progress

0.0.1

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Contents

Chapter 1

README

A library for quantum chemistry solvers.

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

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

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Build Dependencies

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

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

Build and Install Instructions

How to build

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

How to install

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

To specify the Intel Fortran compiler:

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

To build with the gfortran compiler and OpenMP:

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

To build with OpenMP, MPI and testing enabled:

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

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

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

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

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

Citing

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

Chapter 2

Testing the Progress library

Testing program for the progress library

To run the tests:

Go into the build folder and type:

```
make test
```

To run the tests in verbose mode:

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

To run a single test:

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

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

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

- density : Tests the diagonalization routine to build the density.
- sp2_short : Tests the first version of sp2
- sp2_alg1 : Algorithm 1 for sp2
- sp2_alg2 : Algorithm 2 for sp2
- sp2_alg2_ellpack : Algorithm 2 for sp2 with ellpack
- sp2_alg1_seq : See sp2_mod.F90 source file
- sp2_alg2_seq : See sp2_mod.F90 source file
- deorthogonalize_dense: See nonortho.F90 source file
- orthogonalize_dense: See nonortho.F90 source file
- buildzdiag: See genz_mod.F90 source file

To add a test:

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

Chapter 3

Todo List

Module prg_dos_mod

Add LDOS.

Subprogram prg_pulaycomponent_mod::prg_pulaycomponent0 (rho_bml, ham_bml, pcm_bml, threshold, M, bml_type, verbose)

M and bml_type will have to be removed from the input parameter.

Subprogram prg_pulaycomponent_mod::prg_pulaycomponentt (rho_bml, ham_bml, zmat_bml, pcm_bml, threshold, M, bml_type, verbose)

M and bml_type will have to be removed from the input parameter.

Module prg_pulaymixer_mod

add the density matrix mixer.

Module prg_response_mod

Add the response scf

Change name response_SP2 to dm_prt_response

Change name response_rs to rs_prt_response

Subprogram prg_response_mod::prg_pert_from_file (prt_bml, norb)

Add read perturbation from file

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

Integrate this loop in the loop for building the splist.

Chapter 4

Module Index

4.1 Modules

Here is a list of all modules:

Chapter 5

Modules Index

5.1 Modules List

Here is a list of all modules with brief descriptions:

Chapter 6

Data Type Index

6.1 Data Types List

Here are the data types with brief descriptions:

Chapter 7

File Index

7.1 File List

Here is a list of all files with brief descriptions:

Chapter 8

Module Documentation

8.1 (LATTE related routines)

8.2 (PROGRESS related routines)

Modules

- module prg_charges_mod

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

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

  Module to obtain the density matrix by diagonalizing an prg_orthogonalized Hamiltonian.
- module prg_extras_mod

  Extra routines:
- module prg_genz_mod

  To produce a matrix Z which is needed to orthogonalize H.
- module prg_graph_mod

  The graph module.
- module prg_graphsp2parser_mod

  Graph partitioning SP2 parser.
- module prg_homolumo_mod

  The homolumo module.
- module prg_initmatrices_mod

  Initialization module.
- module prg_kernelparser_mod

  Some general parsing functions.
- module prg_nonortho_mod

  Module to prg_orthogonalize and prg_deorthogonalize any operator.
- module prg_openfiles_mod

  Module to handle input output files for the PROGRESS lib.
- module prg_parallel_mod

  The parallel module.
- module prg_progress_mod

  The progress module.
- module prg_ptable_mod

  Periodic table of elements.
- module prg_pulaycomponent_mod

  Produces a matrix to get the Pulay Component of the forces.
- module prg_pulaymixer_mod

  Pulay mixer mode.
- module prg_quantumdynamics_mod

  A module to add in common quantum dynamical operations.
- module prg_response_mod

  Module to compute the density matrix response and related quantities.
- module prg_sp2_fermi_mod

  The SP2 Fermi module.
- module prg_sp2_mod

  The SP2 module.
- module prg_sp2parser_mod

  SP2 parser.
- module prg_syrotation_mod

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

- module prg_system_mod

  A module to read and handle chemical systems.
- module prg_timer_mod

  The timer module.
- module prg_xlbo_mod

  A module to perform XLBO integration.
- module prg_xlkernel_mod

  Add name.

8.2.1 Detailed Description

8.3 (EXTERNAL related routines)

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

Chapter 9

Module Documentation

9.1 prg_charges_mod Module Reference

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

Functions/Subroutines

- subroutine, public prg_get_charges (rho_bml, over_bml, hindex, charges, numel, spindex, mdimin, threshold)

  Constructs the charges from the density matrix.
- subroutine, public prg_get_hscf (ham0_bml, over_bml, ham_bml, spindex, hindex, hubbardu, charges, coulomb_pot_r, coulomb_pot_k, mdimin, threshold)

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

Variables

- integer, parameter dp = kind(1.0d0)

9.1.1 Detailed Description

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

This module contains routines that compute properties related to charges.

9.1.2 Function/Subroutine Documentation

9.1.2.1 subroutine, public prg_charges_mod::prg_get_charges (type(bml_matrix_t), intent(inout) *rho_bml,* type(bml_matrix_t), intent(inout) *over_bml,* integer, dimension(:,:), intent(in) *hindex,* real(dp), dimension(:), intent(inout), allocatable *charges,* real(dp), dimension(:), intent(in) *numel,* integer, dimension(:), intent(in) *spindex,* integer, intent(in) *mdimin,* real(dp), intent(in) *threshold*)

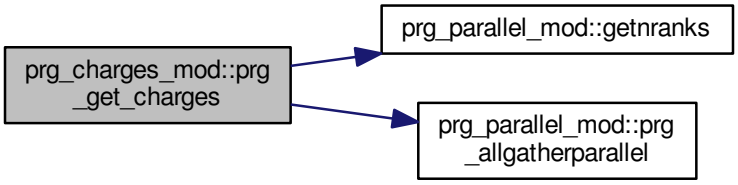
Constructs the charges from the density matrix.

Parameters

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

Definition at line 31 of file prg_charges_mod.F90.

Here is the call graph for this function:



9.1.2.2 subroutine, public prg_charges_mod::prg_get_hscf (type(bml_matrix_t), intent(in) *ham0_bml,* type(bml_matrix_t), intent(in) *over_bml,* type(bml_matrix_t), intent(inout) *ham_bml,* integer, dimension(:), intent(in) *spindex,* integer, dimension(:,:), intent(in) *hindex,* real(**dp**), dimension(:), intent(in) *hubbardu,* real(**dp**), dimension(:), intent(in) *charges,* real(**dp**), dimension(:), intent(in) *coulomb_pot_r,* real(**dp**), dimension(:), intent(in) *coulomb_pot_k,* integer, intent(in) *mdimin,* real(**dp**), intent(in) *threshold*)

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

Parameters

ham_bml	Hamiltonian in bml format.
over_bml	Overlap in bml format.
hindex	Start and end index for every atom in the system.
hubbardu	Hubbard parameter for every atom.
charges	Charges for every atom.
coulomb_pot_r	Coulombic potential (r contribution)
coulomb_pot_k	Coulombic potential (k contribution)
mdim	Maximum nonzeroes elements per row for every row.
threshold	Threshold value for matrix elements.

Definition at line 101 of file prg_charges_mod.F90.

9.1.3 Variable Documentation

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

Definition at line 17 of file prg_charges_mod.F90.

9.2 prg_chebyshev_mod Module Reference

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

Data Types

- type chebdata_type

  General Cheb solver type.

Functions/Subroutines

- subroutine, public prg_parse_cheb (chebdata, filename)

  Chebyshev parser. This module is used to parse all the input variables for the cheb electronic structure solver. Adding a new input keyword to the parser:
- subroutine, public prg_build_density_cheb (ham_bml, rho_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, jon, verbose)

  Builds the density matrix from H_0 for a Fermi function approximated with a Chebyshev polynomial expansion.
- subroutine, public prg_build_density_cheb_fermi (ham_bml, rho_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, getef, fermitol, jon, npts, trkfunc, verbose)

  Builds the density matrix from H_0 for a Fermi function approximated with a Chebyshev polynomial expansion. In this case the self-consistent recursion is applied to converge to the correct number of electrons and obtain the Fermi level.
- real(dp) function jackson (ncoeffs, i, jon)

  Evaluates the Jackson Kernel Coefficients.
- subroutine prg_get_chebcoeffs (npts, kbt, ef, ncoeffs, coeffs, emin, emax)

  Gets the coefficients of the Chebyshev expansion.
- subroutine prg_get_chebcoeffs_fermi_bs (npts, kbt, ef, tracesT, ncoeffs, coeffs, emin, emax, bndfil, norb, tol, jon, verbose)

  Gets the coefficients of the Chebyshev expansion with Ef computation.
- subroutine prg_get_chebcoeffs_fermi_nt (npts, kbt, ef, tracesT, ncoeffs, coeffs, emin, emax, bndfil, norb, tol, jon, verbose)

  Gets the coefficients of the Chebyshev expansion with Ef computation.
- real(dp) function tr (r, x)

  Chebyshev polynomial obtained by recursion.
- real(dp) function fermi (e, ef, kbt)

  Gives the Fermi distribution value for energy e.
- real(dp) function absmaxderivative (func, de)

  Gets the absolute maximum of the derivative of a function.

Variables

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

9.2.1 Detailed Description

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

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

9.2.2 Function/Subroutine Documentation

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

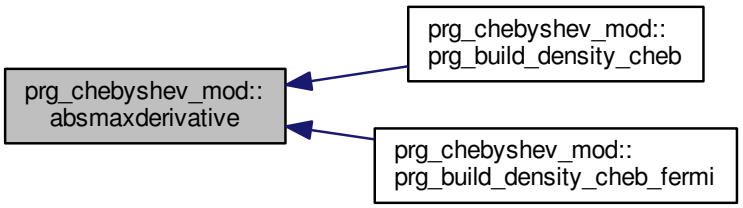
Gets the absolute maximum of the derivative of a function.

Parameters

func.	
de	Energy step.

Definition at line 802 of file prg_chebyshev_mod.F90.

Here is the caller graph for this function:



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

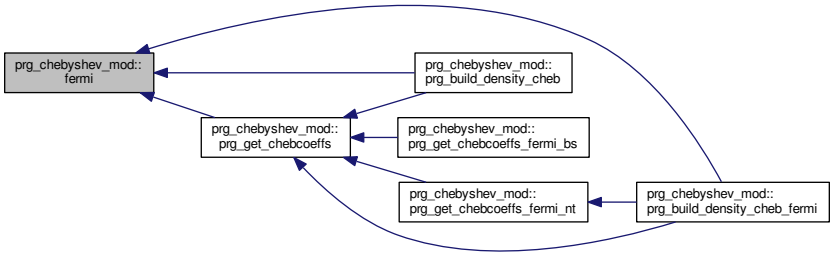
Gives the Fermi distribution value for energy e.

Parameters

e	Energy.
ef	Fermi energy.

Definition at line 790 of file prg_chebyshev_mod.F90.

Here is the caller graph for this function:



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

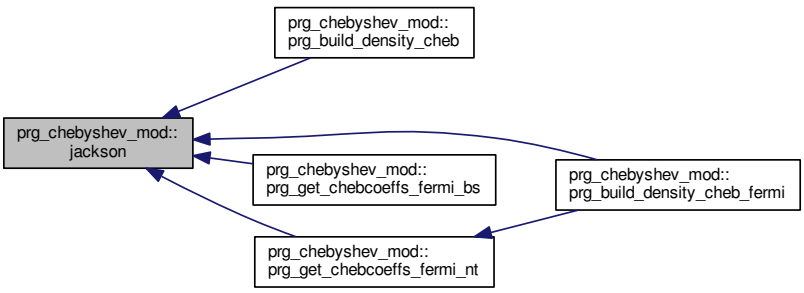
Evaluates the Jackson Kernel Coefficients.

Parameters

ncoeffs	Number of Chebyshev polynomial.
i	Coefficient number i.

Definition at line 532 of file prg_chebyshev_mod.F90.

Here is the caller graph for this function:



9.2.2.4 subroutine, public prg_chebyshev_mod::prg_build_density_cheb (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(inout) *rho_bml,* real(dp), intent(in) *athr,* real(dp), intent(in) *threshold,* integer, intent(in) *ncoeffs,* real(dp), intent(in) *kbt,* real(dp), intent(in) *ef,* real(dp), intent(in) *bndfil,* logical, intent(in) *jon,* integer, intent(in) *verbose*)

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

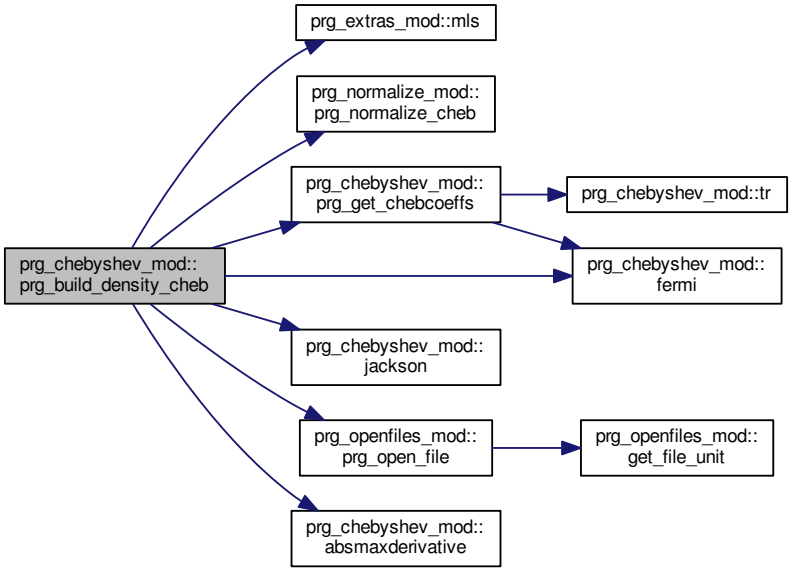
$\rho_{n+1} = b_{n+1}T_{n+1} + \rho_n$ Where, T_n is the nth Chebyshev polynomial and b_n is the nth coefficient of the expansion for the Fermi function. In the sparse version (when ellpack is used) the threshold can be varied linearly with the polynomial degree. The function is the following: $Thresh(n)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

Parameters

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

Definition at line 143 of file prg_chebyshev_mod.F90.

Here is the call graph for this function:



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

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

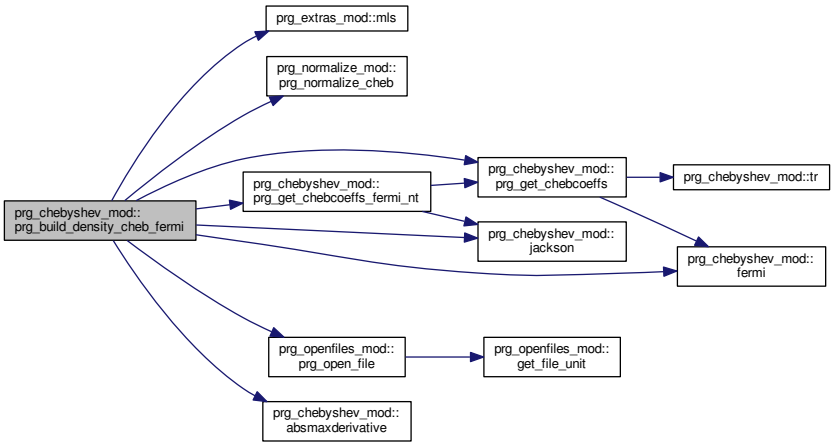
$\rho_{n+1} = b_{n+1}T_{n+1} + \rho_n$ Where, T_n is the nth Chebyshev polynomial and b_n is the nth coefficient of the expansion for the Fermi function. In the sparse version (when ellpack is used) the threshold can be varied linearly with the polynomial degree. The function is the following: $Thresh(n)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

Parameters

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

Definition at line 310 of file prg_chebyshev_mod.F90.

Here is the call graph for this function:



9.2.2.6 subroutine prg_chebyshev_mod::prg_get_chebcoeffs (integer, intent(in) *npts,* real(dp), intent(in) *kbt,* real(dp), intent(in) *ef,* integer, intent(in) *ncoeffs,* real(dp), dimension(:), intent(inout) *coeffs,* real(dp), intent(in) *emin,* real(dp), intent(in) *emax*) [private]

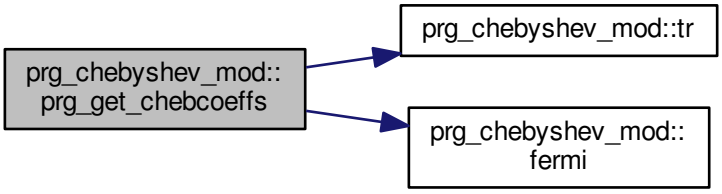
Gets the coefficients of the Chebyshev expansion.

Parameters

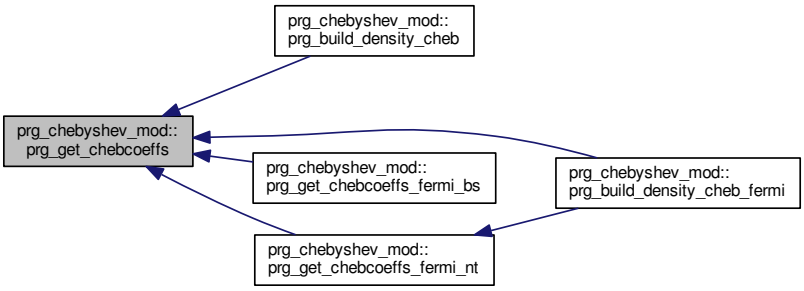
npts	Number of points for discretization.
kbt	Electronic temperature.
ef	Fermi level.
ncoeffs	Number of Chebyshev coefficients.
coeffs	Output vector for the Chebyshev coefficients.
emin	lowest boundary for the eigenvalues of H.
emax	highest boundary for the eigenvalues of H.

Definition at line 568 of file prg_chebyshev_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



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

Gets the coefficients of the Chebyshev expansion with Ef computation.

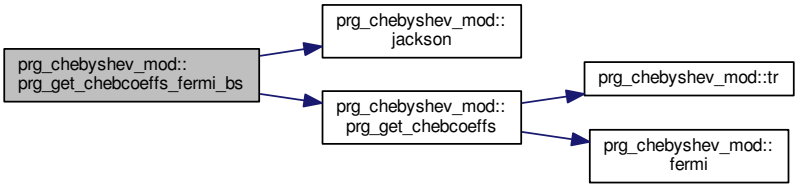
In this case we are applying the bisection method to find the root.

Parameters

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

Definition at line 620 of file prg_chebyshev_mod.F90.

Here is the call graph for this function:



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

Gets the coefficients of the Chebyshev expansion with Ef computation.

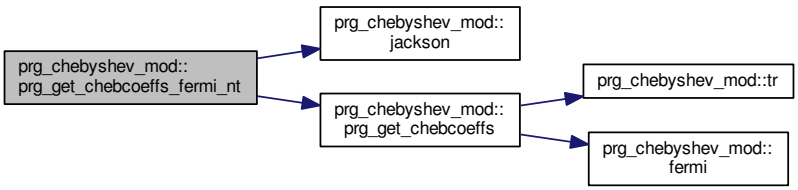
In this case the Newton-Raphson method is applied to find the root.

Parameters

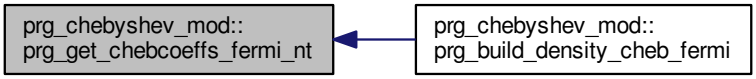
npst	Number of points for the discretization.
kbt	Electronic temperature.
ef	Fermi level.
tracesT	Input traces for matrix polynomials.
ncoeffs	Number of Chebyshev coefficients.
coeffs	Output vector for the Chebyshev coefficients.
emin	lowest boundary for the eigenvalues of H.
emax	highest boundary for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

Definition at line 697 of file prg_chebyshev_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



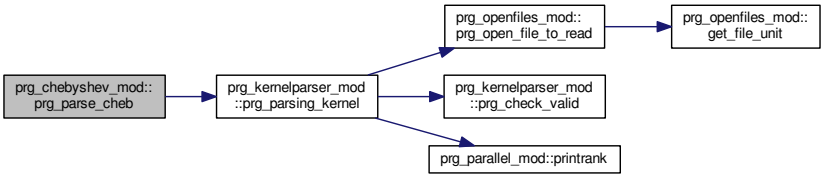
9.2.2.9 subroutine, public prg_chebyshev_mod::prg_parse_cheb (type(chebdata_type), intent(inout) *chebdata,* character(len=∗) *filename*)

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

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

Definition at line 54 of file prg_chebyshev_mod.F90.

Here is the call graph for this function:



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

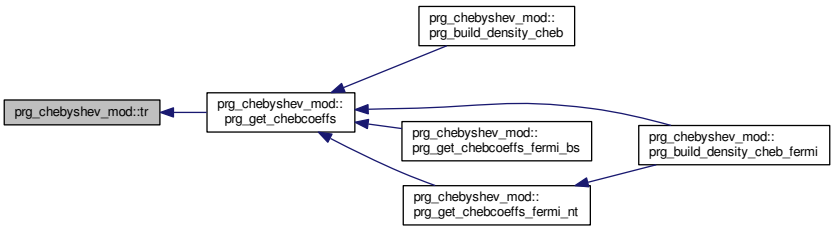
Chebyshev polynomial obtained by recursion.

Parameters

r	rth polynomial.
x	argument the evaluate the polynomial.

Definition at line 777 of file prg_chebyshev_mod.F90.

Here is the caller graph for this function:



9.2.3 Variable Documentation

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

Definition at line 23 of file prg_chebyshev_mod.F90.

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

Definition at line 24 of file prg_chebyshev_mod.F90.

9.3 prg_densitymatrix_mod Module Reference

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

Functions/Subroutines

- subroutine, public prg_build_density_t0 (ham_bml, rho_bml, threshold, bndfil)

  Builds the density matrix from H_0 for zero electronic temperature. $\rho = C\Theta(\mu I - \epsilon)C^\dagger$ Where, C is the matrix eigenvector and ϵ is the matrix eigenvalue. $\Theta()$ is the Heaviside function.
- subroutine, public prg_build_density_t (ham_bml, rho_bml, threshold, bndfil, kbt, ef)

  Builds the density matrix from H_0 for electronic temperature T. $\rho = Cf(\mu I - \epsilon)C^\dagger$ Where, C is the matrix eigenvector and 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. $\rho_{ii} = mathcalZ_{ii}$ Where, $mathcalZ_{ii}$ is the number of electrons for orbital i.
- subroutine, public prg_get_flevel (eigenvalues, kbt, bndfil, tol, Ef)

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

  Gets the eigenvalues of the Orthogonalized Hamiltonian.
- subroutine, public prg_check_idempotency (mat_bml, threshold, idempotency)

  To check the idempotency error of a matrix. This is calculated as the Frobenius norm of $(A - A^2)$.
- real(dp) function fermi (e, ef, kbt)

  Gives the Fermi distribution value for energy e.

Variables

- integer, parameter dp = kind(1.0d0)

9.3.1 Detailed Description

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

9.3.2 Function/Subroutine Documentation

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

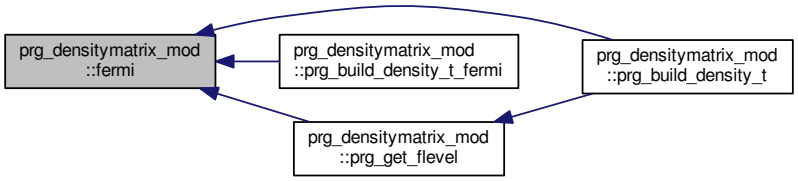
Gives the Fermi distribution value for energy e.

Parameters

e	Energy.
ef	Fermi energy.

Definition at line 413 of file prg_densitymatrix_mod.F90.

Here is the caller graph for this function:



9.3.2.2 subroutine, public prg_densitymatrix_mod::prg_build_atomic_density (type(bml_matrix_t), intent(inout) *rhoat_bml,* real(dp), dimension(:), intent(in) *numel,* integer, dimension(:,:), intent(in) *hindex,* integer, dimension(:), intent(in) *spindex,* integer, intent(in) *norb,* character(len=∗), intent(in) *bml_type*)

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

Parameters

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

Definition at line 215 of file prg_densitymatrix_mod.F90.

9.3.2.3 subroutine, public prg_densitymatrix_mod::prg_build_density_t (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(inout) *rho_bml,* real(8), intent(in) *threshold,* real(8), intent(in) *bndfil,* real(8), intent(in) *kbt,* real(8), intent(inout) *ef*)

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

Parameters

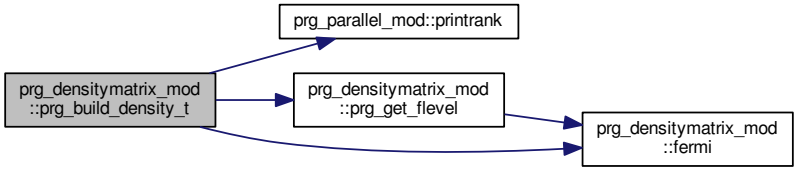
ham_bml	Input Orthogonalized Hamiltonian matrix.
rho_bml	Output density matrix,
threshold	Threshold for sparse matrix algebra.
bndfil	Filing factor.

Warning

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

Definition at line 94 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:



9.3.2.4 subroutine, public prg_densitymatrix_mod::prg_build_density_t0 (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(inout) *rho_bml,* real(8), intent(in) *threshold,* real(8), intent(in) *bndfil*)

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

Parameters

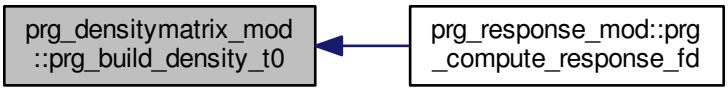
ham_bml	Input Orthogonalized Hamiltonian matrix.
rho_bml	Output density matrix,
threshold	Threshold for sparse matrix algebra.
bndfil	Filing factor.

Warning

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

Definition at line 33 of file prg_densitymatrix_mod.F90.

Here is the caller graph for this function:



9.3.2.5 subroutine, public prg_densitymatrix_mod::prg_build_density_t_fermi (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(inout) *rho_bml,* real(8), intent(in) *threshold,* real(8), intent(in) *kbt,* real(8), intent(in) *ef,* integer, intent(in), optional *verbose*)

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

Parameters

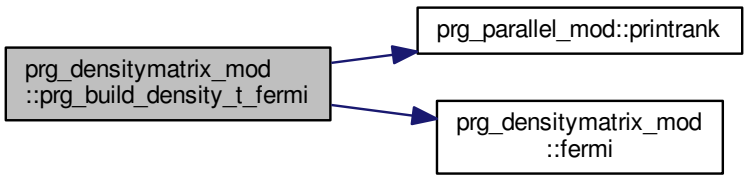
ham_bml	Input Orthogonalized Hamiltonian matrix.
rho_bml	Output density matrix,
threshold	Threshold for sparse matrix algebra.

Warning

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

Definition at line 156 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:



9.3.2.6 subroutine, public prg_densitymatrix_mod::prg_check_idempotency (type(bml_matrix_t), intent(in) *mat_bml,* real(**dp**), intent(in) *threshold,* real(**dp**), intent(out) *idempotency*)

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

Parameters

mat_bml	Some bml matrix
idempotency	(Output value of the idempotency error)

Definition at line 389 of file prg_densitymatrix_mod.F90.

9.3.2.7 subroutine, public prg_densitymatrix_mod::prg_get_eigenvalues (type(bml_matrix_t), intent(in) *ham_bml,* real(**dp**), dimension(:), intent(inout), allocatable *eigenvalues,* integer, intent(in) *verbose*)

Gets the eigenvalues of the Orthogonalized Hamiltonian.

Parameters

ham_bml	Input Orthogonalized Hamiltonian matrix.
eigenvalues	Output eigenvalues of the system.
verbose	Verbosity level.

Definition at line 344 of file prg_densitymatrix_mod.F90.

9.3.2.8 subroutine, public prg_densitymatrix_mod::prg_get_flevel (real(dp), dimension(:), intent(in) *eigenvalues,* real(dp), intent(in) *kbt,* real(dp), intent(in) *bndfil,* real(dp) *tol,* real(dp), intent(inout) *Ef*)

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

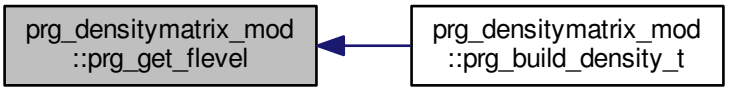
Parameters

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

Definition at line 280 of file prg_densitymatrix_mod.F90.

Here is the call graph for this function:

Here is the caller graph for this function:



9.3.3 Variable Documentation

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

Definition at line 14 of file prg_densitymatrix_mod.F90.

9.4 prg_dos_mod Module Reference

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

Functions/Subroutines

- subroutine, public prg_write_tdos (eigenvals, gamma, npts, emin, emax, filename)

  Writes the total DOS into a file. $DOS(\epsilon) = \sum_k L(\epsilon - \epsilon_k)$ *Where* $\int_{-\infty}^{\infty} DOS(\epsilon) = Nstates.$
- real(dp) function lorentz (energy, eigenvals, loads, Gamma)

  Lorentzian Function.

Variables

- integer, parameter dp = kind(1.0d0)

9.4.1 Detailed Description

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

This module will be used to compute DOS and IDOS.

Todo Add LDOS.

9.4.2 Function/Subroutine Documentation

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

Lorentzian Function.

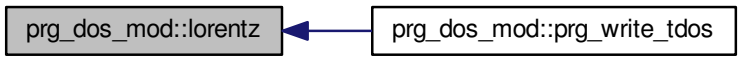
Computes: $L(\epsilon) = \sum_k \frac{\omega(k)\Gamma}{2\pi} \frac{1}{(\epsilon-\epsilon_k)^2+(\Gamma/2)^2}$

Parameters

energy	Energy point.
eigenvals	Eigenvalues of the system.
Gamma	Lorentz function broadening.

Definition at line 78 of file prg_dos_mod.F90.

Here is the caller graph for this function:



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

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

Note

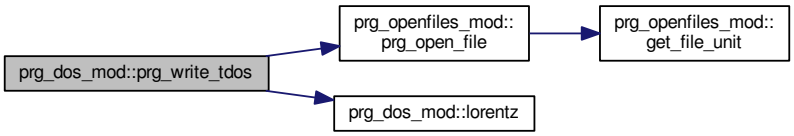
DOS is NOT shifted respect to Ef.

Parameters

eigenvals	Eigenvalues of the system. gamma Lorentzian width.
npts	Number of energy points.
emin	Minimum energy value.
emax	Maximum energy value.
filename	Filename to write the DOS.

Definition at line 36 of file prg_dos_mod.F90.

Here is the call graph for this function:



9.4.3 Variable Documentation

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

Definition at line 17 of file prg_dos_mod.F90.

9.5 prg_extras_mod Module Reference

Extra routines:

Data Types

- interface prg_memory_consumption
- interface to_string

Functions/Subroutines

- character(len=:) function, allocatable to_string_integer (i)

  Convert integer to string.
- character(len=:) function, allocatable to_string_long_long (i)

  Convert integer to string.
- character(len=:) function, allocatable to_string_double (x)

  Convert double to string.
- subroutine, public prg_print_matrix (matname, amat, i1, i2, j1, j2)

  To write a dense matrix to screen.
- real(dp) function, public mls ()

  To get the actual time in milliseconds.
- subroutine, public prg_delta (x, s, nn, dta)

  Delta function ||X^tSX - I||. CFAN, March 2015.
- subroutine, public prg_get_mem (procname, tag)

  Get proc memory.
- subroutine prg_twonorm (a, nn, norm2)

Variables

- integer, parameter dp = kind(1.0d0)

9.5.1 Detailed Description

Extra routines:

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

9.5.2 Function/Subroutine Documentation

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

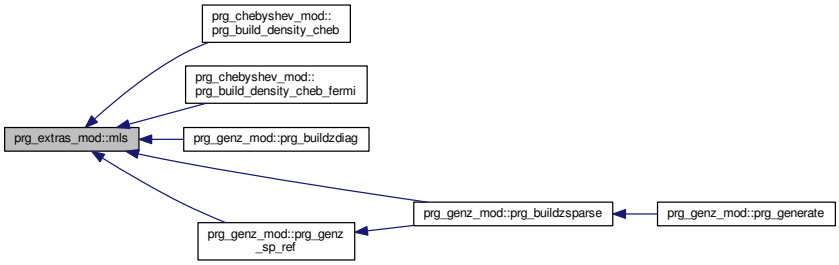
To get the actual time in milliseconds.

Parameters

mls	Output value with the machine time in milliseconds.

Definition at line 139 of file prg_extras_mod.F90.

Here is the caller graph for this function:



9.5.2.2 subroutine, public prg_extras_mod::prg_delta (real(dp), dimension(nn,nn) *x,* real(dp), dimension(nn,nn) *s,* integer *nn,* real(dp) *dta*)

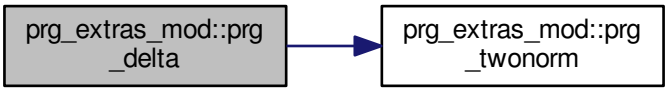
Delta function ||X^tSX - I||. CFAN, March 2015.

Parameters

x	input matrix.
s	overlap matrix.
dta	Delta output value.

Definition at line 155 of file prg_extras_mod.F90.

Here is the call graph for this function:



9.5.2.3 subroutine, public prg_extras_mod::prg_get_mem (character(∗), intent(in) *procname,* character(∗), intent(in) *tag*)

Get proc memory.

Parameters

procname	Process name to get the mem usage.
tag	Tag to pprint the processor mem usage.

Definition at line 191 of file prg_extras_mod.F90.

9.5.2.4 subroutine, public prg_extras_mod::prg_print_matrix (character(len=∗) *matname,* real(dp), dimension(:,:), intent(in) *amat,* integer, intent(in) *i1,* integer, intent(in) *i2,* integer, intent(in) *j1,* integer, intent(in) *j2*)

To write a dense matrix to screen.

Parameters

matname	Matrix name.
amat	Matrix to be printed.
i1	Print from row i1.
i2	Print up to from row i2.
j1	Print from column j1.
j2	Print up to column j2.

Definition at line 100 of file prg_extras_mod.F90.

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

Definition at line 211 of file prg_extras_mod.F90.

Here is the caller graph for this function:

9.5.2.6 character(len=:) function, allocatable prg_extras_mod::to_string_double (double precision, intent(in) *x*) [private]

Convert double to string.

Parameters

x	The double

Returns

The string

Definition at line 80 of file prg_extras_mod.F90.

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

Convert integer to string.

Parameters

i	The integer

Returns

The string

Definition at line 46 of file prg_extras_mod.F90.

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

Convert integer to string.

Parameters

i	The integer

Returns

The string

Definition at line 62 of file prg_extras_mod.F90.

9.5.3 Variable Documentation

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

Definition at line 31 of file prg_extras_mod.F90.

9.6 prg_genz_mod Module Reference

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

Data Types

- type genzspdata

  contains the data for the genZ driver.
- type genzspinp

  Input for the genz driver.

Functions/Subroutines

- subroutine, public prg_parse_zsp (input, filename)

  The parser for genz solver.
- subroutine prg_init (self, input)

  Initializes the genz input variables.
- subroutine prg_allocatezspmat (self, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, norb, bml_↩ type)

  Allocates the matrices for the XI integration of Z.
- subroutine, public prg_init_zspmat (igenz, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, norb, bml_type)

  Initiates the matrices for the XI integration of Z.
- subroutine prg_generate (self, over_bml, zmat_bml, igenz, mdim, bml_type, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml)

  Generates the Z matrix.
- subroutine, public prg_buildzdiag (smat_bml, zmat_bml, threshold, mdimin, bml_type, verbose)

  Usual subroutine involving diagonalization.
- subroutine, public prg_buildzsparse (smat_bml, zmat_bml, igenz, mdim, bml_type, zk1_bml, zk2_bml, zk3↩ _bml, zk4_bml, zk5_bml, zk6_bml, nfirst, nrefi, nreff, thresholdi, thresholdf, integration, verbose)

  Inverse factorization using niklasson's algorithm.
- subroutine, public prg_genz_sp_initialz0 (smat_bml, zmat_bml, norb, mdim, bml_type_f, threshold)
- subroutine, public prg_genz_sp_initial_zmat (smat_bml, zmat_bml, norb, mdim, bml_type_f, threshold)

  Estimate Z matrix.
- subroutine prg_genz_sp_int (zmat_bml, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, igenz, norb, bml_type, threshold)
- subroutine, public prg_genz_sp_ref (smat_bml, zmat_bml, nref, norb, bml_type, threshold)

Variables

- integer, parameter dp = kind(1.0d0)

9.6.1 Detailed Description

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

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

9.6.2 Function/Subroutine Documentation

9.6.2.1 subroutine prg_genz_mod::prg_allocatezspmat (class(genzspdata), intent(in) *self,* type(bml_matrix_t) *zk1_bml,* type(bml_matrix_t) *zk2_bml,* type(bml_matrix_t) *zk3_bml,* type(bml_matrix_t) *zk4_bml,* type(bml_matrix_t) *zk5_bml,* type(bml_matrix_t) *zk6_bml,* integer *norb,* character(20) *bml_type*) [private]

Allocates the matrices for the XI integration of Z.

Parameters

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

Definition at line 174 of file prg_genz_mod.F90.

9.6.2.2 subroutine, public prg_genz_mod::prg_buildzdiag (type(bml_matrix_t), intent(inout) *smat_bml,* type(bml_matrix_t) *zmat_bml,* real(dp) *threshold,* integer, intent(in) *mdimin,* character(len=*) *bml_type,* integer, intent(in), optional *verbose*)

Usual subroutine involving diagonalization.

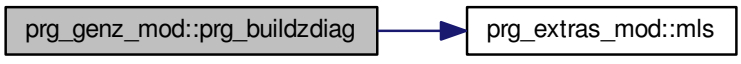
$Z = U\sqrt{s}U^{\dagger}$, where U = eigenvectors and s = eigenvalues. The purpose of this subroutine is to have an exact way of computing z for comparing with the sparse approach.

Parameters

smat_bml	Overlap matrix in bml format.
zmat_bml	Congruence transform in bml format.
threshold	Threshold value to use, in this case, only in the backtranformation to ellpack format.
mdim	Maximun nonzero to use, in this case, only in the backtranformation to ellpack format.
bml_type	the bml type we are passing.

Definition at line 281 of file prg_genz_mod.F90.

Here is the call graph for this function:



9.6.2.3 subroutine, public prg_genz_mod::prg_buildzsparse (type(bml_matrix_t) *smat_bml,* type(bml_matrix_t) *zmat_bml,* integer *igenz,* integer *mdim,* character(20) *bml_type,* type(bml_matrix_t) *zk1_bml,* type(bml_matrix_t) *zk2_bml,* type(bml_matrix_t) *zk3_bml,* type(bml_matrix_t) *zk4_bml,* type(bml_matrix_t) *zk5_bml,* type(bml_matrix_t) *zk6_bml,* integer *nfirst,* integer *nrefi,* integer *nreff,* real(dp) *thresholdi,* real(dp) *thresholdf,* logical *integration,* integer *verbose*)

Inverse factorization using niklasson's algorithm.

Parameters

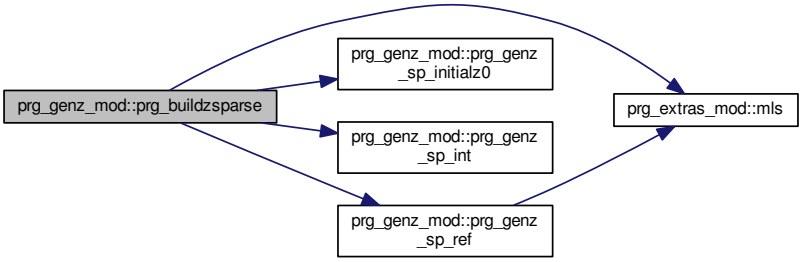
smat_bml	overlap matrix

Parameters

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

Definition at line 421 of file prg_genz_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:

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

Generates the Z matrix.

Parameters

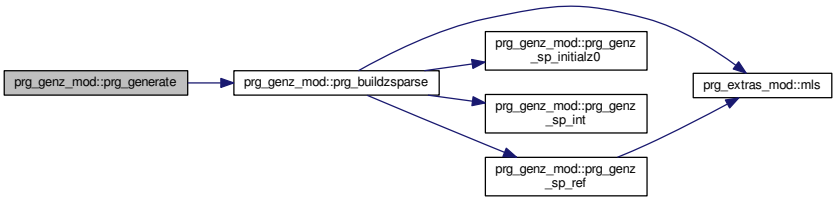
over_bml	Overlap matrix.

Parameters

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

Definition at line 242 of file prg_genz_mod.F90.

Here is the call graph for this function:



9.6.2.5 subroutine, public prg_genz_mod::prg_genz_sp_initial_zmat (type(bml_matrix_t), intent(in) *smat_bml,* type(bml_matrix_t) *zmat_bml,* integer *norb,* integer *mdim,* character(20) *bml_type_f,* real(dp), intent(in) *threshold*)

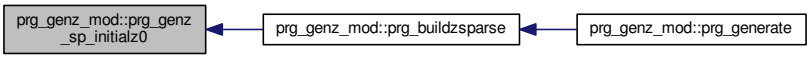
Estimate Z matrix.

Definition at line 600 of file prg_genz_mod.F90.

