation()

```
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 307 of file prg_quantumdynamics_mod.F90.

9.23.2.2 prg_get_sparsity_cplxmat()

```
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 98 of file prg_quantumdynamics_mod.F90.

9.23.2.3 prg_get_sparsity_realmat()

```
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 122 of file prg_quantumdynamics_mod.F90.

9.23.2.4 prg_getcharge()

```
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 247 of file prg_quantumdynamics_mod.F90.

9.23.2.5 prg_getdipole()

```
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 282 of file prg_quantumdynamics_mod.F90.

9.23.2.6 prg_kick_density()

```
subroutine, public prg_quantumdynamics_mod::prg_kick_density (
    integer, intent(in) kick_direc,
    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: $\rho_{kick}^{\hat{}} = \exp \frac{-i}{\hbar} \hat{V} \hat{\rho} \hat{S} \exp \frac{i}{\hbar} \hat{V} S^{-1}$ where \hat{V} is the field disturbance.

Parameters

<i>kick_direc</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 kick_direc
<i>bmltype</i>	type of BML matrix desired for faster computation
<i>thresh</i>	threshold for BML matrix conversion

Definition at line 43 of file prg_quantumdynamics_mod.F90.

9.23.2.7 prg_kick_density_bml()

```
subroutine, public prg_quantumdynamics_mod::prg_kick_density_bml (
    integer, intent(in) kick_direc,
    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 154 of file prg_quantumdynamics_mod.F90.

9.23.2.8 prg_lvni_bml()

```

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: $\frac{\partial \hat{\rho}(t)}{\partial t} = \frac{-i}{\hbar} (S^{-1} \hat{H}(t) \hat{\rho}(t) - \hat{\rho}(t) \hat{H}(t) S^{-1})$.

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 211 of file prg_quantumdynamics_mod.F90.

9.23.3 Variable Documentation

9.23.3.1 dp

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

Definition at line 14 of file prg_quantumdynamics_mod.F90.

9.24 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 λ .

- subroutine, public `prg_pert_sin_pot` (direction, lx, coordinate, lambda, prt_bml, threshold, spindex, norbi, verbose, over_bml)

Apply a sinusoidal length dependent potential ($\sin(\tilde{r}_x)$) 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 λ .

- 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 \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 λ .

- subroutine, public `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_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 α belong to atom i .

Variables

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

9.24.1 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

9.24.2 Function/Subroutine Documentation

9.24.2.1 prg_compute_dipole()

```
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 122 of file prg_response_mod.F90.

9.24.2.2 prg_compute_polarizability()

```
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 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 200 of file prg_response_mod.F90.

9.24.2.3 prg_compute_response_fd()

```
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

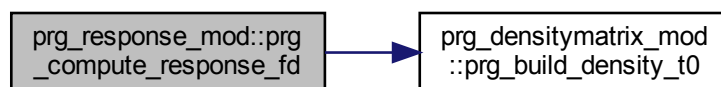
<i>ham_bml</i>	Hamiltonian in bml format ($H^{(0)}$).
<i>prt_bml</i>	Perturbation in bml format ($H^{(1)}$).
<i>rsp_bml</i>	First order response to the perturbation ($\rho^{(1)}$).
<i>bndfil</i>	Filing factor.
<i>threshold</i>	Threshold value for matrix elements.
<i>verbose</i>	Different levels of verbosity.

Warning

This works only for the prg_orthogonalized form of ham_bml.
The response must be in the prg_orthogonalized form.

Definition at line 381 of file prg_response_mod.F90.

Here is the call graph for this function:



9.24.2.4 prg_compute_response_rs()

```

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 251 of file prg_response_mod.F90.

9.24.2.5 prg_compute_response_sp2()

```

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 654 of file prg_response_mod.F90.

9.24.2.6 prg_parse_response()

```
subroutine, public prg_response_mod::prg_parse_response (
    type(respdata_type) RespData,
    character(len=*) filename )
```

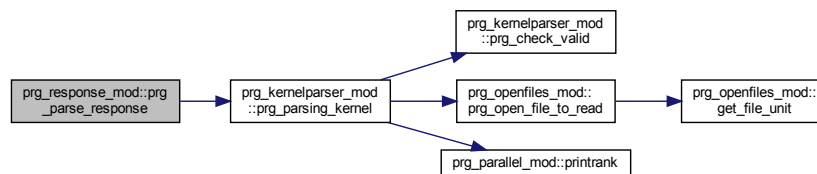
The parser for the calculation of the DM response.

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:



9.24.2.7 prg_pert_constant_field()

```
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 λ .

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} $)..
<i>coordinate</i>	Coordinates of the system (\mathbf{r}).
<i>lambda</i>	Constant to premultiply the perturbation (λ).
<i>prt_bml</i>	Perturbation in bml format ($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 448 of file prg_response_mod.F90.

9.24.2.8 prg_pert_cos_pot()

```
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 λ .

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 (λ).
<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 593 of file prg_response_mod.F90.

9.24.2.9 prg_pert_from_file()

```
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 225 of file prg_response_mod.F90.

9.24.2.10 prg_pert_sin_pot()

```
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 λ .

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 (λ).
<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 (<i>S</i>).

Definition at line 525 of file prg_response_mod.F90.

9.24.2.11 prg_project_response()

```
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 α 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 797 of file prg_response_mod.F90.

9.24.2.12 prg_write_dipole_tcl()

```
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 )
```

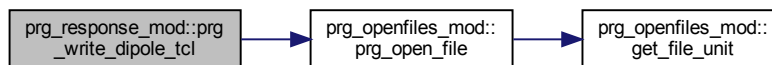
To visualize a dipole moment using VMD. This will prg_generate a .tcl script that could be run using VMD To visualize with VMD: \$ vmd -e dipole.tcl.

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 160 of file prg_response_mod.F90.

Here is the call graph for this function:



9.24.3 Variable Documentation

9.24.3.1 dp

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

Definition at line 18 of file prg_response_mod.F90.

9.24.3.2 pi

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

Definition at line 19 of file prg_response_mod.F90.

9.25 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)`

9.25.1 Detailed Description

The SP2 Fermi module.

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

9.25.2 Function/Subroutine Documentation

9.25.2.1 `absmaxderivative()`

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

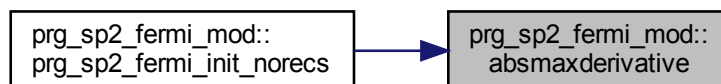
Gets the absolute maximum of the derivative of a function.

Parameters

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

Definition at line 618 of file `prg_sp2_fermi_mod.F90`.

Here is the caller graph for this function:



9.25.2.2 `prg_sp2_entropy_function()`

```
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 )

```

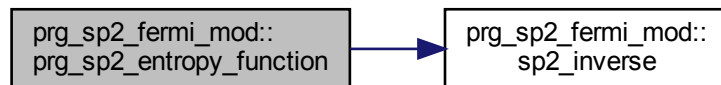
Calculate SP2 entropy function using gaussian quadrature. Note that GG and ee are allocated and returned from this routine.

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 483 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



9.25.2.3 prg_sp2_fermi()

```

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 )

```

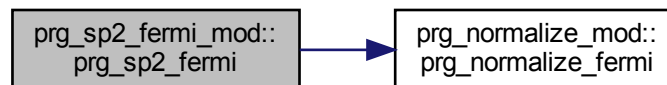
Calculate Truncated SP2.

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 390 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



9.25.2.4 prg_sp2_fermi_init()

```

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

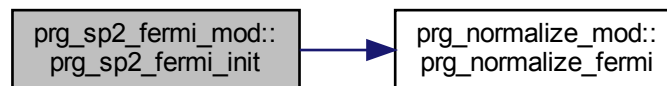
<i>h_bml</i>	Input Hamiltonian matrix.
<i>nsteps</i>	Number of sp2 iterations.
<i>nocc</i>	Number of occupied states.
<i>tscale</i>	Temperature rescaling factor.
<i>threshold</i>	Threshold for multiplication.
<i>occErrLimit</i>	Occupation error limit.
<i>traceLimit</i>	Trace limit.
<i>x_bml</i>	Output 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 45 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



9.25.2.5 prg_sp2_fermi_init_norecs()

```

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

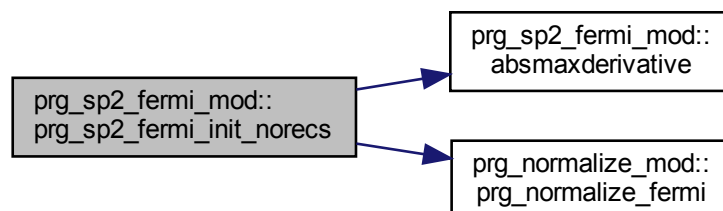
<i>h_bml</i>	Input Hamiltonian matrix.
<i>nsteps</i>	Output number of sp2 iterations.
<i>nocc</i>	Number of occupied states.
<i>tscale</i>	Temperature rescaling factor.
<i>threshold</i>	Threshold for multiplication.
<i>occErrLimit</i>	Occupation error limit.
<i>traceLimit</i>	Trace limit.
<i>x_bml</i>	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 200 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



9.25.2.6 sp2_entropy_ts()

```
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 541 of file prg_sp2_fermi_mod.F90.

9.25.2.7 sp2_inverse()

```
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 593 of file prg_sp2_fermi_mod.F90.

Here is the caller graph for this function:



9.25.3 Variable Documentation

9.25.3.1 dp

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

Definition at line 18 of file prg_sp2_fermi_mod.F90.

9.26 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_basic_tcore](#) (h_bml, rho_bml, rhofull_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)
- 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)
- integer, parameter [dp1](#) = kind(1.0)

9.26.1 Detailed Description

The SP2 module.

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

9.26.2 Function/Subroutine Documentation

9.26.2.1 prg_prg_sp2_alg1_seq_inplace()

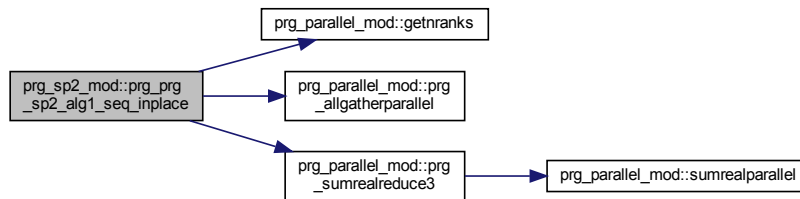
```

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 1099 of file prg_sp2_mod.F90.

Here is the call graph for this function:



9.26.2.2 prg_prg_sp2_alg2_seq_inplace()

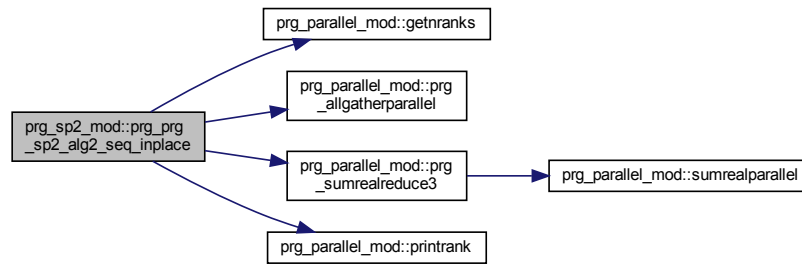
```

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 640 of file prg_sp2_mod.F90.

Here is the call graph for this function:



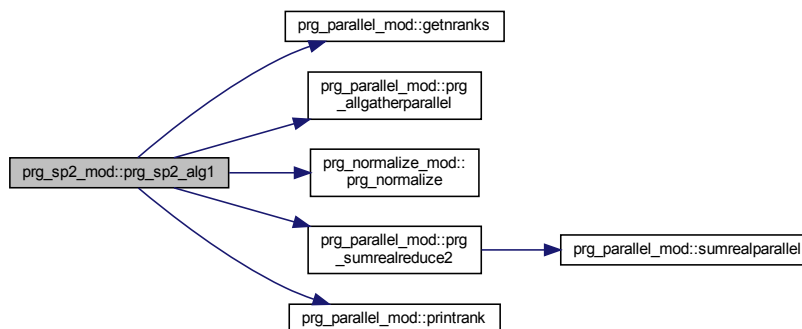
9.26.2.3 prg_sp2_alg1()

```

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 736 of file `prg_sp2_mod.F90`.

Here is the call graph for this function:



9.26.2.4 prg_sp2_alg1_genseq()

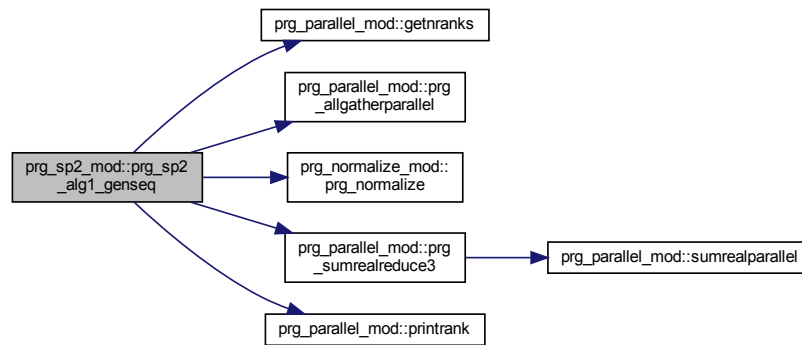
```

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 879 of file prg_sp2_mod.F90.

Here is the call graph for this function:



9.26.2.5 prg_sp2_alg1_seq()

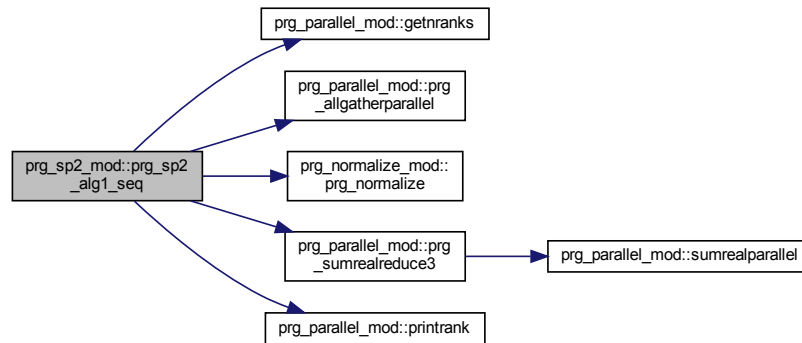
```

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 1008 of file prg_sp2_mod.F90.

Here is the call graph for this function:



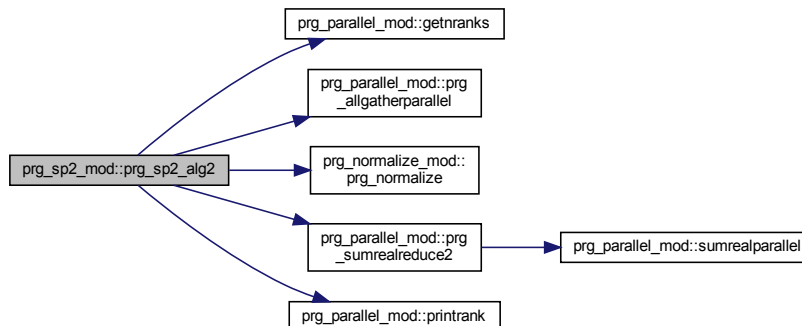
9.26.2.6 prg_sp2_alg2()

```

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 265 of file `prg_sp2_mod.F90`.

Here is the call graph for this function:



9.26.2.7 prg_sp2_alg2_genseq()

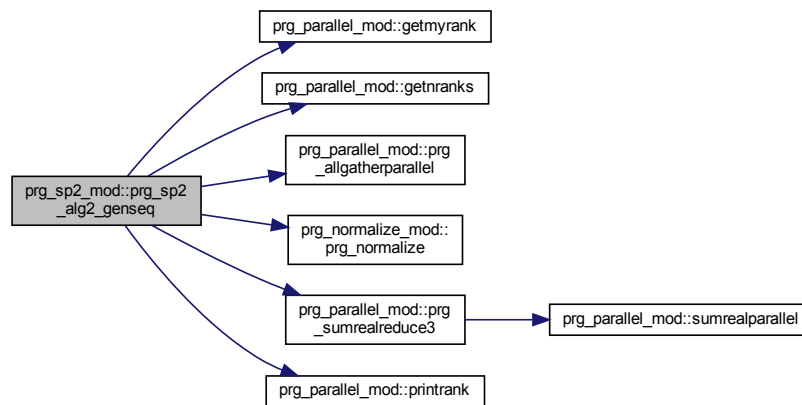
```

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 397 of file prg_sp2_mod.F90.

Here is the call graph for this function:



9.26.2.8 prg_sp2_alg2_seq()

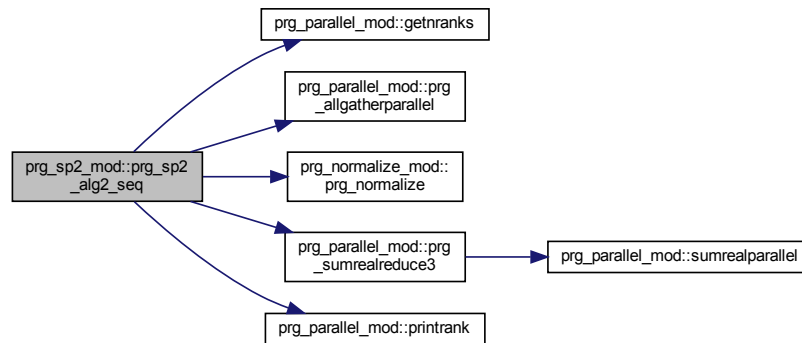
```

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 544 of file prg_sp2_mod.F90.

Here is the call graph for this function:



9.26.2.9 prg_sp2_basic()

```

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) idemtol,
    integer verbose )
  
```

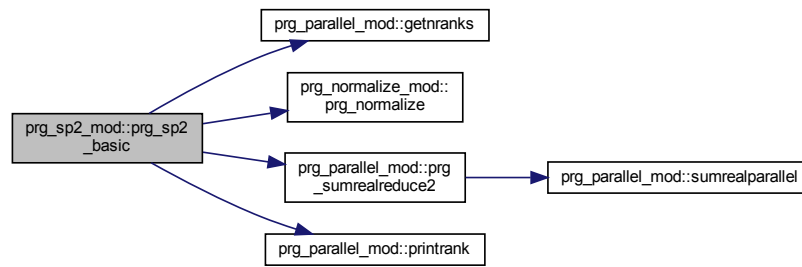
Calculates the density matrix from a Hamiltonian matrix by purification. The method implemented here is the very first version of the SP2 method.

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 51 of file `prg_sp2_mod.F90`.

Here is the call graph for this function:



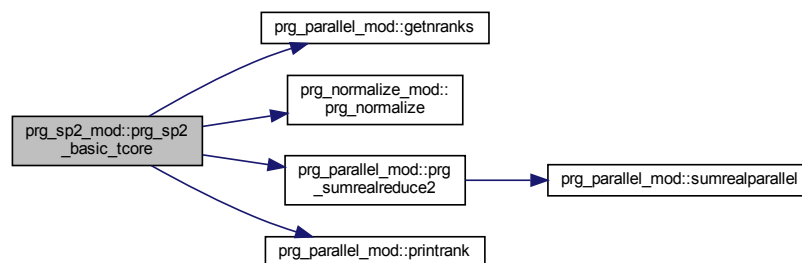
9.26.2.10 prg_sp2_basic_tcore()

```

subroutine, public prg_sp2_mod::prg_sp2_basic_tcore (
    type(bml_matrix_t), intent(in) h_bml,
    type(bml_matrix_t), intent(inout) rho_bml,
    type(bml_matrix_t), intent(inout) rhofull_bml,
    real(dp) threshold,
    real(dp) bndfil,
    integer minsp2iter,
    integer maxsp2iter,
    character(len=*), intent(in) sp2conv,
    real(dp) idemtol,
    integer verbose )
  
```

Definition at line 140 of file `prg_sp2_mod.F90`.

Here is the call graph for this function:



9.26.2.11 prg_sp2_submatrix()

```

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 1189 of file prg_sp2_mod.F90.

9.26.2.12 prg_sp2_submatrix_inplace()

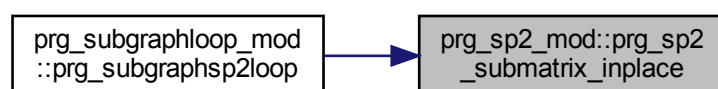
```

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 1258 of file prg_sp2_mod.F90.

Here is the caller graph for this function:



9.26.3 Variable Documentation

9.26.3.1 dp

```
integer, parameter prg_sp2_mod::dp = kind(1.0d0) [private]
```

Definition at line 18 of file prg_sp2_mod.F90.

9.26.3.2 dp1

```
integer, parameter prg_sp2_mod::dp1 = kind(1.0) [private]
```

Definition at line 19 of file prg_sp2_mod.F90.

9.27 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)

9.27.1 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.

9.27.2 Function/Subroutine Documentation

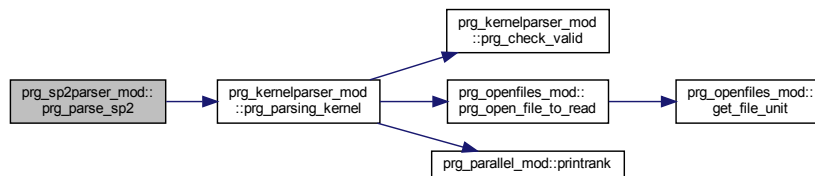
9.27.2.1 prg_parse_sp2()

```
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:



9.27.3 Variable Documentation

9.27.3.1 dp

```
integer, parameter prg_sp2parser_mod::dp = kind(1.0d0) [private]
```

Definition at line 22 of file prg_sp2parser_mod.F90.

9.28 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)`

9.28.1 Detailed Description

The subgraphloop module.

9.28.2 Function/Subroutine Documentation

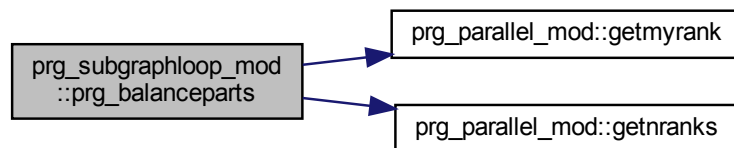
9.28.2.1 prg_balanceparts()

```
subroutine, public prg_subgraphloop_mod::prg_balanceparts (
    type (graph_partitioning_t), intent(inout) gp )
```

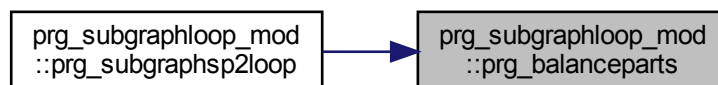
Renumber parts Handle unbalanced numbers of parts.

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:



9.28.2.2 prg_collectmatrixfromparts()

```
subroutine, public prg_subgraphloop_mod::prg_collectmatrixfromparts (
    type (graph_partitioning_t), intent(inout) gp,
    type (bml_matrix_t), intent(inout) rho_bml )
```

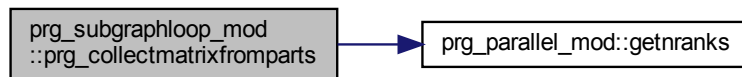
Collect distributed parts into same matrix.

Parameters

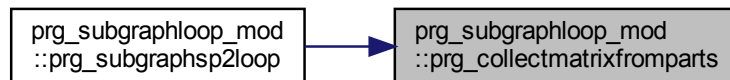
<i>gp</i>	Graph partitioning
<i>rho_bml</i>	Matrix to be collected into

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:



9.28.2.3 prg_getgrouppartitionhalosfromgraph()

```

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.

9.28.2.4 prg_getpartitionhalosfromgraph()

```
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.

9.28.2.5 prg_partordering()

```
subroutine, public prg_subgraphloop_mod::prg_partordering (
    type (graph_partitioning_t), intent(inout) gp )
```

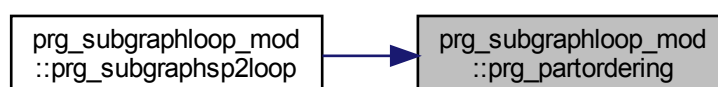
Set row ordering bases on parts.

Parameters

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

Definition at line 263 of file prg_subgraphloop_mod.F90.

Here is the caller graph for this function:

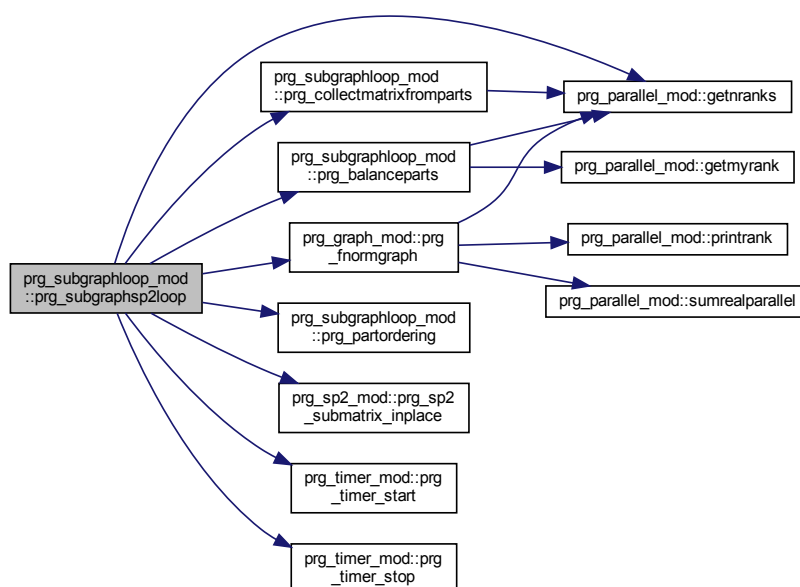


9.28.2.6 prg_subgraphsp2loop()

```
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:



9.28.3 Variable Documentation

9.28.3.1 dp

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

Definition at line 18 of file prg_subgraphloop_mod.F90.