9.6.2.6 subroutine, public prg_genz_mod::prg_genz_sp_initialz0 (type(bml_matrix_t), intent(in) *smat_bml,* type(bml_matrix_t) *zmat_bml,* integer *norb,* integer *mdim,* character(20) *bml_type_f,* real(dp) *threshold*)

Definition at line 476 of file prg_genz_mod.F90.

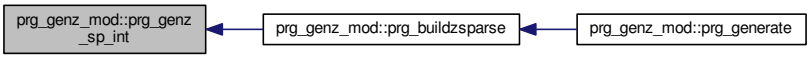
Here is the caller graph for this function:



9.6.2.7 subroutine prg_genz_mod::prg_genz_sp_int (type(bml_matrix_t) *zmat_bml,* type(bml_matrix_t) *zk1_bml,* type(bml_matrix_t) *zk2_bml,* type(bml_matrix_t) *zk3_bml,* type(bml_matrix_t) *zk4_bml,* type(bml_matrix_t) *zk5_bml,* type(bml_matrix_t) *zk6_bml,* integer *igenz,* integer *norb,* character(20) *bml_type,* real(dp) *threshold*) [private]

Definition at line 739 of file prg_genz_mod.F90.

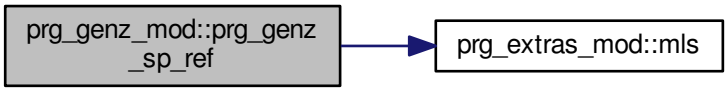
Here is the caller graph for this function:



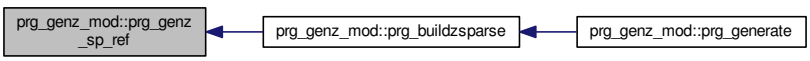
9.6.2.8 subroutine, public prg_genz_mod::prg_genz_sp_ref (type(bml_matrix_t), intent(in) *smat_bml,* type(bml_matrix_t), intent(inout) *zmat_bml,* integer, intent(in) *nref,* integer, intent(inout) *norb,* character(20), intent(in) *bml_type,* real(dp), intent(in) *threshold*)

Definition at line 806 of file prg_genz_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.6.2.9 subroutine prg_genz_mod::prg_init (class(genzspdata), intent(out) *self,* type(genzspinp), intent(in) *input*) [private]

Initializes the genz input variables.

Parameters

self	basic input parameters.
input	basic input parameters from the parser.

Definition at line 152 of file prg_genz_mod.F90.

9.6.2.10 subroutine, public prg_genz_mod::prg_init_zspmat (integer *igenz,* type(bml_matrix_t) *zk1_bml,* type(bml_matrix_t) *zk2_bml,* type(bml_matrix_t) *zk3_bml,* type(bml_matrix_t) *zk4_bml,* type(bml_matrix_t) *zk5_bml,* type(bml_matrix_t) *zk6_bml,* integer *norb,* character(20) *bml_type*)

Initiates the matrices for the XI integration of Z.

Parameters

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

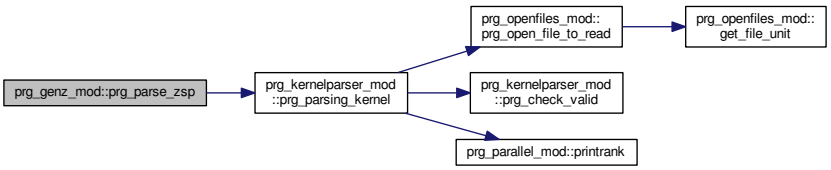
Definition at line 207 of file prg_genz_mod.F90.

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

The parser for genz solver.

Definition at line 88 of file prg_genz_mod.F90.

Here is the call graph for this function:



9.6.3 Variable Documentation

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

Definition at line 20 of file prg_genz_mod.F90.

9.7 prg_graph_mod Module Reference

The graph module.

Data Types

- type graph_partitioning_t
  Trace per iteration.
- type subgraph_t
  Subgraph type.

Functions/Subroutines

- subroutine, public prg_initsubgraph (sg, pnum, hsize)
  Initialize subgraph.
- subroutine, public prg_destroysubgraph (sg)
  Destroy subgraph.
- subroutine, public prg_initgraphpartitioning (gp, pname, np, nnodes, nnodes2)
  Initialize graph partitioning.
- subroutine, public prg_destroygraphpartitioning (gp)
  Destroy graph partitioning.
- subroutine, public prg_printgraphpartitioning (gp)
  Print graph partitioning structure data.
- subroutine, public prg_equalpartition (gp, nodesPerPart, nnodes)
  Create equal graph partitions, based on number of rows/orbitals.
- subroutine, public prg_equalgrouppartition (gp, hindex, ngroup, nodesPerPart, nnodes)
  Create equal group graph partitions, based on number of atoms/groups.
- subroutine, public prg_filepartition (gp, partFile)
  Read graph partitions from a file, based on number of rows/orbitals.
- subroutine prg_readpart (gp, partFile)
  Read parts (core) from part file.
- subroutine, public prg_fnormgraph (gp)
  Accumulate trace norm across all subgraphs.

Variables

- integer, parameter dp = kind(1.0d0)

9.7.1 Detailed Description

The graph module.

9.7.2 Function/Subroutine Documentation

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

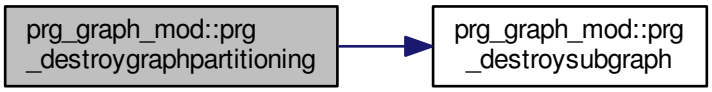
Destroy graph partitioning.

Parameters

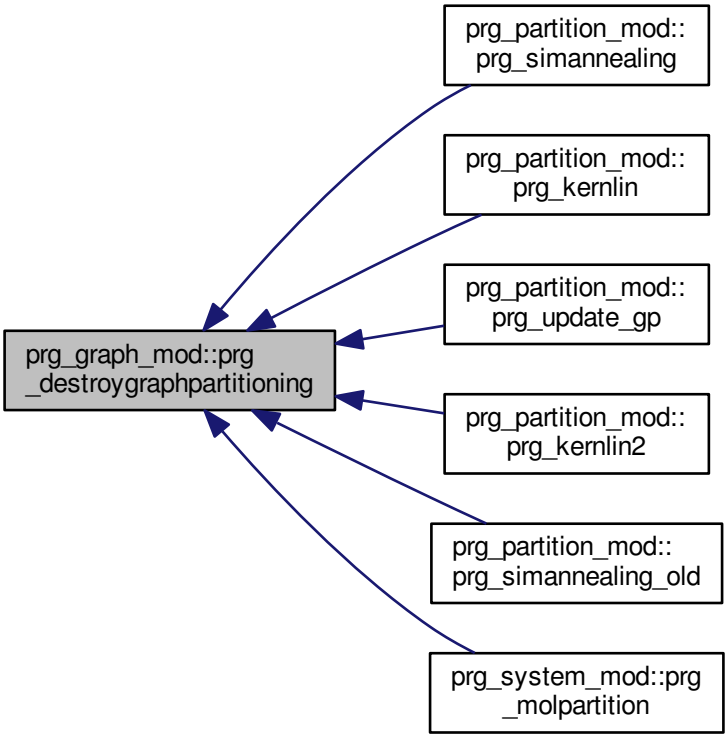
sg	Subgraph

Definition at line 263 of file prg_graph_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



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

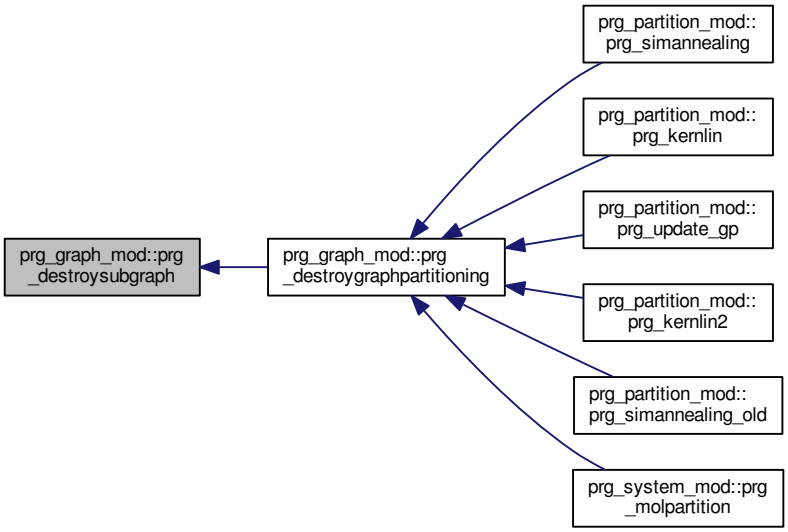
Destroy subgraph.

Parameters

sg	Subgraph

Definition at line 159 of file prg_graph_mod.F90.

Here is the caller graph for this function:



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

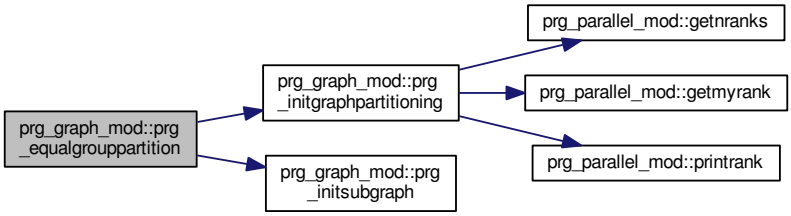
Create equal group graph partitions, based on number of atoms/groups.

Parameters

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

Definition at line 402 of file prg_graph_mod.F90.

Here is the call graph for this function:



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

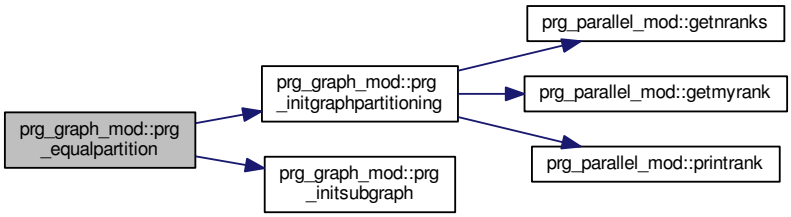
Create equal graph partitions, based on number of rows/orbitals.

Parameters

gp	Graph partitioning‘
nodesPerPart	Number of core nodes per partition
nnodes	Total nodes in Hamiltonian matrix

Definition at line 355 of file prg_graph_mod.F90.

Here is the call graph for this function:



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

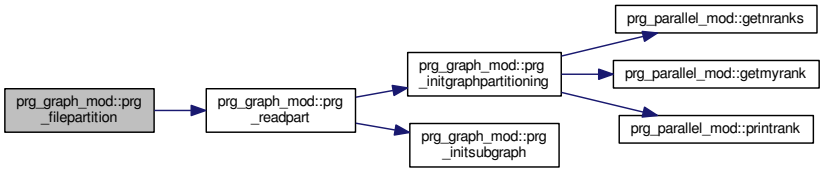
Read graph partitions from a file, based on number of rows/orbitals.

Parameters

partFile	File containing core nodes for each partition
gp	Graph partitioning

Definition at line 463 of file prg_graph_mod.F90.

Here is the call graph for this function:



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

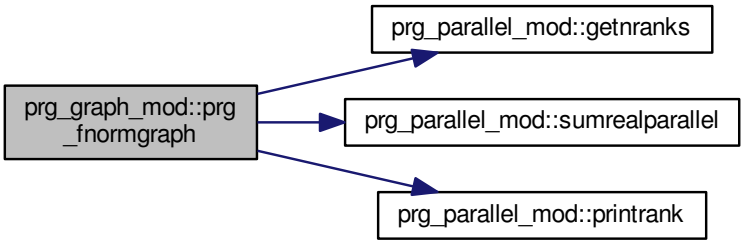
Accumulate trace norm across all subgraphs.

Parameters

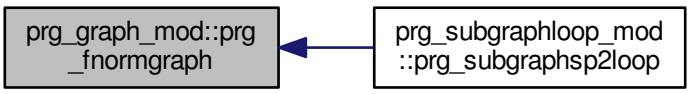
gp	Graph partitioning

Definition at line 516 of file prg_graph_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.7.2.7 subroutine, public prg_graph_mod::prg_initgraphpartitioning (type (graph_partitioning_t), intent(inout) *gp,* character(len=∗), intent(in) *pname,* integer, intent(in) *np,* integer, intent(in) *nnodes,* integer, intent(in) *nnodes2*)

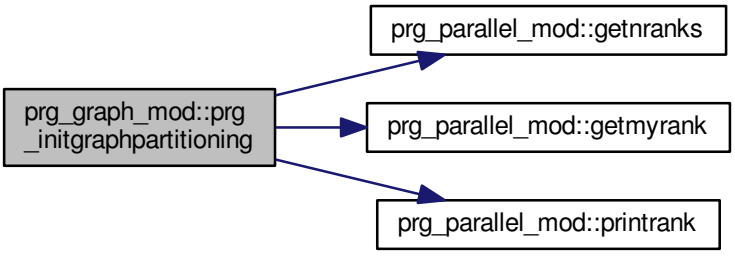
Initialize graph partitioning.

Parameters

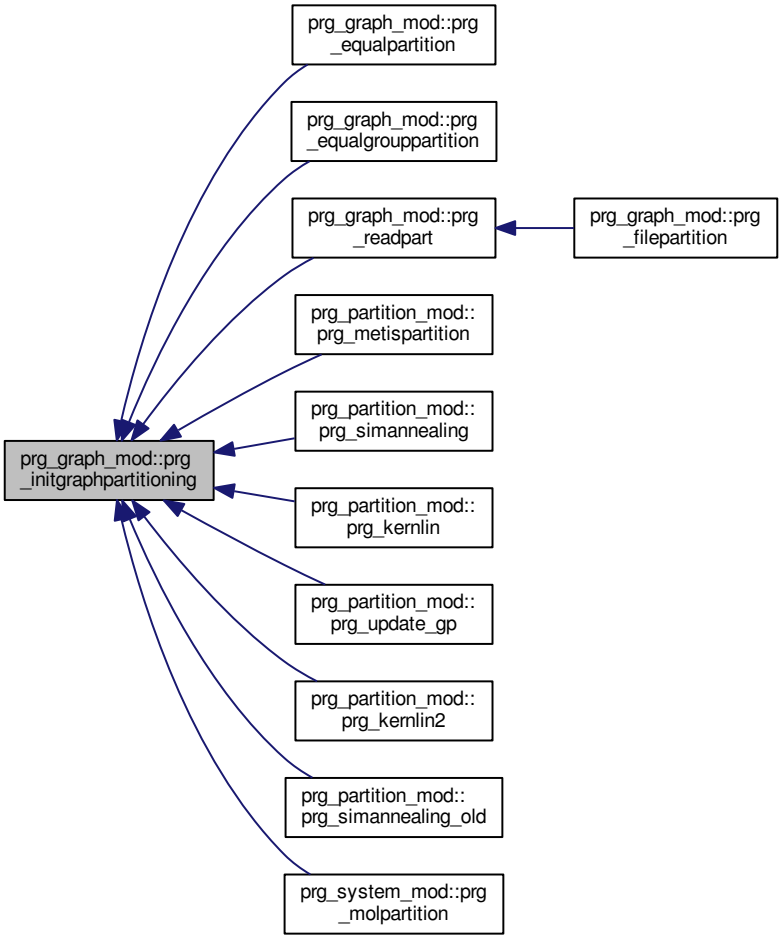
gp	Graph partitioning
pname	Partitioning name
np	Number of partitions
nnodes	Number of groups/nodes
nnodes2	Number of nodes

Definition at line 175 of file prg_graph_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



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

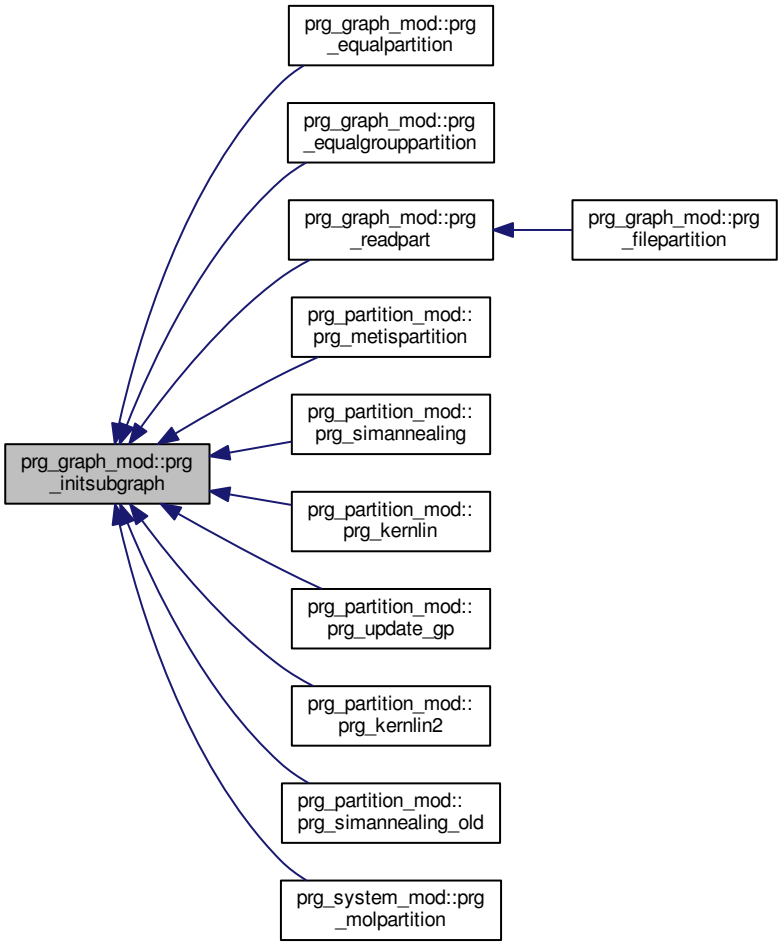
Initialize subgraph.

Parameters

sg	Subgraph
pnum	Part number
hsize	Size of full matrix

Definition at line 143 of file prg_graph_mod.F90.

Here is the caller graph for this function:



9.7.2.9 subroutine, public prg_graph_mod::prg_printgraphpartitioning (type (graph_partitioning_t), intent(in) *gp*)

Print graph partitioning structure data.

Parameters

gp	Graph partitioning

Definition at line 292 of file prg_graph_mod.F90.

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

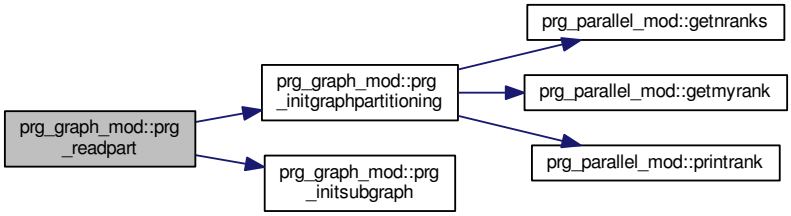
Read parts (core) from part file.

Parameters

gp	Graph partitioning
partFile	Partition file

Definition at line 475 of file prg_graph_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:

9.7.3 Variable Documentation

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

Definition at line 16 of file prg_graph_mod.F90.

9.8 prg_graphsp2parser_mod Module Reference

Graph partitioning SP2 parser.

Data Types

- type gsp2data_type

  General SP2 solver type.

Functions/Subroutines

- subroutine, public prg_parse_gsp2 (gsp2data, filename)

  The parser for SP2 solver.

Variables

- integer, parameter dp = kind(1.0d0)

9.8.1 Detailed Description

Graph partitioning SP2 parser.

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

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

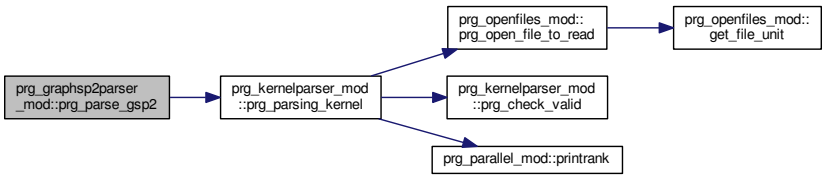
9.8.2 Function/Subroutine Documentation

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

The parser for SP2 solver.

Definition at line 62 of file prg_graphsp2parser_mod.F90.

Here is the call graph for this function:



9.8.3 Variable Documentation

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

Definition at line 22 of file prg_graphsp2parser_mod.F90.

9.9 prg_homolumo_mod Module Reference

The homolumo module.

Functions/Subroutines

- subroutine, public prg_homolumogap (vv, imax, pp, mineval, maxeval, ehomo, elumo, egap, verbose)
- subroutine, public prg_sp2sequence (pp, imax, mineval, maxeval, ehomo, elumo, errlimit, verbose)

Variables

- integer, parameter dp = kind(1.0d0)

9.9.1 Detailed Description

The homolumo module.

9.9.2 Function/Subroutine Documentation

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

Definition at line 24 of file prg_homolumo_mod.F90.

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

Definition at line 94 of file prg_homolumo_mod.F90.

9.9.3 Variable Documentation

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

Definition at line 14 of file prg_homolumo_mod.F90.

9.10 prg_implicit_fermi_mod Module Reference

Functions/Subroutines

- subroutine, public prg_implicit_fermi (h_bml, xi0_bml, p_bml, nsteps, nocc, mu, beta, osteps, occErrLimit, threshold)

  Recursive Implicit Fermi Dirac.

Variables

- integer, parameter dp = kind(1.0d0)

9.10.1 Function/Subroutine Documentation

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

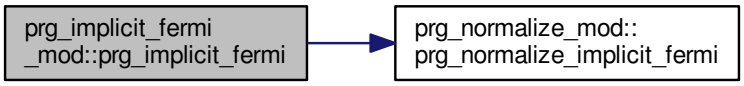
Recursive Implicit Fermi Dirac.

Parameters

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

Definition at line 39 of file prg_implicit_fermi_mod.F90.

Here is the call graph for this function:



9.10.2 Variable Documentation

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

Definition at line 20 of file prg_implicit_fermi_mod.F90.

9.11 prg_initmatrices_mod Module Reference

Initialization module.

Functions/Subroutines

- subroutine, public prg_init_hsmat (ham_bml, over_bml, bml_type, mdim, norb)

  Initialize Hamiltonian and Overlap Matrix.
- subroutine, public prg_init_pzmat (rho_bml, zmat_bml, bml_type, mdim, norb)

  Initialize Density matrix and Inverse square root Overlap.
- subroutine, public prg_init_ortho (orthoh_bml, orthop_bml, bml_type, mdim, norb)

  Initialize The orthogonal versions of Hamiltonian and Density Matrix.

Variables

- integer, parameter dp = kind(1.0d0)

9.11.1 Detailed Description

Initialization module.

Routines in this module are used to prg_initialize several matrices that will be used in the code.

9.11.2 Function/Subroutine Documentation

9.11.2.1 subroutine, public prg_initmatrices_mod::prg_init_hsmat (type(bml_matrix_t), intent(inout) *ham_bml,* type(bml_matrix_t), intent(inout) *over_bml,* character(20) *bml_type,* integer, intent(inout) *mdim,* integer, intent(in) *norb*)

Initialize Hamiltonian and Overlap Matrix.

Allocation of the Hamiltonian and Overlap matrix into bml formats.

Parameters

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

Definition at line 28 of file prg_initmatrices_mod.F90.

9.11.2.2 subroutine, public prg_initmatrices_mod::prg_init_ortho (type(bml_matrix_t), intent(inout) *orthoh_bml,* type(bml_matrix_t), intent(inout) *orthop_bml,* character(20) *bml_type,* integer, intent(inout) *mdim,* integer, intent(in) *norb*)

Initialize The orthogonal versions of Hamiltonian and Density Matrix.

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

Parameters

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

Definition at line 70 of file prg_initmatrices_mod.F90.

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

Initialize Density matrix and Inverse square root Overlap.

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

Parameters

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

Definition at line 49 of file prg_initmatrices_mod.F90.

9.11.3 Variable Documentation

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

Definition at line 14 of file prg_initmatrices_mod.F90.

9.12 prg_kernelparser_mod Module Reference

Some general parsing functions.

Functions/Subroutines

- subroutine, public prg_parsing_kernel (keyvector_char, valvector_char, keyvector_int, valvector_int, keyvector_re, valvector_re, keyvector_log, valvector_log, filename, startstop)

  The general parsing function. It is used to vectorize a set of "keywords" "value" pairs as included in a general input file.
- subroutine prg_check_valid (invalidc)

  Check for valid keywords (checks for an = sign)

Variables

- integer, parameter dp = kind(1.0d0)

9.12.1 Detailed Description

Some general parsing functions.

Author

C. F. A. Negre (cnegre@lanl.gov)

9.12.2 Function/Subroutine Documentation

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

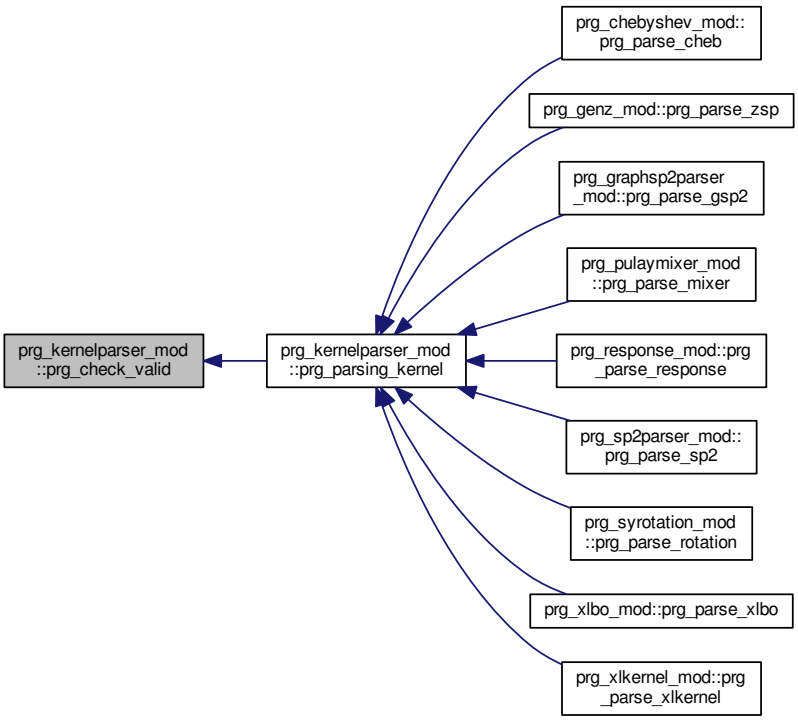
Check for valid keywords (checks for an = sign)

Parameters

invalidc	Keyword to check.

Definition at line 396 of file prg_kernelparser_mod.F90.

Here is the caller graph for this function:



9.12.2.2 subroutine, public prg_kernelparser_mod::prg_parsing_kernel (character(50), dimension(:) *keyvector_char,* character(100), dimension(:) *valvector_char,* character(50), dimension(:) *keyvector_int,* integer, dimension(:) *valvector_int,* character(50), dimension(:) *keyvector_re,* real(dp), dimension(:) *valvector_re,* character(50), dimension(:) *keyvector_log,* logical, dimension(:) *valvector_log,* character(len=*) *filename,* character(len=*), dimension(2), intent(in), optional *startstop*)

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

Note

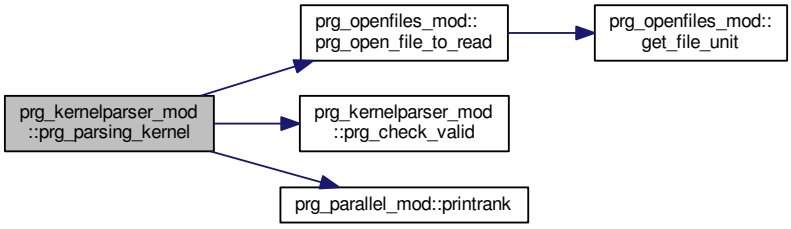
This parsing strategy can only parse a file of 500 lines by 500 words.

Warning

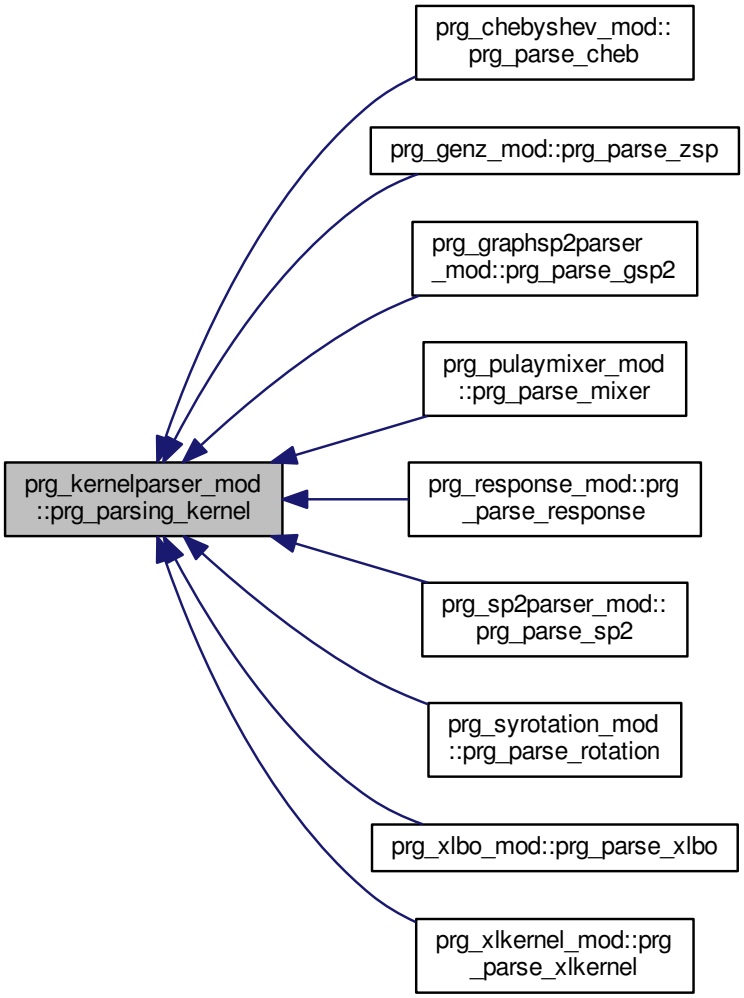
If the length of variable vect is changed, this could produce a segmentation fault.

Definition at line 33 of file prg_kernelparser_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.12.3 Variable Documentation

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

Definition at line 16 of file prg_kernelparser_mod.F90.

9.13 prg_nonortho_mod Module Reference

Module to prg_orthogonalize and prg_deorthogonalize any operator.

Functions/Subroutines

- subroutine, public prg_orthogonalize (A_bml, zmat_bml, orthoA_bml, threshold, bml_type, verbose)

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

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

Variables

- integer, parameter dp = kind(1.0d0)

9.13.1 Detailed Description

Module to prg_orthogonalize and prg_deorthogonalize any operator.

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

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

9.13.2 Function/Subroutine Documentation

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

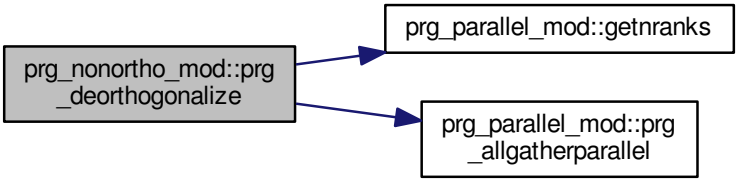
This routine performs: $A = Z A_{ortho} Z^{\dagger}$.

Parameters

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

Definition at line 82 of file prg_nonortho_mod.F90.

Here is the call graph for this function:



9.13.2.2 subroutine, public prg_nonortho_mod::prg_orthogonalize (type(bml_matrix_t), intent(inout) *A_bml,* type(bml_matrix_t), intent(inout) *zmat_bml,* type(bml_matrix_t), intent(inout) *orthoA_bml,* real(dp), intent(in) *threshold,* character(len=∗), intent(in) *bml_type,* integer, intent(in) *verbose*)

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

Parameters

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

Definition at line 36 of file prg_nonortho_mod.F90.

9.13.3 Variable Documentation

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

Definition at line 19 of file prg_nonortho_mod.F90.

9.14 prg_normalize_mod Module Reference

The prg_normalize module.

Functions/Subroutines

- subroutine, public prg_normalize (h_bml)

  Normalize a Hamiltonian matrix prior to running the SP2 algorithm.
- subroutine, public prg_normalize_fermi (h_bml, h1, hN, mu)

  Normalize a Hamiltonian matrix prior to running the truncated SP2 algorithm.
- subroutine, public prg_normalize_implicit_fermi (h_bml, cnst, mu)

  Normalize a Hamiltonian matrix prior to running the implicit fermi dirac algorithm.
- subroutine, public prg_gershgorinreduction (gp)

  Determine gershgorin bounds across all parts, local and distributed.
- subroutine, public prg_normalize_cheb (h_bml, mu, emin, emax, alpha, scaledmu)

  Normalize a Hamiltonian matrix prior to running the Chebyshev algorithm.

Variables

- integer, parameter dp = kind(1.0d0)

9.14.1 Detailed Description

The prg_normalize module.

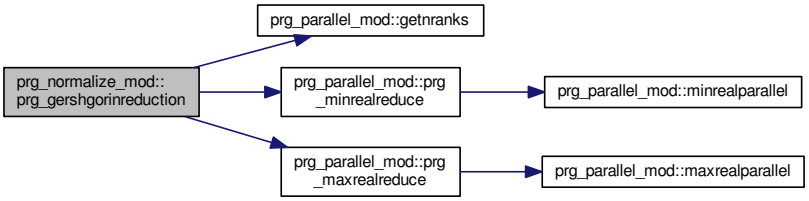
9.14.2 Function/Subroutine Documentation

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

Determine gershgorin bounds across all parts, local and distributed.

Definition at line 101 of file prg_normalize_mod.F90.

Here is the call graph for this function:



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

Normalize a Hamiltonian matrix prior to running the SP2 algorithm.

X0 = (e_max ∗ I - H) / (e_max - e_min)

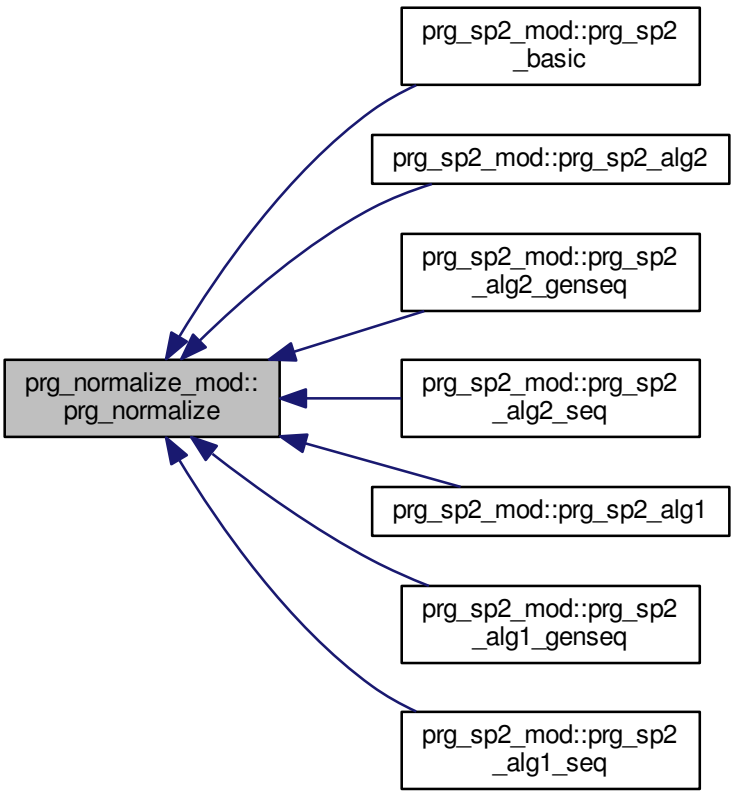
where e_max and e_min are obtained sing the Gershgorin circle theorem.

Parameters

h_bml	Input/Output Hamiltonian matrix

Definition at line 33 of file prg_normalize_mod.F90.

Here is the caller graph for this function:



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

Normalize a Hamiltonian matrix prior to running the Chebyshev algorithm.

X0 = 2∗(H - e_min∗I) / (e_max - e_min) - I

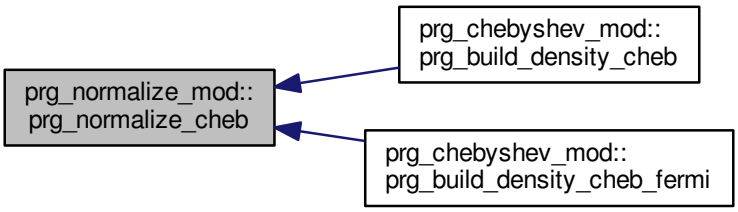
where e_max and e_min are obtained sing the Gershgorin circle theorem.

Parameters

h_bml	Input/Output Hamiltonian matrix

Definition at line 130 of file prg_normalize_mod.F90.

Here is the caller graph for this function:



9.14.2.4 subroutine, public prg_normalize_mod::prg_normalize_fermi (type(bml_matrix_t), intent(inout) *h_bml,* real(dp), intent(in) *h1,* real(dp), intent(in) *hN,* real(dp), intent(in) *mu*)

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

X0 = ((hN-mu) ∗ I - H) / (hN - h1) or X0 = (hN∗I-H0-mu∗I)/(hN-h1)

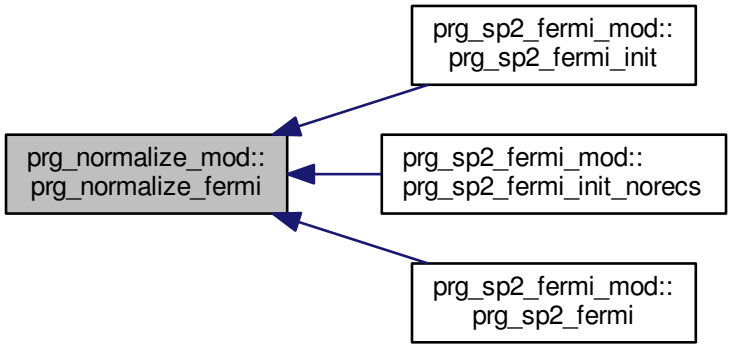
where h1 and hN are scaled Gershgorin bounds.

Parameters

H_bml	Hamiltonian matrix
h1	Scaled minimum Gershgorin bound.
hN	Scaled maximum Gershgorin bound.
mu	Chemical potential

Definition at line 63 of file prg_normalize_mod.F90.

Here is the caller graph for this function:



9.14.2.5 subroutine, public prg_normalize_mod::prg_normalize_implicit_fermi (type(bml_matrix_t), intent(inout) *h_bml,* real(dp), intent(in) *cnst,* real(dp), intent(in) *mu*)

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

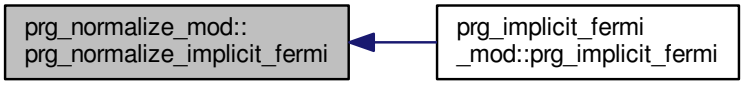
X0 = 0.5∗II - cnst∗(H0-mu0∗II) or X0 = (0.5 + cnst ∗ mu0)∗II -cnst∗ H0

Parameters

H_bml	Hamiltonian matrix
cnst	Constant based on beta and steps
mu	Chemical potential

Definition at line 87 of file prg_normalize_mod.F90.

Here is the caller graph for this function:



9.14.3 Variable Documentation

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

Definition at line 15 of file prg_normalize_mod.F90.

9.15 prg_openfiles_mod Module Reference

Module to handle input output files for the PROGRESS lib.

Functions/Subroutines

- integer function, public get_file_unit (io_max)

  Returns a unit number that is not in use.
- subroutine, public prg_open_file (io, name)

  Opens a file to write.
- subroutine, public prg_open_file_to_read (io, name)

  Opens a file to read.

9.15.1 Detailed Description

Module to handle input output files for the PROGRESS lib.

9.15.2 Function/Subroutine Documentation

9.15.2.1 integer function, public prg_openfiles_mod::get_file_unit (integer *io_max*)

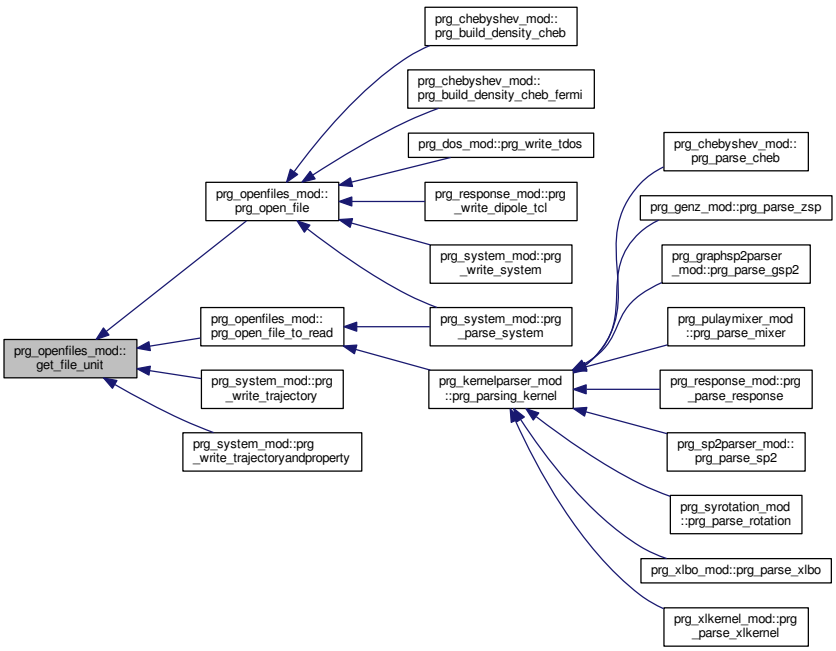
Returns a unit number that is not in use.