9.29 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)

9.29.1 Detailed Description

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

It works by specifying two orientations and a rotation point.

9.29.2 Function/Subroutine Documentation

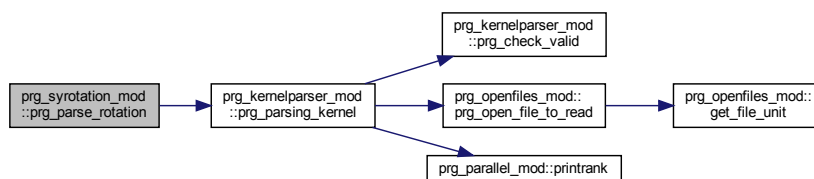
9.29.2.1 `prg_parse_rotation()`

```
subroutine, public prg_syrotation_mod::prg_parse_rotation (  
    type(rotation_type), intent(inout) rot,  
    character(len=*) filename )
```

The parser for rotation.

Definition at line 46 of file `prg_syrotation_mod.F90`.

Here is the call graph for this function:



9.29.2.2 prg_rotate()

```
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 139 of file prg_syrotation_mod.F90.

9.29.3 Variable Documentation

9.29.3.1 dp

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

Definition at line 11 of file prg_syrotation_mod.F90.

9.30 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, extin)
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, public [prg_parameters_to_vectors](#) (abc_angles, lattice_vector)
Transforms the lattice parameters into lattice vectors.
- subroutine, public [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_cleanuprepeatedatoms](#) (nats, coords, symbols, verbose)
Cleanup repeated atoms we might have in the system.
- subroutine, public [prg_get_recip_vects](#) (lattice_vectors, recip_vectors, volr, volk)
Get the volume of the cell and the reciprocal vectors: This soubroutine 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)
- subroutine, public [prg_get_covgraph_h](#) (sy, nnStructMindist, nnStruct, nrrnnstruct, rcut, graph_h, 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)

9.30.1 Detailed Description

A module to read and handle chemical systems.

This module will be used to build and handle a molecular system.

9.30.2 Function/Subroutine Documentation

9.30.2.1 prg_adj2bml()

```
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 2422 of file prg_system_mod.F90.

9.30.2.2 prg_centeratbox()

```
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 system_type).
<i>lattice_vectors</i>	System lattice vectors.
<i>verbose</i>	Verbosity level.

Definition at line 1324 of file prg_system_mod.F90.

9.30.2.3 prg_cleanuprepeatedatoms()

```
subroutine, public prg_system_mod::prg_cleanuprepeatedatoms (
    integer, intent(inout) nats,
    real(dp), dimension(:,:), intent(inout), allocatable coords,
    character(len=*), dimension(:), intent(inout), allocatable symbols,
    integer, intent(in), optional verbose )
```

Cleanup repeated atoms we might have in the system.

Parameters

<i>nats</i>	Number of atoms in the system.
<i>coords</i>	Coordinates of the system (see system_type).
<i>symbols</i>	Atomic symbols (see system_type). \verbose Verbosity level.

Definition at line 1505 of file prg_system_mod.F90.

9.30.2.4 prg_collect_graph_p()

```
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

<i>rho_bml</i>	Density matix in bml format.
<i>nc</i>	Number of core atoms.
<i>nats</i>	Number of atoms.
<i>hindex</i>	Hindex for the small part (see haindex)
<i>chindex</i>	Core-hallo index for the small part.
<i>graph_p</i>	Graph in an "ellpack" format.
<i>threshold</i>	Threshold to buil the density based atom projected graph.
<i>verbose</i>	Verbosity level.

Definition at line 2205 of file prg_system_mod.F90.

9.30.2.5 prg_destroy_subsystems()

```

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

<i>sy</i>	System to de deallocated (see system_type).
-----------	--

Definition at line 1986 of file prg_system_mod.F90.

9.30.2.6 prg_get_covgraph()

```

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) nrrnnstruct,
    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.

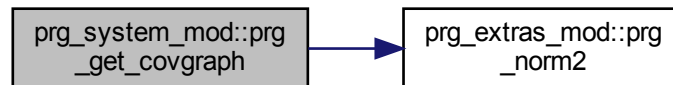
This is the graph composed by the covalent bonds (edges) that are determined with the VDW radius.

Parameters

<i>sy</i>	System structure (see system_type).
<i>nnStructMindist</i>	Minimum distance between atoms.
<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>bml_type</i>	The bml type for constructing the graph.
<i>gconv_bml</i>	Covanlency graph in bml format.
<i>verbose</i>	Verbosity level.

Definition at line 1691 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.2.7 prg_get_covgraph_h()

```

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) nrnnstruct,
    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.

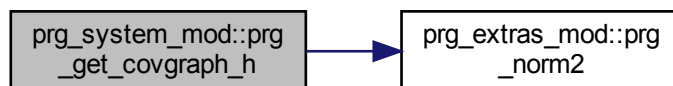
This is the graph composed by the covalent bonds (edges) that are determined with the VDW radius.

Parameters

<i>sy</i>	System structure (see system_type).
<i>nnStructMindist</i>	Minimum distance between atoms.
<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>bml_type</i>	The bml type for constructing the graph.
<i>gconv_bml</i>	Covacency graph in bml format.
<i>verbose</i>	Verbosity level.

Definition at line 1828 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.2.8 prg_get_covgraph_int()

```

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) 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 ) [private]
  
```

Definition at line 1767 of file prg_system_mod.F90.

9.30.2.9 prg_get_dihedral()

```

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

<i>sy</i>	System structure
<i>id1</i>	Atom index 1
<i>id2</i>	Atom index 1
<i>id3</i>	Atom index 1
<i>id4</i>	Atom index 1
<i>dihedral</i>	Output dihedral angle

Definition at line 1635 of file prg_system_mod.F90.

9.30.2.10 prg_get_distancematrix()

```
subroutine, public prg_system_mod::prg_get_distancematrix (
    real(dp), dimension(:,:), intent(in) coords,
    real(dp), dimension(:,:), intent(out), allocatable dmat )
```

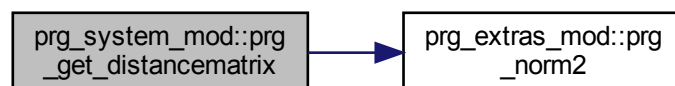
Get the distance matrix.

Parameters

<i>coords</i>	Coordinates of the system (see system_type).
<i>dmat</i>	Distance matrix (nats x nats).

Definition at line 1246 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.2.11 prg_get_nameandext()

```
subroutine, public prg_system_mod::prg_get_nameandext (
    character(len=*), intent(in) fullfilename,
    character(50), intent(inout) filename,
    character(3), intent(inout) ext )
```

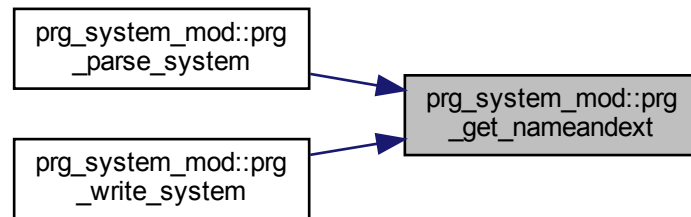
Get the name and extension of a file.

Parameters

<i>fullfilename</i>	Full filename.
<i>filename</i>	Filename of the system.
<i>extension</i>	Extension of the file.

Definition at line 210 of file prg_system_mod.F90.

Here is the caller graph for this function:



9.30.2.12 prg_get_origin()

```

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 teh system (see system_type).
<i>origin</i>	(min(x),min(y),min(z)) set as the origin of the system.

Definition at line 1213 of file prg_system_mod.F90.

9.30.2.13 prg_get_partial_atomgraph()

```

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 matix 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 2139 of file prg_system_mod.F90.

9.30.2.14 prg_get_recip_vects()

```

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 soubroutine 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 1586 of file prg_system_mod.F90.

9.30.2.15 prg_get_subsystem()

```

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 system_type).
<i>lsize</i>	Core+Halo subsystem size.
<i>indices</i>	Partition indices.
<i>sbsy</i>	Subsystem to be extracted.

Definition at line 1897 of file prg_system_mod.F90.

9.30.2.16 prg_graph2bml()

```
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 2456 of file prg_system_mod.F90.

9.30.2.17 prg_graph2vector()

```
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 2499 of file prg_system_mod.F90.

9.30.2.18 prg_make_random_system()

```
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 1089 of file prg_system_mod.F90.

9.30.2.19 prg_merge_graph()

```
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> ↔ <i>_p</i>	Density matix based graph in bml format.
<i>graph</i> ↔ <i>_h</i>	Hamiltonian matix based graph in bml format.

Definition at line 2297 of file prg_system_mod.F90.

9.30.2.20 prg_merge_graph_adj()

```
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_p</i>	Density matix based graph in "ellpack type format".
<i>graph_h</i>	Hamiltonian matix 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 2348 of file prg_system_mod.F90.

9.30.2.21 prg_molpartition()

```
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 )
```

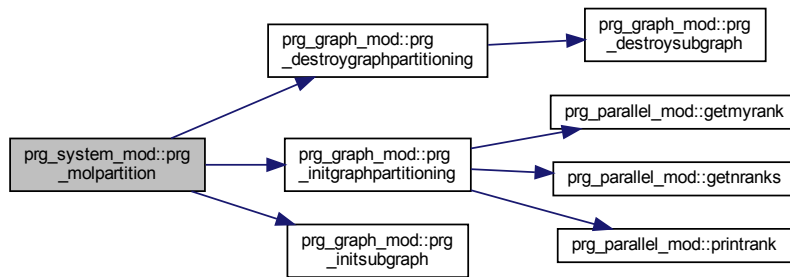
Partition by molecule.

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 2050 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.2.22 prg_parameters_to_vectors()

```

subroutine, public 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 )

```

Transforms the lattice parameters into lattice vectors.

Parameters

<i>abc_angles</i>	2x3 array containing the lattice parameters. $abc_angles(1,1) = a$, $abc_angles(1,2) = b$, and $abc_angles(1,3) = c$ $abc_angles(2,1) = \alpha$, $abc_angles(2,2) = \beta$ and $abc_angles(2,3) = \gamma$
<i>lattice_vector</i>	3x3 array containing the lattice vectors. $lattice_vector(1,:) = \vec{a}$

Definition at line 1135 of file prg_system_mod.F90.

Here is the caller graph for this function:



9.30.2.23 prg_parse_system()

```

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

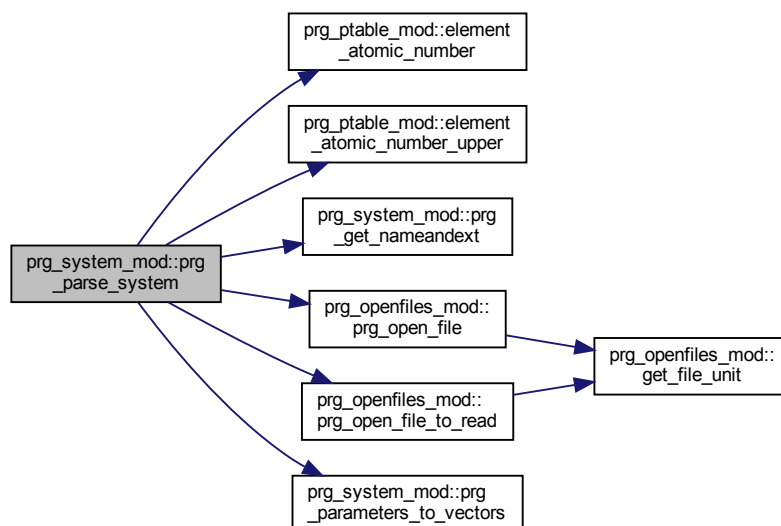
<i>system</i>	System to be constructed.
<i>filename</i>	Filename of the system.
<i>extin</i>	Extension of the file.

Assignment of species index for every atom.

Todo Integrate this loop in the loop for building the splist.

Definition at line 233 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.2.24 prg_replicate()

```
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 system_type).
<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 1450 of file prg_system_mod.F90.

9.30.2.25 prg_sortadj()

```
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 2556 of file prg_system_mod.F90.

9.30.2.26 prg_translateandfoldtobox()

```
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 system_type).
<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 1271 of file prg_system_mod.F90.

9.30.2.27 prg_translatetogeomcandfoldtobox()

```
subroutine, public prg_system_mod::prg_translatetogeomcandfoldtobox (
    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 system_type).
<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 1411 of file prg_system_mod.F90.

9.30.2.28 prg_vector2graph()

```
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 2528 of file prg_system_mod.F90.

9.30.2.29 prg_vectors_to_parameters()

```
subroutine, public 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 )
```

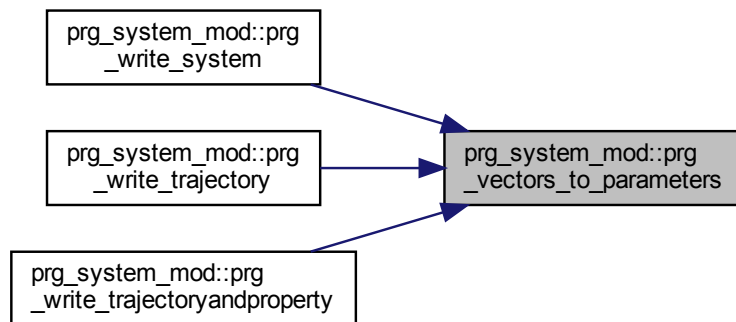
Transforms the lattice vectors into lattice parameters.

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 1177 of file prg_system_mod.F90.

Here is the caller graph for this function:



9.30.2.30 prg_wraparound()

```

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 system_type).
<i>lattice_vectors</i>	System lattice vectors.
<i>index</i>	Index atom to wrap around

Definition at line 1366 of file prg_system_mod.F90.

9.30.2.31 prg_write_system()

```
subroutine, public prg_system_mod::prg_write_system (
    type(system_type), intent(inout) system,
    character(len=*) filename,
    character(3), intent(in), optional extin )
```

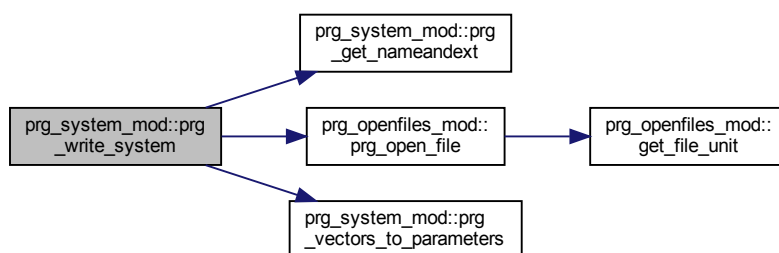
Write system in .xyz, .dat or pdb file.

Parameters

<i>system</i>	System to be constructed.
<i>filename</i>	File name.
<i>extension</i>	Extension of the file.

Definition at line 644 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.2.32 prg_write_trajectory()

```
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(len=*) filename,
    character(3) extension )
```

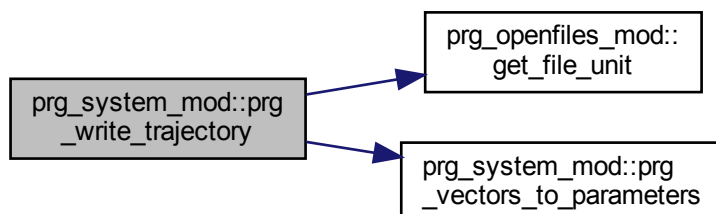
Write trajectory in .xyz, .dat or pdb file.

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 856 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.2.33 prg_write_trajectoryandproperty()

```

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(len=*) filename,
    character(3) extension )
  
```

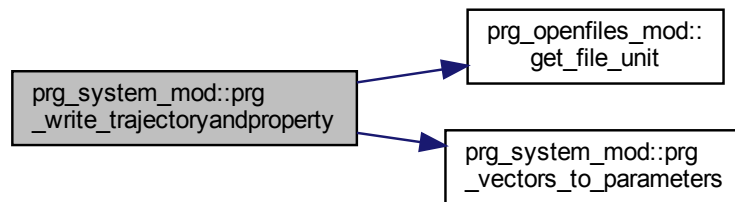
Write trajectory and atomic properties. Only pdb file.

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 979 of file prg_system_mod.F90.

Here is the call graph for this function:



9.30.3 Variable Documentation

9.30.3.1 dp

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

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

9.31 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`

9.31.1 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"

9.31.2 Function/Subroutine Documentation

9.31.2.1 int2char()

```
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:



9.31.2.2 prg_print_date_and_time()

```
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:

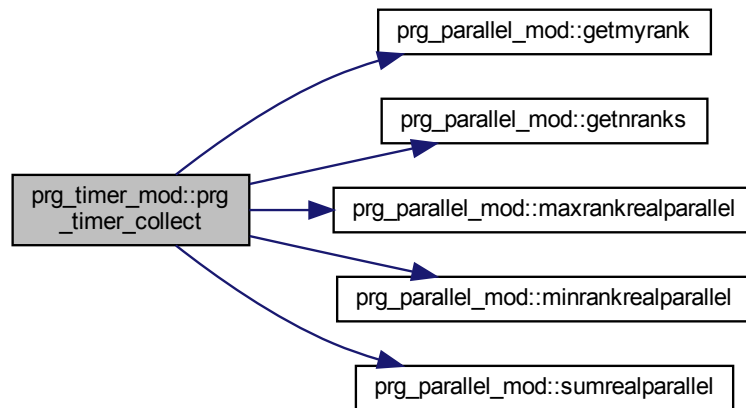


9.31.2.3 prg_timer_collect()

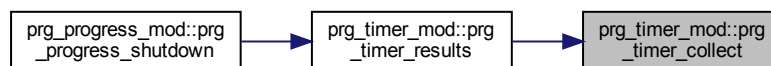
```
subroutine, public prg_timer_mod::prg_timer_collect
```

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:



9.31.2.4 prg_timer_getid()

```
subroutine prg_timer_mod::prg_timer_getid [private]
```

Get timer id.

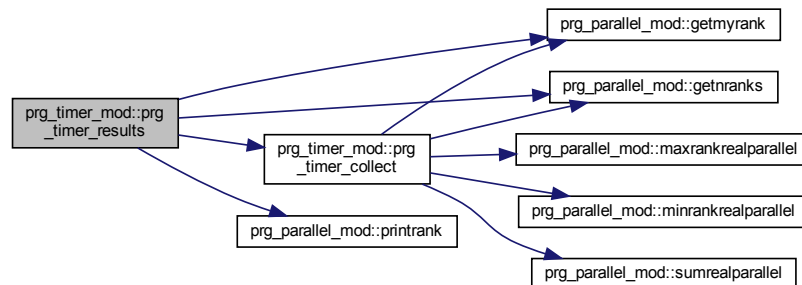
Definition at line 200 of file prg_timer_mod.F90.

9.31.2.5 prg_timer_results()

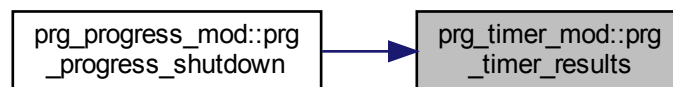
subroutine, public prg_timer_mod::prg_timer_results

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:



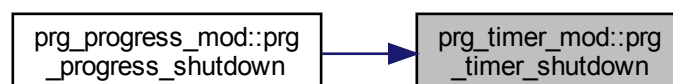
9.31.2.6 prg_timer_shutdown()

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:



9.31.2.7 prg_timer_start()

```
subroutine, public prg_timer_mod::prg_timer_start (
    integer, intent(in) itimer,
    character(len=*), intent(in), optional tag )
```

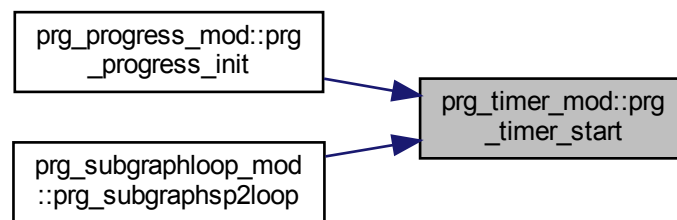
Start Timing.

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:



9.31.2.8 prg_timer_stop()

```
subroutine, public prg_timer_mod::prg_timer_stop (
    integer, intent(in) itimer,
    integer, intent(in), optional verbose )
```

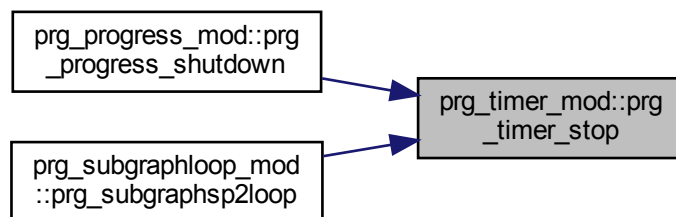
Stop timing.

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:

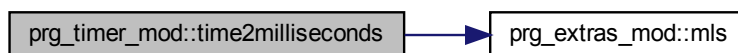


9.31.2.9 time2milliseconds()

```
real(8) function, public prg_timer_mod::time2milliseconds
```

Definition at line 360 of file `prg_timer_mod.F90`.

Here is the call graph for this function:



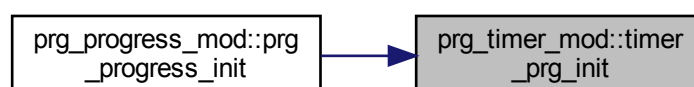
9.31.2.10 timer_prg_init()

```
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:



9.31.3 Variable Documentation

9.31.3.1 badd_timer

```
integer, public prg_timer_mod::badd_timer
```

Definition at line 48 of file prg_timer_mod.F90.

9.31.3.2 bmult_timer

```
integer, public prg_timer_mod::bmult_timer
```

Definition at line 48 of file prg_timer_mod.F90.

9.31.3.3 buildz_timer

```
integer, public prg_timer_mod::buildz_timer
```

Definition at line 49 of file prg_timer_mod.F90.

9.31.3.4 deortho_timer

```
integer, public prg_timer_mod::deortho_timer
```

Definition at line 45 of file prg_timer_mod.F90.

9.31.3.5 dp

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

Definition at line 32 of file prg_timer_mod.F90.

9.31.3.6 dyn_timer

```
integer, public prg_timer_mod::dyn_timer
```

Definition at line 49 of file prg_timer_mod.F90.

9.31.3.7 genx_timer

```
integer, public prg_timer_mod::genx_timer
```

Definition at line 44 of file prg_timer_mod.F90.

9.31.3.8 graphsp2_timer

```
integer, public prg_timer_mod::graphsp2_timer
```

Definition at line 46 of file prg_timer_mod.F90.

9.31.3.9 halfverlet_timer

```
integer, public prg_timer_mod::halfverlet_timer
```

Definition at line 51 of file prg_timer_mod.F90.

9.31.3.10 loop_timer

```
integer, public prg_timer_mod::loop_timer
```

Definition at line 44 of file prg_timer_mod.F90.

9.31.3.11 mdloop_timer

```
integer, public prg_timer_mod::mdloop_timer
```

Definition at line 49 of file prg_timer_mod.F90.

9.31.3.12 nlist_timer

```
integer, public prg_timer_mod::nlist_timer
```

Definition at line 51 of file prg_timer_mod.F90.

9.31.3.13 num_timers

```
integer prg_timer_mod::num_timers [private]
```

Definition at line 122 of file prg_timer_mod.F90.

9.31.3.14 ortho_timer

```
integer, public prg_timer_mod::ortho_timer
```

Definition at line 46 of file prg_timer_mod.F90.

9.31.3.15 pairpot_timer

```
integer, public prg_timer_mod::pairpot_timer
```

Definition at line 50 of file prg_timer_mod.F90.

9.31.3.16 part_timer

```
integer, public prg_timer_mod::part_timer
```

Definition at line 45 of file prg_timer_mod.F90.

9.31.3.17 pos_timer

```
integer, public prg_timer_mod::pos_timer
```

Definition at line 51 of file prg_timer_mod.F90.

9.31.3.18 ptimer

```
type (timer_status_t), dimension(:), allocatable prg_timer_mod::ptimer [private]
```

Definition at line 124 of file prg_timer_mod.F90.

9.31.3.19 realcoul_timer

```
integer, public prg_timer_mod::realcoul_timer
```

Definition at line 50 of file prg_timer_mod.F90.

9.31.3.20 recipcoul_timer

```
integer, public prg_timer_mod::recipcoul_timer
```

Definition at line 50 of file prg_timer_mod.F90.

9.31.3.21 sp2_timer

```
integer, public prg_timer_mod::sp2_timer
```

Definition at line 44 of file prg_timer_mod.F90.

9.31.3.22 suball_timer

```
integer, public prg_timer_mod::suball_timer
```

Definition at line 48 of file prg_timer_mod.F90.

9.31.3.23 subext_timer

```
integer, public prg_timer_mod::subext_timer
```

Definition at line 47 of file prg_timer_mod.F90.

9.31.3.24 subgraph_timer

```
integer, public prg_timer_mod::subgraph_timer
```

Definition at line 45 of file prg_timer_mod.F90.

9.31.3.25 subind_timer

```
integer, public prg_timer_mod::subind_timer
```

Definition at line 47 of file prg_timer_mod.F90.

9.31.3.26 subsp2_timer

```
integer, public prg_timer_mod::subsp2_timer
```

Definition at line 47 of file prg_timer_mod.F90.

9.31.3.27 tclock_max

```
integer prg_timer_mod::tclock_max [private]
```

Definition at line 121 of file prg_timer_mod.F90.

9.31.3.28 tclock_rate

```
integer prg_timer_mod::tclock_rate [private]
```

Definition at line 121 of file prg_timer_mod.F90.

9.31.3.29 tstart_clock

```
integer prg_timer_mod::tstart_clock [private]
```

Definition at line 121 of file prg_timer_mod.F90.

9.31.3.30 tstop_clock

```
integer prg_timer_mod::tstop_clock [private]
```

Definition at line 121 of file prg_timer_mod.F90.

9.31.3.31 zdiag_timer

```
integer, public prg_timer_mod::zdiag_timer
```

Definition at line 46 of file prg_timer_mod.F90.

9.32 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

9.32.1 Detailed Description

A module to perform XLBO integration.

This module will be used to compute integrate the dynamical variable "n" in xlbo.

9.32.2 Function/Subroutine Documentation

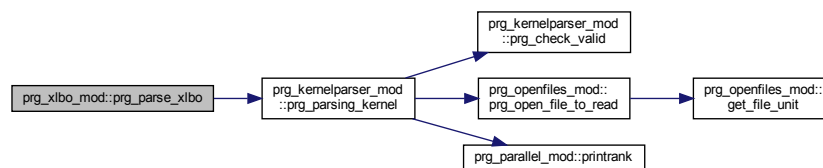
9.32.2.1 prg_parse_xlbo()

```
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:



9.32.2.2 prg_xlbo_fcoulupdate()

```
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.

9.32.2.3 prg_xlbo_nint()

```
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.