Parameters

io_max	Maximum units to search.
get_file_unit	Unit return to use for the file.

Definition at line 19 of file prg_openfiles_mod.F90.

Here is the caller graph for this function:



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

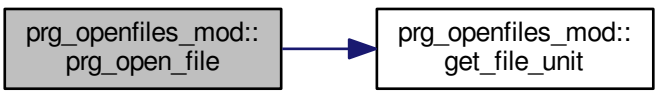
Opens a file to write.

Parameters

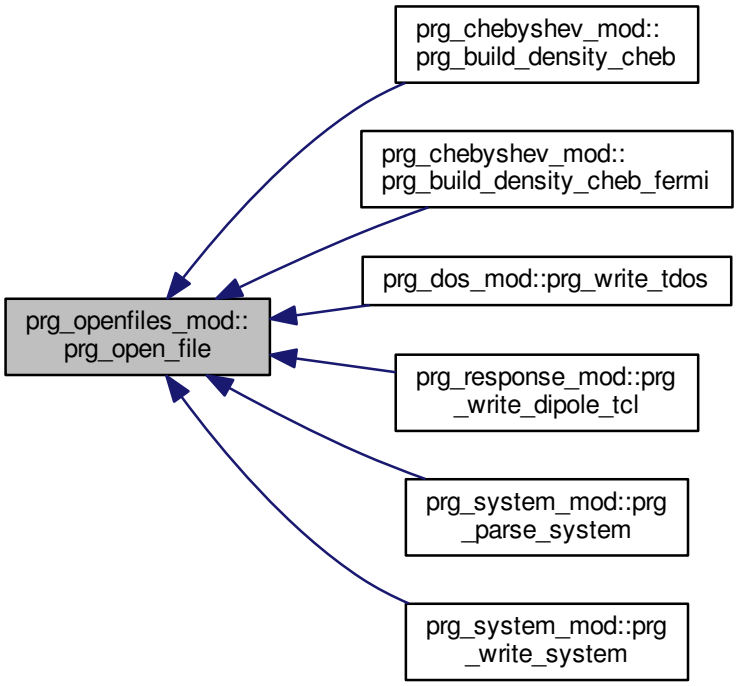
io	Unit for the file.
name	Name of the file.

Definition at line 38 of file prg_openfiles_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



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

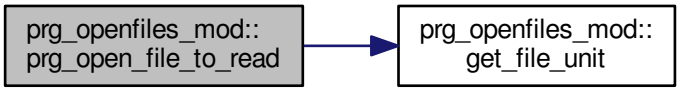
Opens a file to read.

Parameters

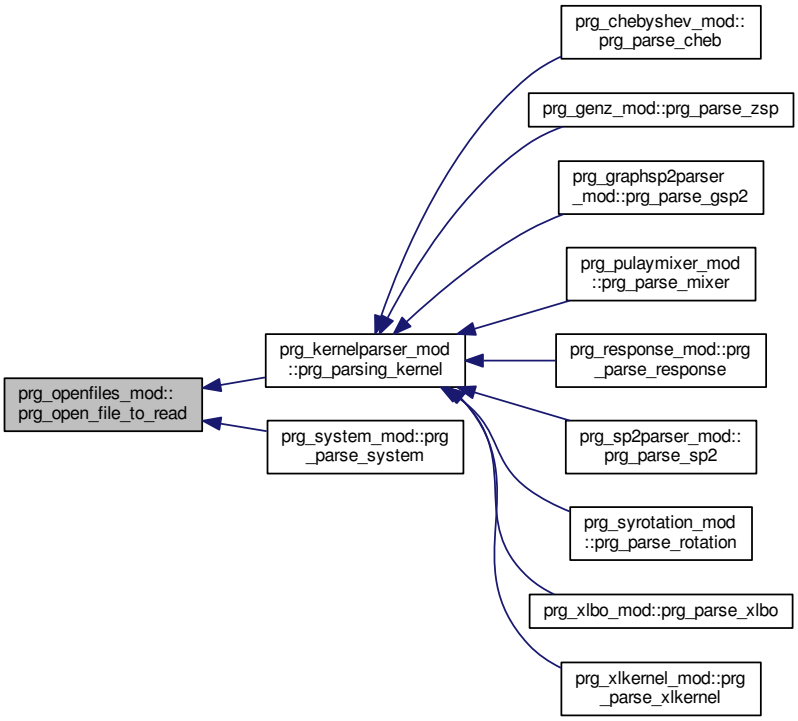
io	Unit for the file.
name	Name of the file.

Definition at line 54 of file prg_openfiles_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.16 prg_parallel_mod Module Reference

The parallel module.

Data Types

- type rankreducedata_t

  Data structure for rection over MPI ranks.

Functions/Subroutines

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

- subroutine, public prg_iprg_recvparallel (recvBuf, recvLen, rind)
- subroutine, public prg_recvparallel (recvBuf, recvLen)
- subroutine, public sumintparallel (sendBuf, recvBuf, icount)
- subroutine, public sumrealparallel (sendBuf, recvBuf, icount)
- subroutine, public maxintparallel (sendBuf, recvBuf, icount)
- subroutine, public maxrealparallel (sendBuf, recvBuf, icount)
- subroutine, public minintparallel (sendBuf, recvBuf, icount)
- subroutine, public minrealparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_minrealreduce (rvalue)
- subroutine, public prg_maxrealreduce (rvalue)
- subroutine, public prg_maxintreduce2 (value1, value2)
- subroutine, public prg_sumintreduce2 (value1, value2)
- subroutine, public prg_sumrealreduce (value1)
- subroutine, public prg_sumrealreduce2 (value1, value2)
- subroutine, public prg_sumrealreduce3 (value1, value2, value3)
- subroutine, public prg_sumrealreducen (valueVec, N)
- subroutine, public prg_sumintreducen (valueVec, N)
- subroutine, public minrankrealparallel (sendBuf, recvBuf, icount)
- subroutine, public maxrankrealparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_bcastparallel (buf, blen, root)
- subroutine, public allgatherrealparallel (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public allgatherintparallel (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public allgathervrealparallel (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public allgathervintparallel (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public prg_allsumrealreduceparallel (buf, buflen)
- subroutine, public prg_allsumintreduceparallel (buf, buflen)
- subroutine, public prg_allgatherparallel (a)
- subroutine, public prg_wait ()

Variables

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

9.16.1 Detailed Description

The parallel module.

9.16.2 Function/Subroutine Documentation

9.16.2.1 subroutine, public prg_parallel_mod::allgatherintparallel (integer, dimension(∗), intent(in) *sendBuf,* integer, intent(in) *sendLen,* integer, dimension(∗), intent(out) *recvBuf,* integer, intent(in) *recvLen*)

Definition at line 660 of file prg_parallel_mod.F90.

9.16.2.2 subroutine, public prg_parallel_mod::allgatherrealparallel (real(dp), dimension(∗), intent(in) *sendBuf,* integer, intent(in) *sendLen,* real(dp), dimension(∗), intent(out) *recvBuf,* integer, intent(in) *recvLen*)

Definition at line 644 of file prg_parallel_mod.F90.

9.16.2.3 subroutine, public prg_parallel_mod::allgathervintparallel (integer, dimension(∗), intent(in) *sendBuf,* integer, intent(in) *sendLen,* integer, dimension(∗), intent(out) *recvBuf,* integer, dimension(∗), intent(in) *recvLen,* integer, dimension(∗), intent(in) *recvDispl*)

Definition at line 696 of file prg_parallel_mod.F90.

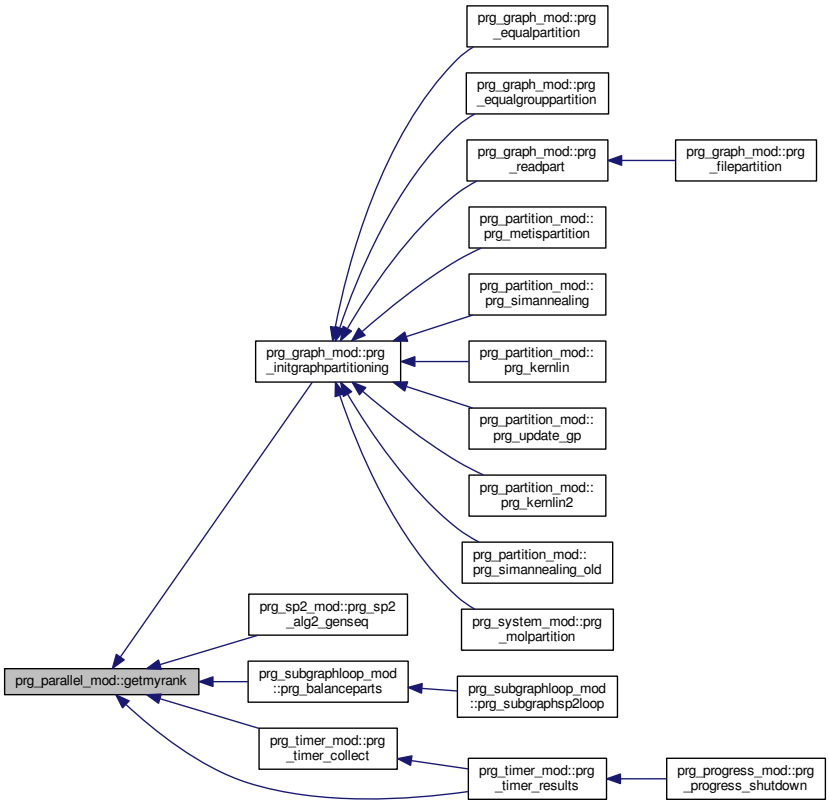
9.16.2.4 subroutine, public prg_parallel_mod::allgathervrealparallel (real(dp), dimension(∗), intent(in) *sendBuf,* integer, intent(in) *sendLen,* real(dp), dimension(∗), intent(out) *recvBuf,* integer, dimension(∗), intent(in) *recvLen,* integer, dimension(∗), intent(in) *recvDispl*)

Definition at line 676 of file prg_parallel_mod.F90.

9.16.2.5 integer function, public prg_parallel_mod::getmyrank ( )

Definition at line 99 of file prg_parallel_mod.F90.

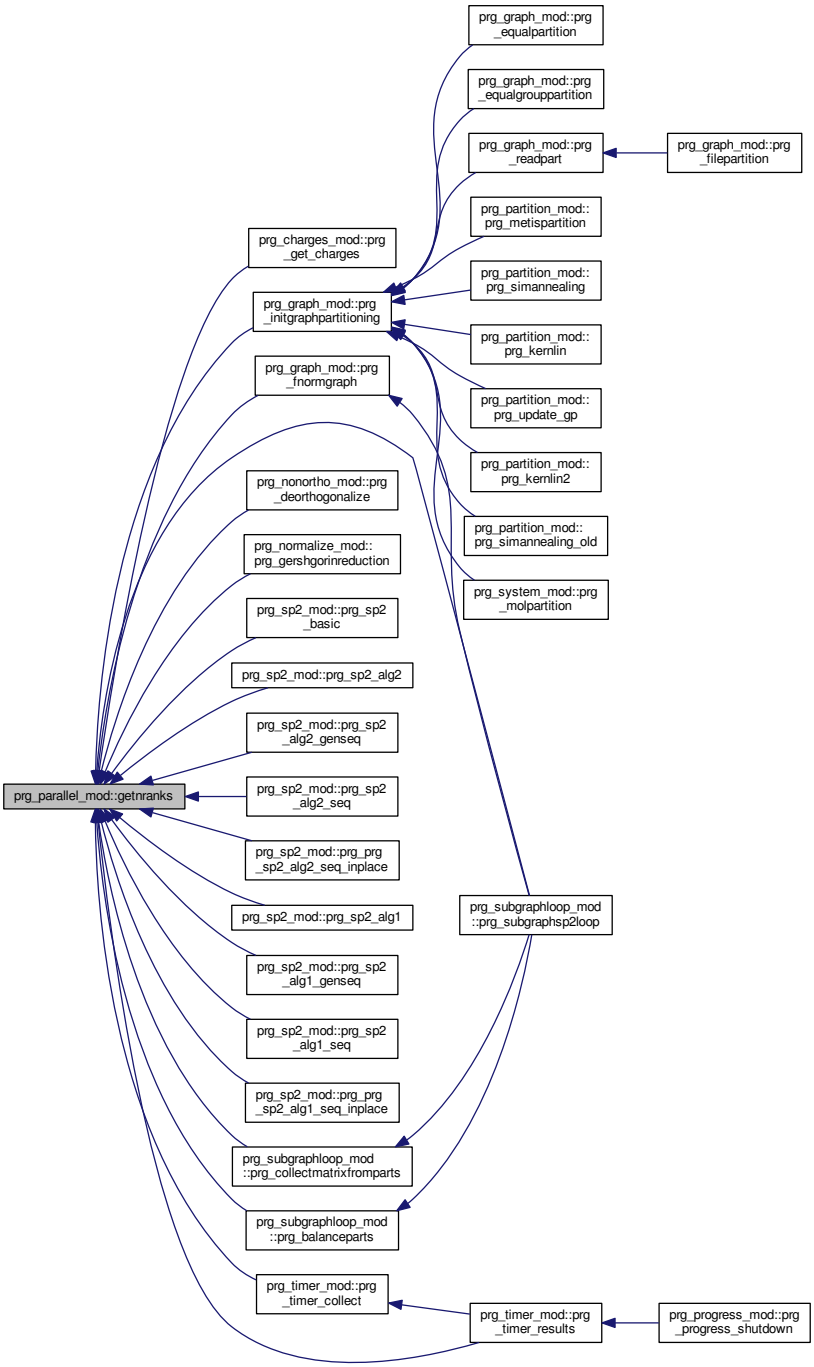
Here is the caller graph for this function:



9.16.2.6 integer function, public prg_parallel_mod::getnranks ( )

Definition at line 88 of file prg_parallel_mod.F90.

Here is the caller graph for this function:



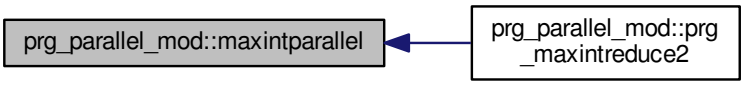
9.16.2.7 subroutine, public prg_parallel_mod::isendparallel (real(dp), dimension(:), intent(in) *sendBuf,* integer, intent(in) *sendLen,* integer, intent(in) *dest*)

Definition at line 230 of file prg_parallel_mod.F90.

9.16.2.8 subroutine, public prg_parallel_mod::maxintparallel (integer, dimension(∗), intent(in) *sendBuf,* integer, dimension(∗), intent(out) *recvBuf,* integer, intent(in) *icount*)

Definition at line 337 of file prg_parallel_mod.F90.

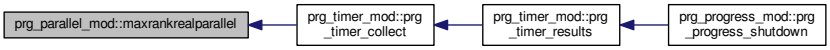
Here is the caller graph for this function:



9.16.2.9 subroutine, public prg_parallel_mod::maxrankrealparallel (type(**rankreducedata_t**), dimension(∗), intent(in) *sendBuf,* type(**rankreducedata_t**), dimension(∗), intent(out) *recvBuf,* integer, intent(in) *icount*)

Definition at line 607 of file prg_parallel_mod.F90.

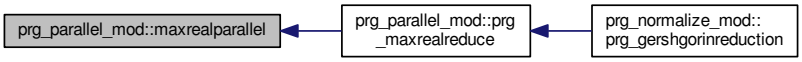
Here is the caller graph for this function:



9.16.2.10 subroutine, public prg_parallel_mod::maxrealparallel (real(**dp**), dimension(∗), intent(in) *sendBuf,* real(**dp**), dimension(∗), intent(out) *recvBuf,* integer, intent(in) *icount*)

Definition at line 358 of file prg_parallel_mod.F90.

Here is the caller graph for this function:



9.16.2.11 subroutine, public prg_parallel_mod::minintparallel (integer, dimension(∗), intent(in) *sendBuf,* integer, dimension(∗), intent(out) *recvBuf,* integer, intent(in) *icount*)

Definition at line 379 of file prg_parallel_mod.F90.

9.16.2.12 subroutine, public prg_parallel_mod::minrankrealparallel (type(**rankreducedata_t**), dimension(∗), intent(in) *sendBuf,* type(**rankreducedata_t**), dimension(∗), intent(out) *recvBuf,* integer, intent(in) *icount*)

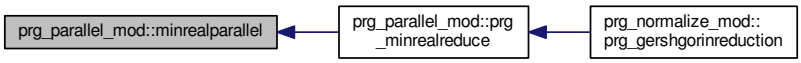
Definition at line 584 of file prg_parallel_mod.F90.

Here is the caller graph for this function:

9.16.2.13 subroutine, public prg_parallel_mod::minrealparallel (real(**dp**), dimension(∗), intent(in) *sendBuf,* real(**dp**), dimension(∗), intent(out) *recvBuf,* integer, intent(in) *icount*)

Definition at line 400 of file prg_parallel_mod.F90.

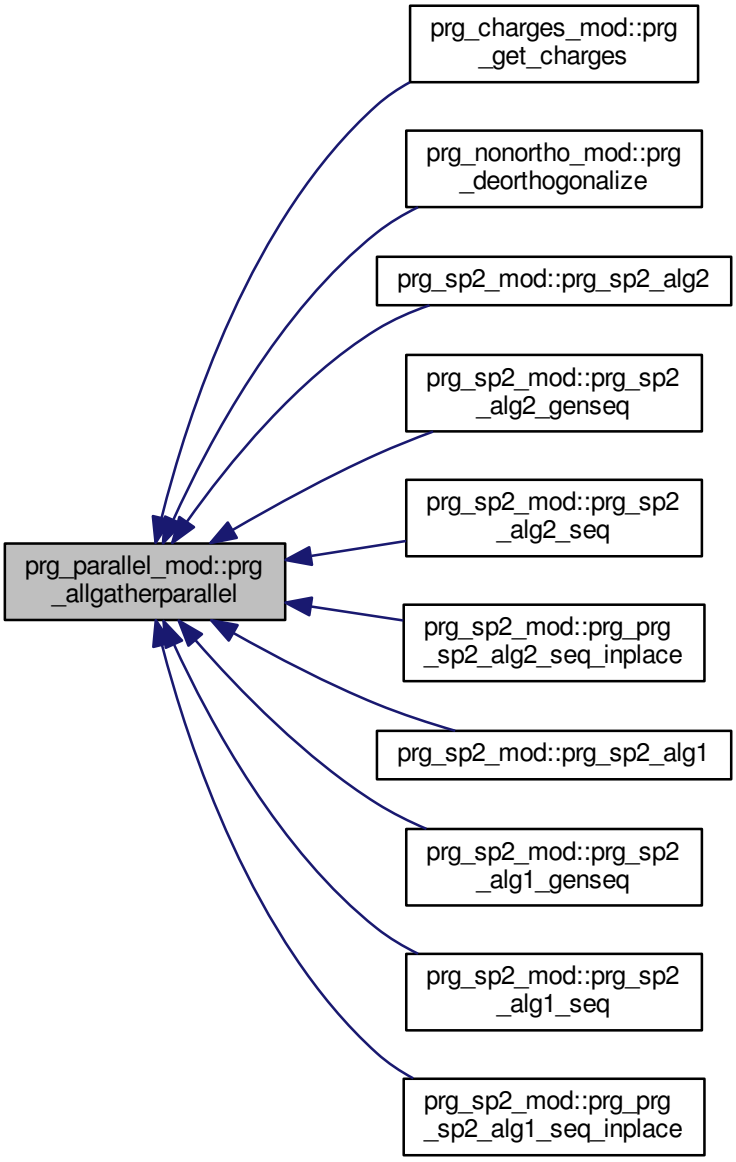
Here is the caller graph for this function:



9.16.2.14 subroutine, public prg_parallel_mod::prg_allgatherparallel (type (bml_matrix_t), intent(inout) *a*)

Definition at line 744 of file prg_parallel_mod.F90.

Here is the caller graph for this function:



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

Definition at line 729 of file prg_parallel_mod.F90.

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

Definition at line 714 of file prg_parallel_mod.F90.

9.16.2.17 subroutine, public prg_parallel_mod::prg_barrierparallel ( )

Definition at line 196 of file prg_parallel_mod.F90.

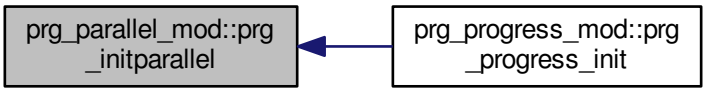
9.16.2.18 subroutine, public prg_parallel_mod::prg_bcastparallel (character, dimension(∗), intent(in) *buf,* integer, intent(in) *blen,* integer, intent(in) *root*)

Definition at line 630 of file prg_parallel_mod.F90.

9.16.2.19 subroutine, public prg_parallel_mod::prg_initparallel ( )

Definition at line 127 of file prg_parallel_mod.F90.

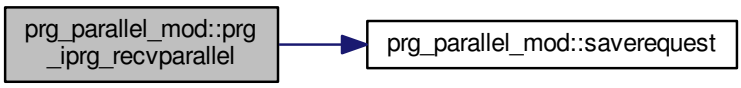
Here is the caller graph for this function:



9.16.2.20 subroutine, public prg_parallel_mod::prg_iprg_recvparallel (real(dp), dimension(∗) *recvBuf,* integer, intent(in) *recvLen,* integer *rind*)

Definition at line 261 of file prg_parallel_mod.F90.

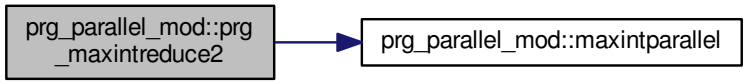
Here is the call graph for this function:



9.16.2.21 subroutine, public prg_parallel_mod::prg_maxintreduce2 (integer, intent(inout) *value1,* integer, intent(inout) *value2*)

Definition at line 453 of file prg_parallel_mod.F90.

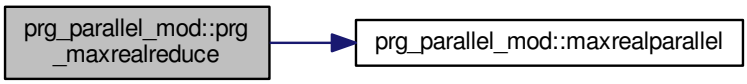
Here is the call graph for this function:



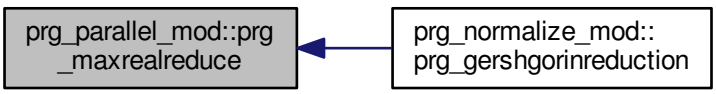
9.16.2.22 subroutine, public prg_parallel_mod::prg_maxrealreduce (real(dp), intent(inout) *rvalue*)

Definition at line 437 of file prg_parallel_mod.F90.

Here is the call graph for this function:



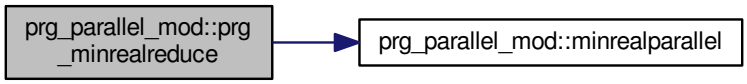
Here is the caller graph for this function:



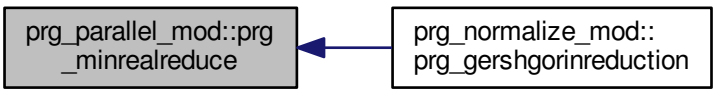
9.16.2.23 subroutine, public prg_parallel_mod::prg_minrealreduce (real(dp), intent(inout) *rvalue*)

Definition at line 421 of file prg_parallel_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



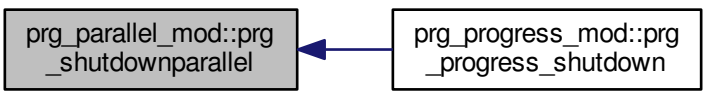
9.16.2.24 subroutine, public prg_parallel_mod::prg_recvparallel (real(dp), dimension(∗) *recvBuf,* integer, intent(in) *recvLen*)

Definition at line 279 of file prg_parallel_mod.F90.

9.16.2.25 subroutine, public prg_parallel_mod::prg_shutdownparallel ( )

Definition at line 154 of file prg_parallel_mod.F90.

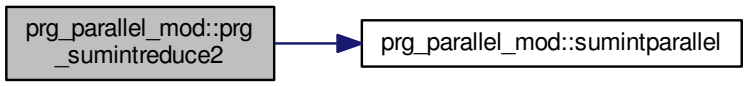
Here is the caller graph for this function:



9.16.2.26 subroutine, public prg_parallel_mod::prg_sumintreduce2 (integer, intent(inout) *value1,* integer, intent(inout) *value2*)

Definition at line 471 of file prg_parallel_mod.F90.

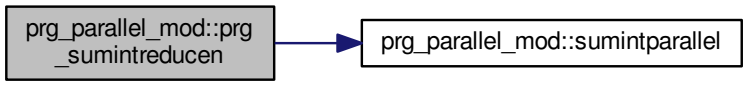
Here is the call graph for this function:



9.16.2.27 subroutine, public prg_parallel_mod::prg_sumintreducen (integer, dimension(n), intent(inout) *valueVec,* integer, intent(in) *N*)

Definition at line 564 of file prg_parallel_mod.F90.

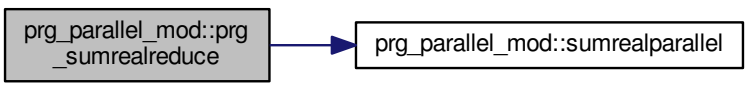
Here is the call graph for this function:



9.16.2.28 subroutine, public prg_parallel_mod::prg_sumrealreduce (real(dp), intent(inout) *value1*)

Definition at line 489 of file prg_parallel_mod.F90.

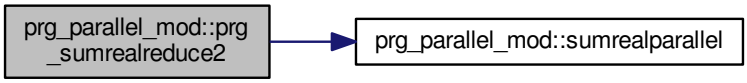
Here is the call graph for this function:



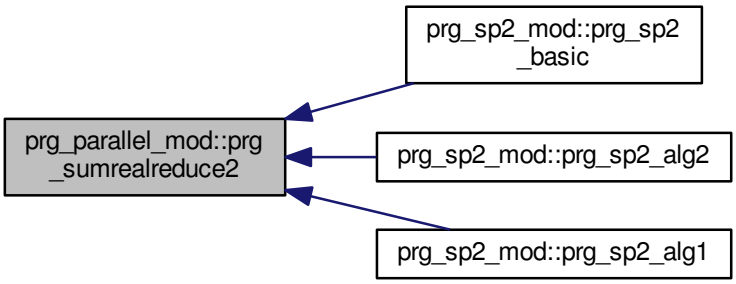
9.16.2.29 subroutine, public prg_parallel_mod::prg_sumrealreduce2 (real(dp), intent(inout) *value1,* real(dp), intent(inout) *value2*)

Definition at line 505 of file prg_parallel_mod.F90.

Here is the call graph for this function:



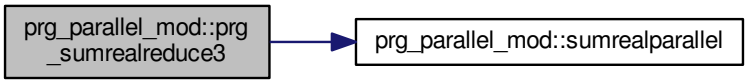
Here is the caller graph for this function:



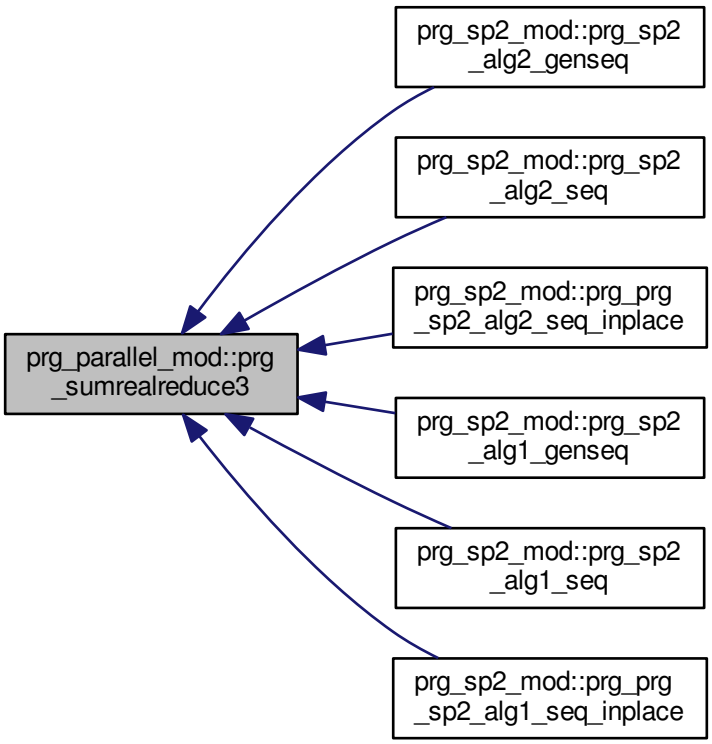
9.16.2.30 subroutine, public prg_parallel_mod::prg_sumrealreduce3 (real(dp), intent(inout) *value1,* real(dp), intent(inout) *value2,* real(dp), intent(inout) *value3*)

Definition at line 523 of file prg_parallel_mod.F90.

Here is the call graph for this function:



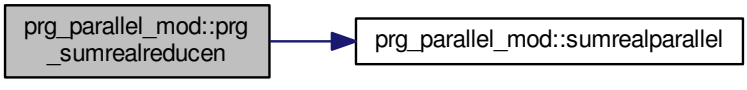
Here is the caller graph for this function:



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

Definition at line 543 of file prg_parallel_mod.F90.

Here is the call graph for this function:



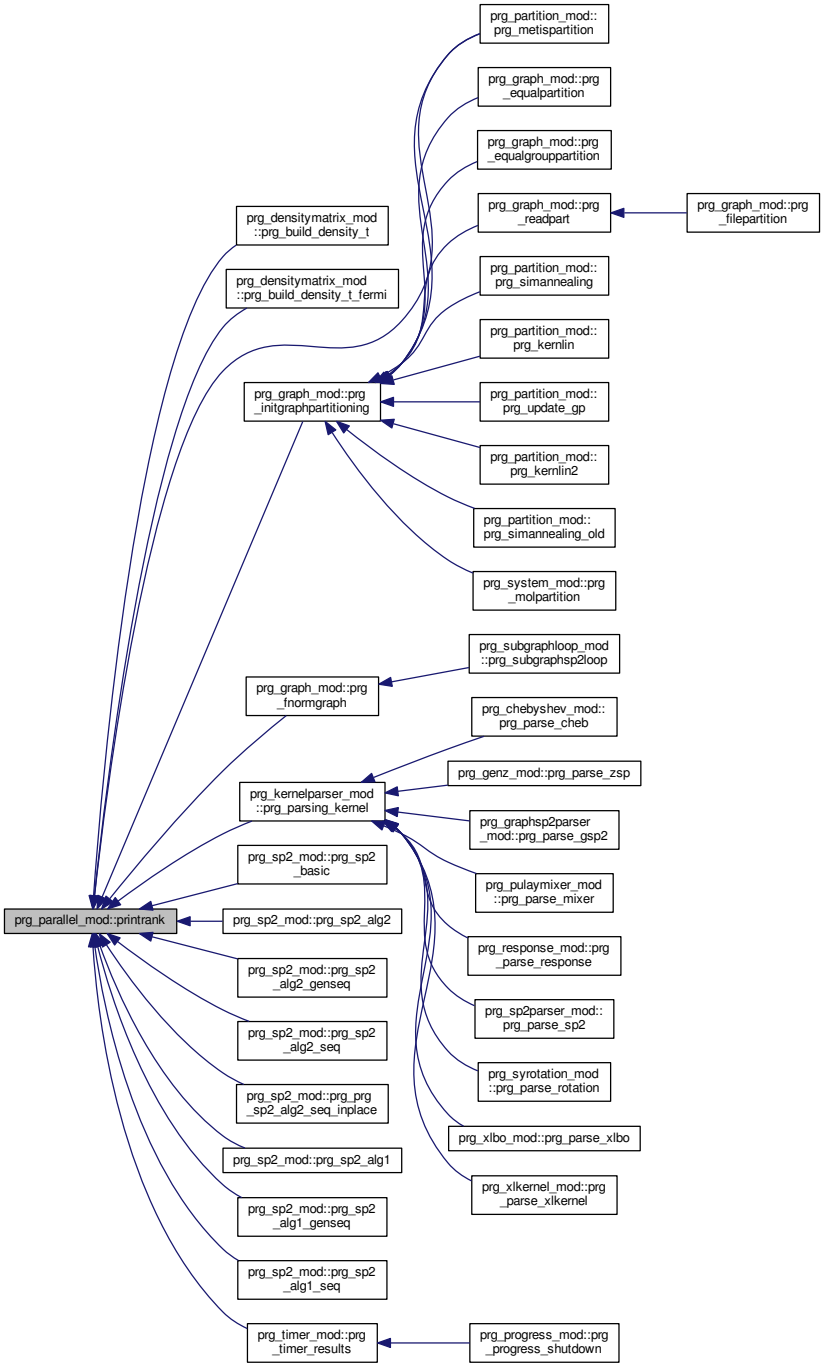
9.16.2.32 subroutine, public prg_parallel_mod::prg_wait ( )

Definition at line 758 of file prg_parallel_mod.F90.

9.16.2.33 integer function, public prg_parallel_mod::printrank ( )

Definition at line 111 of file prg_parallel_mod.F90.

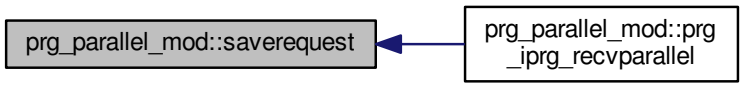
Here is the caller graph for this function:



9.16.2.34 integer function prg_parallel_mod::saverequest (integer, intent(in) *irequest*) [private]

Definition at line 170 of file prg_parallel_mod.F90.

Here is the caller graph for this function:



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

Definition at line 246 of file prg_parallel_mod.F90.

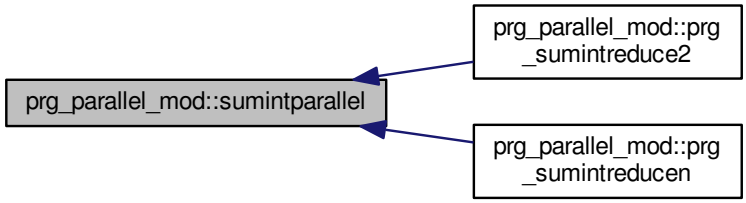
9.16.2.36 subroutine, public prg_parallel_mod::sendreceiveparallel (real(dp), dimension(∗), intent(in) *sendBuf,* integer, intent(in) *sendLen,* integer, intent(in) *dest,* real(dp), dimension(∗), intent(out) *recvBuf,* integer, intent(in) *recvLen,* integer, intent(in) *source,* integer, intent(out)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

Definition at line 207 of file prg_parallel_mod.F90.

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

Definition at line 295 of file prg_parallel_mod.F90.

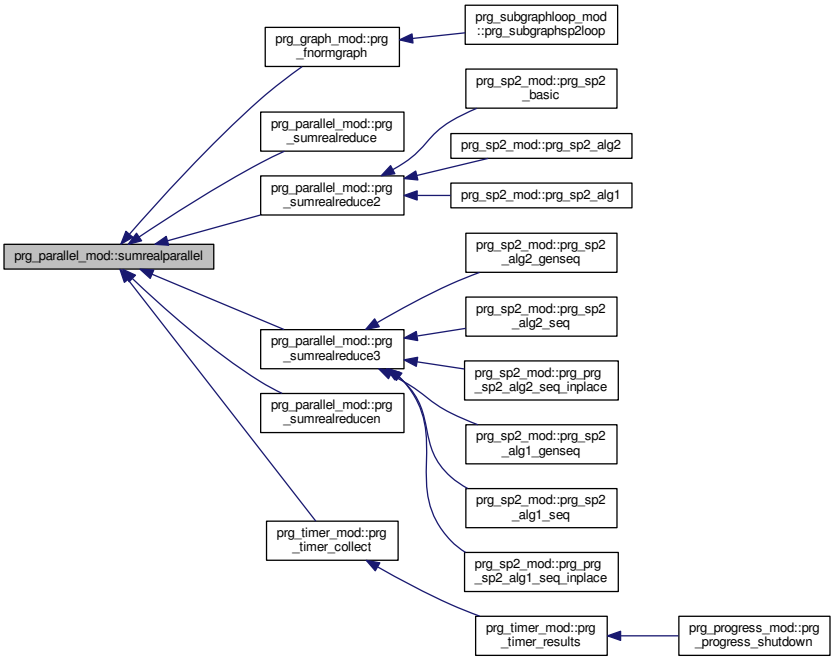
Here is the caller graph for this function:



9.16.2.38 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.

Here is the caller graph for this function:



9.16.3 Variable Documentation

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

Definition at line 26 of file prg_parallel_mod.F90.

9.16.3.2 integer prg_parallel_mod::ierr [private]

Definition at line 29 of file prg_parallel_mod.F90.

9.16.3.3 integer prg_parallel_mod::myrank [private]

Definition at line 28 of file prg_parallel_mod.F90.

9.16.3.4 integer prg_parallel_mod::nranks [private]

Definition at line 28 of file prg_parallel_mod.F90.

9.16.3.5 integer prg_parallel_mod::reqcount [private]

Definition at line 29 of file prg_parallel_mod.F90.

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

Definition at line 30 of file prg_parallel_mod.F90.

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

Definition at line 30 of file prg_parallel_mod.F90.

9.17 prg_partition_mod Module Reference

The partition module.

Functions/Subroutines

- subroutine, public prg_metispartition (gp, ngroups, nnodes, xadj, adjncy, nparts, part, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm)

  Create graph partitions minizing number of cut edges.
- subroutine, public prg_costpartition (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm)

  Compute cost of a partition.
- subroutine, public update_prg_costpartition (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, node, new_part)

  Update cost of partition and the different parameters node is moves into new_part For each neighbor of node, the following cases hold: Case 1: neighbor is in old_part Case 2: neighbor is in new_part Case 3: neighbor is neither in old_ or new_part.
- subroutine prg_accept_prob (it, prg_delta, r)

  Compute acceptance probability for simulated annealing.
- subroutine prg_costindex (cost, sumCubes, maxCH, smooth_maxCH, obj_fun)

  Choose objective function to work with.
- subroutine prg_rand_node (gp, node, seed)

  Pick a random node.
- subroutine, public prg_simannealing (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, niter, seed)

  Graph partitioning based on Simulated Annealing.
- subroutine, public prg_kernlin (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, nconverg, seed)

  Graph partitioning based on inspired by Kernighan-Lin Review METiS manual for description of k-way implementation of KL Pick a core together with its halos Place free vertices on a priority queue with (key, value) =(prg_delta, best_part),with prg_delta = change in obj_value Dequeue and allow hill climbing.
- subroutine, public prg_update_gp (gp, partNumber, core_count)
- subroutine prg_rand_shuffle (array, seed)

  Randomly shuffle array.
- subroutine, public prg_check_arrays (gp, core_count, CH_count, Halo_count)

Error checking Checking that core_count, CH_count, Halo_count match.

- subroutine, public prg_kernlin_queue (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm)

  Greedy algorithm. At each step it chooses the (vertex, new_part) pair with highest gain Currently implementation is very slow.
- subroutine prg_find_best_move (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sum↩ Cubes, 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, sum↩ Cubes, maxCH, smooth_maxCH, pnorm)
- subroutine prg_get_largest_hedge_in_part (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_↩ count, sumCubes, maxCH, smooth_maxCH, pnorm, search_part, largest_Hedge)
- subroutine, public prg_simannealing_old (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, niter, seed)

Variables

- integer, parameter dp = kind(1.0d0)
- integer, parameter metis_index_kind = METIS_INDEX_KIND

  From /usr/include/metis.h.
- integer, parameter metis_real_kind = kind(METIS_REAL_KIND)

  From /usr/include/metis.h.

9.17.1 Detailed Description

The partition module.

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

9.17.2 Function/Subroutine Documentation

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

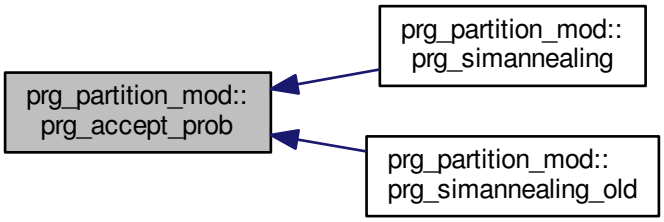
Compute acceptance probability for simulated annealing.

Parameters

it	iteration
prg_delta	(new_obj_value - old_obj_value)
r	acceptance probability

Definition at line 489 of file prg_partition_mod.F90.

Here is the caller graph for this function:



9.17.2.2 subroutine, public prg_partition_mod::prg_check_arrays (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *core_count,* integer, dimension(:), intent(inout), allocatable *CH_count,* integer, dimension(:,:), intent(inout), allocatable *Halo_count*)

Error checking Checking that core_count, CH_count, Halo_count match.

Definition at line 1146 of file prg_partition_mod.F90.

9.17.2.3 subroutine prg_partition_mod::prg_costindex (real(dp), intent(inout) *cost,* real(dp), intent(inout) *sumCubes,* real(dp), intent(inout) *maxCH,* real(dp), intent(inout) *smooth_maxCH,* integer, intent(inout) *obj_fun*) [private]

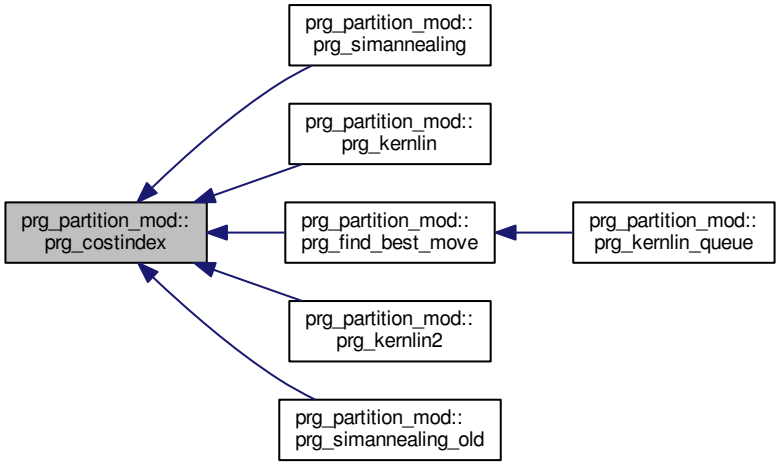
Choose objective function to work with.

Parameters

cost	output according to chosen obj_fun
sumCubes	Sum of cubes obj value
maxCH	maximum core-halo part size obective value
obj_fun	0=sumcubes, 1=maxCH

Definition at line 507 of file prg_partition_mod.F90.

Here is the caller graph for this function:



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

Compute cost of a partition.

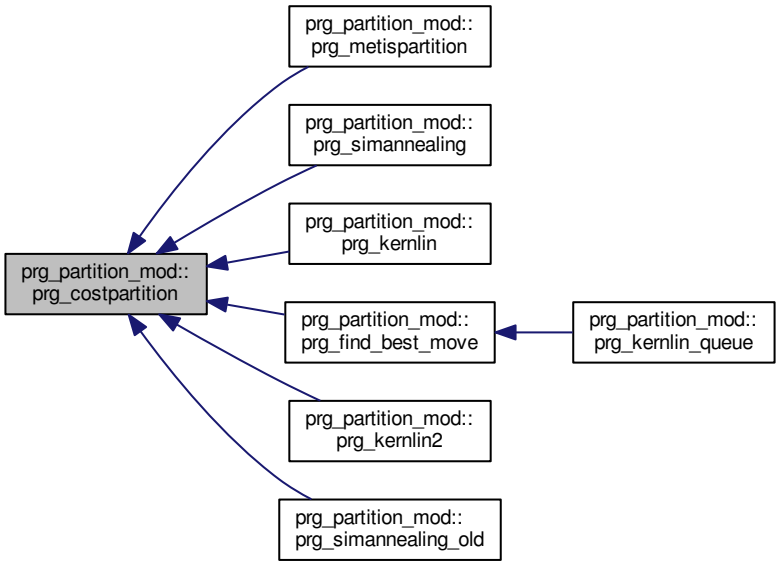
Parameters

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

prg_initialize

Definition at line 327 of file prg_partition_mod.F90.

Here is the caller graph for this function:

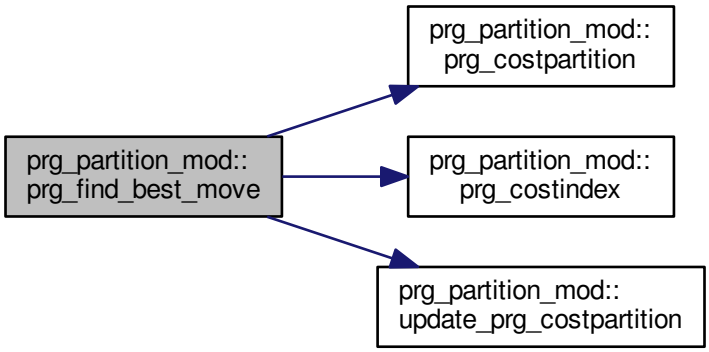


9.17.2.5 subroutine prg_partition_mod::prg_find_best_move (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy,* integer, dimension(:), intent(inout), allocatable *partNumber,* integer, dimension(:), intent(inout), allocatable *core_count,* integer, dimension(:), intent(inout), allocatable *CH_count,* integer, dimension(:,:), intent(inout), allocatable *Halo_count,* real(dp), intent(inout) *sumCubes,* real(dp), intent(inout) *maxCH,* real(dp), intent(inout) *smooth_maxCH,* real(dp), intent(inout) *pnorm,* integer, intent(inout) *best_node,* integer, intent(inout) *best_part*) [private]

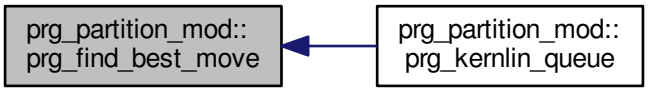
For kerlin_queue to find (vertex, new_part) pair with highest gain.

Definition at line 1209 of file prg_partition_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:

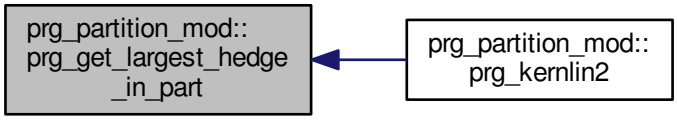


9.17.2.6 subroutine prg_partition_mod::prg_get_largest_hedge_in_part (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy,* integer, dimension(:), intent(inout), allocatable *partNumber,*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

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

Definition at line 1420 of file prg_partition_mod.F90.

Here is the caller graph for this function:



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

Graph partitioning based on inspired by Kernighan-Lin Review METiS manual for description of k-way implementation of KL Pick a core together with its halos Place free vertices on a priority queue with (key, value) =(prg_delta, best_part),with prg_delta = change in obj_value Dequeue and allow hill climbing.

Parameters

gp	Graph partitioning

Parameters

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

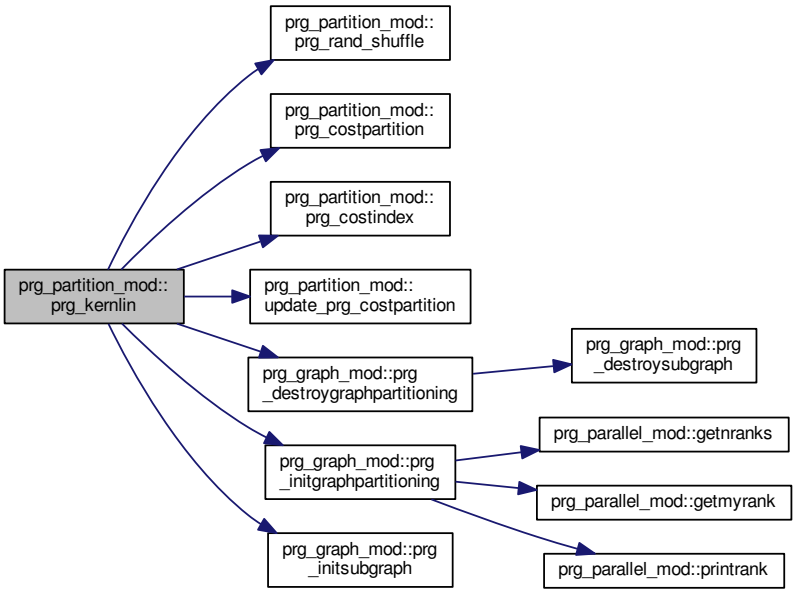
Update graph structure

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:



9.17.2.8 subroutine, public prg_partition_mod::prg_kernlin2 (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy,* integer, dimension(:), intent(inout), allocatable *partNumber,* integer, dimension(:), intent(inout), allocatable *core_count,* integer, dimension(:), intent(inout), allocatable *CH_count,* integer, dimension(:,:), intent(inout), allocatable *Halo_count,* real(dp), intent(inout) *sumCubes,* real(dp), intent(inout) *maxCH,* real(dp), intent(inout) *smooth_maxCH,* real(dp), intent(inout) *pnorm*)

Allocate arrays

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

Find part with smalles size (should be included in update_prg_costPartition

if current part is max, move to min_part then move subsets (neighbors)

Move hyperedges to minCH part

Try and move intersecting hyperedges

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

Check empty part exist move nodes from maxpart to empty part

move it neighbor in the max parts to the newpart

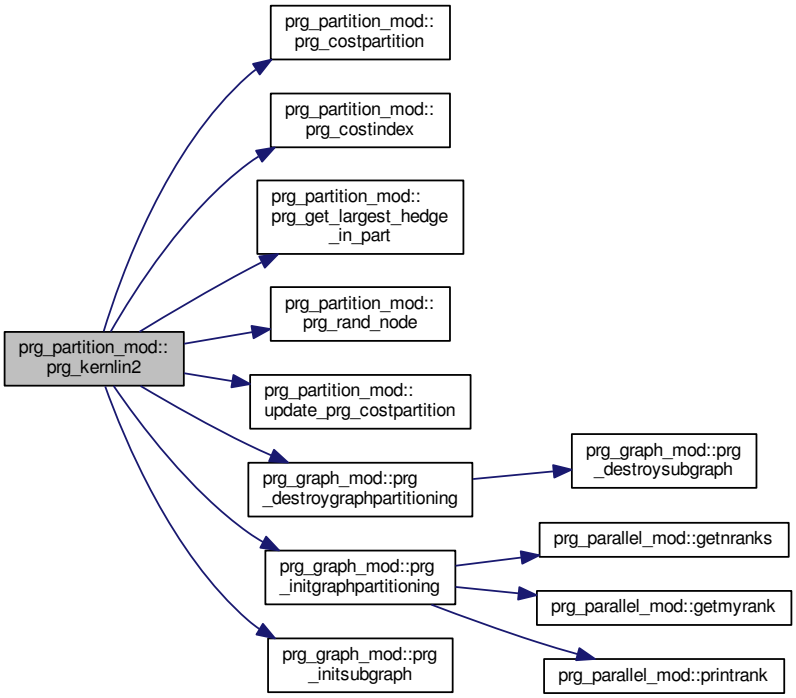
Update graph structure

Allocate subgraph structure

Assign node ids to sgraph

Definition at line 1257 of file prg_partition_mod.F90.

Here is the call graph for this function:

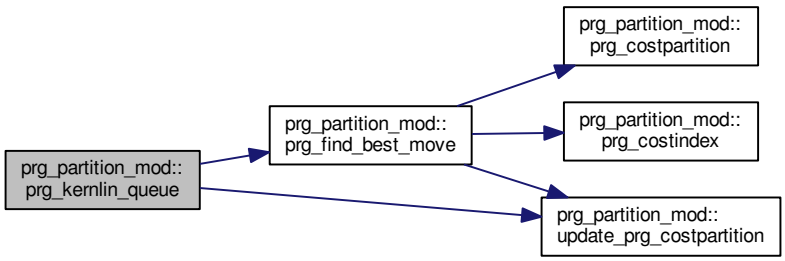


9.17.2.9 **subroutine, public prg_partition_mod::prg_kernlin_queue (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy,* integer, dimension(:), intent(inout), allocatable *partNumber,* integer, dimension(:), intent(inout), allocatable *core_count,* integer, dimension(:), intent(inout), allocatable *CH_count,* integer, dimension(:,:), intent(inout), allocatable *Halo_count,* real(dp), intent(inout) *sumCubes,* real(dp), intent(inout) *maxCH,* real(dp), intent(inout) *smooth_maxCH,* real(dp), intent(inout) *pnorm*)**

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

Definition at line 1173 of file prg_partition_mod.F90.

Here is the call graph for this function:



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

Create graph partitions minizing number of cut edges.

Parameters

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

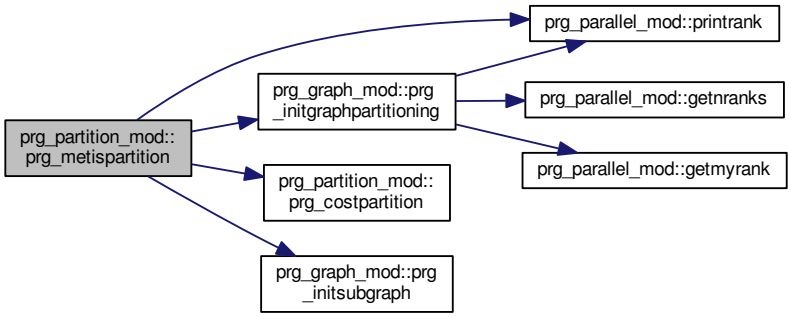
prg_initialize

Partition graph into nparts'

Compute cost of partition

Definition at line 217 of file prg_partition_mod.F90.

Here is the call graph for this function:



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

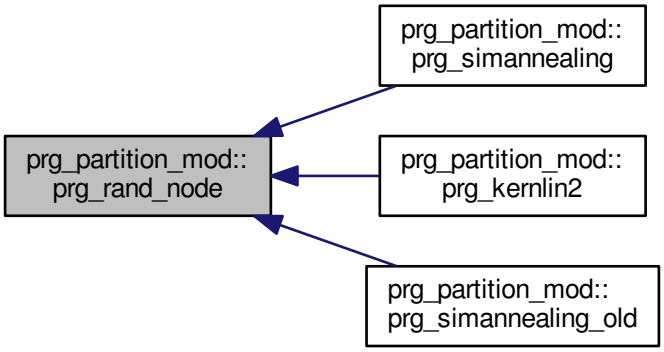
Pick a random node.

Parameters

gp	graph partitioning structure
node	output node
seed	random seed

Definition at line 527 of file prg_partition_mod.F90.

Here is the caller graph for this function:



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

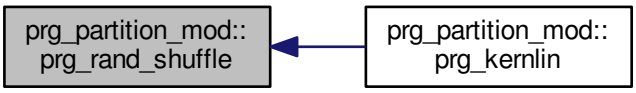
Randomly shuffle array.

Random seed

Shuffle array

Definition at line 1123 of file prg_partition_mod.F90.

Here is the caller graph for this function:



9.17.2.13 subroutine, public prg_partition_mod::prg_simannealing (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy,* integer, dimension(:), intent(inout), allocatable *partNumber,* integer, dimension(:), intent(inout), allocatable *core_count,* integer, dimension(:), intent(inout), allocatable *CH_count,* integer, dimension(:,:), intent(inout), allocatable *Halo_count,* real(dp), intent(inout) *sumCubes,* real(dp), intent(inout) *maxCH,* real(dp), intent(inout) *smooth_maxCH,* real(dp), intent(inout) *pnorm,* integer, intent(in) *niter,* integer, intent(inout) *seed*)

Graph partitioning based on Simulated Annealing.

Parameters

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

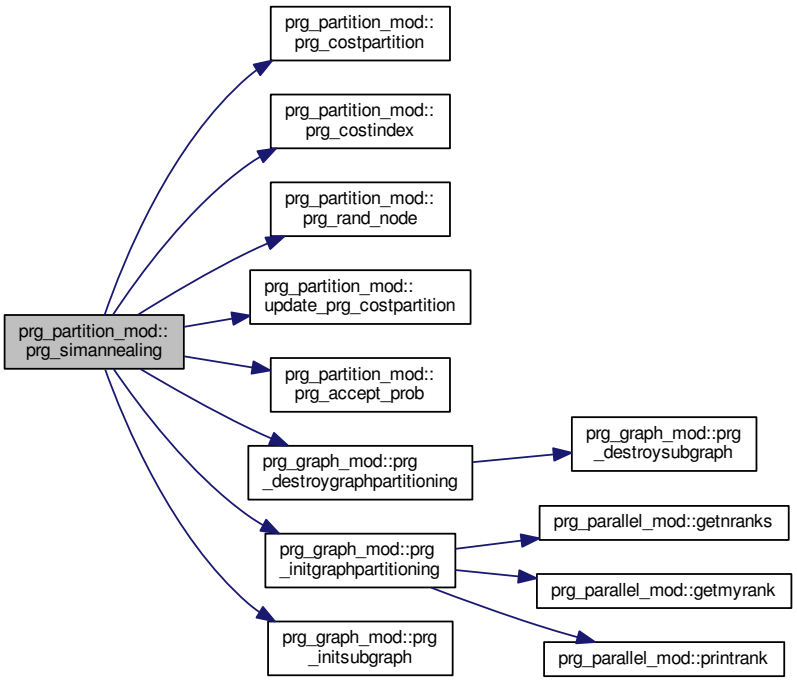
move it neighbor in the max parts to the newpart

Update graph structure

For debuging

Definition at line 552 of file prg_partition_mod.F90.

Here is the call graph for this function:



9.17.2.14 subroutine, public prg_partition_mod::prg_simannealing_old (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy,* integer, dimension(:), intent(inout), allocatable *partNumber,* integer, dimension(:), intent(inout), allocatable *core_count,* integer, dimension(:), intent(inout), allocatable *CH_count,* integer, dimension(:,:), intent(inout), allocatable *Halo_count,* real(dp), intent(inout) *sumCubes,* real(dp), intent(inout) *maxCH,* real(dp), intent(inout) *smooth_maxCH,* real(dp), intent(inout) *pnorm,* integer, intent(in) *niter,* integer, intent(inout) *seed*)

Compute current cost of partition

Choose objective function to minimize

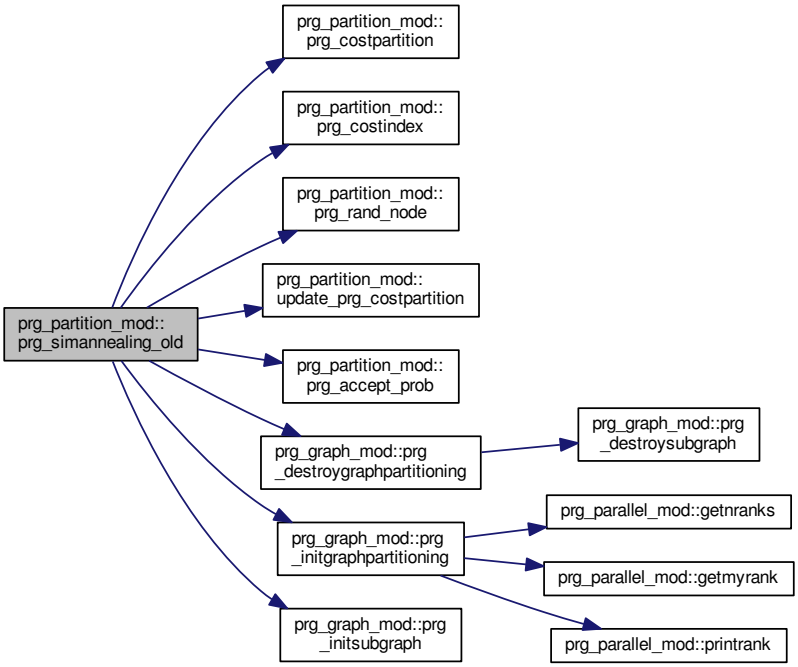
Perform SA

Update graph structure

For debuging

Definition at line 1453 of file prg_partition_mod.F90.

Here is the call graph for this function:



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

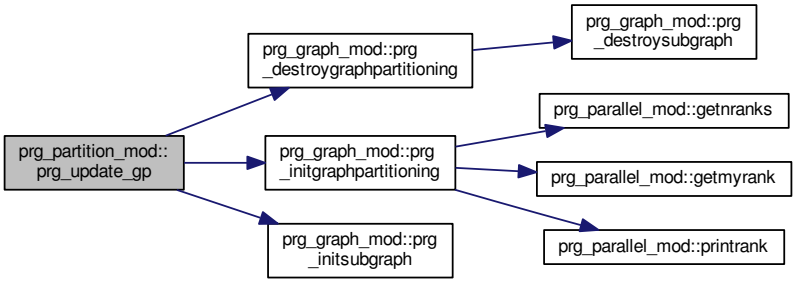
Update graph structure

Allocate subgraph structure

Assign node ids to sgraph

Definition at line 1082 of file prg_partition_mod.F90.

Here is the call graph for this function:



9.17.2.16 **subroutine, public prg_partition_mod::update_prg_costpartition (type (graph_partitioning_t), intent(inout) *gp,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy,* integer, dimension(:), intent(inout), allocatable *partNumber,* integer, dimension(:), intent(inout), allocatable *core_count,* integer, dimension(:), intent(inout), allocatable *CH_count,* integer, dimension(:,:), intent(inout), allocatable *Halo_count,* real(dp), intent(inout) *sumCubes,* real(dp), intent(inout) *maxCH,* real(dp), intent(inout) *smooth_maxCH,* real(dp), intent(inout) *pnorm,* integer, intent(in) *node,* integer, intent(in) *new_part*)**

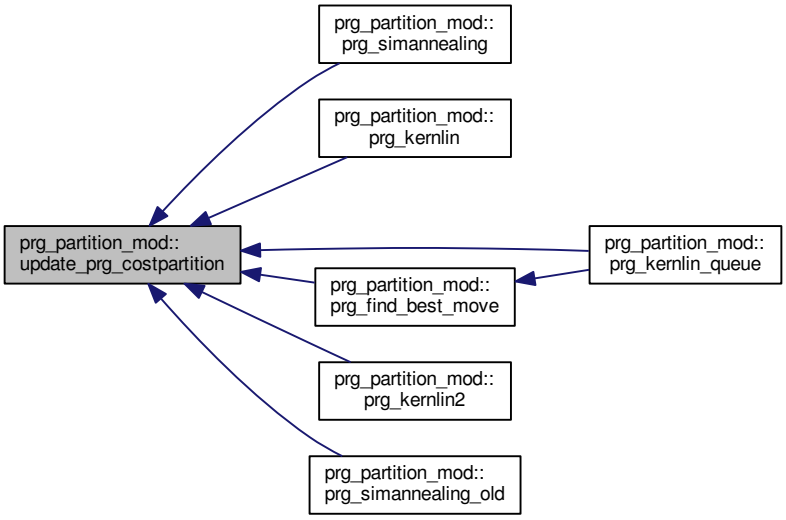
Update cost of partition and the different parameters node is moves into new_part For each neighbor of node, the following cases hold: Case 1: neighbor is in old_part Case 2: neighbor is in new_part Case 3: neighbor is neither in old_ or new_part.

Parameters

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

Definition at line 401 of file prg_partition_mod.F90.

Here is the caller graph for this function:



9.17.3 Variable Documentation

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

Definition at line 18 of file prg_partition_mod.F90.

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

From /usr/include/metis.h.

IDXTYPEWIDTH = 32 –> metis_index_kind = 4 IDXTYPEWIDTH = 64 –> metis_index_kind = 8

Definition at line 24 of file prg_partition_mod.F90.

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

From /usr/include/metis.h.

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

Definition at line 30 of file prg_partition_mod.F90.

9.18 prg_progress_mod Module Reference

The progress module.

Functions/Subroutines

- subroutine, public prg_progress_init ()

  Initialize progress.
- subroutine, public prg_progress_shutdown ()

  Shutdown progress.

Variables

- integer, parameter dp = kind(1.0d0)

9.18.1 Detailed Description

The progress module.

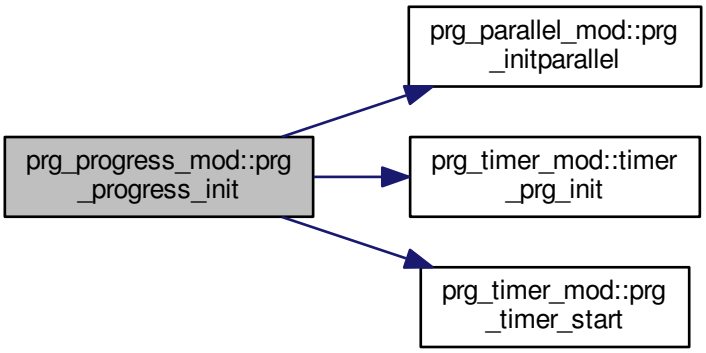
9.18.2 Function/Subroutine Documentation

9.18.2.1 subroutine, public prg_progress_mod::prg_progress_init ( )

Initialize progress.

Definition at line 25 of file prg_progress_mod.F90.

Here is the call graph for this function:

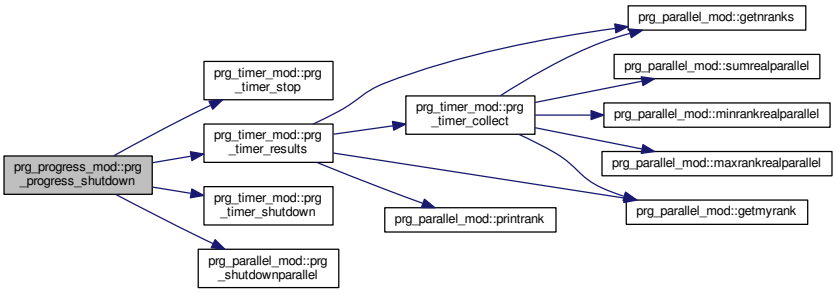


9.18.2.2 subroutine, public prg_progress_mod::prg_progress_shutdown ( )

Shutdown progress.

Definition at line 37 of file prg_progress_mod.F90.

Here is the call graph for this function:



9.18.3 Variable Documentation

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

Definition at line 16 of file prg_progress_mod.F90.

9.19 prg_ptable_mod Module Reference

Periodic table of elements.

Functions/Subroutines

- integer function, public element_atomic_number (symbol)
- integer function element_atomic_number_upper (symbol)

Variables

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

  Element symbol.

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

  Element symbol upper.

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

  Element name.

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

  Element mass in atomic mass units (1.66 x 10-27 kg)

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

  van der Waals radius (in Angstroms)

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

  Covalent radius (in Angstroms)

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

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

Ionization energy (in eV)

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

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

  The Pauling electronegativity for this element.
- integer, dimension(nz), parameter element_maxbonds = (/ 1 , 0 , 1 , 2 , 4 , 4 , 4 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 8 , 6 , 6 , 6 , 6 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 6 , 3 , 4 , 3 , 2 , 1 , 0 , 1 , 2 , 12 , 6 , 6 , 6 , 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 , 6 /)

  The maximum expected number of bonds to this element.
- integer, dimension(nz), parameter element_numel = (/ 1 , 2 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 , 18 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 , 18 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 , 18 , 19 , 20 , 21 , 22 , 23 , 24 , 25 , 26 , 27 , 28 , 29 , 30 , 31 , 32 , 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 , 13 , 14 , 15 , 16 , 17 /)

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

  The electronic configuration.

9.19.1 Detailed Description

Periodic table of elements.

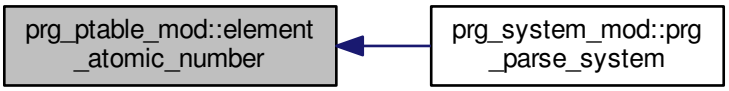
This data was prg_generated with pybabel and openbable packages Openbabel: http://openbabel.org/dev-api/index.shtml Pybel: https://openbabel.org/docs/dev/UseTheLibrary/Python_Pybel.html# Other sources includes NIST: http://www.nist.gov/pml/data/ion_energy.cfm

9.19.2 Function/Subroutine Documentation

9.19.2.1 integer function, public prg_ptable_mod::element_atomic_number (character(len=∗) *symbol*)

Definition at line 394 of file prg_ptable_mod.F90.

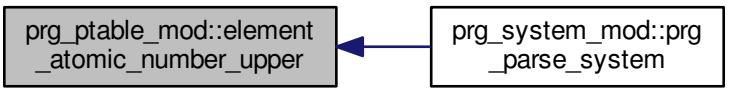
Here is the caller graph for this function:



9.19.2.2 integer function prg_ptable_mod::element_atomic_number_upper (character(len=∗) *symbol*)

Definition at line 408 of file prg_ptable_mod.F90.

Here is the caller graph for this function:



9.19.3 Variable Documentation

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

The Pauling electronegativity for this element.

Definition at line 266 of file prg_ptable_mod.F90.

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

Definition at line 13 of file prg_ptable_mod.F90.

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

Covalent radius (in Angstroms)

Definition at line 173 of file prg_ptable_mod.F90.

9.19.3.4 real(dp), dimension(nz), parameter prg_ptable_mod::element_ea = (/ 0.75420375 , 0.0 , 0.618049 , 0.0 , 0.279723 , 1.262118 , -0.07 , 1.461112 , 3.4011887 , 0.0 , 0.547926 , 0.0 , 0.43283 , 1.389521 , 0.7465 , 2.0771029 , 3.612724 , 0.0 , 0.501459 , 0.02455 , 0.188 , 0.084 , 0.525 , 0.67584 , 0.0 , 0.151 , 0.6633 , 1.15716 , 1.23578 , 0.0 , 0.41 , 1.232712 , 0.814 , 2.02067 , 3.363588 , 0.0 , 0.485916 , 0.05206 , 0.307 , 0.426 , 0.893 , 0.7472 , 0.55 , 1.04638 , 1.14289 , 0.56214 , 1.30447 , 0.0 , 0.404 , 1.112066 , 1.047401 , 1.970875 , 3.059038 , 0.0 , 0.471626 , 0.14462 , 0.47 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 0.5 , 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 , 0.0 , 0.0 /)

Electron affprg_inity (in eV)

Definition at line 235 of file prg_ptable_mod.F90.

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

The electronic configuration.

Definition at line 360 of file prg_ptable_mod.F90.

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

Ionization energy (in eV)

Definition at line 204 of file prg_ptable_mod.F90.

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

Element mass in atomic mass units (1.66 x 10-27 kg)

Definition at line 110 of file prg_ptable_mod.F90.

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

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

Element name.

Definition at line 79 of file prg_ptable_mod.F90.

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

Last shell number of electrons.

Definition at line 329 of file prg_ptable_mod.F90.

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

Element symbol.

Definition at line 17 of file prg_ptable_mod.F90.

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

Element symbol upper.

Definition at line 48 of file prg_ptable_mod.F90.

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

van der Waals radius (in Angstroms)

Definition at line 141 of file prg_ptable_mod.F90.

9.19.3.14 integer, parameter prg_ptable_mod::nz = 103

Definition at line 12 of file prg_ptable_mod.F90.

9.20 prg_pulaycomponent_mod Module Reference

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

Functions/Subroutines

- subroutine, public prg_pulaycomponent0 (rho_bml, ham_bml, pcm_bml, threshold, M, bml_type, verbose)

  At $T = 0K$, $P = \rho H \rho$.
- subroutine, public prg_pulaycomponentt (rho_bml, ham_bml, zmat_bml, pcm_bml, threshold, M, bml_type, verbose)

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

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

Variables

- integer, parameter dp = kind(1.0d0)

9.20.1 Detailed Description

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

For a further explanation please see Niklasson 2008 [3]

9.20.2 Function/Subroutine Documentation

9.20.2.1 subroutine, public prg_pulaycomponent_mod::prg_get_pulayforce (integer, intent(in) *nats,* type(bml_matrix_t), intent(in) *zmat_bml,* type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(in) *rho_bml,* type(bml_matrix_t), intent(in) *dSx_bml,* type(bml_matrix_t), intent(in) *dSy_bml,* type(bml_matrix_t), intent(in) *dSz_bml,* integer, dimension(:,:), intent(in) *hindex,* real(dp), dimension(:,:), intent(inout), allocatable *FPUL,* real(dp), intent(in) *threshold*)

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

Parameters

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

Definition at line 152 of file prg_pulaycomponent_mod.F90.

9.20.2.2 subroutine, public prg_pulaycomponent_mod::prg_pulaycomponent0 (type(bml_matrix_t), intent(in) *rho_bml,* type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(inout) *pcm_bml,* real(dp), intent(in) *threshold,* integer, intent(in) *M,* character(20), intent(in) *bml_type,* integer *verbose*)

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

Parameters

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

Todo M and bml_type will have to be removed from the input parameter.

Definition at line 32 of file prg_pulaycomponent_mod.F90.

9.20.2.3 subroutine, public prg_pulaycomponent_mod::prg_pulaycomponentt (type(bml_matrix_t), intent(in) *rho_bml,* type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(in) *zmat_bml,* type(bml_matrix_t), intent(inout) *pcm_bml,* real(dp), intent(in) *threshold,* integer, intent(in) *M,* character(20), intent(in) *bml_type,* integer *verbose*)

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

Parameters

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

Todo M and bml_type will have to be removed from the input parameter.

Definition at line 83 of file prg_pulaycomponent_mod.F90.

9.20.3 Variable Documentation

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

Definition at line 13 of file prg_pulaycomponent_mod.F90.

9.21 prg_pulaymixer_mod Module Reference

Pulay mixer mode.

Data Types

- type mx_type

Functions/Subroutines

- subroutine, public prg_parse_mixer (input, filename)

  The parser for the mixer routines.
- subroutine, public prg_qmixer (charges, oldcharges, dqin, dqout, scferror, piter, pulaycoef, mpulay, verbose)

  Mixing the charges to acelerate scf convergence.
- subroutine, public prg_linearmixer (charges, oldcharges, scferror, linmixcoef, verbose)

  Routine to perform linear mixing.

Variables

- integer, parameter dp = kind(1.0d0)

9.21.1 Detailed Description

Pulay mixer mode.

Gets the best coefficient for mixing the charges during scf.

Todo add the density matrix mixer.

9.21.2 Function/Subroutine Documentation

9.21.2.1 subroutine, public prg_pulaymixer_mod::prg_linearmixer (real(dp), dimension(:), intent(inout), allocatable *charges,* real(dp), dimension(:), intent(inout), allocatable *oldcharges,* real(dp), intent(inout) *scferror,* real(dp), intent(in) *linmixcoef,* integer, intent(in) *verbose*)

Routine to perform linear mixing.

Parameters

charges	Actual charges of the system.
oldcharges	Previous scf charges.
scferror	SCF error.
linmixcoef	Mixing coefficient.
verbose	Verbosity level.

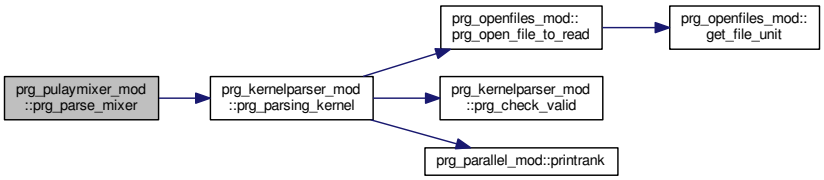
Definition at line 237 of file prg_pulaymixer_mod.F90.

9.21.2.2 subroutine, public prg_pulaymixer_mod::prg_parse_mixer (type(mx_type), intent(inout) *input,* character(len=∗) *filename*)

The parser for the mixer routines.

Definition at line 42 of file prg_pulaymixer_mod.F90.

Here is the call graph for this function:



9.21.2.3 subroutine, public prg_pulaymixer_mod::prg_qmixer (real(dp), dimension(:), intent(inout) *charges,* real(dp), dimension(:), intent(inout), allocatable *oldcharges,* real(dp), dimension(:,:), intent(inout), allocatable *dqin,* real(dp), dimension(:,:), intent(inout), allocatable *dqout,* real(dp), intent(inout) *scferror,* integer *piter,* real(dp), intent(in) *pulaycoef,* integer, intent(in) *mpulay,* integer, intent(in) *verbose*)

Mixing the charges to acelerate scf convergence.

Parameters

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

Definition at line 103 of file prg_pulaymixer_mod.F90.

9.21.3 Variable Documentation

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

Definition at line 14 of file prg_pulaymixer_mod.F90.

9.22 prg_quantumdynamics_mod Module Reference

A module to add in common quantum dynamical operations.

Functions/Subroutines

- subroutine, public prg_kick_density (kick_direc, 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: $\rho_{\hat{kick}} = \exp \frac{-i}{\hbar}\hat{V}\hat{\rho}\hat{S} \exp \frac{i}{\hbar}\hat{V}\hat{S^{-1}}$ *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_direc, 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 matricies in BML format. This routine does: $\rho_{\hat{kick}} = \exp \frac{-i}{\hbar}\hat{V}\hat{\rho}\hat{S} \exp \frac{i}{\hbar}\hat{V}\hat{S^{-1}}$ *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:* $\frac{\partial \hat{\rho}(t)}{\partial t} = \frac{-i}{\hbar}\left(S^{-1}\hat{H}(t)\hat{\rho}(t) - \hat{\rho}(t)\hat{H}(t)S^{-1}\right)$.
- 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_exci)

  Produce an excitation in the initially calculated density matrix to.

Variables

- integer, parameter dp = kind(1.0d0)

9.22.1 Detailed Description

A module to add in common quantum dynamical operations.

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

Author

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Alicia Rae Welden (welden@lanl.gov)

9.22.2 Function/Subroutine Documentation

9.22.2.1 subroutine, public prg_quantumdynamics_mod::prg_excitation (integer, dimension(:), intent(inout) *fill_mat,* integer, intent(in) *orbit_orig,* integer, intent(in) *orbit_exci*)

Produce an excitation in the initially calculated density matrix to.

Definition at line 312 of file prg_quantumdynamics_mod.F90.

9.22.2.2 subroutine, public prg_quantumdynamics_mod::prg_get_sparsity_cplxmat (character(len=$*$), intent(in) *matrix_type,* character(len=$*$), intent(in) *element_type,* real(dp), intent(in) *thresh,* complex(dp), dimension(:,:), intent(in) *a_dense*)

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

Parameters

matrix_type	the BML matrix type
element_type	the BML element type
thresh	the threshold for sparsity evaluation
a_dense	the dense complex matrix to be evaluated for sparsity

Definition at line 103 of file prg_quantumdynamics_mod.F90.

9.22.2.3 subroutine, public prg_quantumdynamics_mod::prg_get_sparsity_realmat (character(len=$*$), intent(in) *matrix_type,* character(len=$*$), intent(in) *element_type,* real(dp), intent(in) *thresh,* real(dp), dimension(:,:), intent(in) *a_dense*)

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

Parameters

matrix_type	the BML matrix type
element_type	the BML element type
thresh	the threshold for sparsity evaluation
a_dense	the dense real matrix to be evaluated for sparsity

Definition at line 127 of file prg_quantumdynamics_mod.F90.

9.22.2.4 subroutine, public prg_quantumdynamics_mod::prg_getcharge (type(bml_matrix_t), intent(in) *rho_bml,* type(bml_matrix_t), intent(in) *s_bml,* real(dp), dimension(:), allocatable *charges,* type(bml_matrix_t) *aux_bml,* real(dp), dimension(:), intent(in) *z,* integer, dimension(:), intent(in), allocatable *spindex,* integer, dimension(:), intent(in), allocatable *N,* integer *nats,* real(dp), intent(in) *thresh*)

Constructs the charges from the density matrix.

Parameters

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

Definition at line 252 of file prg_quantumdynamics_mod.F90.

9.22.2.5 subroutine, public prg_quantumdynamics_mod::prg_getdipole (real(dp), dimension(:), intent(in) *charges,* real(dp), dimension(:,:), intent(in) *r,* real(dp), dimension(3), intent(inout) *mu*)

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

Parameters

charges	Charge on each atom.
r	Coordinate matrix of the atoms.
p	Dipole moment vector.

Definition at line 287 of file prg_quantumdynamics_mod.F90.

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

Parameters

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

Definition at line 48 of file prg_quantumdynamics_mod.F90.

9.22.2.7 subroutine, public prg_quantumdynamics_mod::prg_kick_density_bml (integer, intent(in) *kick_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 matricies in BML format. This routine does: $\rho_{\hat{kick}} = \exp \frac{-i}{\hbar}\hat{V}\hat{\rho}\hat{S} \exp \frac{i}{\hbar}\hat{V}\hat{S^{-1}}$ where $\hat{V}$ is the field disturbance.

Parameters

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

Definition at line 159 of file prg_quantumdynamics_mod.F90.

9.22.2.8 subroutine, public prg_quantumdynamics_mod::prg_lvni_bml (type(bml_matrix_t) *h1_bml,* type(bml_matrix_t) *sinv_bml,* real(**dp**) *dt,* real(**dp**) *hbar,* type(bml_matrix_t) *rhoold_bml,* type(bml_matrix_t) *rho_bml,* type(bml_matrix_t) *aux_bml,* character(len=$*$), intent(in) *matrix_type,* integer *mdim,* real(**dp**), intent(in) *thresh*)

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

Parameters

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

Definition at line 216 of file prg_quantumdynamics_mod.F90.

9.22.3 Variable Documentation

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

Definition at line 19 of file prg_quantumdynamics_mod.F90.

9.23 prg_response_mod Module Reference

Module to compute the density matrix response and related quantities.

Data Types

- type respdata_type

Functions/Subroutines

- subroutine, public prg_parse_response (RespData, filename)

  The parser for the calculation of the DM response.
- subroutine, public prg_compute_dipole (charges, coordinate, dipoleMoment, factor, verbose)

  To compute the dipole moment of the system. The units of the dipole moment are determined by the units of the coordinates and charges that are given.
- subroutine, public prg_write_dipole_tcl (dipoleMoment, file, factor, verbose)

  To visualize a dipole moment using VMD. This will prg_generate a .tcl script that could be run using VMD To visualize with VMD: $ vmd -e dipole.tcl.
- subroutine, public prg_compute_polarizability (rsp_bml, prt_bml, polarizability, factor, verbose)

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

  Read perturbation from file.
- subroutine, public prg_compute_response_rs (ham_bml, prt_bml, rsp_bml, lambda, bndfil, threshold, verbose)

  Computes the first order response density matrix using Rayleigh Schrodinger Perturbation theory The transformation hereby performed are:
- subroutine, public prg_compute_response_fd (ham_bml, prt_bml, rsp_bml, prg_delta, bndfil, threshold, verbose)

  Computes the first order response density matrix using finite differences. The transformation hereby performed are:
- subroutine, public prg_pert_constant_field (field, intensity, coordinate, lambda, prt_bml, threshold, spindex, norbi, verbose, over_bml)

  Apply a constant field perturbation through the dipole moment operator ($\hat{\mu} = e\hat{\boldsymbol{r}}$). In the matrix representation, this is: $H^{(1)} = \lambda\frac{1}{2}(\, S\, e\boldsymbol{r}\cdot\boldsymbol{E} + e\boldsymbol{r}\cdot\boldsymbol{E}S)$. 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 ($\sin(\tilde{\boldsymbol{r}}_x)$) where $\boldsymbol{r}_x$ is the x coordinate. The Hamiltonian gets modified as follows: $H^{(1)} = \frac{1}{2}\lambda(S\sin(\tilde{\boldsymbol{r}}_x) + \sin(\tilde{\boldsymbol{r}}_x)S)$. $\tilde{\boldsymbol{r}}_x = 2\pi(\boldsymbol{r}/l_x) - \pi$. 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 ($\cos(\tilde{\mathbf{r}}_x)$) 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.
- subroutine, public prg_compute_response_sp2 (ham_bml, prt_bml, rsp_bml, rho_bml, lambda, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, 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: $rsp(i) = \sum_{\alpha \in i} \rho^{(1)}_{\alpha\alpha}$, where orbital α belong to atom i.