9.32.3 Variable Documentation

9.32.3.1 alpha

```
real(dp), parameter prg_xlbo_mod::alpha = 0.018_dp [private]
```

Definition at line 28 of file prg_xlbo_mod.F90.

9.32.3.2 c0

```
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.

9.32.3.3 c1

```
real(dp), parameter prg_xlbo_mod::c1 = 14.0_dp [private]
```

Definition at line 20 of file prg_xlbo_mod.F90.

9.32.3.4 c2

```
real(dp), parameter prg_xlbo_mod::c2 = -8.0_dp [private]
```

Definition at line 21 of file prg_xlbo_mod.F90.

9.32.3.5 c3

```
real(dp), parameter prg_xlbo_mod::c3 = -3.0_dp [private]
```

Definition at line 22 of file prg_xlbo_mod.F90.

9.32.3.6 c4

```
real(dp), parameter prg_xlbo_mod::c4 = 4.0_dp [private]
```

Definition at line 23 of file prg_xlbo_mod.F90.

9.32.3.7 c5

```
real(dp), parameter prg_xlbo_mod::c5 = -1.0_dp [private]
```

Definition at line 24 of file prg_xlbo_mod.F90.

9.32.3.8 cc

```
real(dp), parameter prg_xlbo_mod::cc = 0.9_dp [private]
```

Definition at line 29 of file prg_xlbo_mod.F90.

9.32.3.9 dp

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

Definition at line 16 of file prg_xlbo_mod.F90.

9.32.3.10 kappa

```
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.

9.33 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)

9.33.1 Detailed Description

Add name.

XL kernel (To be integrated)

Note

This module is still not functional

9.33.2 Function/Subroutine Documentation

9.33.2.1 prg_eig()

```
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]
```

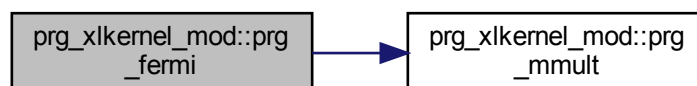
Definition at line 385 of file prg_xlkernel_mod.F90.

9.33.2.2 prg_fermi()

```
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 89 of file prg_xlkernel_mod.F90.

Here is the call graph for this function:



9.33.2.3 prg_get_deriv_finite_temp()

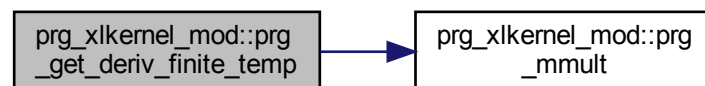
```

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 307 of file prg_xlkernel_mod.F90.

Here is the call graph for this function:



9.33.2.4 prg_inv()

```

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 412 of file prg_xlkernel_mod.F90.

9.33.2.5 prg_kernel_fermi_full()

```

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,

```

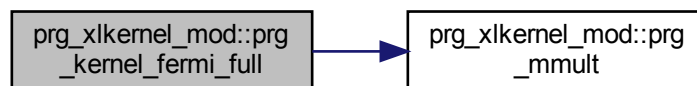
```

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) nrnnlist,
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 145 of file prg_xlkernel_mod.F90.

Here is the call graph for this function:



9.33.2.6 prg_mmult()

```

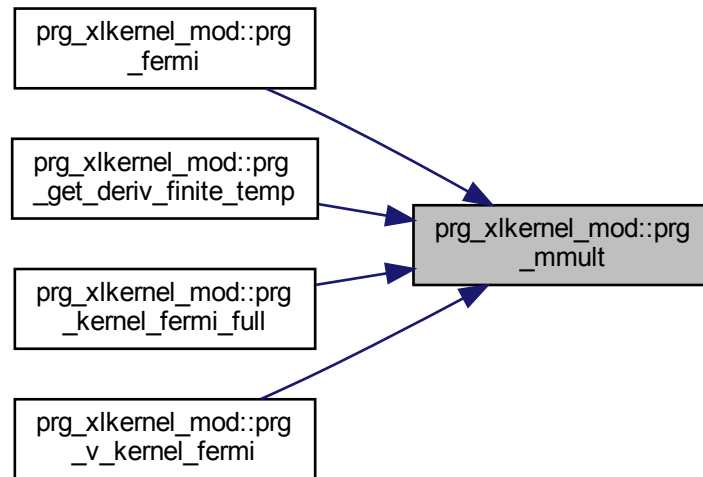
subroutine, private prg_xlkernel_mod::prg_mmult (
    real(prec), intent(in) alpha,
    real(prec), dimension(hdim,hdim), intent(in) A,
    real(prec), dimension(hdim,hdim), intent(in) B,
    real(prec), intent(in) beta,
    real(prec), dimension(hdim,hdim), intent(inout) C,
    character(1), intent(in) TA,

```

```
character(1), intent(in) TB,
integer(prec), intent(in) HDIM ) [private]
```

Definition at line 367 of file prg_xlkernel_mod.F90.

Here is the caller graph for this function:



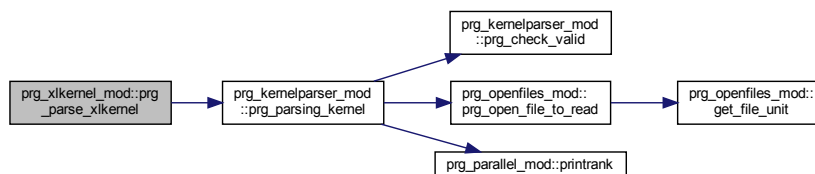
9.33.2.7 prg_parse_xlkernel()

```
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 40 of file prg_xlkernel_mod.F90.

Here is the call graph for this function:



9.33.2.8 prg_rank1()

```
subroutine, public prg_xlkernel_mod::prg_rank1 (
    integer, intent(in) verbose )
```

Rank1 kernel

Parameters

<i>param1</i>	..
<i>verbose</i>	Different levels of verbosity.

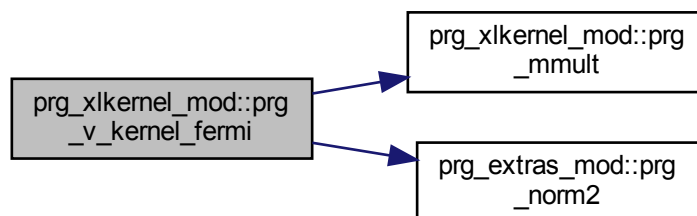
Definition at line 440 of file prg_xlkernel_mod.F90.

9.33.2.9 prg_v_kernel_fermi()

```
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) nrnnlist,
    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 236 of file prg_xlkernel_mod.F90.

Here is the call graph for this function:



9.33.3 Variable Documentation

9.33.3.1 dp

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

Definition at line 16 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 atr

```
real(dp) prg_chebyshev_mod::chebdata_type::atr
```

Definition at line 33 of file prg_chebyshev_mod.F90.

10.1.2.2 bml_type

```
character(100) prg_chebyshev_mod::chebdata_type::bml_type
```

Definition at line 30 of file prg_chebyshev_mod.F90.

10.1.2.3 bndfil

```
real(dp) prg_chebyshev_mod::chebdata_type::bndfil
```

Definition at line 33 of file prg_chebyshev_mod.F90.

10.1.2.4 ef

```
real(dp) prg_chebyshev_mod::chebdata_type::ef
```

Definition at line 33 of file prg_chebyshev_mod.F90.

10.1.2.5 estep

```
real(dp) prg_chebyshev_mod::chebdata_type::estep
```

Definition at line 33 of file prg_chebyshev_mod.F90.

10.1.2.6 fermitol

```
real(dp) prg_chebyshev_mod::chebdata_type::fermitol
```

Definition at line 34 of file prg_chebyshev_mod.F90.

10.1.2.7 flavor

```
character(100) prg_chebyshev_mod::chebdata_type::flavor
```

Definition at line 29 of file prg_chebyshev_mod.F90.

10.1.2.8 getef

```
logical prg_chebyshev_mod::chebdata_type::getef
```

Definition at line 35 of file prg_chebyshev_mod.F90.

10.1.2.9 jobname

```
character(100) prg_chebyshev_mod::chebdata_type::jobname
```

Definition at line 30 of file prg_chebyshev_mod.F90.

10.1.2.10 jon

```
logical prg_chebyshev_mod::chebdata_type::jon
```

Definition at line 35 of file prg_chebyshev_mod.F90.

10.1.2.11 kbt

```
real(dp) prg_chebyshev_mod::chebdata_type::kbt
```

Definition at line 34 of file prg_chebyshev_mod.F90.

10.1.2.12 mdim

```
integer prg_chebyshev_mod::chebdata_type::mdim
```

Definition at line 31 of file prg_chebyshev_mod.F90.

10.1.2.13 ncoeffs

```
integer prg_chebyshev_mod::chebdata_type::ncoeffs
```

Definition at line 31 of file prg_chebyshev_mod.F90.

10.1.2.14 ndim

```
integer prg_chebyshev_mod::chebdata_type::ndim
```

Definition at line 31 of file prg_chebyshev_mod.F90.

10.1.2.15 npts

```
integer prg_chebyshev_mod::chebdata_type::npts
```

Definition at line 32 of file prg_chebyshev_mod.F90.

10.1.2.16 threshold

```
real(dp) prg_chebyshev_mod::chebdata_type::threshold
```

Definition at line 34 of file prg_chebyshev_mod.F90.

10.1.2.17 trkfunc

```
logical prg_chebyshev_mod::chebdata_type::trkfunc
```

Definition at line 35 of file prg_chebyshev_mod.F90.