Variables

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

9.23.1 Detailed Description

Module to compute the density matrix response and related quantities.

Todo Add the response scf

Change name response_SP2 to dm_prt_response

Change name response_rs to rs_prt_response

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

9.23.2 Function/Subroutine Documentation

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

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

Parameters

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

Definition at line 120 of file prg_response_mod.F90.

9.23.2.2 subroutine, public prg_response_mod::prg_compute_polarizability (type(bml_matrix_t), intent(in) *rsp_bml,* type(bml_matrix_t), intent(in) *prt_bml,* real(dp), intent(inout) *polarizability,* real(dp), intent(in) *factor,* integer *verbose*)

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

Parameters

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

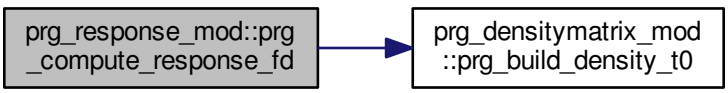
Definition at line 198 of file prg_response_mod.F90.

9.23.2.3 subroutine, public prg_response_mod::prg_compute_response_fd (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(in) *prt_bml,* type(bml_matrix_t), intent(inout) *rsp_bml,* real(dp) *prg_delta,* real(dp), intent(in) *bndfil,* real(dp), intent(in) *threshold,* integer *verbose*)

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

Definition at line 379 of file prg_response_mod.F90.

Here is the call graph for this function:



9.23.2.4 subroutine, public prg_response_mod::prg_compute_response_rs (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(in) *prt_bml,* type(bml_matrix_t), intent(inout) *rsp_bml,* real(dp) *lambda,* real(dp), intent(in) *bndfil,* real(dp), intent(in) *threshold,* integer *verbose*)

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

Definition at line 249 of file prg_response_mod.F90.

9.23.2.5 subroutine, public prg_response_mod::prg_compute_response_sp2 (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(in) *prt_bml,* type(bml_matrix_t), intent(inout) *rsp_bml,* type(bml_matrix_t), intent(inout) *rho_bml,* real(dp) *lambda,* real(dp), intent(in) *bndfil,* integer, intent(in) *minsp2iter,* integer, intent(in) *maxsp2iter,* character(len=$*$), intent(in) *sp2conv,* real(dp), intent(in) *idemtol,* real(dp), intent(in) *threshold,* integer *verbose*)

Finds the first order response matrix from a Hamiltonian matrix.

Definition at line 652 of file prg_response_mod.F90.

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

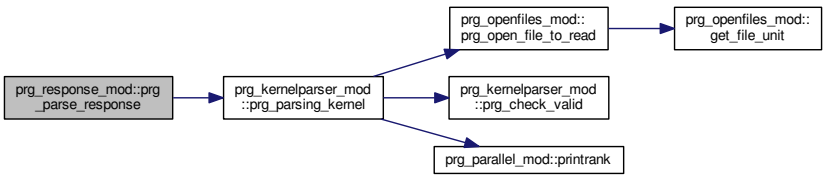
The parser for the calculation of the DM response.

Parameters

RespData	Response data type.
filename	Name of the file to parse.

Definition at line 45 of file prg_response_mod.F90.

Here is the call graph for this function:



9.23.2.7 subroutine, public prg_response_mod::prg_pert_constant_field (real(dp), dimension(3), intent(in) *field,* real(dp) *intensity,* real(dp), dimension(:,:), intent(in) *coordinate,* real(dp) *lambda,* type(bml_matrix_t), intent(inout) *prt_bml,* real(dp) *threshold,* integer, dimension(:), intent(in) *spindex,* integer, dimension(:), intent(in) *norbi,* integer, intent(in) *verbose,* type(bml_matrix_t), intent(in), optional *over_bml*)

Apply a constant field perturbation through the dipole moment operator ($\hat{\mu} = e\hat{\mathbf{r}}$). In the matrix representation, this is: $H^{(1)} = \lambda\frac{1}{2}(S\, e\mathbf{r}\cdot\mathbf{E} + e\mathbf{r}\cdot\mathbf{E}S)$. 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.

Note

If the Hamiltonian is already in the prg_orthogonalized form, then parameter over_bml can be omitted.

Parameters

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

Definition at line 446 of file prg_response_mod.F90.

9.23.2.8 subroutine, public prg_response_mod::prg_pert_cos_pot (character *direction,* real(dp) *lx,* real(dp), dimension(:,:), intent(in) *coordinate,* real(dp) *lambda,* type(bml_matrix_t), intent(inout) *prt_bml,* real(dp) *threshold,* integer, dimension(:), intent(in) *spindex,* integer, dimension(:), intent(in) *norbi,* integer, intent(in) *verbose,* type(bml_matrix_t), intent(in), optional *over_bml*)

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

Note

If the Hamiltonian is already in the prg_orthogonalized form, then parameter over_bml can be omitted.

Parameters

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

Definition at line 591 of file prg_response_mod.F90.

9.23.2.9 subroutine, public prg_response_mod::prg_pert_from_file (type(bml_matrix_t), intent(inout) *prt_bml,* integer *norb*)

Read perturbation from file.

Todo Add read perturbation from file

Definition at line 223 of file prg_response_mod.F90.

9.23.2.10 subroutine, public prg_response_mod::prg_pert_sin_pot (character *direction,* real(dp) *lx,* real(dp), dimension(:,:), intent(in) *coordinate,* real(dp) *lambda,* type(bml_matrix_t), intent(inout) *prt_bml,* real(dp) *threshold,* integer, dimension(:), intent(in) *spindex,* integer, dimension(:), intent(in) *norbi,* integer, intent(in) *verbose,* type(bml_matrix_t), intent(in), optional *over_bml*)

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

Note

If the Hamiltonian is already in the prg_orthogonalized form, then parameter over_bml can be omitted.

Parameters

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

Definition at line 523 of file prg_response_mod.F90.

9.23.2.11 subroutine, public prg_response_mod::prg_project_response (type(bml_matrix_t), intent(inout) *rsp_bml,* type(bml_matrix_t), intent(in) *over_bml,* integer, dimension(:), intent(in) *spindex,* integer, dimension(:), intent(in) *norbi,* real(dp), dimension(:,:), intent(in) *coordinates,* real(dp), dimension(:), intent(inout), allocatable *rspfunc,* integer, intent(in) *verbose*)

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

Parameters

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

Definition at line 795 of file prg_response_mod.F90.

9.23.2.12 subroutine, public prg_response_mod::prg_write_dipole_tcl (real(dp), dimension(3), intent(in) *dipoleMoment,* character(∗), intent(in) *file,* real(dp), intent(in) *factor,* integer *verbose*)

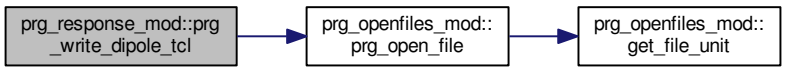
To visualize a dipole moment using VMD. This will prg_generate a .tcl script that could be run using VMD To visualize with VMD: $ vmd -e dipole.tcl.

Parameters

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

Definition at line 158 of file prg_response_mod.F90.

Here is the call graph for this function:



9.23.3 Variable Documentation

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

Definition at line 18 of file prg_response_mod.F90.

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

Definition at line 19 of file prg_response_mod.F90.

9.24 prg_sp2_fermi_mod Module Reference

The SP2 Fermi module.

Functions/Subroutines

- subroutine, public prg_sp2_fermi_init (h_bml, nsteps, nocc, tscale, threshold, occErrLimit, traceLimit, x_bml, mu, beta, h1, hN, sgnlist)

  Truncated SP2 prg_initialization.
- subroutine, public prg_sp2_fermi_init_norecs (h_bml, nsteps, nocc, tscale, threshold, occErrLimit, traceLimit, x_bml, mu, beta, h1, hN, sgnlist, verbose)

  Truncated SP2 prg_initialization. This routine also gives back the Number of SP2 recursive steps that gets a Pseudo-Fermi distribution with a temperature close to the target temperature which is entered using parameter beta = (1/KbT).
- subroutine, public prg_sp2_fermi (h_bml, osteps, nsteps, nocc, mu, beta, h1, hN, sgnlist, threshold, eps, traceLimit, x_bml)

  Calculate Truncated SP2.
- subroutine, public prg_sp2_entropy_function (mu, h1, hN, nsteps, sgnlist, GG, ee)

  Calculate SP2 entropy function using gaussian quadrature. Note that GG and ee are allocated and returned from this routine.
- real(dp) function, public sp2_entropy_ts (D0_bml, GG, ee)

  Test SP2 entropy. Get the entropy contribution TS to the total free energy.
- real(dp) function, public sp2_inverse (f, mu, h1, hN, nsteps, sgnlist)

  Calculate the SP2 inverse.
- real(dp) function absmaxderivative (func, de)

  Gets the absolute maximum of the derivative of a function.

Variables

- integer, parameter dp = kind(1.0d0)

9.24.1 Detailed Description

The SP2 Fermi module.

9.24.2 Function/Subroutine Documentation

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

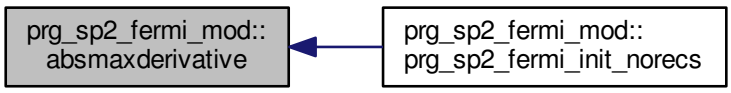
Gets the absolute maximum of the derivative of a function.

Parameters

func.	
de	Energy step.

Definition at line 615 of file prg_sp2_fermi_mod.F90.

Here is the caller graph for this function:



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

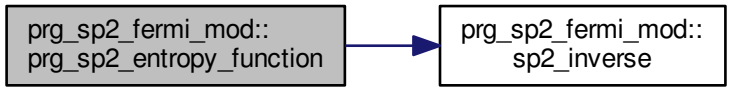
Calculate SP2 entropy function using gaussian quadrature. Note that GG and ee are allocated and returned from this routine.

Parameters

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

Definition at line 480 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



9.24.2.3 subroutine, public prg_sp2_fermi_mod::prg_sp2_fermi (type(bml_matrix_t), intent(in) *h_bml,* integer, intent(in) *osteps,* integer, intent(in) *nsteps,* real(dp), intent(in) *nocc,* real(dp), intent(inout) *mu,* real(dp), intent(inout) *beta,* real(dp), intent(inout) *h1,* real(dp), intent(inout) *hN,* integer, dimension(:), intent(in) *sgnlist,* real(dp), intent(in) *threshold,* real(dp), intent(in) *eps,* real(dp), intent(in) *traceLimit,* type(bml_matrix_t), intent(inout) *x_bml*)

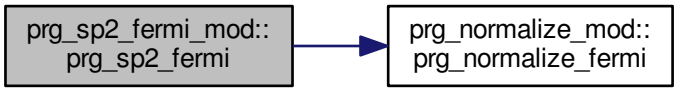
Calculate Truncated SP2.

Parameters

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

Definition at line 387 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



9.24.2.4 subroutine, public prg_sp2_fermi_mod::prg_sp2_fermi_init (type(bml_matrix_t), intent(in) *h_bml,* integer, intent(in) *nsteps,* real(**dp**), intent(in) *nocc,* real(**dp**), intent(in) *tscale,* real(**dp**), intent(in) *threshold,* real(**dp**), intent(in) *occErrLimit,* real(**dp**), intent(in) *traceLimit,* type(bml_matrix_t), intent(inout) *x_bml,* real(**dp**), intent(inout) *mu,* real(**dp**), intent(inout) *beta,* real(**dp**), intent(inout) *h1,* real(**dp**), intent(inout) *hN,* integer, dimension(:), intent(inout) *sgnlist*)

Truncated SP2 prg_initialization.

Parameters

h_bml	Input Hamiltonian matrix.
nsteps	Number of sp2 iterations.
nocc	Number of occupied states.
tscale	Temperature rescaling factor.
threshold	Threshold for multiplication.
occErrLimit	Occupation error limit.
traceLimit	Trace limit.
x_bml	Output prg_initial matrix.
mu	Shifted chemical potential

Parameters

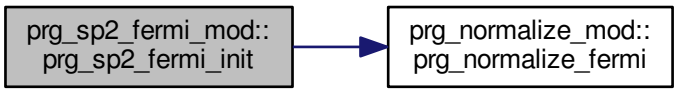
beta	Output inverse temperature.
h1	Output temperature-scaled minimum gershgorin bound.
hN	Output temperature-scaled maximum gershgorin bound.
sgnlist	SP2 sequence

Calculate Gershgorin bounds and rescale

Determine sequence branching first time through

Definition at line 46 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



9.24.2.5 subroutine, public prg_sp2_fermi_mod::prg_sp2_fermi_init_norecs (type(bml_matrix_t), intent(in) *h_bml,* integer, intent(inout) *nsteps,* real(dp), intent(in) *nocc,* real(dp), intent(in) *tscale,* real(dp), intent(in) *threshold,* real(dp), intent(in) *occErrLimit,* real(dp), intent(in) *traceLimit,* type(bml_matrix_t), intent(inout) *x_bml,* real(dp), intent(inout) *mu,* real(dp), intent(inout) *beta,* real(dp), intent(inout) *h1,* real(dp), intent(inout) *hN,* integer, dimension(:), intent(inout) *sgnlist,* integer, optional *verbose*)

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

Parameters

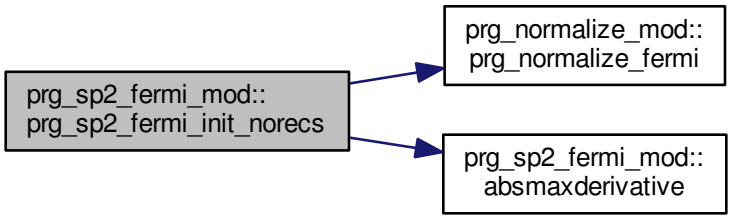
h_bml	Input Hamiltonian matrix.
nsteps	Output number of sp2 iterations.
nocc	Number of occupied states.
tscale	Temperature rescaling factor.
threshold	Threshold for multiplication.
occErrLimit	Occupation error limit.
traceLimit	Trace limit.
x_bml	Output prg_initial matrix.
mu	Shifted chemical potential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

Calculate Gershgorin bounds and rescale

Determine sequence branching first time through

Definition at line 201 of file prg_sp2_fermi_mod.F90.

Here is the call graph for this function:



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

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

Parameters

D0_bml	BML matrix
GG	Entropy function
ee	1D mesh
TS	Energy contribution

Definition at line 538 of file prg_sp2_fermi_mod.F90.

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

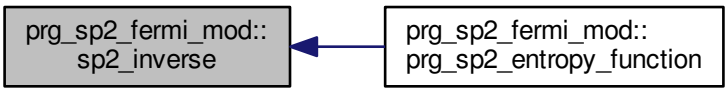
Calculate the SP2 inverse.

Parameters

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

Definition at line 590 of file prg_sp2_fermi_mod.F90.

Here is the caller graph for this function:



9.24.3 Variable Documentation

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

Definition at line 19 of file prg_sp2_fermi_mod.F90.

9.25 prg_sp2_mod Module Reference

The SP2 module.

Functions/Subroutines

- subroutine, public prg_sp2_basic (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)

  Calculates the density matrix from a Hamiltonian matrix by purification. The method implemented here is the very first verion of the SP2 method.
- subroutine, public prg_sp2_alg2 (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)
- subroutine, public prg_sp2_alg2_genseq (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, pp, icount, vv, verbose)
- subroutine, public prg_sp2_alg2_seq (h_bml, rho_bml, threshold, pp, icount, vv, verbose)
- subroutine, public prg_prg_sp2_alg2_seq_inplace (rho_bml, threshold, pp, icount, vv, mineval, maxeval, verbose)
- subroutine, public prg_sp2_alg1 (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)
- subroutine, public prg_sp2_alg1_genseq (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, pp, icount, vv)
- subroutine, public prg_sp2_alg1_seq (h_bml, rho_bml, threshold, pp, icount, vv)
- subroutine, public prg_prg_sp2_alg1_seq_inplace (rho_bml, threshold, pp, icount, vv, mineval, maxeval)
- subroutine, public prg_sp2_submatrix (ham_bml, rho_bml, threshold, pp, icount, vv, mineval, maxeval, core↩_size)

  Perform SP2 algorithm using sequence and calculate norm for a submatrix.
- subroutine, public prg_sp2_submatrix_inplace (rho_bml, threshold, pp, icount, vv, mineval, maxeval, core_↩size)

Variables

- integer, parameter dp = kind(1.0d0)

9.25.1 Detailed Description

The SP2 module.

Author

S. Mniszewski (smn@lanl.gov)

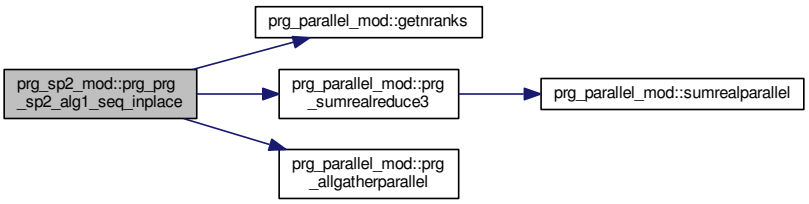
This subroutine implements Niklasson's SP2 density matrix purification algorithm.

9.25.2 Function/Subroutine Documentation

9.25.2.1 subroutine, public prg_sp2_mod::prg_prg_sp2_alg1_seq_inplace (type(bml_matrix_t), intent(inout) *rho_bml,* real(dp), intent(in) *threshold,* integer, dimension(:), intent(inout) *pp,* integer, intent(inout) *icount,* real(dp), dimension(:), intent(inout) *vv,* real(dp), intent(in) *mineval,* real(dp), intent(in) *maxeval*)

Definition at line 971 of file prg_sp2_mod.F90.

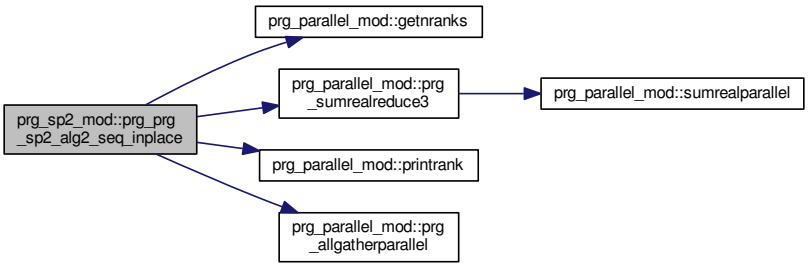
Here is the call graph for this function:



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

Definition at line 528 of file prg_sp2_mod.F90.

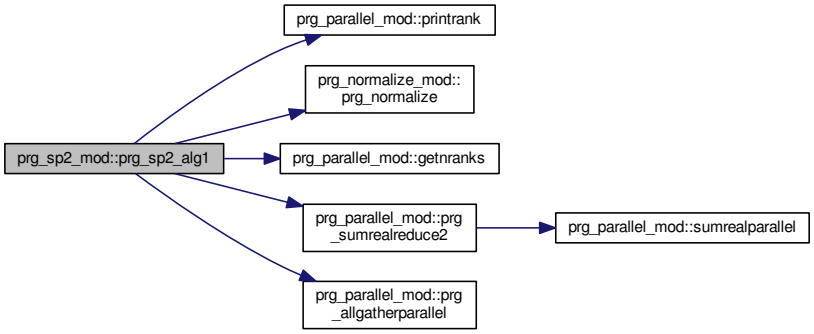
Here is the call graph for this function:



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

Definition at line 624 of file prg_sp2_mod.F90.

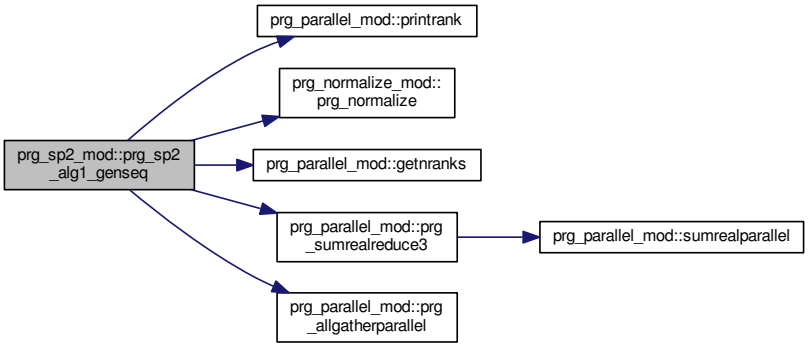
Here is the call graph for this function:



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

Definition at line 751 of file prg_sp2_mod.F90.

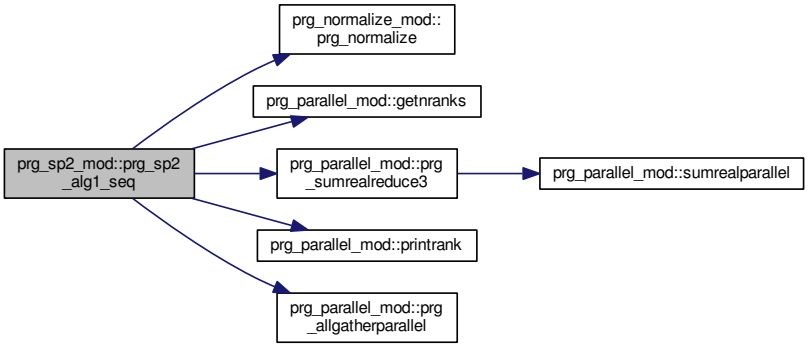
Here is the call graph for this function:



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

Definition at line 880 of file prg_sp2_mod.F90.

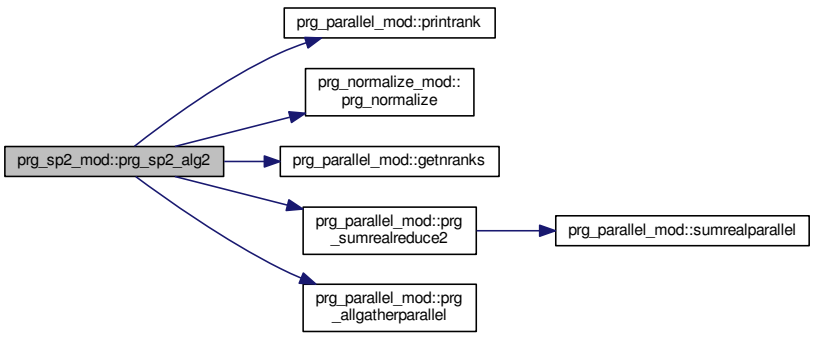
Here is the call graph for this function:



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

Definition at line 153 of file prg_sp2_mod.F90.

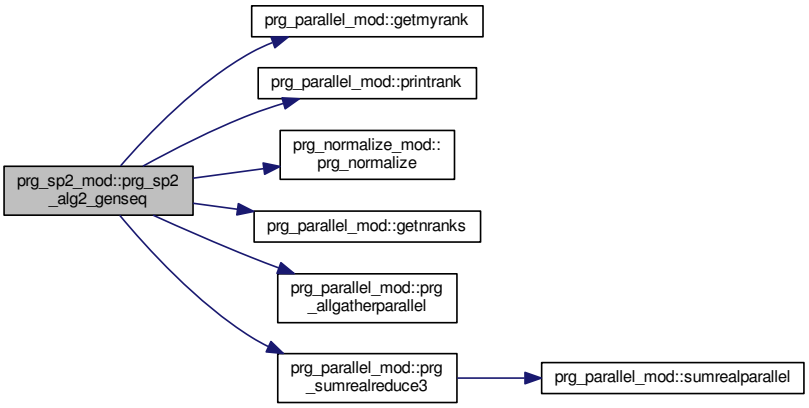
Here is the call graph for this function:



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

Definition at line 285 of file prg_sp2_mod.F90.

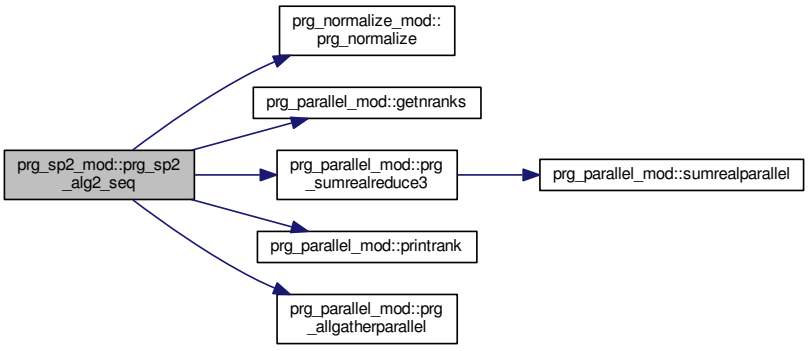
Here is the call graph for this function:



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

Definition at line 432 of file prg_sp2_mod.F90.

Here is the call graph for this function:



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

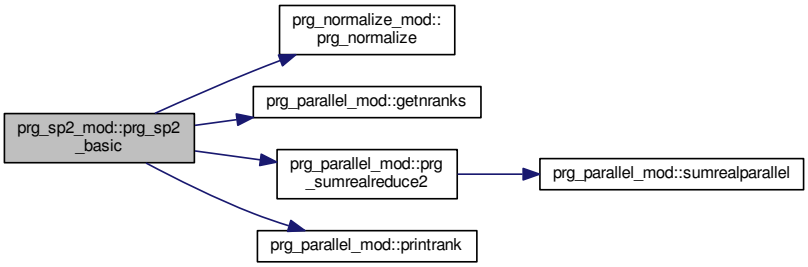
Calculates the density matrix from a Hamiltonian matrix by purification. The method implemented here is the very first verion of the SP2 method.

Parameters

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

Definition at line 52 of file prg_sp2_mod.F90.

Here is the call graph for this function:



9.25.2.10 subroutine, public prg_sp2_mod::prg_sp2_submatrix (type(bml_matrix_t), intent(in) *ham_bml,* type(bml_matrix_t), intent(inout) *rho_bml,* real(dp), intent(in) *threshold,* integer, dimension(:), intent(in) *pp,* integer, intent(in) *icount,* real(dp), dimension(:), intent(inout) *vv,* real(dp), intent(in) *mineval,* real(dp), intent(in) *maxeval,* integer, intent(in) *core_size*)

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

Parameters

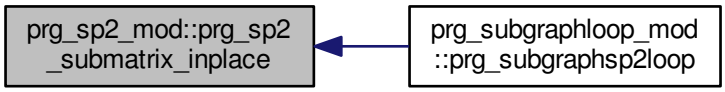
rho_bml	Input Hamiltonian/Output density matrix
threshold	Threshold for sparse matrix algebra
pp	Vector containing sequence of 0s and 1s
icount	Sequence count
vv	Vector of sum of squares per iteration
mineval	Min value used for normalization (optional)
maxeval	Max value used for normalization (optional)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

Definition at line 1061 of file prg_sp2_mod.F90.

9.25.2.11 subroutine, public prg_sp2_mod::prg_sp2_submatrix_inplace (type(bml_matrix_t), intent(inout) *rho_bml,* real(dp), intent(in) *threshold,* integer, dimension(:), intent(inout) *pp,* integer, intent(inout) *icount,* real(dp), dimension(:), intent(inout) *vv,* real(dp), intent(in) *mineval,* real(dp), intent(in) *maxeval,* integer, intent(in) *core_size*)

Definition at line 1130 of file prg_sp2_mod.F90.

Here is the caller graph for this function:



9.25.3 Variable Documentation

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

Definition at line 21 of file prg_sp2_mod.F90.

9.26 prg_sp2parser_mod Module Reference

SP2 parser.

Data Types

- type sp2data_type

  General SP2 solver type.

Functions/Subroutines

- subroutine, public prg_parse_sp2 (sp2data, filename)

  The parser for SP2 solver.

Variables

- integer, parameter dp = kind(1.0d0)

9.26.1 Detailed Description

SP2 parser.

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

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

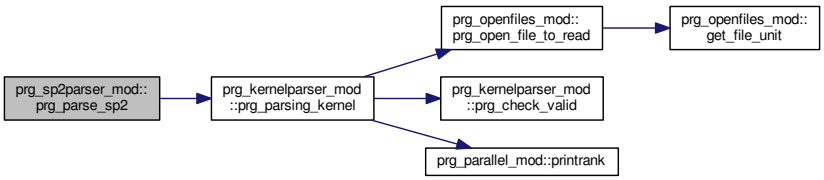
9.26.2 Function/Subroutine Documentation

9.26.2.1 subroutine, public prg_sp2parser_mod::prg_parse_sp2 (type(sp2data_type), intent(inout) *sp2data,* character(len=∗) *filename*)

The parser for SP2 solver.

Definition at line 50 of file prg_sp2parser_mod.F90.

Here is the call graph for this function:



9.26.3 Variable Documentation

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

Definition at line 22 of file prg_sp2parser_mod.F90.

9.27 prg_subgraphloop_mod Module Reference

The subgraphloop module.

Functions/Subroutines

- subroutine, public prg_subgraphsp2loop (h_bml, g_bml, rho_bml, gp, threshold)
- subroutine, public prg_collectmatrixfromparts (gp, rho_bml)

  Collect distributed parts into same matrix.
- subroutine, public prg_balanceparts (gp)
- subroutine, public prg_partordering (gp)

  Set row ordering bases on parts.
- subroutine, public prg_getgrouppartitionhalosfromgraph (gp, g_bml, hnode, djflag)

  Get core+halo indeces for all partitions only using the graph.
- subroutine, public prg_getpartitionhalosfromgraph (gp, g_bml, djflag)

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

Variables

- integer, parameter dp = kind(1.0d0)

9.27.1 Detailed Description

The subgraphloop module.

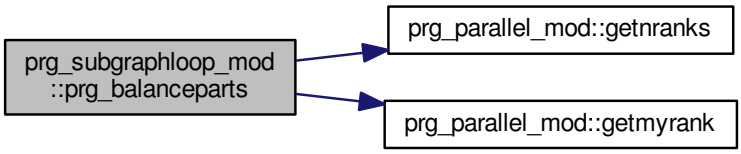
9.27.2 Function/Subroutine Documentation

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

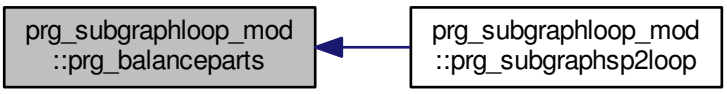
Renumber parts Handle unbalanced numbers of parts.

Definition at line 165 of file prg_subgraphloop_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



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

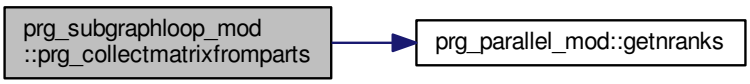
Collect distributed parts into same matrix.

Parameters

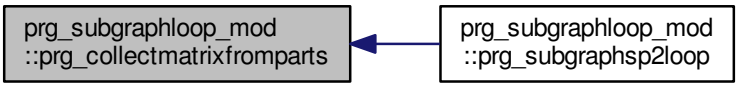
gp	Graph partitioning
rho_bml	Matrix to be collected into

Definition at line 133 of file prg_subgraphloop_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.27.2.3 subroutine, public prg_subgraphloop_mod::prg_getgrouppartitionhalosfromgraph (type (graph_partitioning_t), intent(inout) *gp,* type (bml_matrix_t), intent(in) *g_bml,* integer, dimension(∗), intent(in) *hnode,* logical, intent(in) *djflag*)

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

Parameters

gp	Graph partitioning
g_bml	Graph
hnode	Group start indeces
djflg	Double jump flag (true/false)

Determine halo elements for each subgraph

Definition at line 292 of file prg_subgraphloop_mod.F90.

9.27.2.4 subroutine, public prg_subgraphloop_mod::prg_getpartitionhalosfromgraph (type (graph_partitioning_t), intent(inout) *gp,* type (bml_matrix_t), intent(in) *g_bml,* logical, intent(in) *djflag*)

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

Parameters

gp	Graph partitioning
g_bml	Graph
djflg	Double jump flag (true/false)

Determine halo elements for each subgraph

Definition at line 337 of file prg_subgraphloop_mod.F90.

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

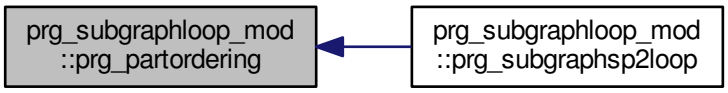
Set row ordering bases on parts.

Parameters

gp	Graph partitioning

Definition at line 263 of file prg_subgraphloop_mod.F90.

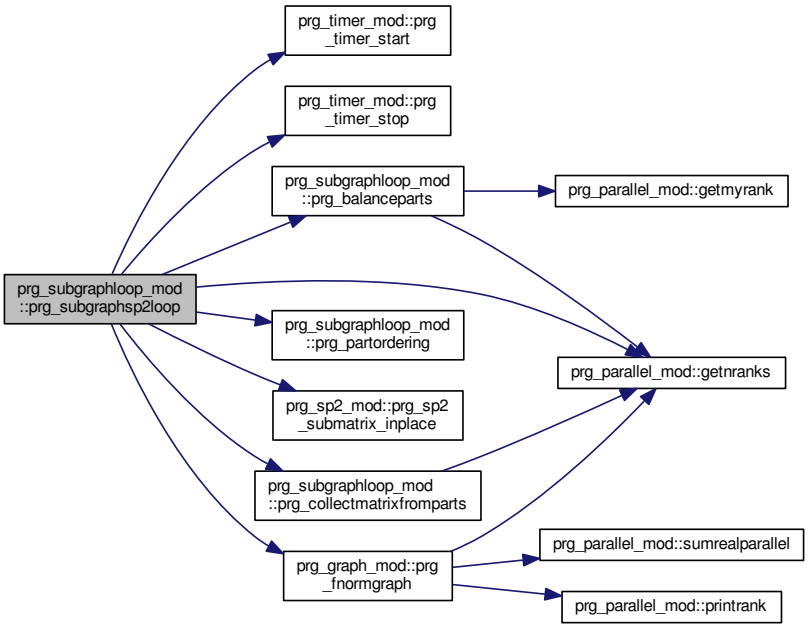
Here is the caller graph for this function:



9.27.2.6 subroutine, public prg_subgraphloop_mod::prg_subgraphsp2loop (type (bml_matrix_t), intent(in) *h_bml,* type (bml_matrix_t), intent(in) *g_bml,* type (bml_matrix_t), intent(inout) *rho_bml,* type (graph_partitioning_t), intent(inout) *gp,* real(dp), intent(in) *threshold*)

Definition at line 37 of file prg_subgraphloop_mod.F90.

Here is the call graph for this function:



9.27.3 Variable Documentation

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

Definition at line 18 of file prg_subgraphloop_mod.F90.

9.28 prg_syrotation_mod Module Reference

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

Data Types

- type rotation_type

  Rotation type.

Functions/Subroutines

- subroutine, public prg_parse_rotation (rot, filename)

  The parser for rotation.
- subroutine, public prg_rotate (rot, r, verbose)

  Rotation routine.

Variables

- integer, parameter dp = kind(1.0d0)

9.28.1 Detailed Description

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

It works by specifying two orientations and a rotation point.

Author

C. F. A. Negre (cnegre@lanl.gov)

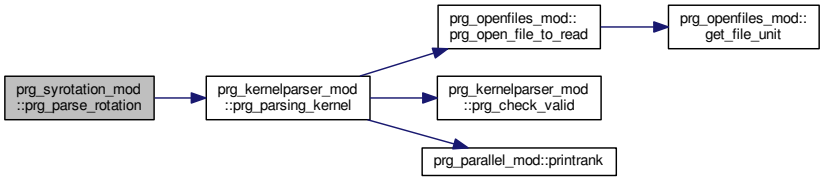
9.28.2 Function/Subroutine Documentation

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

The parser for rotation.

Definition at line 49 of file prg_syrotation_mod.F90.

Here is the call graph for this function:



9.28.2.2 subroutine, public prg_syrotation_mod::prg_rotate (type(rotation_type), intent(in) *rot,* real(dp), dimension(:,:), intent(inout) *r,* integer, intent(in) *verbose*)

Rotation routine.

It works by indicating the orientations (v1 and v1) and a rotation center. The orientation can be passed either directly by setting v1 and v2 or by indicating two points pQ1 and pQ2. Orientation can also be specified with an atom position if patom1 and patom2 indices are not zero this atoms are used to determine the initial and final orientation.

Parameters

rot	Rotation type
r	Coordinates to be rotated
verbose	Verbosity level

Example:

```
rot%patom1 = 4
rot%patom2 = 0
rot%catom2 = 6
rot%v2 = 0.0 ; rot%v2(1) = 1
call prg_rotate(rot,r)
```

The latter will orient the system such that atom 4 points to the (1,0,0) direction.

Definition at line 142 of file prg_syrotation_mod.F90.

9.28.3 Variable Documentation

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

Definition at line 14 of file prg_syrotation_mod.F90.

9.29 prg_system_mod Module Reference

A module to read and handle chemical systems.

Data Types

- type estruct_type

  Electronic structure type.
- type system_type

  System type.

Functions/Subroutines

- subroutine, public prg_get_nameandext (fullfilename, filename, ext)

  Get the name and extension of a file.
- subroutine, public prg_parse_system (system, filename, extin)

  The parser for the chemical system.
- subroutine, public prg_write_system (system, filename, extension)

  Write system in .xyz, .dat or pdb file.
- subroutine, public prg_write_trajectory (system, iter, each, prg_deltat, filename, extension)

  Write trajectory in .xyz, .dat or pdb file.
- subroutine, public prg_write_trajectoryandproperty (system, iter, each, prg_deltat, scalarprop, filename, extension)

  Write trajectory and atomic properties. Only pdb file.
- subroutine, public prg_make_random_system (system, nats, seed, lx, ly, lz)

  Make random Xx system.
- subroutine prg_parameters_to_vectors (abc_angles, lattice_vector)

  Transforms the lattice parameters into lattice vectors.
- subroutine prg_vectors_to_parameters (lattice_vector, abc_angles)

Transforms the lattice vectors into lattice parameters.

- subroutine, public prg_get_origin (coords, origin)

  Get the origin of the coordinates.
- subroutine, public prg_get_distancematrix (coords, dmat)

  Get the distance matrix.
- subroutine, public prg_translateandfoldtobox (coords, lattice_vectors, origin, verbose)

  Translate and fold to box.
- subroutine, public prg_centeratbox (coords, lattice_vectors, verbose)

  Translate geometric center to the center of the box.
- subroutine, public prg_wraparound (coords, lattice_vectors, index, verbose)

  Wrap around atom i using pbc.
- subroutine, public prg_translatetogeomcandfoldtobox (coords, lattice_vectors, origin)

  Translate to geometric center.
- subroutine, public prg_replicate (coords, symbols, lattice_vectors, nx, ny, nz)

  Extend/replicate system along lattice vectors.
- subroutine, public prg_get_recip_vects (lattice_vectors, recip_vectors, volr, volk)

  Get the volume of the cell and the reciprocal vectors: This 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, nrnnstruct, bml_type, factor, gcov_bml, mdimin, verbose)

  Get the covalency graph in bml format.
- subroutine prg_get_covgraph_int (sy, nnStructMindist, nnStruct, nrnnstruct, bml_type, factor, gcov_bml, mdimin, verbose)
- subroutine, public prg_get_covgraph_h (sy, nnStructMindist, nnStruct, nrnnstruct, 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, nrnnstruct, 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 anymre since the bml_get_adj routine is sorting the values.

Variables

- integer, parameter dp = kind(1.0d0)

9.29.1 Detailed Description

A module to read and handle chemical systems.

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

Author

C. F. A. Negre (cnegre@lanl.gov)

9.29.2 Function/Subroutine Documentation

9.29.2.1 subroutine, public prg_system_mod::prg_adj2bml (integer, dimension(:), intent(in) *xadj,* integer, dimension(:), intent(in) *adjncy,* character(20), intent(in) *bml_type,* type(bml_matrix_t), intent(inout) *g_bml*)

prg_adj2bml

Parameters

xadj	CSR start values for the adjacency matrix.
adjncy	CSR positions of adjacency matrix.
bml_type	bml format.
g_bml	graph in bml format.

Definition at line 2299 of file prg_system_mod.F90.

9.29.2.2 subroutine, public prg_system_mod::prg_centeratbox (real(dp), dimension(:,:), intent(inout), allocatable *coords,* real(dp), dimension(:,:), intent(in) *lattice_vectors,* integer, intent(in), optional *verbose*)

Translate geometric center to the center of the box.

Parameters

coords	Coordinates of the system (see system_type).
lattice_vectors	System lattice vectors.
verbose	Verbosity level.

Definition at line 1293 of file prg_system_mod.F90.

9.29.2.3 subroutine, public prg_system_mod::prg_collect_graph_p (type(bml_matrix_t), intent(in) *rho_bml,* integer, intent(in) *nc,* integer, intent(in) *nats,* integer, dimension(:,:), intent(in) *hindex,* integer, dimension(:), intent(in) *chindex,* integer, dimension(:,:), intent(inout), allocatable *graph_p,* real(dp), intent(in) *threshold,* integer, intent(in) *mdimin,* integer, intent(in), optional *verbose*)

Collect the small graph to build the full graph.

Parameters

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

Definition at line 2082 of file prg_system_mod.F90.

9.29.2.4 subroutine, public prg_system_mod::prg_destroy_subsystems (type(system_type), intent(inout) *sbsy,* integer, intent(in), optional *verbose*)

Destroy allocated subsystem.

This routine will deallocate all the arrays of the structures.

Parameters

sy	System to de deallocated (see system_type).

Definition at line 1867 of file prg_system_mod.F90.

9.29.2.5 subroutine, public prg_system_mod::prg_get_covgraph (type(system_type), intent(in) *sy,* real(dp), dimension(:,:), intent(in) *nnStructMindist,* integer, dimension(:,:), intent(in) *nnStruct,* integer, dimension(:), intent(in) *nrnnstruct,* character(20), intent(in) *bml_type,* real(dp) *factor,* type(bml_matrix_t), intent(inout) *gcov_bml,* integer, intent(in) *mdimin,* integer, intent(in), optional *verbose*)

Get the covalency graph in bml format.

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

Parameters

sy	System structure (see system_type).
nnStructMindist	Minimun distance between atoms.
nnStruct	The neigbors J to I within Rcut that are all within the box.
nrnnstruct	Number of neigbors to I within Rcut that are all within the box.
bml_type	The bml type for constructing the graph.
gconv_bml	Covanlency graph in bml format.
verbose	Verbosity level.

Definition at line 1582 of file prg_system_mod.F90.

9.29.2.6 subroutine, public prg_system_mod::prg_get_covgraph_h (type(system_type), intent(in) *sy,* real(dp), dimension(:,:), intent(in) *nnStructMindist,* integer, dimension(:,:), intent(in) *nnStruct,* integer, dimension(:), intent(in) *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

sy	System structure (see system_type).
nnStructMindist	Minimun distance between atoms.
nnStruct	The neigbors J to I within Rcut that are all within the box.
nrnnstruct	Number of neigbors to I within Rcut that are all within the box.
bml_type	The bml type for constructing the graph.
gconv_bml	Covanlency graph in bml format.
verbose	Verbosity level.

Definition at line 1715 of file prg_system_mod.F90.

9.29.2.7 subroutine prg_system_mod::prg_get_covgraph_int (type(system_type), intent(in) *sy,* real(dp), dimension(:,:), intent(in) *nnStructMindist,* integer, dimension(:,:), intent(in) *nnStruct,* integer, dimension(:), intent(in) *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 1656 of file prg_system_mod.F90.

9.29.2.8 subroutine, public prg_system_mod::prg_get_dihedral (real(dp), dimension(:,:), intent(in) *coords,* integer, intent(in) *id1,* integer, intent(in) *id2,* integer, intent(in) *id3,* integer, intent(in) *id4,* real(dp), intent(out) *dihedral*)

Get the dihedral angle given four atomic positions.

Parameters

sy	System structure
id1	Atom index 1
id2	Atom index 1
id3	Atom index 1
id4	Atom index 1
dihedral	Output dihedral angle

Definition at line 1526 of file prg_system_mod.F90.

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

Get the distance matrix.

Parameters

coords	Coordinates of the system (see system_type).
dmat	Distance matrix (nats x nats).

Definition at line 1219 of file prg_system_mod.F90.

9.29.2.10 subroutine, public prg_system_mod::prg_get_nameandext (character(30), intent(in) *fullfilename,* character(30), intent(inout) *filename,* character(3), intent(inout) *ext*)

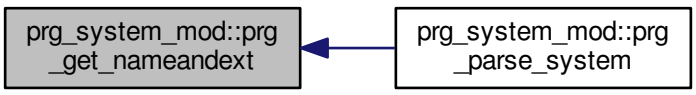
Get the name and extension of a file.

Parameters

fullfilename	Full filename.
filename	Filename of the system.
extension	Extension of the file.

Definition at line 206 of file prg_system_mod.F90.

Here is the caller graph for this function:



9.29.2.11 subroutine, public prg_system_mod::prg_get_origin (real(dp), dimension(:,:), intent(in) *coords,* real(dp), dimension(:), intent(inout), allocatable *origin*)

Get the origin of the coordinates.

Parameters

coords	Coordinates of teh system (see system_type).
origin	(min(x),min(y),min(z)) set as the origin of the system.

Definition at line 1183 of file prg_system_mod.F90.

9.29.2.12 subroutine, public prg_system_mod::prg_get_partial_atomgraph (type(bml_matrix_t), intent(in) *rho_bml,* integer, dimension(:,:), intent(in) *hindex,* type(bml_matrix_t), intent(inout) *gch_bml,* real(dp), intent(in) *threshold,* integer, intent(in), optional *verbose*)

Get partial subgraph based on the Density matrix.

Parameters

rho_bml	Density matix in bml format.
hindex	Start and end index for every atom in the system.
gch_bml	Atom based graph in bml format.
threshold	Threshold value for constructing the graph.
verbose	Verbosity levels.

Definition at line 2016 of file prg_system_mod.F90.

9.29.2.13 subroutine, public prg_system_mod::prg_get_recip_vects (real(dp), dimension(:,:), intent(in) *lattice_vectors,* real(dp), dimension(:,:), intent(inout), allocatable *recip_vectors,* real(dp), intent(inout) *volr,* real(dp), intent(inout) *volk*)

Get the volume of the cell and the reciprocal vectors: This 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

lattice_vectors	Lattice vectors for the system.
recip_vectors	Reciprocal vectors of the system.
volr	Volume of the cell.
volk	Volume of the reciprocal cell.

Definition at line 1477 of file prg_system_mod.F90.

9.29.2.14 subroutine, public prg_system_mod::prg_get_subsystem (type(system_type), intent(in) *sy,* integer, intent(in) *lsize,* integer, dimension(:), intent(in) *indices,* type(system_type), intent(inout) *sbsy,* integer, intent(in), optional *verbose*)

Get a subsystem out of the total system.

This will get a subsystem from the total system guided by a partition.

Parameters

sy	System structure (see system_type).
lsize	Core+Hallo subsystem size.
indices	Partition indices.
sbsy	Subsystem to be extracted.

Definition at line 1780 of file prg_system_mod.F90.

9.29.2.15 subroutine, public prg_system_mod::prg_graph2bml (integer, dimension(:,:), intent(inout), allocatable *graph,* character(20), intent(in) *bml_type,* type(bml_matrix_t), intent(inout) *g_bml*)

Graph2bml.

Parameters

graph	Atom based graph in "ellpack" like format.
bml_type	Bml type (usually ellpack for graph starage)
g_bml	Graph in bml format.

Definition at line 2333 of file prg_system_mod.F90.

9.29.2.16 subroutine, public prg_system_mod::prg_graph2vector (integer, dimension(:,:), intent(inout) *graph,* integer, dimension(:), allocatable *vector,* integer *maxnz*)

Vectorize graph.

Parameters

graph	Ellpack graph.
vector	Vector to store the graph.

Definition at line 2376 of file prg_system_mod.F90.

9.29.2.17 subroutine, public prg_system_mod::prg_make_random_system (type(system_type), intent(out) *system,* integer *nats,* integer *seed,* real(dp) *lx,* real(dp) *ly,* real(dp) *lz*)

Make random Xx system.

Parameters

system	System to be construucted.
nats	Number of atoms.
lx	length of the box for the x coordinate.
ly	length of the box for the y coordinate.
lz	length of the box for the z coordinate.

Definition at line 1059 of file prg_system_mod.F90.

9.29.2.18 subroutine, public prg_system_mod::prg_merge_graph (integer, dimension(:,:), intent(inout) *graph_p,* integer, dimension(:,:), intent(inout) *graph_h*)

Get partial subgraph based on the Density matrix.

Parameters

graph_p	Density matix based graph in bml format.
graph_h	Hamiltonian matix based graph in bml format.

Definition at line 2174 of file prg_system_mod.F90.

9.29.2.19 subroutine, public prg_system_mod::prg_merge_graph_adj (integer, dimension(:,:), intent(inout), allocatable *graph_p,* integer, dimension(:,:), intent(inout), allocatable *graph_h,* integer, dimension(:), intent(inout), allocatable *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy*)

Get partial subgraph based on the Density matrix.

Parameters

graph_p	Density matix based graph in "ellpack type format".
graph_h	Hamiltonian matix based graph in "ellpack type format".
xadj	CSR start values for the adjacency matrix.
adjncy	CSR positions of adjacency matrix.

Definition at line 2225 of file prg_system_mod.F90.

9.29.2.20 subroutine, public prg_system_mod::prg_molpartition (type(system_type), intent(in) *sy,* integer, intent(inout) *npart,* real(dp), dimension(:,:), intent(in) *nnStructMindist,* integer, dimension(:,:), intent(in) *nnStruct,* integer, dimension(:), intent(in) *nrnnstruct,* character(2), intent(in) *hetatm,* type(graph_partitioning_t), intent(inout) *gp,* integer, intent(inout), optional *verbose*)

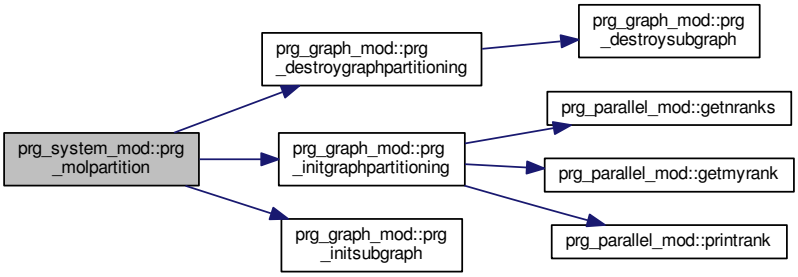
Partition by molecule.

Parameters

sy	System structure.
npart	Number of parts.
nnStructMindist	Minimum distance between neighbors.
nnStruct	The neighbors J to I within Rcut that are all within the box.
nrnnstruct	Number of neighbors to I within Rcut that are all within the box.
hetatm	Atom to be taken as the "center" of the by molecule partition.
gp	Graph partition structure.
verbose	Verbosity level.

Definition at line 1929 of file prg_system_mod.F90.

Here is the call graph for this function:



9.29.2.21 subroutine prg_system_mod::prg_parameters_to_vectors (real(dp), dimension(2,3), intent(in) *abc_angles,* real(dp), dimension(3,3), intent(out) *lattice_vector*) [private]

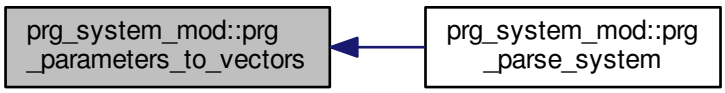
Transforms the lattice parameters into lattice vectors.

Parameters

abc_angles	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) = α , abc_angles(2,2) = β and abc_angles(2,3) = γ
lattice_vector	3x3 array containing the lattice vectors. lattice_vector(1,:) = $\vec{a}$

Definition at line 1105 of file prg_system_mod.F90.

Here is the caller graph for this function:



9.29.2.22 subroutine, public prg_system_mod::prg_parse_system (type(system_type), intent(out) *system,* character(len=$*$) *filename,* character(3), intent(in), optional *extin*)

The parser for the chemical system.

Parameters

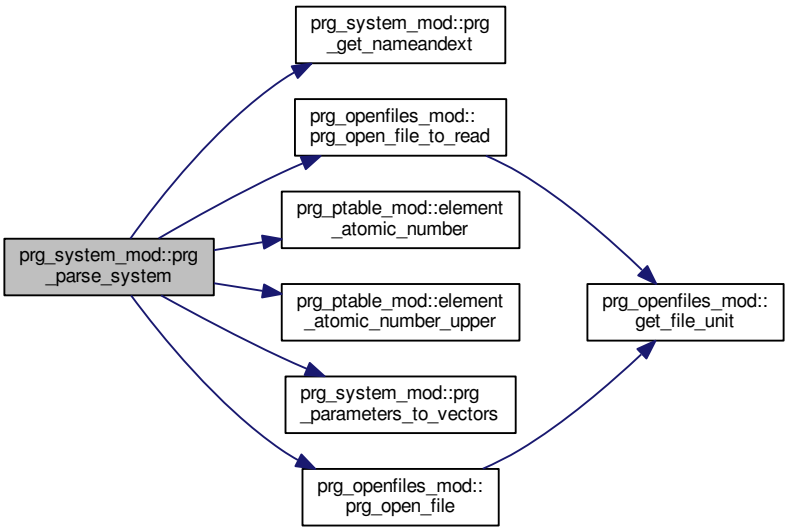
system	System to be constructed.
filename	Filename of the system.
extin	Extension of the file.

Assignment of species index for every atom.

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

Definition at line 229 of file prg_system_mod.F90.

Here is the call graph for this function:



9.29.2.23 **subroutine, public prg_system_mod::prg_replicate (real(dp), dimension(:,:), intent(inout), allocatable *coords,* character(2), dimension(:), intent(inout), allocatable *symbols,* real(dp), dimension(:,:), intent(inout) *lattice_vectors,* integer, intent(in) *nx,* integer, intent(in) *ny,* integer, intent(in) *nz*)**

Extend/replicate system along lattice vectors.

Parameters

coords	Coordinates of the system (see system_type).
symbols	Symbols for elements.
lattice_vectors	System lattice vectors.
nx	Number of lattice points in the v1 direction.
ny	Number of lattice points in the v2 direction.
nz	Number of lattice points in the v2 direction.

Definition at line 1417 of file prg_system_mod.F90.

9.29.2.24 subroutine, public prg_system_mod::prg_sortadj (integer, dimension(:), intent(inout) *xadj,* integer, dimension(:), intent(inout), allocatable *adjncy*)

Sort adj NOTE: this might not be needed anymre since the bml_get_adj routine is sorting the values.

Definition at line 2433 of file prg_system_mod.F90.

9.29.2.25 subroutine, public prg_system_mod::prg_translateandfoldtobox (real(dp), dimension(:,:), intent(inout), allocatable *coords,* real(dp), dimension(:,:), intent(in) *lattice_vectors,* real(dp), dimension(:), intent(inout), allocatable *origin,* integer, intent(in), optional *verbose*)

Translate and fold to box.

Parameters

coords	Coordinates of the system (see system_type).
lattice_vectors	System lattice vectors.
origin	(min(x),min(y),min(z)) set as the origin of the system.

Definition at line 1243 of file prg_system_mod.F90.

9.29.2.26 subroutine, public prg_system_mod::prg_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

coords	Coordinates of the system (see system_type).
lattice_vectors	System lattice vectors.
origin	(min(x),min(y),min(z)) set as the origin of the system.

Definition at line 1376 of file prg_system_mod.F90.

9.29.2.27 subroutine, public prg_system_mod::prg_vector2graph (integer, dimension(:), intent(inout), allocatable *vector,* integer, dimension(:,:), intent(inout) *graph,* integer *maxnz*)

Back to graph.

Parameters

vector	Vector to store the graph.
graph	Ellpack graph.

Definition at line 2405 of file prg_system_mod.F90.

9.29.2.28 subroutine prg_system_mod::prg_vectors_to_parameters (real(dp), dimension(3,3), intent(in) *lattice_vector,* real(dp), dimension(2,3), intent(out) *abc_angles*) [private]

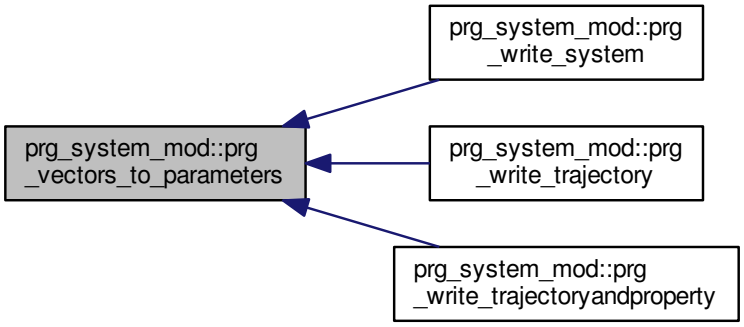
Transforms the lattice vectors into lattice parameters.

Parameters

lattice_vector	3x3 array containing the lattice vectors. lattice_vector(1,:) = $\vec{a}$
abc_angles	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) = α, abc_angles(2,2) = β, and abc_angles(2,3) = γ.

Definition at line 1147 of file prg_system_mod.F90.

Here is the caller graph for this function:



9.29.2.29 subroutine, public prg_system_mod::prg_wraparound (real(dp), dimension(:,:), intent(inout), allocatable *coords,* real(dp), dimension(:,:), intent(in) *lattice_vectors,* integer, intent(in) *index,* integer, intent(in), optional *verbose*)

Wrap around atom i using pbc.

Parameters

coords	Coordinates of the system (see system_type).
lattice_vectors	System lattice vectors.
index	Index atom to wrap around

Definition at line 1333 of file prg_system_mod.F90.

9.29.2.30 subroutine, public prg_system_mod::prg_write_system (type(system_type), intent(in) *system,* character(∗) *filename,* character(3) *extension*)

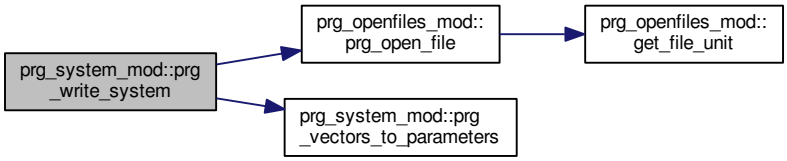
Write system in .xyz, .dat or pdb file.

Parameters

system	System to be constructed.
filename	File name.
extension	Extension of the file.

Definition at line 638 of file prg_system_mod.F90.

Here is the call graph for this function:



9.29.2.31 subroutine, public prg_system_mod::prg_write_trajectory (type(system_type), intent(in) *system,* integer, intent(in) *iter,* integer, intent(in) *each,* real(dp), intent(in) *prg_deltat,* character(∗) *filename,* character(3) *extension*)

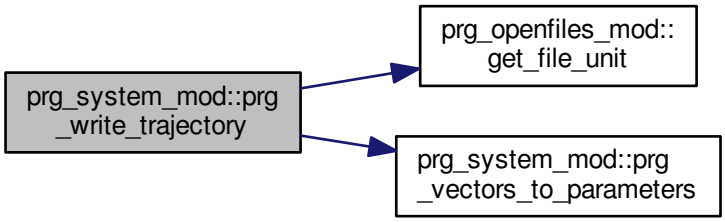
Write trajectory in .xyz, .dat or pdb file.

Parameters

system	System to be appended to the trajectory file.
iter	Simulation step.
each	Writing frequency.
filename	File name for the trajectory.
extension	Extension of the file.

Definition at line 826 of file prg_system_mod.F90.

Here is the call graph for this function:



9.29.2.32 subroutine, public prg_system_mod::prg_write_trajectoryandproperty (type(system_type), intent(in) *system,* integer, intent(in) *iter,* integer, intent(in) *each,* real(dp), intent(in) *prg_deltat,* real(dp), dimension(:), intent(in) *scalarprop,* character(∗) *filename,* character(3) *extension*)

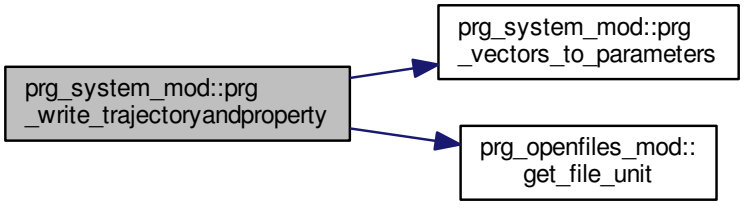
Write trajectory and atomic properties. Only pdb file.

Parameters

system	System to be appended to the trajectory file.
iter	Simulation step.
each	Writing frequency.
prg_deltat	Integration step.
scalarprop	Scalar property to plot on atoms.
filename	File name for the trajectory.
extension	Extension of the file.

Definition at line 949 of file prg_system_mod.F90.

Here is the call graph for this function:



9.29.3 Variable Documentation

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

Definition at line 19 of file prg_system_mod.F90.

9.30 prg_timer_mod Module Reference

The timer module.

Data Types

- type timer_status_t
  Timer status type.

Functions/Subroutines

- subroutine, public timer_prg_init ()
  Initialize timers.
- subroutine prg_timer_getid ()
  Get timer id.
- subroutine, public prg_timer_shutdown ()
  Done with timers.
- subroutine, public prg_timer_start (itimer, tag)
  Start Timing.
- subroutine, public prg_timer_stop (itimer, verbose)
  Stop timing.
- subroutine, public prg_timer_collect ()
- subroutine, public prg_timer_results ()
- real(8) function, public time2milliseconds ()
- subroutine, public prg_print_date_and_time (tag)
- character(2) function, private int2char (ival)

Variables

- integer, parameter dp = kind(1.0d0)
- integer, public loop_timer
- integer, public sp2_timer
- integer, public genx_timer
- integer, public part_timer
- integer, public subgraph_timer
- integer, public deortho_timer
- integer, public ortho_timer
- integer, public zdiag_timer
- integer, public graphsp2_timer
- integer, public subind_timer
- integer, public subext_timer
- integer, public subsp2_timer

- integer, public suball_timer
- integer, public bmult_timer
- integer, public badd_timer
- integer, public dyn_timer
- integer, public mdloop_timer
- integer, public buildz_timer
- integer, public realcoul_timer
- integer, public recipcoul_timer
- integer, public pairpot_timer
- integer, public halfverlet_timer
- integer, public pos_timer
- integer, public nlist_timer
- integer tstart_clock
- integer tstop_clock
- integer tclock_rate
- integer tclock_max
- integer num_timers
- type(timer_status_t), dimension(:), allocatable ptimer

9.30.1 Detailed Description

The timer module.

Sets up timers that can be used to time other routines.

Example use of dynamic timing:

call timer_prg_init()

call prg_timer_start(dyn_timer,"timer_tag")

.... code lines ...

call prg_timer_stop(dyn_timer,1)

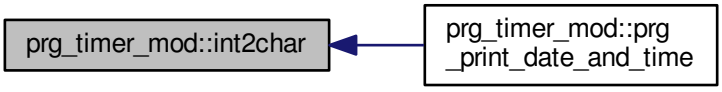
This will write the time it takes to execute "code lines" and it will name it "timer_tag"

9.30.2 Function/Subroutine Documentation

9.30.2.1 character(2) function, private prg_timer_mod::int2char (integer, intent(in) *ival*) [private]

Definition at line 394 of file prg_timer_mod.F90.

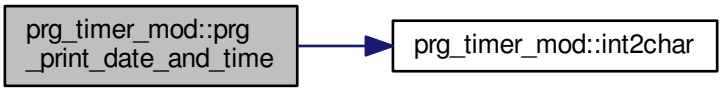
Here is the caller graph for this function:



9.30.2.2 subroutine, public prg_timer_mod::prg_print_date_and_time (character(len=*), intent(in) *tag*)

Definition at line 371 of file prg_timer_mod.F90.

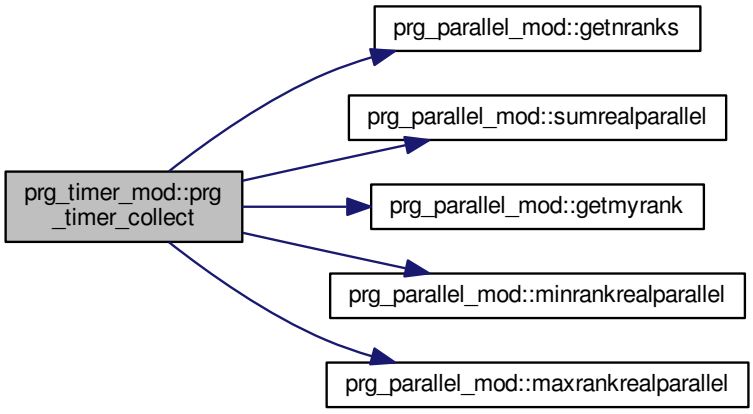
Here is the call graph for this function:



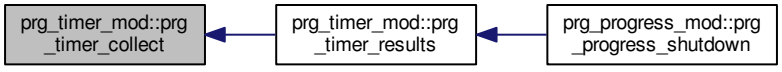
9.30.2.3 subroutine, public prg_timer_mod::prg_timer_collect ( )

Definition at line 253 of file prg_timer_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:



9.30.2.4 subroutine prg_timer_mod::prg_timer_getid ( ) [private]

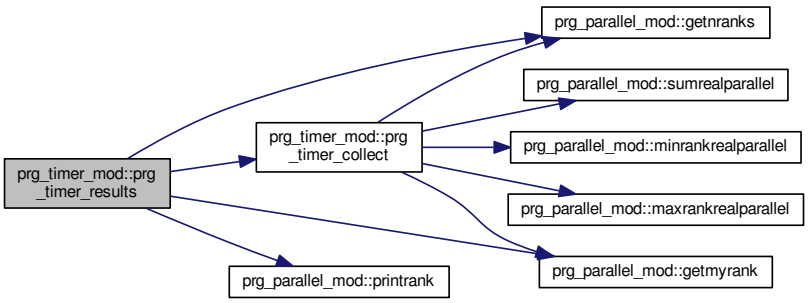
Get timer id.

Definition at line 200 of file prg_timer_mod.F90.

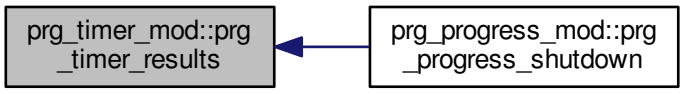
9.30.2.5 subroutine, public prg_timer_mod::prg_timer_results ( )

Definition at line 317 of file prg_timer_mod.F90.

Here is the call graph for this function:



Here is the caller graph for this function:

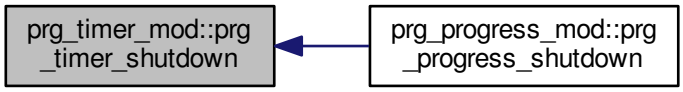


9.30.2.6 subroutine, public prg_timer_mod::prg_timer_shutdown ( )

Done with timers.

Definition at line 205 of file prg_timer_mod.F90.

Here is the caller graph for this function:



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

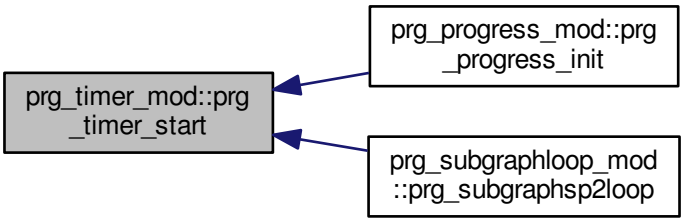
Start Timing.

Parameters

itimer	The index of the timer to start.
tag	Optional parameter to retag the timer on the fly.

Definition at line 215 of file prg_timer_mod.F90.

Here is the caller graph for this function:



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

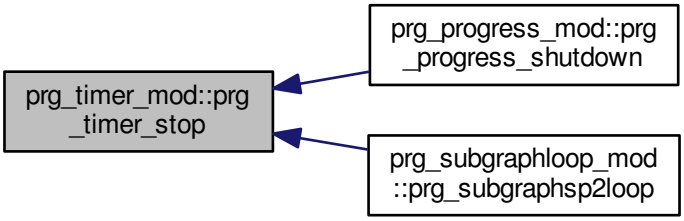
Stop timing.

Parameters

itimer	The index of the timer to stop.
verbose	Optional parameters to print partial times.

Definition at line 233 of file prg_timer_mod.F90.

Here is the caller graph for this function:



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

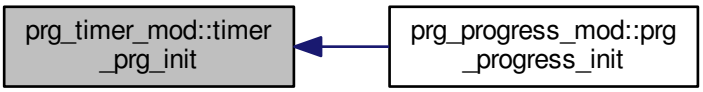
Definition at line 360 of file prg_timer_mod.F90.

9.30.2.10 subroutine, public prg_timer_mod::timer_prg_init ( )

Initialize timers.

Definition at line 132 of file prg_timer_mod.F90.

Here is the caller graph for this function:



9.30.3 Variable Documentation

9.30.3.1 integer, public prg_timer_mod::badd_timer

Definition at line 48 of file prg_timer_mod.F90.

9.30.3.2 integer, public prg_timer_mod::bmult_timer

Definition at line 48 of file prg_timer_mod.F90.

9.30.3.3 integer, public prg_timer_mod::buildz_timer

Definition at line 49 of file prg_timer_mod.F90.

9.30.3.4 integer, public prg_timer_mod::deortho_timer

Definition at line 45 of file prg_timer_mod.F90.

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

Definition at line 32 of file prg_timer_mod.F90.

9.30.3.6 integer, public prg_timer_mod::dyn_timer

Definition at line 49 of file prg_timer_mod.F90.

9.30.3.7 integer, public prg_timer_mod::genx_timer

Definition at line 44 of file prg_timer_mod.F90.

9.30.3.8 integer, public prg_timer_mod::graphsp2_timer

Definition at line 46 of file prg_timer_mod.F90.

9.30.3.9 integer, public prg_timer_mod::halfverlet_timer

Definition at line 51 of file prg_timer_mod.F90.

9.30.3.10 integer, public prg_timer_mod::loop_timer

Definition at line 44 of file prg_timer_mod.F90.

9.30.3.11 integer, public prg_timer_mod::mdloop_timer

Definition at line 49 of file prg_timer_mod.F90.

9.30.3.12 integer, public prg_timer_mod::nlist_timer

Definition at line 51 of file prg_timer_mod.F90.

9.30.3.13 integer prg_timer_mod::num_timers [private]

Definition at line 122 of file prg_timer_mod.F90.

9.30.3.14 integer, public prg_timer_mod::ortho_timer

Definition at line 46 of file prg_timer_mod.F90.

9.30.3.15 integer, public prg_timer_mod::pairpot_timer

Definition at line 50 of file prg_timer_mod.F90.

9.30.3.16 integer, public prg_timer_mod::part_timer

Definition at line 45 of file prg_timer_mod.F90.

9.30.3.17 integer, public prg_timer_mod::pos_timer

Definition at line 51 of file prg_timer_mod.F90.

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

Definition at line 124 of file prg_timer_mod.F90.

9.30.3.19 integer, public prg_timer_mod::realcoul_timer

Definition at line 50 of file prg_timer_mod.F90.

9.30.3.20 integer, public prg_timer_mod::recipcoul_timer

Definition at line 50 of file prg_timer_mod.F90.

9.30.3.21 integer, public prg_timer_mod::sp2_timer

Definition at line 44 of file prg_timer_mod.F90.

9.30.3.22 integer, public prg_timer_mod::suball_timer

Definition at line 48 of file prg_timer_mod.F90.

9.30.3.23 integer, public prg_timer_mod::subext_timer

Definition at line 47 of file prg_timer_mod.F90.

9.30.3.24 integer, public prg_timer_mod::subgraph_timer

Definition at line 45 of file prg_timer_mod.F90.

9.30.3.25 integer, public prg_timer_mod::subind_timer

Definition at line 47 of file prg_timer_mod.F90.

9.30.3.26 integer, public prg_timer_mod::subsp2_timer

Definition at line 47 of file prg_timer_mod.F90.

9.30.3.27 integer prg_timer_mod::tclock_max [private]

Definition at line 121 of file prg_timer_mod.F90.

9.30.3.28 integer prg_timer_mod::tclock_rate [private]

Definition at line 121 of file prg_timer_mod.F90.

9.30.3.29 integer prg_timer_mod::tstart_clock [private]

Definition at line 121 of file prg_timer_mod.F90.

9.30.3.30 integer prg_timer_mod::tstop_clock [private]

Definition at line 121 of file prg_timer_mod.F90.

9.30.3.31 integer, public prg_timer_mod::zdiag_timer

Definition at line 46 of file prg_timer_mod.F90.

9.31 prg_xlbo_mod Module Reference

A module to perform XLBO integration.

Data Types

- type xlbo_type

  General xlbo solver type.

Functions/Subroutines

- subroutine, public prg_parse_xlbo (xlbo, filename)

  The parser for XLBO parser.
- subroutine, public prg_xlbo_nint (charges, n, n_0, n_1, n_2, n_3, n_4, n_5, mdstep, xl)

  This routine integrates the dynamical variable "n".
- subroutine, public prg_xlbo_fcoulupdate (fcoul, charges, n)

  Adjust forces for the linearized XLBOMD functional.

Variables

- integer, parameter dp = kind(1.0d0)
- real(dp), parameter c0 = -6.0_dp

  Coefficients for modified Verlet integration.
- real(dp), parameter c1 = 14.0_dp
- real(dp), parameter c2 = -8.0_dp
- real(dp), parameter c3 = -3.0_dp
- real(dp), parameter c4 = 4.0_dp
- real(dp), parameter c5 = -1.0_dp
- real(dp), parameter kappa = 1.82_dp

  Coefficients for modified Verlet integration.
- real(dp), parameter alpha = 0.018_dp
- real(dp), parameter cc = 0.9_dp

9.31.1 Detailed Description

A module to perform XLBO integration.

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

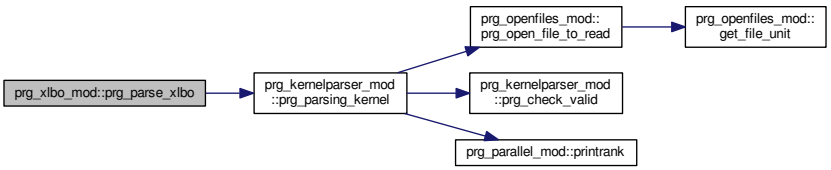
9.31.2 Function/Subroutine Documentation

9.31.2.1 subroutine, public prg_xlbo_mod::prg_parse_xlbo (type(xlbo_type), intent(inout) *xlbo,* character(len=∗) *filename*)

The parser for XLBO parser.

Definition at line 62 of file prg_xlbo_mod.F90.

Here is the call graph for this function:



9.31.2.2 subroutine, public prg_xlbo_mod::prg_xlbo_fcoulupdate (real(dp), dimension(:,:), intent(inout) *fcoul,* real(dp), dimension(:), intent(inout) *charges,* real(dp), dimension(:), intent(inout) *n*)

Adjust forces for the linearized XLBOMD functional.

Parameters

charges	

Definition at line 158 of file prg_xlbo_mod.F90.

9.31.2.3 subroutine, public prg_xlbo_mod::prg_xlbo_nint (real(dp), dimension(:), intent(in), allocatable *charges,* real(dp), dimension(:), intent(inout), allocatable *n,* real(dp), dimension(:), intent(inout), allocatable *n_0,* real(dp), dimension(:), intent(inout), allocatable *n_1,* real(dp), dimension(:), intent(inout), allocatable *n_2,* real(dp), dimension(:), intent(inout), allocatable *n_3,* real(dp), dimension(:), intent(inout), allocatable *n_4,* real(dp), dimension(:), intent(inout), allocatable *n_5,* integer, intent(in) *mdstep,* type(xlbo_type), intent(in) *xl*)

This routine integrates the dynamical variable "n".

Parameters

charges	

Definition at line 118 of file prg_xlbo_mod.F90.

9.31.3 Variable Documentation

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

Definition at line 28 of file prg_xlbo_mod.F90.

9.31.3.2 real(dp), parameter prg_xlbo_mod::c0 = -6.0_dp [private]

Coefficients for modified Verlet integration.

Definition at line 19 of file prg_xlbo_mod.F90.

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

Definition at line 20 of file prg_xlbo_mod.F90.

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

Definition at line 21 of file prg_xlbo_mod.F90.

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

Definition at line 22 of file prg_xlbo_mod.F90.

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

Definition at line 23 of file prg_xlbo_mod.F90.

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

Definition at line 24 of file prg_xlbo_mod.F90.

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

Definition at line 29 of file prg_xlbo_mod.F90.

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

Definition at line 16 of file prg_xlbo_mod.F90.

9.31.3.10 real(dp), parameter prg_xlbo_mod::kappa = 1.82_dp [private]

Coefficients for modified Verlet integration.

Definition at line 27 of file prg_xlbo_mod.F90.

9.32 prg_xlkernel_mod Module Reference

Add name.

Data Types

- type xlk_type

Functions/Subroutines

- subroutine, public prg_parse_xlkernel (input, filename)

  The parser for the mixer routines.
- subroutine, public prg_fermi (D0, QQ, ee, gap, Fe_vec, mu0, H, Z, Nocc, T, OccErrLim, MaxIt, HDIM)
- subroutine, public prg_kernel_fermi_full (KK, JJ, D0, mu0, mu1, T, RX, RY, RZ, LBox, Hubbard_U, Element_Type, Nr_atoms, MaxIt, eps, m, HDIM, Max_Nr_Neigh, Coulomb_acc, TIMERATIO, nnRx, nnRy, nnRz, nrnnlist, nnType, H_INDEX_START, H_INDEX_END, H, S, Z, Nocc, Znuc, QQ, ee, Fe_vec)
- subroutine, public prg_v_kernel_fermi (D0, dq_dv, v, mu0, mu1, T, RX, RY, RZ, LBox, Hubbard_U, Element_Type, Nr_atoms, MaxIt, eps, m, HDIM, Max_Nr_Neigh, Coulomb_acc, TIMERATIO, nnRx, nnRy, nnRz, nrnnlist, nnType, H_INDEX_START, H_INDEX_END, H, S, Z, Nocc, Znuc, QQ, ee, Fe_vec)
- subroutine, private prg_get_deriv_finite_temp (P1, H0, H1, Nocc, T, Q, ev, fe, mu0, eps, HDIM)
- subroutine, private prg_mmult (alpha, A, B, beta, C, TA, TB, HDIM)
- subroutine, private prg_eig (A, Q, ee, type, HDIM)
- subroutine, private prg_inv (X, XI, HDIM)
- subroutine, public prg_rank1 (verbose)

  Rank1 kernel ....

Variables

- integer, parameter dp = kind(1.0d0)

9.32.1 Detailed Description

Add name.

XL kernel (To be integrated)

Note

This module is still not functional

9.32.2 Function/Subroutine Documentation

9.32.2.1 subroutine, private prg_xlkernel_mod::prg_eig (real(prec), dimension(hdim,hdim), intent(in) *A,* real(prec), dimension(hdim,hdim), intent(out) *Q,* real(prec), dimension(hdim), intent(out) *ee,* character(1), intent(in) *type,* integer(prec), intent(in) *HDIM*) [private]

Definition at line 384 of file prg_xlkernel_mod.F90.

9.32.2.2 subroutine, public prg_xlkernel_mod::prg_fermi (real(prec), dimension(hdim,hdim), intent(out) *D0,* real(prec), dimension(hdim,hdim), intent(out) *QQ,* real(prec), dimension(hdim), intent(out) *ee,* real(prec), intent(out) *gap,* real(prec), dimension(hdim), intent(out) *Fe_vec,* real(prec), intent(inout) *mu0,* real(prec), dimension(hdim,hdim), intent(in) *H,* real(prec), dimension(hdim,hdim), intent(in) *Z,* integer(prec), intent(in) *Nocc,* real(prec), intent(in) *T,* real(prec), intent(in) *OccErrLim,* integer(prec), intent(in) *MaxIt,* integer(prec), intent(in) *HDIM*)

Definition at line 88 of file prg_xlkernel_mod.F90.

9.32.2.3 subroutine, private prg_xlkernel_mod::prg_get_deriv_finite_temp (real(prec), dimension(hdim,hdim), intent(out) *P1,* real(prec), dimension(hdim,hdim), intent(in) *H0,* real(prec), dimension(hdim,hdim), intent(in) *H1,* integer(prec), intent(in) *Nocc,* real(prec), intent(in) *T,* real(prec), dimension(hdim,hdim), intent(in) *Q,* real(prec), dimension(hdim), intent(in) *ev,* real(prec), dimension(hdim), intent(in) *fe,* real(prec), intent(inout) *mu0,* real(prec), intent(in) *eps,* integer(prec), intent(in) *HDIM*) [private]

Definition at line 306 of file prg_xlkernel_mod.F90.

9.32.2.4 subroutine, private prg_xlkernel_mod::prg_inv (real(prec), dimension(hdim,hdim), intent(in) *X,* real(prec), dimension(hdim,hdim), intent(out) *XI,* integer(prec), intent(in) *HDIM*) [private]

Definition at line 411 of file prg_xlkernel_mod.F90.

9.32.2.5 subroutine, public prg_xlkernel_mod::prg_kernel_fermi_full (real(prec), dimension(nr_atoms,nr_atoms), intent(out) *KK,* real(prec), dimension(nr_atoms,nr_atoms), intent(out) *JJ,* real(prec), dimension(hdim,hdim), intent(inout) *D0,* real(prec), intent(inout) *mu0,* real(prec), intent(inout) *mu1,* real(prec), intent(in) *T,* real(prec), dimension(nr_atoms), intent(in) *RX,* real(prec), dimension(nr_atoms), intent(in) *RY,* real(prec), dimension(nr_atoms), intent(in) *RZ,* real(prec), dimension(3), intent(in) *LBox,* real(prec), dimension(nr_atoms), intent(in) *Hubbard_U,* character(10), dimension(nr_atoms), intent(in) *Element_Type,* integer(prec), intent(in) *Nr_atoms,* integer(prec), intent(in) *MaxIt,* real(prec), intent(in) *eps,* integer(prec), intent(in) *m,* integer(prec), intent(in) *HDIM,* integer(prec), intent(in) *Max_Nr_Neigh,* real(prec), intent(in) *Coulomb_acc,* real(prec), intent(in) *TIMERATIO,* real(prec), dimension(nr_atoms,max_nr_neigh), intent(in) *nnRx,* real(prec), dimension(nr_atoms,max_nr_neigh), intent(in) *nnRy,* real(prec), dimension(nr_atoms,max_nr_neigh), intent(in) *nnRz,* integer(prec), dimension(nr_atoms), intent(in) *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 144 of file prg_xlkernel_mod.F90.