10.1.2.18 verbose

```
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:

- [/tmp/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 20 of file prg_system_mod.F90.

10.2.2 Member Data Documentation

10.2.2.1 coul_pot_k

```
real(dp), dimension(:), allocatable prg_system_mod::estruct_type::coul_pot_k
```

Reciprocal Coulombic contribution.

Definition at line 56 of file prg_system_mod.F90.

10.2.2.2 coul_pot_r

```
real(dp), dimension(:), allocatable prg_system_mod::estruct_type::coul_pot_r
```

Real Coulombic contribution.

Definition at line 53 of file prg_system_mod.F90.

10.2.2.3 eband

```
real(dp) prg_system_mod::estruct_type::eband
```

Band energy.

Definition at line 68 of file prg_system_mod.F90.

10.2.2.4 fpul

```
real(dp), dimension(:, :), allocatable prg_system_mod::estruct_type::fpul
```

Pulay force.

Definition at line 62 of file prg_system_mod.F90.

10.2.2.5 fscoul

```
real(dp), dimension(:, :), allocatable prg_system_mod::estruct_type::fscoul
```

Nonorthogonal Coulombic force.

Definition at line 65 of file prg_system_mod.F90.

10.2.2.6 ham

```
type(bml_matrix_t) prg_system_mod::estruct_type::ham
```

SCC-Hamiltonian of the system.

Definition at line 32 of file prg_system_mod.F90.

10.2.2.7 ham0

```
type(bml_matrix_t) prg_system_mod::estruct_type::ham0
```

Hamiltonian of the system.

Definition at line 35 of file prg_system_mod.F90.

10.2.2.8 hindex

```
integer, dimension(:, :), allocatable prg_system_mod::estruct_type::hindex
```

Hindex.

Definition at line 29 of file prg_system_mod.F90.

10.2.2.9 nel

```
integer prg_system_mod::estruct_type::nel
```

Number of electrons.

Definition at line 26 of file prg_system_mod.F90.

10.2.2.10 norbs

```
integer prg_system_mod::estruct_type::norbs
```

Number of orbitals of the system.

Definition at line 23 of file prg_system_mod.F90.

10.2.2.11 oham

```
type(bml_matrix_t) prg_system_mod::estruct_type::oham
```

Orthogonalized Hamiltonian.

Definition at line 38 of file prg_system_mod.F90.

10.2.2.12 orho

```
type(bml_matrix_t) prg_system_mod::estruct_type::orho
```

Orthogonalized density matrix.

Definition at line 47 of file prg_system_mod.F90.

10.2.2.13 over

```
type(bml_matrix_t) prg_system_mod::estruct_type::over
```

Overlap matrix of the system.

Definition at line 41 of file prg_system_mod.F90.

10.2.2.14 rho

```
type(bml_matrix_t) prg_system_mod::estruct_type::rho
```

Density matrix of the system.

Definition at line 44 of file prg_system_mod.F90.

10.2.2.15 skforce

```
real(dp), dimension(:, :), allocatable prg_system_mod::estruct_type::skforce
```

Slater Koster force.

Definition at line 59 of file prg_system_mod.F90.

10.2.2.16 zmat

```
type(bml_matrix_t) prg_system_mod::estruct_type::zmat
```

Congruence transformation.

Definition at line 50 of file prg_system_mod.F90.

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

- /tmp/qmd-progress/src/prg_system_mod.F90

10.3 prg_genz_mod::genzspin Type Reference

Input for the genz driver. This type controls all the variables that are needed by genz.

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).

10.3.1 Detailed Description

Input for the genz driver. This type controls all the variables that are needed by genz.

Definition at line 26 of file prg_genz_mod.F90.

10.3.2 Member Data Documentation

10.3.2.1 bml_type

```
character(20) prg_genz_mod::genzspinp::bml_type
```

Matrix format (Dense or Ellpack).

Definition at line 59 of file prg_genz_mod.F90.

10.3.2.2 igenz

```
integer prg_genz_mod::genzspinp::igenz
```

To keep track of the genz iterations.

Definition at line 50 of file prg_genz_mod.F90.

10.3.2.3 integration

```
logical prg_genz_mod::genzspinp::integration
```

If we want to do XL integration scheme for Z.

Definition at line 47 of file prg_genz_mod.F90.

10.3.2.4 mdim

```
integer prg_genz_mod::genzspinp::mdim
```

Max nonzero elements per row for every row see [\[1\]](#) .

Definition at line 56 of file prg_genz_mod.F90.

10.3.2.5 nfirst

```
integer prg_genz_mod::genzspinp::nfirst
```

!Lentgth of the "firsts iteration period".

Definition at line 32 of file prg_genz_mod.F90.

10.3.2.6 nreff

```
integer prg_genz_mod::genzspinp::nreff
```

!Initial number of recursive refinements.

Definition at line 38 of file prg_genz_mod.F90.

10.3.2.7 nrefi

```
integer prg_genz_mod::genzspinp::nrefi
```

!Initial number of recursive refinements.

Definition at line 35 of file prg_genz_mod.F90.

10.3.2.8 numthresf

```
real(dp) prg_genz_mod::genzspinp::numthresf
```

Final threshold value.

Definition at line 44 of file prg_genz_mod.F90.

10.3.2.9 numthresi

```
real(dp) prg_genz_mod::genzspinp::numthresi
```

Initial threshold value.

Definition at line 41 of file prg_genz_mod.F90.

10.3.2.10 verbose

```
integer prg_genz_mod::genzspinp::verbose
```

To have different levels of verbose.

Definition at line 29 of file prg_genz_mod.F90.

10.3.2.11 zsp

```
logical prg_genz_mod::genzspinp::zsp
```

Logical variable to compute in sparse or dense mode.

Definition at line 53 of file prg_genz_mod.F90.

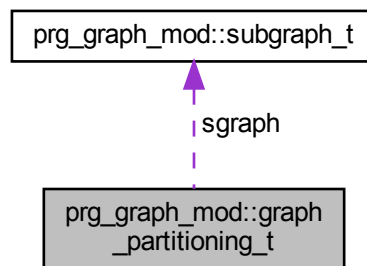
The documentation for this type was generated from the following file:

- /tmp/qmd-progress/src/[prg_genz_mod.F90](#)

10.4 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](#)) [elumo](#)
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.

10.4.1 Detailed Description

Trace per iteration.

Graph partitioning type

Definition at line 57 of file prg_graph_mod.F90.

10.4.2 Member Data Documentation

10.4.2.1 ehomo

```
real(dp) prg_graph_mod::graph_partitioning_t::ehomo [private]
```

Homo value.

Definition at line 117 of file prg_graph_mod.F90.

10.4.2.2 elumo

```
real(dp) prg_graph_mod::graph_partitioning_t::elumo [private]
```

Lumo value.

Definition at line 120 of file prg_graph_mod.F90.

10.4.2.3 globalpartextent

```
integer prg_graph_mod::graph_partitioning_t::globalpartextent [private]
```

Total global parts.

Definition at line 84 of file prg_graph_mod.F90.

10.4.2.4 globalpartmax

```
integer prg_graph_mod::graph_partitioning_t::globalpartmax [private]
```

Maximum global part number.

Definition at line 81 of file prg_graph_mod.F90.

10.4.2.5 globalpartmin

```
integer prg_graph_mod::graph_partitioning_t::globalpartmin [private]
```

Minimum global part number.

Definition at line 78 of file prg_graph_mod.F90.

10.4.2.6 localpartextent

`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.

10.4.2.7 localpartmax

`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.

10.4.2.8 localpartmin

`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.

10.4.2.9 maxeval

`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.

10.4.2.10 maxiter

`integer prg_graph_mod::graph_partitioning_t::maxiter [private]`

Number of SP2 iterations.

Definition at line 114 of file prg_graph_mod.F90.

10.4.2.11 mineval

```
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.

10.4.2.12 myrank

```
integer prg_graph_mod::graph_partitioning_t::myrank [private]
```

Local processor.

Definition at line 63 of file prg_graph_mod.F90.

10.4.2.13 nnodesinpart

```
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.

10.4.2.14 nnodesinpartall

```
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.

10.4.2.15 nparts

```
integer prg_graph_mod::graph_partitioning_t::nparts [private]
```

Total number of local partitions.

Definition at line 102 of file prg_graph_mod.F90.

10.4.2.16 order

```
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.

10.4.2.17 pname

```
character(len=100) prg_graph_mod::graph_partitioning_t::pname [private]
```

Partition name.

Definition at line 60 of file prg_graph_mod.F90.

10.4.2.18 pp

```
integer, dimension(100) prg_graph_mod::graph_partitioning_t::pp [private]
```

Sequence for SP2.

Definition at line 111 of file prg_graph_mod.F90.

10.4.2.19 reorder

```
integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::reorder [private]
```

Reordering if required.

Definition at line 99 of file prg_graph_mod.F90.

10.4.2.20 sgraph

```
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.

10.4.2.21 totalnodes

```
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.

10.4.2.22 totalnodes2

```
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.

10.4.2.23 totalparts

```
integer prg_graph_mod::graph_partitioning_t::totalparts [private]
```

Total number of global partitions.

Definition at line 69 of file prg_graph_mod.F90.

10.4.2.24 totalprocs

```
integer prg_graph_mod::graph_partitioning_t::totalprocs [private]
```

Number of processors.

Definition at line 66 of file prg_graph_mod.F90.

10.4.2.25 vv

```
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:

- [/tmp/qmd-progress/src/prg_graph_mod.F90](#)

10.5 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](#)

10.5.1 Detailed Description

General SP2 solver type.

Definition at line 26 of file prg_graphsp2parser_mod.F90.

10.5.2 Member Data Documentation

10.5.2.1 bml_type

```
character(20) prg_graphsp2parser_mod::gsp2data_type::bml_type
```

Definition at line 44 of file prg_graphsp2parser_mod.F90.

10.5.2.2 bndfil

```
real(dp) prg_graphsp2parser_mod::gsp2data_type::bndfil
```

Definition at line 37 of file prg_graphsp2parser_mod.F90.

10.5.2.3 covgfact

```
real(dp) prg_graphsp2parser_mod::gsp2data_type::covgfact
```

Definition at line 50 of file prg_graphsp2parser_mod.F90.

10.5.2.4 double_jump

```
logical prg_graphsp2parser_mod::gsp2data_type::double_jump
```

Definition at line 49 of file prg_graphsp2parser_mod.F90.

10.5.2.5 errlimit

```
real(dp) prg_graphsp2parser_mod::gsp2data_type::errlimit
```

Definition at line 39 of file prg_graphsp2parser_mod.F90.

10.5.2.6 graph_element

```
character(10) prg_graphsp2parser_mod::gsp2data_type::graph_element
```

Definition at line 46 of file prg_graphsp2parser_mod.F90.

10.5.2.7 gthreshold

```
real(dp) prg_graphsp2parser_mod::gsp2data_type::gthreshold
```

Definition at line 38 of file prg_graphsp2parser_mod.F90.

10.5.2.8 hamfile

```
character(50) prg_graphsp2parser_mod::gsp2data_type::hamfile
```

Definition at line 28 of file prg_graphsp2parser_mod.F90.

10.5.2.9 jobname

```
character(20) prg_graphsp2parser_mod::gsp2data_type::jobname
```

Definition at line 27 of file prg_graphsp2parser_mod.F90.

10.5.2.10 maxsp2iter

```
integer prg_graphsp2parser_mod::gsp2data_type::maxsp2iter
```

Definition at line 31 of file prg_graphsp2parser_mod.F90.

10.5.2.11 mdim

```
integer prg_graphsp2parser_mod::gsp2data_type::mdim
```

Definition at line 40 of file prg_graphsp2parser_mod.F90.

10.5.2.12 minsp2iter

```
integer prg_graphsp2parser_mod::gsp2data_type::minsp2iter
```

Definition at line 30 of file prg_graphsp2parser_mod.F90.

10.5.2.13 natoms

```
integer prg_graphsp2parser_mod::gsp2data_type::natoms
```

Definition at line 33 of file prg_graphsp2parser_mod.F90.

10.5.2.14 ndim

```
integer prg_graphsp2parser_mod::gsp2data_type::ndim
```

Definition at line 41 of file prg_graphsp2parser_mod.F90.

10.5.2.15 nlgcut

```
real(dp) prg_graphsp2parser_mod::gsp2data_type::nlgcut
```

Definition at line 51 of file prg_graphsp2parser_mod.F90.

10.5.2.16 nodesperpart

```
integer prg_graphsp2parser_mod::gsp2data_type::nodesperpart
```

Definition at line 32 of file prg_graphsp2parser_mod.F90.

10.5.2.17 parteach

```
integer prg_graphsp2parser_mod::gsp2data_type::parteach
```

Definition at line 52 of file prg_graphsp2parser_mod.F90.

10.5.2.18 partition_count

```
integer prg_graphsp2parser_mod::gsp2data_type::partition_count
```

Definition at line 34 of file prg_graphsp2parser_mod.F90.

10.5.2.19 partition_refinement

```
character(10) prg_graphsp2parser_mod::gsp2data_type::partition_refinement
```

Definition at line 48 of file prg_graphsp2parser_mod.F90.

10.5.2.20 partition_type

```
character(10) prg_graphsp2parser_mod::gsp2data_type::partition_type
```

Definition at line 47 of file prg_graphsp2parser_mod.F90.

10.5.2.21 pdim

```
real(dp), dimension(3) prg_graphsp2parser_mod::gsp2data_type::pdim
```

Definition at line 43 of file prg_graphsp2parser_mod.F90.

10.5.2.22 sdim

```
character, dimension(3) prg_graphsp2parser_mod::gsp2data_type::sdim
```

Definition at line 42 of file prg_graphsp2parser_mod.F90.

10.5.2.23 sp2conv

```
character(10) prg_graphsp2parser_mod::gsp2data_type::sp2conv
```

Definition at line 45 of file prg_graphsp2parser_mod.F90.

10.5.2.24 sp2tol

```
real(dp) prg_graphsp2parser_mod::gsp2data_type::sp2tol
```

Definition at line 35 of file prg_graphsp2parser_mod.F90.

10.5.2.25 threshold

```
real(dp) prg_graphsp2parser_mod::gsp2data_type::threshold
```

Definition at line 36 of file prg_graphsp2parser_mod.F90.

10.5.2.26 verbose

```
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:

- /tmp/qmd-progress/src/[prg_graphsp2parser_mod.F90](#)

10.6 prg_modelham_mod::mham_type Type Reference

General ModelHam type.

Public Attributes

- integer [norbs](#)
- integer [seed](#)
- character(100) [jobname](#)
- character(100) [bml_type](#)
- real(dp) [ea](#)
- real(dp) [eb](#)
- real(dp) [dab](#)
- real(dp) [daiaj](#)
- real(dp) [dbibj](#)
- real(dp) [dec](#)
- real(dp) [rcoeff](#)
- logical [reshuffle](#)

10.6.1 Detailed Description

General ModelHam type.

Definition at line 18 of file prg_modelham_mod.F90.

10.6.2 Member Data Documentation

10.6.2.1 bml_type

```
character(100) prg_modelham_mod::mham_type::bml_type
```

Definition at line 21 of file prg_modelham_mod.F90.

10.6.2.2 dab

```
real(dp) prg_modelham_mod::mham_type::dab
```

Definition at line 24 of file prg_modelham_mod.F90.

10.6.2.3 daiaj

```
real(dp) prg_modelham_mod::mham_type::daiaj
```

Definition at line 25 of file prg_modelham_mod.F90.

10.6.2.4 dbibj

```
real(dp) prg_modelham_mod::mham_type::dbibj
```

Definition at line 26 of file prg_modelham_mod.F90.

10.6.2.5 dec

```
real(dp) prg_modelham_mod::mham_type::dec
```

Definition at line 27 of file prg_modelham_mod.F90.

10.6.2.6 ea

```
real(dp) prg_modelham_mod::mham_type::ea
```

Definition at line 22 of file prg_modelham_mod.F90.

10.6.2.7 eb

```
real(dp) prg_modelham_mod::mham_type::eb
```

Definition at line 23 of file prg_modelham_mod.F90.

10.6.2.8 jobname

```
character(100) prg_modelham_mod::mham_type::jobname
```

Definition at line 20 of file prg_modelham_mod.F90.

10.6.2.9 norbs

```
integer prg_modelham_mod::mham_type::norbs
```

Definition at line 19 of file prg_modelham_mod.F90.

10.6.2.10 rcoeff

```
real(dp) prg_modelham_mod::mham_type::rcoeff
```

Definition at line 27 of file prg_modelham_mod.F90.

10.6.2.11 reshuffle

```
logical prg_modelham_mod::mham_type::reshuffle
```

Definition at line 28 of file prg_modelham_mod.F90.

10.6.2.12 seed

```
integer prg_modelham_mod::mham_type::seed
```

Definition at line 19 of file prg_modelham_mod.F90.

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

- [/tmp/qmd-progress/src/prg_modelham_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 17 of file prg_pulaymixer_mod.F90.

10.7.2 Member Data Documentation

10.7.2.1 mixcoeff

```
real(dp) prg_pulaymixer_mod::mx_type::mixcoeff
```

Coefficient for mixing.

Definition at line 29 of file prg_pulaymixer_mod.F90.

10.7.2.2 mixeron

```
logical prg_pulaymixer_mod::mx_type::mixeron
```

Mixer on or off (Not implemented)

Definition at line 32 of file prg_pulaymixer_mod.F90.

10.7.2.3 mixertype

```
character(20) prg_pulaymixer_mod::mx_type::mixertype
```

Type or mixing scheme to be used (Linear or Pulay)

Definition at line 20 of file prg_pulaymixer_mod.F90.

10.7.2.4 mpulay

```
integer prg_pulaymixer_mod::mx_type::mpulay
```

Pulay dimension for matrix.

Definition at line 26 of file prg_pulaymixer_mod.F90.

10.7.2.5 verbose

```
integer prg_pulaymixer_mod::mx_type::verbose
```

Verbosity level.

Definition at line 23 of file prg_pulaymixer_mod.F90.

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

- [/tmp/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 prg_memory_consumption()

```
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:

- /tmp/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 rank

```
integer prg_parallel_mod::rankreducedata_t::rank [private]
```

MPI rank.

Definition at line 78 of file prg_parallel_mod.F90.

10.9.2.2 val

```
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:

- /tmp/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 bmltype

```
character(20) prg_response_mod::respdata_type::bmltype
```

Definition at line 24 of file prg_response_mod.F90.

10.10.2.2 computedipole

```
logical prg_response_mod::respdata_type::computedipole
```

Definition at line 27 of file prg_response_mod.F90.

10.10.2.3 field

```
real(dp), dimension(3) prg_response_mod::respdata_type::field
```

Definition at line 30 of file prg_response_mod.F90.

10.10.2.4 fieldintensity

```
real(dp) prg_response_mod::respdata_type::fieldintensity
```

Definition at line 29 of file prg_response_mod.F90.

10.10.2.5 getresponse

```
logical prg_response_mod::respdata_type::getresponse
```

Definition at line 28 of file prg_response_mod.F90.

10.10.2.6 mdim

```
integer prg_response_mod::respdata_type::mdim
```

Definition at line 25 of file prg_response_mod.F90.

10.10.2.7 numthresh

```
real(dp) prg_response_mod::respdata_type::numthresh
```

Definition at line 26 of file prg_response_mod.F90.

10.10.2.8 respmode

```
character(20) prg_response_mod::respdata_type::respmode
```

Definition at line 22 of file prg_response_mod.F90.

10.10.2.9 typeofpert

```
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:

- /tmp/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 14 of file prg_syrotation_mod.F90.

10.11.2 Member Data Documentation

10.11.2.1 catom

```
integer prg_syrotation_mod::rotation_type::catom
```

Atomic point to determine the rotation center.

Definition at line 22 of file prg_syrotation_mod.F90.

10.11.2.2 catom2

```
integer prg_syrotation_mod::rotation_type::catom2
```

Atomic point to determine a second rotation center.

Definition at line 24 of file prg_syrotation_mod.F90.

10.11.2.3 jobname

```
character(20) prg_syrotation_mod::rotation_type::jobname
```

Definition at line 15 of file prg_syrotation_mod.F90.

10.11.2.4 patom1

```
integer prg_syrotation_mod::rotation_type::patom1
```

Atomic point to determine the initial orientation.

Definition at line 18 of file prg_syrotation_mod.F90.

10.11.2.5 patom2

```
integer prg_syrotation_mod::rotation_type::patom2
```

Atomic point to determine initial orientation.

Definition at line 20 of file prg_syrotation_mod.F90.

10.11.2.6 pq1

```
real(dp), dimension(3) prg_syrotation_mod::rotation_type::pq1
```

Point to determine initial orientation.

Definition at line 26 of file prg_syrotation_mod.F90.

10.11.2.7 pq2

```
real(dp), dimension(3) prg_syrotation_mod::rotation_type::pq2
```

Point to determine final orientation.

Definition at line 28 of file prg_syrotation_mod.F90.

10.11.2.8 rotate_atoms

```
integer, dimension(2) prg_syrotation_mod::rotation_type::rotate_atoms
```

First and last rotated atom in the list.

Definition at line 36 of file prg_syrotation_mod.F90.

10.11.2.9 typeofrot

```
character(50) prg_syrotation_mod::rotation_type::typeofrot
```

Definition at line 16 of file prg_syrotation_mod.F90.

10.11.2.10 v1

```
real(dp), dimension(3) prg_syrotation_mod::rotation_type::v1
```

Initial orientation.

Definition at line 30 of file prg_syrotation_mod.F90.

10.11.2.11 v2

```
real(dp), dimension(3) prg_syrotation_mod::rotation_type::v2
```

Final orientation.

Definition at line 32 of file prg_syrotation_mod.F90.

10.11.2.12 vq

```
real(dp), dimension(3) prg_syrotation_mod::rotation_type::vq
```

Center of rotation.

Definition at line 34 of file prg_syrotation_mod.F90.

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

- /tmp/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 bml_type

```
character(20) prg_sp2parser_mod::sp2data_type::bml_type
```

Definition at line 38 of file prg_sp2parser_mod.F90.

10.12.2.2 bndfil

```
real(dp) prg_sp2parser_mod::sp2data_type::bndfil
```

Definition at line 33 of file prg_sp2parser_mod.F90.

10.12.2.3 flavor

```
character(10) prg_sp2parser_mod::sp2data_type::flavor
```

Definition at line 40 of file prg_sp2parser_mod.F90.

10.12.2.4 jobname

```
character(20) prg_sp2parser_mod::sp2data_type::jobname
```

Definition at line 27 of file prg_sp2parser_mod.F90.

10.12.2.5 maxsp2iter

```
integer prg_sp2parser_mod::sp2data_type::maxsp2iter
```

Definition at line 30 of file prg_sp2parser_mod.F90.

10.12.2.6 mdim

```
integer prg_sp2parser_mod::sp2data_type::mdim
```

Definition at line 34 of file prg_sp2parser_mod.F90.

10.12.2.7 minsp2iter

```
integer prg_sp2parser_mod::sp2data_type::minsp2iter
```

Definition at line 29 of file prg_sp2parser_mod.F90.

10.12.2.8 ndim

```
integer prg_sp2parser_mod::sp2data_type::ndim
```

Definition at line 35 of file prg_sp2parser_mod.F90.

10.12.2.9 pdim

```
real(dp), dimension(3) prg_sp2parser_mod::sp2data_type::pdim
```

Definition at line 37 of file prg_sp2parser_mod.F90.

10.12.2.10 sdim

```
character, dimension(3) prg_sp2parser_mod::sp2data_type::sdim
```

Definition at line 36 of file prg_sp2parser_mod.F90.

10.12.2.11 sp2conv

```
character(10) prg_sp2parser_mod::sp2data_type::sp2conv
```

Definition at line 39 of file prg_sp2parser_mod.F90.

10.12.2.12 sp2tol

```
real(dp) prg_sp2parser_mod::sp2data_type::sp2tol
```

Definition at line 31 of file prg_sp2parser_mod.F90.

10.12.2.13 threshold

```
real(dp) prg_sp2parser_mod::sp2data_type::threshold
```

Definition at line 32 of file prg_sp2parser_mod.F90.

10.12.2.14 verbose

```
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:

- /tmp/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](#)
Indices 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 core_halo_index

```
integer, dimension(:), allocatable prg_graph_mod::subgraph_t::core_halo_index [private]
```

Indices from original matrix for subgraph core+halo extraction.

Definition at line 46 of file prg_graph_mod.F90.

10.13.2.2 hsize

```
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 lsize

```
integer prg_graph_mod::subgraph_t::lsize [private]
```

Size of core subgraph.

Definition at line 43 of file prg_graph_mod.F90.

10.13.2.4 isize

```
integer prg_graph_mod::subgraph_t::isize [private]
```

Size of full subgraph (l x l)

Definition at line 40 of file prg_graph_mod.F90.

10.13.2.5 nodeinpart

```
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 part

```
integer prg_graph_mod::subgraph_t::part [private]
```

Partition number.

Definition at line 34 of file prg_graph_mod.F90.

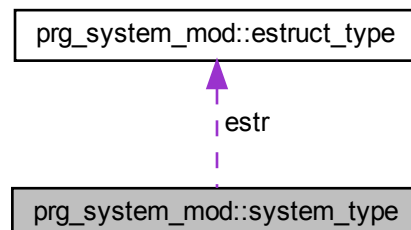
The documentation for this type was generated from the following file:

- [/tmp/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.
- character(3), dimension(:), allocatable **resname**
Residue name.
- character(3), dimension(:), allocatable **atomname**
Atom name (to distinguish atoms with same symbol)
- type(**estruct_type**) **estr**
Electronic structure.

10.14.1 Detailed Description

System type.

The molecular system type.

Definition at line 73 of file prg_system_mod.F90.

10.14.2 Member Data Documentation

10.14.2.1 atomic_number

```
integer, dimension(:), allocatable prg_system_mod::system_type::atomic_number
```

Atomic number for every atom in the system.

Definition at line 87 of file prg_system_mod.F90.

10.14.2.2 atomname

```
character(3), dimension(:), allocatable prg_system_mod::system_type::atomname
```

Atom name (to distinguish atoms with same symbol)

Definition at line 188 of file prg_system_mod.F90.

10.14.2.3 coordinate

```
real(dp), dimension(:, :), allocatable prg_system_mod::system_type::coordinate
```

Coordinates of every atom in the system. Allocation:

```
coordinate(3,nats)
```

Definition at line 92 of file prg_system_mod.F90.

10.14.2.4 estr

```
type(estruct_type) prg_system_mod::system_type::estr
```

Electronic structure.

Definition at line 191 of file prg_system_mod.F90.

10.14.2.5 force

```
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 102 of file prg_system_mod.F90.

10.14.2.6 lattice_vector

```
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 124 of file prg_system_mod.F90.

10.14.2.7 mass

```
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 114 of file prg_system_mod.F90.

10.14.2.8 nats

```
integer prg_system_mod::system_type::nats
```

Number of atoms of the system.

Definition at line 76 of file prg_system_mod.F90.

10.14.2.9 net_charge

```
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 107 of file prg_system_mod.F90.