9.32.2.6 subroutine, private prg_xlkernel_mod::prg_mmult (real(prec), intent(in) *alpha,* real(prec), dimension(hdim,hdim), intent(in) *A,* real(prec), dimension(hdim,hdim), intent(in) *B,* real(prec), intent(in) *beta,* real(prec), dimension(hdim,hdim), intent(inout) *C,* character(1), intent(in) *TA,* character(1), intent(in) *TB,* integer(prec), intent(in) *HDIM*) [private]

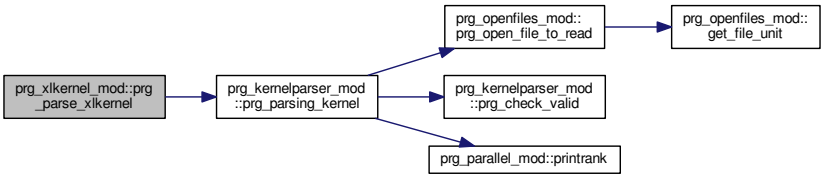
Definition at line 366 of file prg_xlkernel_mod.F90.

9.32.2.7 subroutine, public prg_xlkernel_mod::prg_parse_xlkernel (type(xlk_type), intent(inout) *input,* character(len=*) *filename*)

The parser for the mixer routines.

Definition at line 39 of file prg_xlkernel_mod.F90.

Here is the call graph for this function:



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

Rank1 kernel ....

Parameters

param1	..
verbose	Different levels of verbosity.

Definition at line 439 of file prg_xlkernel_mod.F90.

9.32.2.9 subroutine, public prg_xlkernel_mod::prg_v_kernel_fermi (real(prec), dimension(hdim,hdim), intent(inout) *D0,* real(prec), dimension(nr_atoms), intent(out) *dq_dv,* real(prec), dimension(nr_atoms), intent(in) *v,* real(prec), intent(inout) *mu0,* real(prec), intent(inout) *mu1,* real(prec), intent(in) *T,* real(prec), dimension(nr_atoms), intent(in) *RX,* real(prec), dimension(nr_atoms), intent(in) *RY,* real(prec), dimension(nr_atoms), intent(in) *RZ,* real(prec), dimension(3), intent(in) *LBox,* real(prec), dimension(nr_atoms), intent(in) *Hubbard_U,* character(10), dimension(nr_atoms), intent(in) *Element_Type,* integer(prec), intent(in) *Nr_atoms,* integer(prec), intent(in) *MaxIt,* real(prec), intent(in) *eps,* integer(prec), intent(in) *m,* integer(prec), intent(in) *HDIM,* integer(prec), intent(in) *Max_Nr_Neigh,* real(prec), intent(in) *Coulomb_acc,* real(prec), intent(in) *TIMERATIO,* real(prec), dimension(nr_atoms,max_nr_neigh), intent(in) *nnRx,* real(prec), dimension(nr_atoms,max_nr_neigh), intent(in) *nnRy,* real(prec), dimension(nr_atoms,max_nr_neigh), intent(in) *nnRz,* integer(prec), dimension(nr_atoms), intent(in) *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 235 of file prg_xlkernel_mod.F90.

9.32.3 Variable Documentation

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

Definition at line 15 of file prg_xlkernel_mod.F90.

Chapter 10

Data Type Documentation

10.1 prg_chebyshev_mod::chebdata_type Type Reference

General Cheb solver type.

Public Attributes

- character(100) flavor
- character(100) bml_type
- character(100) jobname
- integer mdim
- integer ncoeffs
- integer ndim
- integer verbose
- integer npts
- real(dp) atr
- real(dp) bndfil
- real(dp) ef
- real(dp) estep
- real(dp) fermitol
- real(dp) kbt
- real(dp) threshold
- logical getef
- logical jon
- logical trkfunc

10.1.1 Detailed Description

General Cheb solver type.

Definition at line 28 of file prg_chebyshev_mod.F90.

10.1.2 Member Data Documentation

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

Definition at line 33 of file prg_chebyshev_mod.F90.

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

Definition at line 30 of file prg_chebyshev_mod.F90.

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

Definition at line 33 of file prg_chebyshev_mod.F90.

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

Definition at line 33 of file prg_chebyshev_mod.F90.

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

Definition at line 33 of file prg_chebyshev_mod.F90.

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

Definition at line 34 of file prg_chebyshev_mod.F90.

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

Definition at line 29 of file prg_chebyshev_mod.F90.

10.1.2.8 logical prg_chebyshev_mod::chebdata_type::getef

Definition at line 35 of file prg_chebyshev_mod.F90.

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

Definition at line 30 of file prg_chebyshev_mod.F90.

10.1.2.10 logical prg_chebyshev_mod::chebdata_type::jon

Definition at line 35 of file prg_chebyshev_mod.F90.

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

Definition at line 34 of file prg_chebyshev_mod.F90.

10.1.2.12 integer prg_chebyshev_mod::chebdata_type::mdim

Definition at line 31 of file prg_chebyshev_mod.F90.

10.1.2.13 integer prg_chebyshev_mod::chebdata_type::ncoeffs

Definition at line 31 of file prg_chebyshev_mod.F90.

10.1.2.14 integer prg_chebyshev_mod::chebdata_type::ndim

Definition at line 31 of file prg_chebyshev_mod.F90.

10.1.2.15 integer prg_chebyshev_mod::chebdata_type::npts

Definition at line 32 of file prg_chebyshev_mod.F90.

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

Definition at line 34 of file prg_chebyshev_mod.F90.

10.1.2.17 logical prg_chebyshev_mod::chebdata_type::trkfunc

Definition at line 35 of file prg_chebyshev_mod.F90.

10.1.2.18 integer prg_chebyshev_mod::chebdata_type::verbose

Definition at line 31 of file prg_chebyshev_mod.F90.

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

- /home/christian/qmd-progress/src/prg_chebyshev_mod.F90

10.2 prg_system_mod::estruct_type Type Reference

Electronic structure type.

Public Attributes

- integer norbs
  Number of orbitals of the system.
- integer nel
  Number of electrons.
- integer, dimension(:,:), allocatable hindex
  Hindex.
- type(bml_matrix_t) ham
  SCC-Hamiltonian of the system.
- type(bml_matrix_t) ham0
  Hamiltonian of the system.
- type(bml_matrix_t) oham
  Orthogonalized Hamiltonian.
- type(bml_matrix_t) over
  Overlap matrix of the system.
- type(bml_matrix_t) rho
  Density matrix of the system.
- type(bml_matrix_t) orho
  Orthogonalized density matrix.
- type(bml_matrix_t) zmat
  Congruence transformation.
- real(dp), dimension(:), allocatable coul_pot_r
  Real Coulombic contribution.
- real(dp), dimension(:), allocatable coul_pot_k
  Reciprocal Coulombic contribution.
- real(dp), dimension(:,:), allocatable skforce
  Slater Koster force.
- real(dp), dimension(:,:), allocatable fpul
  Pulay force.
- real(dp), dimension(:,:), allocatable fscoul
  Nonorthogonal Coulombic force.
- real(dp) eband
  Band energy.

10.2.1 Detailed Description

Electronic structure type.

The electronic structure type.

Definition at line 22 of file prg_system_mod.F90.

10.2.2 Member Data Documentation

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

Reciprocal Coulombic contribution.

Definition at line 58 of file prg_system_mod.F90.

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

Real Coulombic contribution.

Definition at line 55 of file prg_system_mod.F90.

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

Band energy.

Definition at line 70 of file prg_system_mod.F90.

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

Pulay force.

Definition at line 64 of file prg_system_mod.F90.

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

Nonorthogonal Coulombic force.

Definition at line 67 of file prg_system_mod.F90.

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

SCC-Hamiltonian of the system.

Definition at line 34 of file prg_system_mod.F90.

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

Hamiltonian of the system.

Definition at line 37 of file prg_system_mod.F90.

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

Hindex.

Definition at line 31 of file prg_system_mod.F90.

10.2.2.9 integer prg_system_mod::estruct_type::nel

Number of electrons.

Definition at line 28 of file prg_system_mod.F90.

10.2.2.10 integer prg_system_mod::estruct_type::norbs

Number of orbitals of the system.

Definition at line 25 of file prg_system_mod.F90.

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

Orthogonalized Hamiltonian.

Definition at line 40 of file prg_system_mod.F90.

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

Orthogonalized density matrix.

Definition at line 49 of file prg_system_mod.F90.

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

Overlap matrix of the system.

Definition at line 43 of file prg_system_mod.F90.

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

Density matrix of the system.

Definition at line 46 of file prg_system_mod.F90.

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

Slater Koster force.

Definition at line 61 of file prg_system_mod.F90.

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

Congruence transformation.

Definition at line 52 of file prg_system_mod.F90.

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

- /home/christian/qmd-progress/src/prg_system_mod.F90

10.3 prg_genz_mod::genzspdata Type Reference

contains the data for the genZ driver.

Public Member Functions

- procedure prg_init
- procedure prg_generate
- procedure prg_allocatezspmat

Public Attributes

- integer verbose
- integer nfirst
- integer nrefi
- integer nreff
- real(dp) numthresi
- real(dp) numthresf
- logical integration

10.3.1 Detailed Description

contains the data for the genZ driver.

Definition at line 67 of file prg_genz_mod.F90.

10.3.2 Member Function/Subroutine Documentation

10.3.2.1 procedure prg_genz_mod::genzspdata::prg_allocatezspmat ( )

Definition at line 79 of file prg_genz_mod.F90.

10.3.2.2 procedure prg_genz_mod::genzspdata::prg_generate ( )

Definition at line 78 of file prg_genz_mod.F90.

10.3.2.3 procedure prg_genz_mod::genzspdata::prg_init ( )

Definition at line 77 of file prg_genz_mod.F90.

10.3.3 Member Data Documentation

10.3.3.1 logical prg_genz_mod::genzspdata::integration

Definition at line 75 of file prg_genz_mod.F90.

10.3.3.2 integer prg_genz_mod::genzspdata::nfirst

Definition at line 70 of file prg_genz_mod.F90.

10.3.3.3 integer prg_genz_mod::genzspdata::nreff

Definition at line 72 of file prg_genz_mod.F90.

10.3.3.4 integer prg_genz_mod::genzspdata::nrefi

Definition at line 71 of file prg_genz_mod.F90.

10.3.3.5 real(dp) prg_genz_mod::genzspdata::numthresf

Definition at line 74 of file prg_genz_mod.F90.

10.3.3.6 real(dp) prg_genz_mod::genzspdata::numthresi

Definition at line 73 of file prg_genz_mod.F90.

10.3.3.7 integer prg_genz_mod::genzspdata::verbose

Definition at line 69 of file prg_genz_mod.F90.

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

- /home/christian/qmd-progress/src/prg_genz_mod.F90

10.4 prg_genz_mod::genzspinp Type Reference

Input for the genz driver.

Public Attributes

- integer verbose

  To have different levels of verbose.
- integer nfirst

  !Lentgth of the "firsts iteration period".
- integer nrefi

  !Initial number of recursive refinements.
- integer nreff

  !Initial number of recursive refinements.
- real(dp) numthresi

  Initial threshold value.
- real(dp) numthresf

  Final threshold value.
- logical integration

  If we want to do XL integration scheme for Z.
- integer igenz

  To keep track of the genz iterations.
- logical zsp

  Logical variable to compute in sparse or dense mode.
- integer mdim

  Max nonzero elements per row for every row see [1] .
- character(20) bml_type

  Matrix format (Dense or Ellpack).

10.4.1 Detailed Description

Input for the genz driver.

This type controlls all the variables that are needed by genz

Definition at line 28 of file prg_genz_mod.F90.

10.4.2 Member Data Documentation

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

Matrix format (Dense or Ellpack).

Definition at line 61 of file prg_genz_mod.F90.

10.4.2.2 integer prg_genz_mod::genzspinp::igenz

To keep track of the genz iterations.

Definition at line 52 of file prg_genz_mod.F90.

10.4.2.3 logical prg_genz_mod::genzspinp::integration

If we want to do XL integration scheme for Z.

Definition at line 49 of file prg_genz_mod.F90.

10.4.2.4 integer prg_genz_mod::genzspinp::mdim

Max nonzero elements per row for every row see [1] .

Definition at line 58 of file prg_genz_mod.F90.

10.4.2.5 integer prg_genz_mod::genzspinp::nfirst

!Lentgth of the "firsts iteration period".

Definition at line 34 of file prg_genz_mod.F90.

10.4.2.6 integer prg_genz_mod::genzspinp::nreff

!Initial number of recursive refinements.

Definition at line 40 of file prg_genz_mod.F90.

10.4.2.7 integer prg_genz_mod::genzspinp::nrefi

!Initial number of recursive refinements.

Definition at line 37 of file prg_genz_mod.F90.

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

Final threshold value.

Definition at line 46 of file prg_genz_mod.F90.

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

Initial threshold value.

Definition at line 43 of file prg_genz_mod.F90.

10.4.2.10 integer prg_genz_mod::genzspinp::verbose

To have different levels of verbose.

Definition at line 31 of file prg_genz_mod.F90.

10.4.2.11 logical prg_genz_mod::genzspinp::zsp

Logical variable to compute in sparse or dense mode.

Definition at line 55 of file prg_genz_mod.F90.

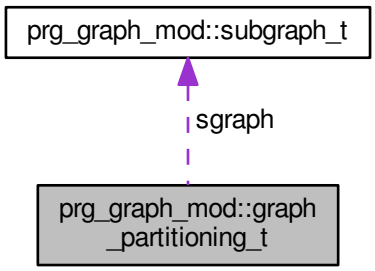
The documentation for this type was generated from the following file:

- /home/christian/qmd-progress/src/prg_genz_mod.F90

10.5 prg_graph_mod::graph_partitioning_t Type Reference

Trace per iteration.

Collaboration diagram for prg_graph_mod::graph_partitioning_t:



Private Attributes

- character(len=100) pname
  Partition name.
- integer myrank
  Local processor.
- integer totalprocs
  Number of processors.
- integer totalparts
  Total number of global partitions.
- integer totalnodes
  Total number of global groups, nodes (or matrix rows)
- integer totalnodes2
  Total number of global nodes (or matrix rows)
- integer globalpartmin
  Minimum global part number.
- integer globalpartmax
  Maximum global part number.

- integer globalpartextent
  Total global parts.
- integer, dimension(:), allocatable localpartmin
  Minimum part per processor.
- integer, dimension(:), allocatable localpartmax
  Maximum part per processor.
- integer, dimension(:), allocatable localpartextent
  Number of parts per processor.
- integer, dimension(:), allocatable order
  Original ordering if required.
- integer, dimension(:), allocatable reorder
  Reordering if required.
- integer nparts
  Total number of local partitions.
- integer, dimension(:), allocatable nnodesinpart
  Number of nodes in each local partition.
- integer, dimension(:), allocatable nnodesinpartall
  Number of nodes in each partition.
- integer, dimension(100) pp
  Sequence for SP2.
- integer maxiter
  Number of SP2 iterations.
- real(dp) ehomo
  Homo value.
- real(dp) 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.

10.5.1 Detailed Description

Trace per iteration.

Graph partitioning type

Definition at line 57 of file prg_graph_mod.F90.

10.5.2 Member Data Documentation

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

Homo value.

Definition at line 117 of file prg_graph_mod.F90.

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

Lumo value.

Definition at line 120 of file prg_graph_mod.F90.

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

Total global parts.

Definition at line 84 of file prg_graph_mod.F90.

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

Maximum global part number.

Definition at line 81 of file prg_graph_mod.F90.

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

Minimum global part number.

Definition at line 78 of file prg_graph_mod.F90.

10.5.2.6 integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::localpartextent [private]

Number of parts per processor.

Definition at line 93 of file prg_graph_mod.F90.

10.5.2.7 integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::localpartmax [private]

Maximum part per processor.

Definition at line 90 of file prg_graph_mod.F90.

10.5.2.8 integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::localpartmin [private]

Minimum part per processor.

Definition at line 87 of file prg_graph_mod.F90.

10.5.2.9 real(dp) prg_graph_mod::graph_partitioning_t::maxeval [private]

Max eval for prg_normalize.

Definition at line 126 of file prg_graph_mod.F90.

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

Number of SP2 iterations.

Definition at line 114 of file prg_graph_mod.F90.

10.5.2.11 real(dp) prg_graph_mod::graph_partitioning_t::mineval [private]

Min eval for prg_normalize.

Definition at line 123 of file prg_graph_mod.F90.

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

Local processor.

Definition at line 63 of file prg_graph_mod.F90.

10.5.2.13 integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::nnodesinpart [private]

Number of nodes in each local partition.

Definition at line 105 of file prg_graph_mod.F90.

10.5.2.14 integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::nnodesinpartall [private]

Number of nodes in each partition.

Definition at line 108 of file prg_graph_mod.F90.

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

Total number of local partitions.

Definition at line 102 of file prg_graph_mod.F90.

10.5.2.16 integer, dimension(:), allocatable prg_graph_mod::graph_partitioning_t::order [private]

Original ordering if required.

Definition at line 96 of file prg_graph_mod.F90.

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

Partition name.

Definition at line 60 of file prg_graph_mod.F90.

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

Sequence for SP2.

Definition at line 111 of file prg_graph_mod.F90.

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

Reordering if required.

Definition at line 99 of file prg_graph_mod.F90.

10.5.2.20 type (subgraph_t), dimension(:), allocatable prg_graph_mod::graph_partitioning_t::sgraph [private]

Subgraph details.

Definition at line 132 of file prg_graph_mod.F90.

10.5.2.21 integer prg_graph_mod::graph_partitioning_t::totalnodes [private]

Total number of global groups, nodes (or matrix rows)

Definition at line 72 of file prg_graph_mod.F90.

10.5.2.22 integer prg_graph_mod::graph_partitioning_t::totalnodes2 [private]

Total number of global nodes (or matrix rows)

Definition at line 75 of file prg_graph_mod.F90.

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

Total number of global partitions.

Definition at line 69 of file prg_graph_mod.F90.

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

Number of processors.

Definition at line 66 of file prg_graph_mod.F90.

10.5.2.25 real(dp), dimension(100) prg_graph_mod::graph_partitioning_t::vv [private]

Trace per iteration.

Definition at line 129 of file prg_graph_mod.F90.

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

- /home/christian/qmd-progress/src/prg_graph_mod.F90

10.6 prg_graphsp2parser_mod::gsp2data_type Type Reference

General SP2 solver type.

Public Attributes

- character(20) jobname
- character(50) hamfile
- integer verbose
- integer minsp2iter
- integer maxsp2iter
- integer nodesperpart
- integer natoms
- integer partition_count
- real(dp) sp2tol
- real(dp) threshold
- real(dp) bndfil
- real(dp) gthreshold
- real(dp) errlimit
- integer mdim
- integer ndim
- character, dimension(3) sdim
- real(dp), dimension(3) pdim
- character(20) bml_type
- character(10) sp2conv
- character(10) graph_element
- character(10) partition_type
- character(10) partition_refinement
- logical double_jump
- real(dp) covgfact
- real(dp) nlgcut
- integer parteach

10.6.1 Detailed Description

General SP2 solver type.

Definition at line 26 of file prg_graphsp2parser_mod.F90.

10.6.2 Member Data Documentation

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

Definition at line 44 of file prg_graphsp2parser_mod.F90.

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

Definition at line 37 of file prg_graphsp2parser_mod.F90.

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

Definition at line 50 of file prg_graphsp2parser_mod.F90.

10.6.2.4 logical prg_graphsp2parser_mod::gsp2data_type::double_jump

Definition at line 49 of file prg_graphsp2parser_mod.F90.

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

Definition at line 39 of file prg_graphsp2parser_mod.F90.

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

Definition at line 46 of file prg_graphsp2parser_mod.F90.

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

Definition at line 38 of file prg_graphsp2parser_mod.F90.

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

Definition at line 28 of file prg_graphsp2parser_mod.F90.

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

Definition at line 27 of file prg_graphsp2parser_mod.F90.

10.6.2.10 integer prg_graphsp2parser_mod::gsp2data_type::maxsp2iter

Definition at line 31 of file prg_graphsp2parser_mod.F90.

10.6.2.11 integer prg_graphsp2parser_mod::gsp2data_type::mdim

Definition at line 40 of file prg_graphsp2parser_mod.F90.

10.6.2.12 integer prg_graphsp2parser_mod::gsp2data_type::minsp2iter

Definition at line 30 of file prg_graphsp2parser_mod.F90.

10.6.2.13 integer prg_graphsp2parser_mod::gsp2data_type::natoms

Definition at line 33 of file prg_graphsp2parser_mod.F90.

10.6.2.14 integer prg_graphsp2parser_mod::gsp2data_type::ndim

Definition at line 41 of file prg_graphsp2parser_mod.F90.

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

Definition at line 51 of file prg_graphsp2parser_mod.F90.

10.6.2.16 integer prg_graphsp2parser_mod::gsp2data_type::nodesperpart

Definition at line 32 of file prg_graphsp2parser_mod.F90.

10.6.2.17 integer prg_graphsp2parser_mod::gsp2data_type::parteach

Definition at line 52 of file prg_graphsp2parser_mod.F90.

10.6.2.18 integer prg_graphsp2parser_mod::gsp2data_type::partition_count

Definition at line 34 of file prg_graphsp2parser_mod.F90.

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

Definition at line 48 of file prg_graphsp2parser_mod.F90.

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

Definition at line 47 of file prg_graphsp2parser_mod.F90.

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

Definition at line 43 of file prg_graphsp2parser_mod.F90.

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

Definition at line 42 of file prg_graphsp2parser_mod.F90.

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

Definition at line 45 of file prg_graphsp2parser_mod.F90.

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

Definition at line 35 of file prg_graphsp2parser_mod.F90.

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

Definition at line 36 of file prg_graphsp2parser_mod.F90.

10.6.2.26 integer prg_graphsp2parser_mod::gsp2data_type::verbose

Definition at line 29 of file prg_graphsp2parser_mod.F90.

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

- /home/christian/qmd-progress/src/prg_graphsp2parser_mod.F90

10.7 prg_pulaymixer_mod::mx_type Type Reference

Public Attributes

- character(20) mixertype

  Type or mixing scheme to be used (Linear or Pulay)
- integer verbose

  Verbosity level.
- integer mpulay

  Pulay dimension for matrix.
- real(dp) mixcoeff

  Coefficient for mixing.
- logical mixeron

  Mixer on or off (Not implemented)

10.7.1 Detailed Description

Definition at line 16 of file prg_pulaymixer_mod.F90.

10.7.2 Member Data Documentation

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

Coefficient for mixing.

Definition at line 28 of file prg_pulaymixer_mod.F90.

10.7.2.2 logical prg_pulaymixer_mod::mx_type::mixeron

Mixer on or off (Not implemented)

Definition at line 31 of file prg_pulaymixer_mod.F90.

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

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

Definition at line 19 of file prg_pulaymixer_mod.F90.

10.7.2.4 integer prg_pulaymixer_mod::mx_type::mpulay

Pulay dimension for matrix.

Definition at line 25 of file prg_pulaymixer_mod.F90.

10.7.2.5 integer prg_pulaymixer_mod::mx_type::verbose

Verbosity level.

Definition at line 22 of file prg_pulaymixer_mod.F90.

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

- /home/christian/qmd-progress/src/prg_pulaymixer_mod.F90

10.8 prg_extras_mod::prg_memory_consumption Interface Reference

Private Member Functions

- subroutine prg_memory_consumption (vm_peak, vm_size, pid, ppid)

10.8.1 Detailed Description

Definition at line 15 of file prg_extras_mod.F90.

10.8.2 Constructor & Destructor Documentation

10.8.2.1 subroutine prg_extras_mod::prg_memory_consumption::prg_memory_consumption (integer(c_long_long), intent(inout) *vm_peak,* integer(c_long_long), intent(inout) *vm_size,* integer(c_long_long), intent(inout) *pid,* integer(c_long_long), intent(inout) *ppid*) [private]

Definition at line 17 of file prg_extras_mod.F90.

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

- /home/christian/qmd-progress/src/prg_extras_mod.F90

10.9 prg_parallel_mod::rankreducedata_t Type Reference

Data structure for rection over MPI ranks.

Private Attributes

- real(dp) val
  Data value.
- integer rank
  MPI rank.

10.9.1 Detailed Description

Data structure for rection over MPI ranks.

Definition at line 72 of file prg_parallel_mod.F90.

10.9.2 Member Data Documentation

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

MPI rank.

Definition at line 78 of file prg_parallel_mod.F90.

10.9.2.2 real(dp) prg_parallel_mod::rankreducedata_t::val [private]

Data value.

Definition at line 75 of file prg_parallel_mod.F90.

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

- /home/christian/qmd-progress/src/prg_parallel_mod.F90

10.10 prg_response_mod::respdata_type Type Reference

Public Attributes

- character(20) respmode
- character(20) typeofpert
- character(20) bmltype
- integer mdim
- real(dp) numthresh
- logical computedipole
- logical getresponse
- real(dp) fieldintensity
- real(dp), dimension(3) field

10.10.1 Detailed Description

Definition at line 21 of file prg_response_mod.F90.

10.10.2 Member Data Documentation

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

Definition at line 24 of file prg_response_mod.F90.

10.10.2.2 logical prg_response_mod::respdata_type::computedipole

Definition at line 27 of file prg_response_mod.F90.

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

Definition at line 30 of file prg_response_mod.F90.

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

Definition at line 29 of file prg_response_mod.F90.

10.10.2.5 logical prg_response_mod::respdata_type::getresponse

Definition at line 28 of file prg_response_mod.F90.

10.10.2.6 integer prg_response_mod::respdata_type::mdim

Definition at line 25 of file prg_response_mod.F90.

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

Definition at line 26 of file prg_response_mod.F90.

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

Definition at line 22 of file prg_response_mod.F90.

10.10.2.9 character(20) prg_response_mod::respdata_type::typeofpert

Definition at line 23 of file prg_response_mod.F90.

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

- /home/christian/qmd-progress/src/prg_response_mod.F90

10.11 prg_syrotation_mod::rotation_type Type Reference

Rotation type.

Public Attributes

- character(20) jobname
- character(50) typeofrot
- integer patom1
  Atomic point to determine the initial orientation.
- integer patom2
  Atomic point to determine initial orientation.
- integer catom
  Atomic point to determine the rotation center.
- integer catom2
  Atomic point to determine a second rotation center.
- real(dp), dimension(3) pq1
  Point to determine initial orientation.
- real(dp), dimension(3) pq2
  Point to determine final orientation.
- real(dp), dimension(3) v1
  Initial orientation.
- real(dp), dimension(3) v2
  Final orientation.
- real(dp), dimension(3) vq
  Center of rotation.
- integer, dimension(2) rotate_atoms
  First and last rotated atom in the list.

10.11.1 Detailed Description

Rotation type.

Definition at line 17 of file prg_syrotation_mod.F90.

10.11.2 Member Data Documentation

10.11.2.1 integer prg_syrotation_mod::rotation_type::catom

Atomic point to determine the rotation center.

Definition at line 25 of file prg_syrotation_mod.F90.

10.11.2.2 integer prg_syrotation_mod::rotation_type::catom2

Atomic point to determine a second rotation center.

Definition at line 27 of file prg_syrotation_mod.F90.

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

Definition at line 18 of file prg_syrotation_mod.F90.

10.11.2.4 integer prg_syrotation_mod::rotation_type::patom1

Atomic point to determine the initial orientation.

Definition at line 21 of file prg_syrotation_mod.F90.

10.11.2.5 integer prg_syrotation_mod::rotation_type::patom2

Atomic point to determine initial orientation.

Definition at line 23 of file prg_syrotation_mod.F90.

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

Point to determine initial orientation.

Definition at line 29 of file prg_syrotation_mod.F90.

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

Point to determine final orientation.

Definition at line 31 of file prg_syrotation_mod.F90.

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

First and last rotated atom in the list.

Definition at line 39 of file prg_syrotation_mod.F90.

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

Definition at line 19 of file prg_syrotation_mod.F90.

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

Initial orientation.

Definition at line 33 of file prg_syrotation_mod.F90.

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

Final orientation.

Definition at line 35 of file prg_syrotation_mod.F90.

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

Center of rotation.

Definition at line 37 of file prg_syrotation_mod.F90.

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

- /home/christian/qmd-progress/src/prg_syrotation_mod.F90

10.12 prg_sp2parser_mod::sp2data_type Type Reference

General SP2 solver type.

Public Attributes

- character(20) jobname
- integer verbose
- integer minsp2iter
- integer maxsp2iter
- real(dp) sp2tol
- real(dp) threshold
- real(dp) bndfil
- integer mdim
- integer ndim
- character, dimension(3) sdim
- real(dp), dimension(3) pdim
- character(20) bml_type
- character(10) sp2conv
- character(10) flavor

10.12.1 Detailed Description

General SP2 solver type.

Definition at line 26 of file prg_sp2parser_mod.F90.

10.12.2 Member Data Documentation

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

Definition at line 38 of file prg_sp2parser_mod.F90.

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

Definition at line 33 of file prg_sp2parser_mod.F90.

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

Definition at line 40 of file prg_sp2parser_mod.F90.

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

Definition at line 27 of file prg_sp2parser_mod.F90.

10.12.2.5 integer prg_sp2parser_mod::sp2data_type::maxsp2iter

Definition at line 30 of file prg_sp2parser_mod.F90.

10.12.2.6 integer prg_sp2parser_mod::sp2data_type::mdim

Definition at line 34 of file prg_sp2parser_mod.F90.

10.12.2.7 integer prg_sp2parser_mod::sp2data_type::minsp2iter

Definition at line 29 of file prg_sp2parser_mod.F90.

10.12.2.8 integer prg_sp2parser_mod::sp2data_type::ndim

Definition at line 35 of file prg_sp2parser_mod.F90.

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

Definition at line 37 of file prg_sp2parser_mod.F90.

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

Definition at line 36 of file prg_sp2parser_mod.F90.

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

Definition at line 39 of file prg_sp2parser_mod.F90.

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

Definition at line 31 of file prg_sp2parser_mod.F90.

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

Definition at line 32 of file prg_sp2parser_mod.F90.

10.12.2.14 integer prg_sp2parser_mod::sp2data_type::verbose

Definition at line 28 of file prg_sp2parser_mod.F90.

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

- /home/christian/qmd-progress/src/prg_sp2parser_mod.F90

10.13 prg_graph_mod::subgraph_t Type Reference

Subgraph type.

Private Attributes

- integer part
  Partition number.
- integer hsize
  Size of original matrix (h x h)
- integer lsize
  Size of full subgraph (l x l)
- integer llsize
  Size of core subgraph.
- integer, dimension(:), allocatable core_halo_index
  Indeces from original matrix for subgraph core+halo extraction.
- integer, dimension(:), allocatable nodeinpart
  Nodes in this partition.

10.13.1 Detailed Description

Subgraph type.

Definition at line 31 of file prg_graph_mod.F90.

10.13.2 Member Data Documentation

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

Indeces from original matrix for subgraph core+halo extraction.

Definition at line 46 of file prg_graph_mod.F90.

10.13.2.2 integer prg_graph_mod::subgraph_t::hsize [private]

Size of original matrix (h x h)

Definition at line 37 of file prg_graph_mod.F90.

10.13.2.3 integer prg_graph_mod::subgraph_t::llsize [private]

Size of core subgraph.

Definition at line 43 of file prg_graph_mod.F90.

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

Size of full subgraph (l x l)

Definition at line 40 of file prg_graph_mod.F90.

10.13.2.5 integer, dimension(:), allocatable prg_graph_mod::subgraph_t::nodeinpart [private]

Nodes in this partition.

Definition at line 49 of file prg_graph_mod.F90.

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

Partition number.

Definition at line 34 of file prg_graph_mod.F90.

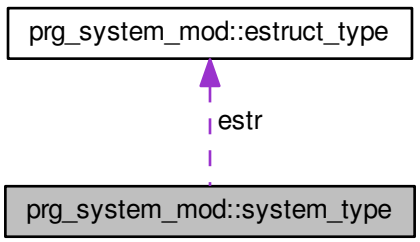
The documentation for this type was generated from the following file:

- /home/christian/qmd-progress/src/prg_graph_mod.F90

10.14 prg_system_mod::system_type Type Reference

System type.

Collaboration diagram for prg_system_mod::system_type:



Public Attributes

- integer nats

  Number of atoms of the system.
- character(2), dimension(:), allocatable symbol

  Chemical Symbols for every atom of the system. Symbol can be recovered using ptable module and calling the following routine:
- integer, dimension(:), allocatable atomic_number

  Atomic number for every atom in the system.
- real(dp), dimension(:,:), allocatable coordinate

  Coordinates of every atom in the system. Allocation:
- real(dp), dimension(:,:), allocatable velocity

  Velocities for every atom in the system. Allocation:
- real(dp), dimension(:,:), allocatable force

  Forces acting on every atom in the system. Allocation:
- real(dp), dimension(:), allocatable net_charge

  Charges of every atom in the system. Allocation:
- real(dp), dimension(:), allocatable mass

  Mass of every atom in the system. These can be automatically loaded by using the structures of the ptable mod:
- real(dp), dimension(:,:), allocatable lattice_vector

  Lattice vectors of the system. Use the prg_vectors_to_parameters and parameters_to_vector to transform from lattice vector to lattice parameters. Allocation:
- real(dp), dimension(:,:), allocatable recip_vector

  Reciprocal vectors of the system. Allocation:
- real(dp) volr

  Volume of the system (direct space).
- real(dp) volk

  Volume of the system (direct space).
- integer nsp

  Number of different species. Number of species or number of differet antom types (symbols) in the system. This integer is alwas less or equal than the total number of atoms (nsp <= nats). This information can also be found in tbparams structure and the following equality holds:
- integer, dimension(:), allocatable spindex

  Species index. It gives the species index of a particulat 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 appearence in systemsymbol. Allocation:
- integer, dimension(:), allocatable spatnum

  Species atomic number list. A list with the atomic numbers for every species Allocation:
- real(dp), dimension(:), allocatable spmass

  Species mass list. A list with the atomic mass for every species Allocation:
- real(dp), dimension(:), allocatable userdef

  User define field.
- integer, dimension(:), allocatable resindex

  Residue index.
- type(estruct_type) estr

  Electronic structure.

10.14.1 Detailed Description

System type.

The molecular system type.

Definition at line 75 of file prg_system_mod.F90.

10.14.2 Member Data Documentation

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

Atomic number for every atom in the system.

Definition at line 89 of file prg_system_mod.F90.

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

Coordinates of every atom in the system. Allocation:

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

Definition at line 94 of file prg_system_mod.F90.

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

Electronic structure.

Definition at line 187 of file prg_system_mod.F90.

10.14.2.4 real(dp), dimension(:,:), allocatable prg_system_mod::system_type::force

Forces acting on every atom in the system. Allocation:

```
force(3,nats)
```

Definition at line 104 of file prg_system_mod.F90.

10.14.2.5 real(dp), dimension(:,:), allocatable prg_system_mod::system_type::lattice_vector

Lattice vectors of the system. Use the prg_vectors_to_parameters and parameters_to_vector to transform from lattice vector to lattice parameters. Allocation:

```
lattice_vector(3,3)
```

```
v1 = lattice_vector(1,:)
```

```
v2 = lattice_vector(2,:)
```

```
v3 = lattice_vector(3,:)
```

Definition at line 126 of file prg_system_mod.F90.

10.14.2.6 real(dp), dimension(:), allocatable prg_system_mod::system_type::mass

Mass of every atom in the system. These can be automatically loaded by using the structures of the ptable mod:

```
system%mass(i) = mass(mystem%atomic_number(i))
```

Allocation:

```
mass(nats)
```

Definition at line 116 of file prg_system_mod.F90.

10.14.2.7 integer prg_system_mod::system_type::nats

Number of atoms of the system.

Definition at line 78 of file prg_system_mod.F90.

10.14.2.8 real(dp), dimension(:), allocatable prg_system_mod::system_type::net_charge

Charges of every atom in the system. Allocation:

```
net_charge(nats)
```

Definition at line 109 of file prg_system_mod.F90.

10.14.2.9 integer prg_system_mod::system_type::nsp

Number of different species. Number of species or number of differet antom types (symbols) in the system. This integer is alwas less or equal than the total number of atoms (nsp <= nats). This information can also be found in tbparams structure and the following equality holds:

```
system%nsp = tbparams%nsp
```

Definition at line 149 of file prg_system_mod.F90.

10.14.2.10 real(dp), dimension(:,:), allocatable prg_system_mod::system_type::recip_vector

Reciprocal vectors of the system. Allocation:

```
recip_vector(3,3)
```

```
v1 = recip_vector(1,:)
```

```
v2 = recip_vector(2,:)
```

```
v3 = recip_vector(3,:)
```

Definition at line 134 of file prg_system_mod.F90.

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

Residue index.

Definition at line 184 of file prg_system_mod.F90.

10.14.2.12 integer, dimension(:), allocatable prg_system_mod::system_type::spatnum

Species atomic number list. A list with the atomic numbers for every species Allocation:

```
spatnum(nsp)
```

Definition at line 172 of file prg_system_mod.F90.

10.14.2.13 integer, dimension(:), allocatable prg_system_mod::system_type::spindex

Species index. It gives the species index of a particulat atom. Allocation:

```
spindex(nats)
```

If we need the index of atom 30 then:

```
system%spindex(30)
```

Definition at line 157 of file prg_system_mod.F90.

10.14.2.14 character(2), dimension(:), allocatable prg_system_mod::system_type::splist

Species symbol list. A list with the different species e.g. H, C, N, etc with the order corresponding to the appearence in systemsymbol. Allocation:

```
splist(nsp)
```

Definition at line 165 of file prg_system_mod.F90.

10.14.2.15 real(dp), dimension(:), allocatable prg_system_mod::system_type::spmass

Species mass list. A list with the atomic mass for every species Allocation:

```
spmass(nsp)
```

Definition at line 178 of file prg_system_mod.F90.

10.14.2.16 character(2), dimension(:), allocatable prg_system_mod::system_type::symbol

Chemical Symbols for every atom of the system. Symbol can be recovered using ptable module and calling the following routine:

```
system%symbol(i) = element_symbol(system%atomic_number(i))
```

Allocation:

```
symbol(nats)
```

Definition at line 86 of file prg_system_mod.F90.

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

User define field.

Definition at line 181 of file prg_system_mod.F90.

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

Velocities for every atom in the system. Allocation:

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

Definition at line 99 of file prg_system_mod.F90.

10.14.2.19 real(dp) prg_system_mod::system_type::volk

Volume of the system (direct space).

Note

use prg_get_recip_vects in coulomb_latte_mod to compute this.

Definition at line 142 of file prg_system_mod.F90.

10.14.2.20 real(dp) prg_system_mod::system_type::volr

Volume of the system (direct space).

Note

use prg_get_recip_vects in coulomb_latte_mod to compute this.

Definition at line 138 of file prg_system_mod.F90.

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

- /home/christian/qmd-progress/src/prg_system_mod.F90

10.15 prg_timer_mod::timer_status_t Type Reference

Timer status type.

Private Attributes

- character(len=20) tname
  Timer name.
- integer tstart
  Start time.
- integer ttotal
  Current total time.
- integer tcount
  Current call count.
- integer minrank
  Rank with min value.
- integer maxrank
  Rank with max value.
- real(dp) tsum
  Sum time - total time in secs.
- real(dp) minvalue
  Minimum value over all ranks.
- real(dp) maxvalue
  Maximum value over all ranks.
- real(dp) tavg
  Average value over all ranks.
- real(dp) tstdev
  Stdev across all ranks.
- real(dp) tpercent
  Percent of time across all timers.

10.15.1 Detailed Description

Timer status type.

Definition at line 54 of file prg_timer_mod.F90.

10.15.2 Member Data Documentation

10.15.2.1 integer prg_timer_mod::timer_status_t::maxrank [private]

Rank with max value.

Definition at line 72 of file prg_timer_mod.F90.

10.15.2.2 real(dp) prg_timer_mod::timer_status_t::maxvalue [private]

Maximum value over all ranks.

Definition at line 81 of file prg_timer_mod.F90.

10.15.2.3 integer prg_timer_mod::timer_status_t::minrank [private]

Rank with min value.

Definition at line 69 of file prg_timer_mod.F90.

10.15.2.4 real(dp) prg_timer_mod::timer_status_t::minvalue [private]

Minimum value over all ranks.

Definition at line 78 of file prg_timer_mod.F90.

10.15.2.5 real(dp) prg_timer_mod::timer_status_t::tavg [private]

Average value over all ranks.

Definition at line 84 of file prg_timer_mod.F90.

10.15.2.6 integer prg_timer_mod::timer_status_t::tcount [private]

Current call count.

Definition at line 66 of file prg_timer_mod.F90.