10.14.2.10 nsp

```
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 147 of file prg_system_mod.F90.

10.14.2.11 recip_vector

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 132 of file prg_system_mod.F90.

10.14.2.12 resindex

integer, dimension(:), allocatable prg_system_mod::system_type::resindex

Residue index.

Definition at line 182 of file prg_system_mod.F90.

10.14.2.13 resname

character(3), dimension(:), allocatable prg_system_mod::system_type::resname

Residue name.

Definition at line 185 of file prg_system_mod.F90.

10.14.2.14 spatnum

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 170 of file prg_system_mod.F90.

10.14.2.15 spindex

```
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 155 of file prg_system_mod.F90.

10.14.2.16 splist

```
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 163 of file prg_system_mod.F90.

10.14.2.17 spmass

```
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 176 of file prg_system_mod.F90.

10.14.2.18 symbol

```
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 84 of file prg_system_mod.F90.

10.14.2.19 userdef

```
real(dp), dimension(:), allocatable prg_system_mod::system_type::userdef
```

User define field.

Definition at line 179 of file prg_system_mod.F90.

10.14.2.20 velocity

```
real(dp), dimension(:, :), allocatable prg_system_mod::system_type::velocity
```

Velocities for every atom in the system. Allocation:

```
velocity(3,nats)
```

Definition at line 97 of file prg_system_mod.F90.

10.14.2.21 volk

```
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 140 of file prg_system_mod.F90.

10.14.2.22 volr

```
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 136 of file `prg_system_mod.F90`.

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

- `/tmp/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 `total`
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 maxrank

```
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 maxvalue

```
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 minrank

```
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 minvalue

```
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 tavg

```
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 tcount

```
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 tname

```
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 tpercent

```
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 tstart

```
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 tstdev

```
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 tsum

```
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 ttotal

```
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:

- /tmp/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 to_string_double()**

```
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 81 of file prg_extras_mod.F90.

10.16.2.2 to_string_integer()

```
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 47 of file prg_extras_mod.F90.

10.16.2.3 to_string_long_long()

```
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 63 of file prg_extras_mod.F90.

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

- [/tmp/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 cc

```
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 jobname

```
character(20) prg_xlbo_mod::xlbo_type::jobname
```

Definition at line 35 of file prg_xlbo_mod.F90.

10.17.2.3 maxscfinititer

```
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 maxscfiter

```
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 minit

```
integer prg_xlbo_mod::xlbo_type::minit
```

Use SCF the first M_prg_init MD steps.

Definition at line 48 of file prg_xlbo_mod.F90.

10.17.2.6 threshold

```
real(dp) prg_xlbo_mod::xlbo_type::threshold
```

Definition at line 45 of file prg_xlbo_mod.F90.

10.17.2.7 verbose

```
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:

- [/tmp/qmd-progress/src/prg_xlbo_mod.F90](#)

10.18 prg_xlkernel_mod::xlk_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 18 of file prg_xlkernel_mod.F90.

10.18.2 Member Data Documentation

10.18.2.1 kerneltype

```
character(20) prg_xlkernel_mod::xlk_type::kerneltype
```

Kernel type.

Definition at line 21 of file prg_xlkernel_mod.F90.

10.18.2.2 nrank

```
integer prg_xlkernel_mod::xlk_type::nrank
```

Definition at line 24 of file prg_xlkernel_mod.F90.

10.18.2.3 scalecoeff

```
real(dp) prg_xlkernel_mod::xlk_type::scalecoeff
```

Coefficient for mixing.

Definition at line 27 of file prg_xlkernel_mod.F90.

10.18.2.4 verbose

```
integer prg_xlkernel_mod::xlk_type::verbose
```

Verbosity level.

Definition at line 24 of file prg_xlkernel_mod.F90.

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

- [/tmp/qmd-progress/src/prg_xlkernel_mod.F90](#)

Chapter 11

File Documentation

11.1 /tmp/qmd-progress/README.md File Reference

11.2 /tmp/qmd-progress/tests/README.md File Reference

11.3 /tmp/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 /tmp/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 Ef 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 Ef 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 /tmp/qmd-progress/src/prg_densitymatrix_mod.F90 File Reference

Modules

- module [prg_densitymatrix_mod](#)

Module to obtain the density matrix by diagonalizing an orthogonalized Hamiltonian.

Functions/Subroutines

- subroutine, public [prg_densitymatrix_mod::prg_build_density_t0](#) (ham_bml, rho_bml, threshold, bndfil, eigenvalues_out)
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 ϵ 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, eigenvalues_out)
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 ϵ is the matrix eigenvalue. f is the Fermi function.
- subroutine, public [prg_densitymatrix_mod::prg_build_density_t_fulldata](#) (ham_bml, rho_bml, threshold, bndfil, kbt, ef, eigenvalues_out, evecs_bml, fvals)
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 ϵ 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 ϵ 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_flevel_nt](#) (eigenvalues, kbt, bndfil, tol, ef, verbose)
Routine to compute the Fermi level given a set of eigenvalues and a temperature. It applies the Newton-Raphson 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 /tmp/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 /tmp/qmd-progress/src/prg_doxy_mod.F90 File Reference

11.8 /tmp/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 $||X^tSX - I||$.
- subroutine, public `prg_extras_mod::prg_get_mem` (procname, tag)
Get proc memory.
- subroutine `prg_extras_mod::prg_twonorm` (a, nn, norm2)
Gets the norm2 of a square matrix.
- real(dp) function, public `prg_extras_mod::prg_norm2` (a)
Gets the norm2 of a vector.

Variables

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

11.9 /tmp/qmd-progress/src/prg_genz_mod.F90 File Reference

Data Types

- type `prg_genz_mod::genzspinp`
Input for the genz driver. This type controls all the variables that are needed by genz.

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, public `prg_genz_mod::prg_init_zspmat` (igenz, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, norb, bml_type, bml_element_type)
Initiates the matrices for the XI integration of Z .
- subroutine, public `prg_genz_mod::prg_buildzdiag` (smat_bml, zmat_bml, threshold, mdimin, bml_type, 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.
- 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)
Initial estimation of Z .
- subroutine, public `prg_genz_mod::prg_genz_sp_initial_zmat` (smat_bml, zmat_bml, norb, mdim, bml_type, f, threshold)
Initial estimation of Z .
- 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)
Inverse factorization using Niklasson's algorithm.
- subroutine, public `prg_genz_mod::prg_genz_sp_ref` (smat_bml, zmat_bml, nref, norb, bml_type, threshold)
Iterative refinement.

Variables

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

11.10 /tmp/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_equalgrouppartition](#) (gp, hindex, ngroup, nodesPerPart, nnodes)
Create equal group graph partitions, based on number of atoms/groups.
- subroutine, public [prg_graph_mod::prg_filepartition](#) (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 /tmp/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 /tmp/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 /tmp/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, p_bml, nsteps, k, nocc, mu, beta, method, osteps, occErrLimit, threshold, tol)
Recursive Implicit Fermi Dirac for finite temperature.
- subroutine, public [prg_implicit_fermi_mod::prg_implicit_fermi_zero](#) (h_bml, p_bml, nsteps, mu, method, threshold, tol)
Recursive Implicit Fermi Dirac for zero temperature.
- subroutine, public [prg_implicit_fermi_mod::prg_implicit_fermi_response](#) (H0_bml, H1_bml, H2_bml, H3_bml, P0_bml, P1_bml, P2_bml, P3_bml, nsteps, mu0, mu, beta, nocc, occ_tol, lin_tol, order, threshold)
Calculate density matrix response to perturbations using Implicit Fermi Dirac.
- subroutine, public [prg_implicit_fermi_mod::prg_finite_diff](#) (H0_bml, H_list, mu0, mu_list, beta, order, lambda, h, threshold)
Calculate density matrix response from perturbations in the Hamiltonian.
- subroutine [prg_implicit_fermi_mod::prg_setup_linsys](#) (p_bml, A_bml, b_bml, p2_bml, y_bml, aux_bml, aux1_bml, k, threshold)
Set up linear system for Implicit Fermi Dirac.
- subroutine [prg_implicit_fermi_mod::prg_newtonschulz](#) (a_bml, ai_bml, r_bml, tmp_bml, tol, threshold)
Find the inverse of the matrix A with Newton-Schulz iteration.
- subroutine [prg_implicit_fermi_mod::prg_pcg](#) (A_bml, p_bml, p2_bml, d_bml, wtmp_bml, cg_tol, threshold)
Solve the system $AX = B$ with conjugate gradient.
- subroutine [prg_implicit_fermi_mod::prg_conjgrad](#) (A_bml, p_bml, p2_bml, d_bml, w_bml, cg_tol, threshold)
Solve the system $AX = B$ with conjugate gradient.
- subroutine [prg_implicit_fermi_mod::prg_get_density_matrix](#) (ham_bml, p_bml, beta, mu, threshold)
Calculate the density matrix with diagonalization.
- subroutine, public [prg_implicit_fermi_mod::prg_test_density_matrix](#) (ham_bml, p_bml, beta, mu, nocc, osteps, occErrLimit, threshold)
Calculate the density matrix with diagonalization and converge chemical.
- real(dp) function [prg_implicit_fermi_mod::fermi](#) (e, mu, beta)
Gives the Fermi distribution value for energy e.

Variables

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

11.14 /tmp/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 /tmp/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 /tmp/qmd-progress/src/prg_modelham_mod.F90 File Reference

Data Types

- type `prg_modelham_mod::mham_type`
General ModelHam type.

Modules

- module `prg_modelham_mod`
The prg_hamiltonian module.

Functions/Subroutines

- subroutine, public `prg_modelham_mod::prg_parse_mham` (mham, filename)
Model Ham parse.
- subroutine, public `prg_modelham_mod::prg_twolevel_model` (ea, eb, dab, daiaj, dbibj, dec, rcoeff, reshuffle, seed, h_bml, verbose)
Construct a two-level model Hamiltonian.

Variables

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

11.17 /tmp/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` \leftrightarrow `_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` \leftrightarrow `_type`, `verbose`)
This routine performs: $A = Z A_{ortho} Z^\dagger$.

Variables

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

11.18 /tmp/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)

11.19 /tmp/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.

11.20 /tmp/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_rcvparallel](#) (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](#)

11.21 /tmp/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 kernlin_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, CH_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.

11.22 /tmp/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)

11.23 /tmp/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 10⁻²⁷ kg)

- 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, 2.0, 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)

- 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 /)

Covalent radius (in Angstroms)

- 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)

Functions/Subroutines

- subroutine, public [prg_pulaycomponent_mod::prg_pulaycomponent0](#) (rho_bml, ham_bml, pcm_bml, threshold, M, bml_type, verbose)

$$\text{At } T = 0K, P = \rho H \rho.$$
- subroutine, public [prg_pulaycomponent_mod::prg_pulaycomponentt](#) (rho_bml, ham_bml, zmat_bml, pcm_bml, threshold, M, bml_type, verbose)

$$\text{At } T > 0K, P = \rho H S^{-1} + S^{-1} H \rho.$$
- subroutine, public [prg_pulaycomponent_mod::prg_get_pulayforce](#) (nats, zmat_bml, ham_bml, rho_bml, dSx_bml, dSy_bml, dSz_bml, hindex, FPUL, threshold)

$$\text{Pulay Force FPUL from } 2Tr[Z Z' H D \frac{dS}{dR}].$$

Variables

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

11.25 /tmp/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, pulaycoef, 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)

11.26 /tmp/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: $\rho_{kick} = \exp\left(-\frac{i}{\hbar}\hat{V}\hat{\rho}\hat{S}\right)\exp\left(\frac{i}{\hbar}\hat{V}\hat{S}^{-1}\right)$ 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: $\rho_{kick} = \exp\left(-\frac{i}{\hbar}\hat{V}\hat{\rho}\hat{S}\right)\exp\left(\frac{i}{\hbar}\hat{V}\hat{S}^{-1}\right)$ 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_exci)

Produce an excitation in the initially calculated density matrix to.

Variables

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

11.27 /tmp/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 λ .
- 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 λ .
- 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 λ .
- 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 α belong to atom i .

Variables

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

11.28 /tmp/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)

11.29 /tmp/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 version of the SP2 method.

- subroutine, public [prg_sp2_mod::prg_sp2_basic_tcore](#) (h_bml, rho_bml, rho_full_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemt看, verbose)
- 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)
- integer, parameter [prg_sp2_mod::dp1](#) = kind(1.0)

11.30 /tmp/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)

11.31 /tmp/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)

11.32 /tmp/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)

11.33 /tmp/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, extin)
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, public `prg_system_mod::prg_parameters_to_vectors` (abc_angles, lattice_vector)
Transforms the lattice parameters into lattice vectors.
- subroutine, public `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_cleanuprepeatedatoms](#) (nats, coords, symbols, verbose)

Cleanup repeated atoms we might have in the system.

 - 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 subroutine 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 anymre since the bml_get_adj routine is sorting the values.

Variables

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

11.34 /tmp/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](#)

11.35 /tmp/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

11.36 /tmp/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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