10.15.2.7 character(len=20) prg_timer_mod::timer_status_t::tname [private]

Timer name.

Definition at line 57 of file prg_timer_mod.F90.

10.15.2.8 real(dp) prg_timer_mod::timer_status_t::tpercent [private]

Percent of time across all timers.

Definition at line 90 of file prg_timer_mod.F90.

10.15.2.9 integer prg_timer_mod::timer_status_t::tstart [private]

Start time.

Definition at line 60 of file prg_timer_mod.F90.

10.15.2.10 real(dp) prg_timer_mod::timer_status_t::tstdev [private]

Stdev across all ranks.

Definition at line 87 of file prg_timer_mod.F90.

10.15.2.11 real(dp) prg_timer_mod::timer_status_t::tsum [private]

Sum time - total time in secs.

Definition at line 75 of file prg_timer_mod.F90.

10.15.2.12 integer prg_timer_mod::timer_status_t::ttotal [private]

Current total time.

Definition at line 63 of file prg_timer_mod.F90.

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

- /home/christian/qmd-progress/src/prg_timer_mod.F90

10.16 prg_extras_mod::to_string Interface Reference

Private Member Functions

- character(len=:) function, allocatable to_string_integer (i)
  Convert integer to string.
- character(len=:) function, allocatable to_string_long_long (i)
  Convert integer to string.
- character(len=:) function, allocatable to_string_double (x)
  Convert double to string.

10.16.1 Detailed Description

Definition at line 25 of file prg_extras_mod.F90.

10.16.2 Member Function/Subroutine Documentation

10.16.2.1 character(len=:) function, allocatable prg_extras_mod::to_string::to_string_double (double precision, intent(in) *x*) [private]

Convert double to string.

Parameters

x	The double

Returns

The string

Definition at line 80 of file prg_extras_mod.F90.

10.16.2.2 character(len=:) function, allocatable prg_extras_mod::to_string::to_string_integer (integer, intent(in) *i*) [private]

Convert integer to string.

Parameters

i	The integer

Returns

The string

Definition at line 46 of file prg_extras_mod.F90.

10.16.2.3 character(len=:) function, allocatable prg_extras_mod::to_string::to_string_long_long (integer(kind=c_long_long), intent(in) *i*) [private]

Convert integer to string.

Parameters

i	The integer

Returns

The string

Definition at line 62 of file prg_extras_mod.F90.

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

- /home/christian/qmd-progress/src/prg_extras_mod.F90

10.17 prg_xlbo_mod::xlbo_type Type Reference

General xlbo solver type.

Public Attributes

- character(20) jobname
- integer verbose
- integer maxscfiter

  Max SCF iterations at every XLBO MD step.
- integer maxscfinititer

  Max SCF iterations for the first minit steps.
- real(dp) threshold
- integer minit

  Use SCF the first M_prg_init MD steps.
- real(dp) cc

  Scaled prg_delta Kernel.

10.17.1 Detailed Description

General xlbo solver type.

Definition at line 33 of file prg_xlbo_mod.F90.

10.17.2 Member Data Documentation

10.17.2.1 real(dp) prg_xlbo_mod::xlbo_type::cc

Scaled prg_delta Kernel.

Definition at line 51 of file prg_xlbo_mod.F90.

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

Definition at line 35 of file prg_xlbo_mod.F90.

10.17.2.3 integer prg_xlbo_mod::xlbo_type::maxscfinititer

Max SCF iterations for the first minit steps.

Definition at line 43 of file prg_xlbo_mod.F90.

10.17.2.4 integer prg_xlbo_mod::xlbo_type::maxscfiter

Max SCF iterations at every XLBO MD step.

Definition at line 40 of file prg_xlbo_mod.F90.

10.17.2.5 integer prg_xlbo_mod::xlbo_type::minit

Use SCF the first M_prg_init MD steps.

Definition at line 48 of file prg_xlbo_mod.F90.

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

Definition at line 45 of file prg_xlbo_mod.F90.

10.17.2.7 integer prg_xlbo_mod::xlbo_type::verbose

Definition at line 37 of file prg_xlbo_mod.F90.

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

- /home/christian/qmd-progress/src/prg_xlbo_mod.F90

10.18 prg_xlkernel_mod::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 17 of file prg_xlkernel_mod.F90.

10.18.2 Member Data Documentation

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

Kernel type.

Definition at line 20 of file prg_xlkernel_mod.F90.

10.18.2.2 integer prg_xlkernel_mod::xlk_type::nrank

Definition at line 23 of file prg_xlkernel_mod.F90.

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

Coefficient for mixing.

Definition at line 26 of file prg_xlkernel_mod.F90.

10.18.2.4 integer prg_xlkernel_mod::xlk_type::verbose

Verbosity level.

Definition at line 23 of file prg_xlkernel_mod.F90.

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

- /home/christian/qmd-progress/src/prg_xlkernel_mod.F90

Chapter 11

File Documentation

11.1 /home/christian/qmd-progress/README.md File Reference

11.2 /home/christian/qmd-progress/tests/README.md File Reference

11.3 /home/christian/qmd-progress/src/prg_charges_mod.F90 File Reference

Modules

- module prg_charges_mod

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

Functions/Subroutines

- subroutine, public prg_charges_mod::prg_get_charges (rho_bml, over_bml, hindex, charges, numel, spindex, mdimin, threshold)

  Constructs the charges from the density matrix.
- subroutine, public prg_charges_mod::prg_get_hscf (ham0_bml, over_bml, ham_bml, spindex, hindex, 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 prg_charges_mod::dp = kind(1.0d0)

11.4 /home/christian/qmd-progress/src/prg_chebyshev_mod.F90 File Reference

Data Types

- type prg_chebyshev_mod::chebdata_type

  General Cheb solver type.

Modules

- module prg_chebyshev_mod

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

Functions/Subroutines

- subroutine, public prg_chebyshev_mod::prg_parse_cheb (chebdata, filename)

  Chebyshev parser. This module is used to parse all the input variables for the cheb electronic structure solver. Adding a new input keyword to the parser:
- subroutine, public prg_chebyshev_mod::prg_build_density_cheb (ham_bml, rho_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, jon, verbose)

  Builds the density matrix from H_0 for a Fermi function approximated with a Chebyshev polynomial expansion.
- subroutine, public prg_chebyshev_mod::prg_build_density_cheb_fermi (ham_bml, rho_bml, athr, threshold, ncoeffs, kbt, ef, bndfil, getef, fermitol, jon, npts, trkfunc, verbose)

  Builds the density matrix from H_0 for a Fermi function approximated with a Chebyshev polynomial expansion. In this case the self-consistent recursion is applied to converge to the correct number of electrons and obtain the Fermi level.
- real(dp) function prg_chebyshev_mod::jackson (ncoeffs, i, jon)

  Evaluates the Jackson Kernel Coefficients.
- subroutine prg_chebyshev_mod::prg_get_chebcoeffs (npts, kbt, ef, ncoeffs, coeffs, emin, emax)

  Gets the coefficients of the Chebyshev expansion.
- subroutine prg_chebyshev_mod::prg_get_chebcoeffs_fermi_bs (npts, kbt, ef, tracesT, ncoeffs, coeffs, emin, emax, bndfil, norb, tol, jon, verbose)

  Gets the coefficients of the Chebyshev expansion with 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 /home/christian/qmd-progress/src/prg_densitymatrix_mod.F90 File Reference

Modules

- module prg_densitymatrix_mod

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

Functions/Subroutines

- subroutine, public prg_densitymatrix_mod::prg_build_density_t0 (ham_bml, rho_bml, threshold, bndfil)

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

  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. $\rho_{ii} = mathcalZ_{ii}$ Where, $mathcalZ_{ii}$ is the number of electrons for orbital i.
- subroutine, public prg_densitymatrix_mod::prg_get_flevel (eigenvalues, kbt, bndfil, tol, Ef)

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

  Gets the eigenvalues of the Orthogonalized Hamiltonian.
- subroutine, public prg_densitymatrix_mod::prg_check_idempotency (mat_bml, threshold, idempotency)

  To check the idempotency error of a matrix. This is calculated as the Frobenius norm of $(A - A^2)$.
- real(dp) function prg_densitymatrix_mod::fermi (e, ef, kbt)

  Gives the Fermi distribution value for energy e.

Variables

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

11.6 /home/christian/qmd-progress/src/prg_dos_mod.F90 File Reference

Modules

- module prg_dos_mod

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

Functions/Subroutines

- subroutine, public prg_dos_mod::prg_write_tdos (eigenvals, gamma, npts, emin, emax, filename)

  Writes the total DOS into a file. $DOS(\epsilon) = \sum_k L(\epsilon - \epsilon_k)$ Where $\int_{-\infty}^{\infty} DOS(\epsilon) = Nstates.$
- real(dp) function prg_dos_mod::lorentz (energy, eigenvals, loads, Gamma)

  Lorentzian Function.

Variables

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

11.7 /home/christian/qmd-progress/src/prg_doxy_mod.F90 File Reference

11.8 /home/christian/qmd-progress/src/prg_extras_mod.F90 File Reference

Data Types

- interface prg_extras_mod::prg_memory_consumption
- interface prg_extras_mod::to_string

Modules

- module prg_extras_mod

  Extra routines:

Functions/Subroutines

- character(len=:) function, allocatable prg_extras_mod::to_string_integer (i)

  Convert integer to string.
- character(len=:) function, allocatable prg_extras_mod::to_string_long_long (i)

  Convert integer to string.
- character(len=:) function, allocatable prg_extras_mod::to_string_double (x)

  Convert double to string.
- subroutine, public prg_extras_mod::prg_print_matrix (matname, amat, i1, i2, j1, j2)

  To write a dense matrix to screen.
- real(dp) function, public prg_extras_mod::mls ()

  To get the actual time in milliseconds.
- subroutine, public prg_extras_mod::prg_delta (x, s, nn, dta)

  Delta function ||X^tSX - I||. CFAN, March 2015.
- subroutine, public prg_extras_mod::prg_get_mem (procname, tag)

  Get proc memory.
- subroutine prg_extras_mod::prg_twonorm (a, nn, norm2)

Variables

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

11.9 /home/christian/qmd-progress/src/prg_genz_mod.F90 File Reference

Data Types

- type prg_genz_mod::genzspinp

  Input for the genz driver.
- type prg_genz_mod::genzspdata

  contains the data for the genZ driver.

Modules

- module prg_genz_mod

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

Functions/Subroutines

- subroutine, public prg_genz_mod::prg_parse_zsp (input, filename)

  The parser for genz solver.
- subroutine prg_genz_mod::prg_init (self, input)

  Initializes the genz input variables.
- subroutine prg_genz_mod::prg_allocatezspmat (self, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, norb, bml_type)

  Allocates the matrices for the Xl integration of Z.
- subroutine, public prg_genz_mod::prg_init_zspmat (igenz, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, norb, bml_type)

  Initiates the matrices for the Xl integration of Z.
- subroutine prg_genz_mod::prg_generate (self, over_bml, zmat_bml, igenz, mdim, bml_type, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml)

  Generates the Z matrix.
- subroutine, public prg_genz_mod::prg_buildzdiag (smat_bml, zmat_bml, threshold, mdimin, bml_type, verbose)

  Usual subroutine involving diagonalization.
- subroutine, public prg_genz_mod::prg_buildzsparse (smat_bml, zmat_bml, igenz, mdim, bml_type, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, nfirst, nrefi, nreff, thresholdi, thresholdf, integration, verbose)

  Inverse factorization using niklasson's algorithm.
- subroutine, public prg_genz_mod::prg_genz_sp_initialz0 (smat_bml, zmat_bml, norb, mdim, bml_type_f, threshold)
- subroutine, public prg_genz_mod::prg_genz_sp_initial_zmat (smat_bml, zmat_bml, norb, mdim, bml_type_f, threshold)

  Estimate Z matrix.
- subroutine prg_genz_mod::prg_genz_sp_int (zmat_bml, zk1_bml, zk2_bml, zk3_bml, zk4_bml, zk5_bml, zk6_bml, igenz, norb, bml_type, threshold)
- subroutine, public prg_genz_mod::prg_genz_sp_ref (smat_bml, zmat_bml, nref, norb, bml_type, threshold)

Variables

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

11.10 /home/christian/qmd-progress/src/prg_graph_mod.F90 File Reference

Data Types

- type prg_graph_mod::subgraph_t

  Subgraph type.
- type prg_graph_mod::graph_partitioning_t

  Trace per iteration.

Modules

- module prg_graph_mod

  The graph module.

Functions/Subroutines

- subroutine, public prg_graph_mod::prg_initsubgraph (sg, pnum, hsize)

  Initialize subgraph.
- subroutine, public prg_graph_mod::prg_destroysubgraph (sg)

  Destroy subgraph.
- subroutine, public prg_graph_mod::prg_initgraphpartitioning (gp, pname, np, nnodes, nnodes2)

  Initialize graph partitioning.
- subroutine, public prg_graph_mod::prg_destroygraphpartitioning (gp)

  Destroy graph partitioning.
- subroutine, public prg_graph_mod::prg_printgraphpartitioning (gp)

  Print graph partitioning structure data.
- subroutine, public prg_graph_mod::prg_equalpartition (gp, nodesPerPart, nnodes)

  Create equal graph partitions, based on number of rows/orbitals.
- subroutine, public prg_graph_mod::prg_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 /home/christian/qmd-progress/src/prg_graphsp2parser_mod.F90 File Reference

Data Types

- type prg_graphsp2parser_mod::gsp2data_type

  General SP2 solver type.

Modules

- module prg_graphsp2parser_mod

  Graph partitioning SP2 parser.

Functions/Subroutines

- subroutine, public prg_graphsp2parser_mod::prg_parse_gsp2 (gsp2data, filename)

  The parser for SP2 solver.

Variables

- integer, parameter prg_graphsp2parser_mod::dp = kind(1.0d0)

11.12 /home/christian/qmd-progress/src/prg_homolumo_mod.F90 File Reference

Modules

- module prg_homolumo_mod

  The homolumo module.

Functions/Subroutines

- subroutine, public prg_homolumo_mod::prg_homolumogap (vv, imax, pp, mineval, maxeval, ehomo, elumo, egap, verbose)
- subroutine, public prg_homolumo_mod::prg_sp2sequence (pp, imax, mineval, maxeval, ehomo, elumo, errlimit, verbose)

Variables

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

11.13 /home/christian/qmd-progress/src/prg_implicit_fermi_mod.F90 File Reference

Modules

- module prg_implicit_fermi_mod

Functions/Subroutines

- subroutine, public prg_implicit_fermi_mod::prg_implicit_fermi (h_bml, xi0_bml, p_bml, nsteps, nocc, mu, beta, osteps, occErrLimit, threshold)

  Recursive Implicit Fermi Dirac.

Variables

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

11.14 /home/christian/qmd-progress/src/prg_initmatrices_mod.F90 File Reference

Modules

- module prg_initmatrices_mod

  Initialization module.

Functions/Subroutines

- subroutine, public prg_initmatrices_mod::prg_init_hsmat (ham_bml, over_bml, bml_type, mdim, norb)

  Initialize Hamiltonian and Overlap Matrix.
- subroutine, public prg_initmatrices_mod::prg_init_pzmat (rho_bml, zmat_bml, bml_type, mdim, norb)

  Initialize Density matrix and Inverse square root Overlap.
- subroutine, public prg_initmatrices_mod::prg_init_ortho (orthoh_bml, orthop_bml, bml_type, mdim, norb)

  Initialize The orthogonal versions of Hamiltonian and Density Matrix.

Variables

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

11.15 /home/christian/qmd-progress/src/prg_kernelparser_mod.F90 File Reference

Modules

- module prg_kernelparser_mod

  Some general parsing functions.

Functions/Subroutines

- subroutine, public prg_kernelparser_mod::prg_parsing_kernel (keyvector_char, valvector_char, keyvector_↩ int, valvector_int, keyvector_re, valvector_re, keyvector_log, valvector_log, filename, startstop)

  The general parsing function. It is used to vectorize a set of "keywords" "value" pairs as included in a general input file.
- subroutine prg_kernelparser_mod::prg_check_valid (invalidc)

  Check for valid keywords (checks for an = sign)

Variables

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

11.16 /home/christian/qmd-progress/src/prg_nonortho_mod.F90 File Reference

Modules

- module prg_nonortho_mod

  Module to prg_orthogonalize and prg_deorthogonalize any operator.

Functions/Subroutines

- subroutine, public prg_nonortho_mod::prg_orthogonalize (A_bml, zmat_bml, orthoA_bml, threshold, bml_↩ type, verbose)

  This routine performs: $A_{ortho} = Z^{\dagger} A Z$.
- subroutine, public prg_nonortho_mod::prg_deorthogonalize (orthoA_bml, zmat_bml, a_bml, threshold, bml↩ _type, verbose)

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

Variables

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

11.17 /home/christian/qmd-progress/src/prg_normalize_mod.F90 File Reference

Modules

- module prg_normalize_mod

  The prg_normalize module.

Functions/Subroutines

- subroutine, public prg_normalize_mod::prg_normalize (h_bml)

  Normalize a Hamiltonian matrix prior to running the SP2 algorithm.
- subroutine, public prg_normalize_mod::prg_normalize_fermi (h_bml, h1, hN, mu)

  Normalize a Hamiltonian matrix prior to running the truncated SP2 algorithm.
- subroutine, public prg_normalize_mod::prg_normalize_implicit_fermi (h_bml, cnst, mu)

  Normalize a Hamiltonian matrix prior to running the implicit fermi dirac algorithm.
- subroutine, public prg_normalize_mod::prg_gershgorinreduction (gp)

  Determine gershgorin bounds across all parts, local and distributed.
- subroutine, public prg_normalize_mod::prg_normalize_cheb (h_bml, mu, emin, emax, alpha, scaledmu)

  Normalize a Hamiltonian matrix prior to running the Chebyshev algorithm.

Variables

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

11.18 /home/christian/qmd-progress/src/prg_openfiles_mod.F90 File Reference

Modules

- module prg_openfiles_mod

  Module to handle input output files for the PROGRESS lib.

Functions/Subroutines

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

  Returns a unit number that is not in use.
- subroutine, public prg_openfiles_mod::prg_open_file (io, name)

  Opens a file to write.
- subroutine, public prg_openfiles_mod::prg_open_file_to_read (io, name)

  Opens a file to read.

11.19 /home/christian/qmd-progress/src/prg_parallel_mod.F90 File Reference

Data Types

- type prg_parallel_mod::rankreducedata_t

  Data structure for rection over MPI ranks.

Modules

- module prg_parallel_mod

  The parallel module.

Functions/Subroutines

- integer function, public prg_parallel_mod::getnranks ()
- integer function, public prg_parallel_mod::getmyrank ()
- integer function, public prg_parallel_mod::printrank ()
- subroutine, public prg_parallel_mod::prg_initparallel ()
- subroutine, public prg_parallel_mod::prg_shutdownparallel ()
- integer function prg_parallel_mod::saverequest (irequest)
- subroutine, public prg_parallel_mod::prg_barrierparallel ()
- subroutine, public prg_parallel_mod::sendreceiveparallel (sendBuf, sendLen, dest, recvBuf, recvLen, source, nreceived)
- subroutine, public prg_parallel_mod::isendparallel (sendBuf, sendLen, dest)
- subroutine, public prg_parallel_mod::sendparallel (sendBuf, sendLen, dest)
- subroutine, public prg_parallel_mod::prg_iprg_recvparallel (recvBuf, recvLen, rind)
- subroutine, public prg_parallel_mod::prg_recvparallel (recvBuf, recvLen)
- subroutine, public prg_parallel_mod::sumintparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::sumrealparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::maxintparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::maxrealparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::minintparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::minrealparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::prg_minrealreduce (rvalue)
- subroutine, public prg_parallel_mod::prg_maxrealreduce (rvalue)
- subroutine, public prg_parallel_mod::prg_maxintreduce2 (value1, value2)
- subroutine, public prg_parallel_mod::prg_sumintreduce2 (value1, value2)
- subroutine, public prg_parallel_mod::prg_sumrealreduce (value1)
- subroutine, public prg_parallel_mod::prg_sumrealreduce2 (value1, value2)
- subroutine, public prg_parallel_mod::prg_sumrealreduce3 (value1, value2, value3)
- subroutine, public prg_parallel_mod::prg_sumrealreducen (valueVec, N)
- subroutine, public prg_parallel_mod::prg_sumintreducen (valueVec, N)
- subroutine, public prg_parallel_mod::minrankrealparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::maxrankrealparallel (sendBuf, recvBuf, icount)
- subroutine, public prg_parallel_mod::prg_bcastparallel (buf, blen, root)
- subroutine, public prg_parallel_mod::allgatherrealparallel (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public prg_parallel_mod::allgatherintparallel (sendBuf, sendLen, recvBuf, recvLen)
- subroutine, public prg_parallel_mod::allgathervrealparallel (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public prg_parallel_mod::allgathervintparallel (sendBuf, sendLen, recvBuf, recvLen, recvDispl)
- subroutine, public prg_parallel_mod::prg_allsumrealreduceparallel (buf, buflen)
- subroutine, public prg_parallel_mod::prg_allsumintreduceparallel (buf, buflen)
- subroutine, public prg_parallel_mod::prg_allgatherparallel (a)
- subroutine, public prg_parallel_mod::prg_wait ()

Variables

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

11.20 /home/christian/qmd-progress/src/prg_partition_mod.F90 File Reference

Modules

- module prg_partition_mod

  The partition module.

Functions/Subroutines

- subroutine, public prg_partition_mod::prg_metispartition (gp, ngroups, nnodes, xadj, adjncy, nparts, part, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm)

  Create graph partitions minizing number of cut edges.
- subroutine, public prg_partition_mod::prg_costpartition (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm)

  Compute cost of a partition.
- subroutine, public prg_partition_mod::update_prg_costpartition (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, node, new_part)

  Update cost of partition and the different parameters node is moves into new_part For each neighbor of node, the following cases hold: Case 1: neighbor is in old_part Case 2: neighbor is in new_part Case 3: neighbor is neither in old_ or new_part.
- subroutine prg_partition_mod::prg_accept_prob (it, prg_delta, r)

  Compute acceptance probability for simulated annealing.
- subroutine prg_partition_mod::prg_costindex (cost, sumCubes, maxCH, smooth_maxCH, obj_fun)

  Choose objective function to work with.
- subroutine prg_partition_mod::prg_rand_node (gp, node, seed)

  Pick a random node.
- subroutine, public prg_partition_mod::prg_simannealing (gp, xadj, adjncy, partNumber, core_count, CH_↩ count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, niter, seed)

  Graph partitioning based on Simulated Annealing.
- subroutine, public prg_partition_mod::prg_kernlin (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, nconverg, seed)

  Graph partitioning based on inspired by Kernighan-Lin Review METiS manual for description of k-way implementation of KL Pick a core together with its halos Place free vertices on a priority queue with (key, value) =(prg_delta, best_↩ part),with prg_delta = change in obj_value Dequeue and allow hill climbing.
- subroutine, public prg_partition_mod::prg_update_gp (gp, partNumber, core_count)
- subroutine prg_partition_mod::prg_rand_shuffle (array, seed)

  Randomly shuffle array.
- subroutine, public prg_partition_mod::prg_check_arrays (gp, core_count, CH_count, Halo_count)

  Error checking Checking that core_count, CH_count, Halo_count match.
- subroutine, public prg_partition_mod::prg_kernlin_queue (gp, xadj, adjncy, partNumber, core_count, CH_↩ count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm)

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

- subroutine prg_partition_mod::prg_find_best_move (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, best_node, best_part)

  For kerlin_queue to find (vertex, new_part) pair with highest gain.
- subroutine, public prg_partition_mod::prg_kernlin2 (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm)
- subroutine prg_partition_mod::prg_get_largest_hedge_in_part (gp, xadj, adjncy, partNumber, core_count, CH_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, search_part, largest_Hedge)
- subroutine, public prg_partition_mod::prg_simannealing_old (gp, xadj, adjncy, partNumber, core_count, C↩H_count, Halo_count, sumCubes, maxCH, smooth_maxCH, pnorm, niter, seed)

Variables

- integer, parameter prg_partition_mod::dp = kind(1.0d0)
- integer, parameter prg_partition_mod::metis_index_kind = METIS_INDEX_KIND

  From /usr/include/metis.h.
- integer, parameter prg_partition_mod::metis_real_kind = kind(METIS_REAL_KIND)

  From /usr/include/metis.h.

11.21 /home/christian/qmd-progress/src/prg_progress_mod.F90 File Reference

Modules

- module prg_progress_mod

  The progress module.

Functions/Subroutines

- subroutine, public prg_progress_mod::prg_progress_init ()

  Initialize progress.
- subroutine, public prg_progress_mod::prg_progress_shutdown ()

  Shutdown progress.

Variables

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

11.22 /home/christian/qmd-progress/src/prg_ptable_mod.F90 File Reference

Modules

- module prg_ptable_mod

  Periodic table of elements.

Functions/Subroutines

- integer function, public prg_ptable_mod::element_atomic_number (symbol)
- integer function prg_ptable_mod::element_atomic_number_upper (symbol)

Variables

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

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

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

  Element name.
- real(dp), dimension(nz), parameter prg_ptable_mod::element_mass = (/ 1.007825032 , 4.002603254 , 7.↩ 01600455 , 9.0121822 , 11.0093054 , 12.0 , 14.003074005 , 15.99491462 , 18.99840322 , 19.992440175 , 22.989769281 , 23.9850417 , 26.98153863 , 27.976926532 , 30.97376163 , 31.972071 , 34.96885268 , 39.962383123 , 38.96370668 , 39.96259098 , 44.9559119 , 47.9479463 , 50.9439595 , 51.9405075 , 54.↩ 9380451 , 55.9349375 , 58.933195 , 57.9353429 , 62.9295975 , 63.929142 , 68.925573 , 73.921177 , 74.↩ 921596 , 79.916521 , 78.918337 , 83.911507 , 84.911789 , 87.905612 , 88.905848 , 89.904704 , 92.906378 , 97.905408 , 97.907216 , 101.904349 , 102.905504 , 105.903486 , 106.905097 , 113.903358 , 114.903878 , 119.902194 , 120.903815 , 129.906224 , 126.904473 , 131.904153 , 132.905451 , 137.905247 , 138.↩ 906353 , 139.905438 , 140.907652 , 141.907723 , 144.912749 , 151.919732 , 152.92123 , 157.924103 , 158.925346 , 163.929174 , 164.930322 , 165.930293 , 168.934213 , 173.938862 , 174.940771 , 179.94655 , 180.947995 , 183.950931 , 186.955753 , 191.96148 , 192.962926 , 194.964791 , 196.966568 , 201.970643 , 204.974427 , 207.976652 , 208.980398 , 208.98243 , 209.987148 , 222.017577 , 223.019735 , 226.025409 , 227.027752 , 232.038055 , 231.035884 , 238.050788 , 237.048173 , 244.064204 , 243.061381 , 247.070354 , 247.070307 , 251.079587 , 252.08298 , 257.095105 , 258.098431 , 259.10103 , 262.10963 /)

  Element mass in atomic mass units (1.66 x 10-27 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 , 2.05 , 2.0 , 2.0 , 2.0 , 2.1 , 1.87 , 2.11 , 1.85 , 1.9 , 1.83 , 2.02 , 3.03 , 2.49 , 2.4 , 2.3 , 2.15 , 2.1 , 2.05 , 2.05 , 2.0 , 2.05 , 2.1 , 2.2 , 2.2 , 1.93 , 2.17 , 2.06 , 1.98 , 2.16 , 3.43 , 2.68 , 2.5 , 2.48 , 2.47 , 2.45 , 2.43 , 2.42 , 2.4 , 2.38 , 2.37 , 2.35 , 2.33 , 2.32 , 2.3 , 2.28 , 2.27 , 2.25 , 2.2 , 2.1 , 2.05 , 2.0 , 2.0 , 2.05 , 2.1 , 2.05 , 1.96 , 2.02 , 2.07 , 1.97 , 2.02 , 2.2 , 3.48 , 2.83 , 2.0 , 2.4 , 2.0 , 2.3 , 2.0 , 2.0 , 2.0 , 2.0 , 2.0 , 2.0 , 2.0 , 2.0 , 2.0 , 2.0 , 2.0 /)

  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 , 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)

- 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 , 0.0 , 0.0 /)

  Electron affprg_inity (in eV)

- 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.

- 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 , 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 , 6 /)

  The maximum expected number of bonds to this element.

- 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.

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

  The electronic configuration.

11.23 /home/christian/qmd-progress/src/prg_pulaycomponent_mod.F90 File Reference

Modules

- module prg_pulaycomponent_mod

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

Functions/Subroutines

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

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

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

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

Variables

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

11.24 /home/christian/qmd-progress/src/prg_pulaymixer_mod.F90 File Reference

Data Types

- type prg_pulaymixer_mod::mx_type

Modules

- module prg_pulaymixer_mod

  Pulay mixer mode.

Functions/Subroutines

- subroutine, public prg_pulaymixer_mod::prg_parse_mixer (input, filename)

  The parser for the mixer routines.
- subroutine, public prg_pulaymixer_mod::prg_qmixer (charges, oldcharges, dqin, dqout, scferror, piter, pulaycoef, mpulay, verbose)

  Mixing the charges to acelerate scf convergence.
- subroutine, public prg_pulaymixer_mod::prg_linearmixer (charges, oldcharges, scferror, linmixcoef, verbose)

  Routine to perform linear mixing.

Variables

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

11.25 /home/christian/qmd-progress/src/prg_quantumdynamics_mod.F90 File Reference

Modules

- module prg_quantumdynamics_mod

  A module to add in common quantum dynamical operations.

Functions/Subroutines

- subroutine, public prg_quantumdynamics_mod::prg_kick_density (kick_direc, 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: $\rho_{\hat{kick}} = \exp\frac{-i}{\hbar}\hat{V}\hat{\rho}\hat{S}\exp\frac{i}{\hbar}\hat{V}\hat{S^{-1}}$ *where* $\hat{V}$ *is the field disturbance.*
- subroutine, public prg_quantumdynamics_mod::prg_get_sparsity_cplxmat (matrix_type, element_type, thresh, a_dense)

  This computes the sparsity of a complex matrix given a threshold value This routine does: $f = \frac{N_0}{N_{tot}}$ *where* f *is the sparsity,* N_0 *is the number of values less than the threshold, and* N_{tot} *is the total number of values. The sparsity and threshold are printed to the screen.*
- subroutine, public prg_quantumdynamics_mod::prg_get_sparsity_realmat (matrix_type, element_type, thresh, a_dense)

  This computes the sparsity of a real matrix given a threshold value This routine does: $f = \frac{N_0}{N_{tot}}$ *where* f *is the sparsity,* N_0 *is the number of values less than the threshold, and* N_{tot} *is the total number of values. The sparsity and threshold are printed to the screen.*
- subroutine, public prg_quantumdynamics_mod::prg_kick_density_bml (kick_direc, 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 matricies in BML format. This routine does: $\rho_{\hat{kick}} = \exp\frac{-i}{\hbar}\hat{V}\hat{\rho}\hat{S}\exp\frac{i}{\hbar}\hat{V}\hat{S^{-1}}$ *where* $\hat{V}$ *is the field disturbance.*
- subroutine, public prg_quantumdynamics_mod::prg_lvni_bml (h1_bml, sinv_bml, dt, hbar, rhoold_bml, rho↩ _bml, aux_bml, matrix_type, mdim, thresh)

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

- subroutine, public prg_quantumdynamics_mod::prg_getcharge (rho_bml, s_bml, charges, aux_bml, z, spindex, 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)

11.26 /home/christian/qmd-progress/src/prg_response_mod.F90 File Reference

Data Types

- type prg_response_mod::respdata_type

Modules

- module prg_response_mod

  Module to compute the density matrix response and related quantities.

Functions/Subroutines

- subroutine, public prg_response_mod::prg_parse_response (RespData, filename)

  The parser for the calculation of the DM response.
- subroutine, public prg_response_mod::prg_compute_dipole (charges, coordinate, dipoleMoment, factor, verbose)

  To compute the dipole moment of the system. The units of the dipole moment are determined by the units of the coordinates and charges that are given.
- subroutine, public prg_response_mod::prg_write_dipole_tcl (dipoleMoment, file, factor, verbose)

  To visualize a dipole moment using VMD. This will prg_generate a .tcl script that could be run using VMD To visualize with VMD: $ vmd -e dipole.tcl.
- subroutine, public prg_response_mod::prg_compute_polarizability (rsp_bml, prt_bml, polarizability, factor, verbose)

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

  Read perturbation from file.
- subroutine, public prg_response_mod::prg_compute_response_rs (ham_bml, prt_bml, rsp_bml, lambda, bndfil, threshold, verbose)

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

- subroutine, public prg_response_mod::prg_compute_response_fd (ham_bml, prt_bml, rsp_bml, prg_delta, bndfil, threshold, verbose)

  Computes the first order response density matrix using finite differences. The transformation hereby performed are:
- subroutine, public prg_response_mod::prg_pert_constant_field (field, intensity, coordinate, lambda, prt_bml, threshold, spindex, norbi, verbose, over_bml)

  Apply a constant field perturbation through the dipole moment operator ($\hat{\mu} = e\hat{\boldsymbol{r}}$). In the matrix representation, this is: $H^{(1)} = \lambda\frac{1}{2}(S\, e\boldsymbol{r}\cdot\boldsymbol{E} + e\boldsymbol{r}\cdot\boldsymbol{E}S)$. 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 ($\sin(\tilde{\boldsymbol{r}}_x)$) where $\boldsymbol{r}_x$ is the x coordinate. The Hamiltonian gets modified as follows: $H^{(1)} = \frac{1}{2}\lambda(S\sin(\tilde{\boldsymbol{r}}_x) + \sin(\tilde{\boldsymbol{r}}_x)S)$. $\tilde{\boldsymbol{r}}_x = 2\pi(\boldsymbol{r}/l_x) - \pi$. 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 ($\cos(\tilde{\boldsymbol{r}}_x)$) where $\boldsymbol{r}_x$ is the x coordinate. The Hamiltonian gets modified as follows: $H^{(1)} = \frac{1}{2}\lambda(S\sin(\tilde{\boldsymbol{r}}_x) + \sin(\tilde{\boldsymbol{r}}_x)S)$. $\tilde{\boldsymbol{r}}_x = 2\pi(\boldsymbol{r}/l_x) - \pi$. 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, idemtol, 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: $rsp(i) = \sum_{\alpha\in i}\rho^{(1)}_{\alpha\alpha}$, 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

11.27 /home/christian/qmd-progress/src/prg_sp2_fermi_mod.F90 File Reference

Modules

- module prg_sp2_fermi_mod

  The SP2 Fermi module.

Functions/Subroutines

- subroutine, public prg_sp2_fermi_mod::prg_sp2_fermi_init (h_bml, nsteps, nocc, tscale, threshold, occErr↩Limit, traceLimit, x_bml, mu, beta, h1, hN, sgnlist)

  Truncated SP2 prg_initialization.
- subroutine, public prg_sp2_fermi_mod::prg_sp2_fermi_init_norecs (h_bml, nsteps, nocc, tscale, threshold, occErrLimit, traceLimit, x_bml, mu, beta, h1, hN, sgnlist, verbose)

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

- subroutine, public prg_sp2_fermi_mod::prg_sp2_fermi (h_bml, osteps, nsteps, nocc, mu, beta, h1, hN, sgnlist, threshold, eps, traceLimit, x_bml)

  Calculate Truncated SP2.
- subroutine, public prg_sp2_fermi_mod::prg_sp2_entropy_function (mu, h1, hN, nsteps, sgnlist, GG, ee)

  Calculate SP2 entropy function using gaussian quadrature. Note that GG and ee are allocated and returned from this routine.
- real(dp) function, public prg_sp2_fermi_mod::sp2_entropy_ts (D0_bml, GG, ee)

  Test SP2 entropy. Get the entropy contribution TS to the total free energy.
- real(dp) function, public prg_sp2_fermi_mod::sp2_inverse (f, mu, h1, hN, nsteps, sgnlist)

  Calculate the SP2 inverse.
- real(dp) function prg_sp2_fermi_mod::absmaxderivative (func, de)

  Gets the absolute maximum of the derivative of a function.

Variables

- integer, parameter prg_sp2_fermi_mod::dp = kind(1.0d0)

11.28 /home/christian/qmd-progress/src/prg_sp2_mod.F90 File Reference

Modules

- module prg_sp2_mod

  The SP2 module.

Functions/Subroutines

- subroutine, public prg_sp2_mod::prg_sp2_basic (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)

  Calculates the density matrix from a Hamiltonian matrix by purification. The method implemented here is the very first verion of the SP2 method.
- subroutine, public prg_sp2_mod::prg_sp2_alg2 (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, verbose)
- subroutine, public prg_sp2_mod::prg_sp2_alg2_genseq (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, 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, idemtol, verbose)
- subroutine, public prg_sp2_mod::prg_sp2_alg1_genseq (h_bml, rho_bml, threshold, bndfil, minsp2iter, maxsp2iter, sp2conv, idemtol, pp, icount, vv)
- subroutine, public prg_sp2_mod::prg_sp2_alg1_seq (h_bml, rho_bml, threshold, pp, icount, vv)
- subroutine, public prg_sp2_mod::prg_prg_sp2_alg1_seq_inplace (rho_bml, threshold, pp, icount, vv, mineval, maxeval)
- subroutine, public prg_sp2_mod::prg_sp2_submatrix (ham_bml, rho_bml, threshold, pp, icount, vv, mineval, maxeval, core_size)

  Perform SP2 algorithm using sequence and calculate norm for a submatrix.
- subroutine, public prg_sp2_mod::prg_sp2_submatrix_inplace (rho_bml, threshold, pp, icount, vv, mineval, maxeval, core_size)

Variables

- integer, parameter prg_sp2_mod::dp = kind(1.0d0)

11.29 /home/christian/qmd-progress/src/prg_sp2parser_mod.F90 File Reference

Data Types

- type prg_sp2parser_mod::sp2data_type
  General SP2 solver type.

Modules

- module prg_sp2parser_mod
  SP2 parser.

Functions/Subroutines

- subroutine, public prg_sp2parser_mod::prg_parse_sp2 (sp2data, filename)
  The parser for SP2 solver.

Variables

- integer, parameter prg_sp2parser_mod::dp = kind(1.0d0)

11.30 /home/christian/qmd-progress/src/prg_subgraphloop_mod.F90 File Reference

Modules

- module prg_subgraphloop_mod
  The subgraphloop module.

Functions/Subroutines

- subroutine, public prg_subgraphloop_mod::prg_subgraphsp2loop (h_bml, g_bml, rho_bml, gp, threshold)
- subroutine, public prg_subgraphloop_mod::prg_collectmatrixfromparts (gp, rho_bml)
  Collect distributed parts into same matrix.
- subroutine, public prg_subgraphloop_mod::prg_balanceparts (gp)
- subroutine, public prg_subgraphloop_mod::prg_partordering (gp)
  Set row ordering bases on parts.
- subroutine, public prg_subgraphloop_mod::prg_getgrouppartitionhalosfromgraph (gp, g_bml, hnode, djflag)
  Get core+halo indeces for all partitions only using the graph.
- subroutine, public prg_subgraphloop_mod::prg_getpartitionhalosfromgraph (gp, g_bml, djflag)
  Get core+halo indeces for all partitions only using the graph.

Variables

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

11.31 /home/christian/qmd-progress/src/prg_syrotation_mod.F90 File Reference

Data Types

- type prg_syrotation_mod::rotation_type

  Rotation type.

Modules

- module prg_syrotation_mod

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

Functions/Subroutines

- subroutine, public prg_syrotation_mod::prg_parse_rotation (rot, filename)

  The parser for rotation.
- subroutine, public prg_syrotation_mod::prg_rotate (rot, r, verbose)

  Rotation routine.

Variables

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

11.32 /home/christian/qmd-progress/src/prg_system_mod.F90 File Reference

Data Types

- type prg_system_mod::estruct_type

  Electronic structure type.
- type prg_system_mod::system_type

  System type.

Modules

- module prg_system_mod

  A module to read and handle chemical systems.

Functions/Subroutines

- subroutine, public prg_system_mod::prg_get_nameandext (fullfilename, filename, ext)

  Get the name and extension of a file.
- subroutine, public prg_system_mod::prg_parse_system (system, filename, extin)

  The parser for the chemical system.
- subroutine, public prg_system_mod::prg_write_system (system, filename, extension)

  Write system in .xyz, .dat or pdb file.
- subroutine, public prg_system_mod::prg_write_trajectory (system, iter, each, prg_deltat, filename, extension)

  Write trajectory in .xyz, .dat or pdb file.
- subroutine, public prg_system_mod::prg_write_trajectoryandproperty (system, iter, each, prg_deltat, scalarprop, filename, extension)

  Write trajectory and atomic properties. Only pdb file.
- subroutine, public prg_system_mod::prg_make_random_system (system, nats, seed, lx, ly, lz)

  Make random Xx system.
- subroutine prg_system_mod::prg_parameters_to_vectors (abc_angles, lattice_vector)

  Transforms the lattice parameters into lattice vectors.
- subroutine prg_system_mod::prg_vectors_to_parameters (lattice_vector, abc_angles)

  Transforms the lattice vectors into lattice parameters.
- subroutine, public prg_system_mod::prg_get_origin (coords, origin)

  Get the origin of the coordinates.
- subroutine, public prg_system_mod::prg_get_distancematrix (coords, dmat)

  Get the distance matrix.
- subroutine, public prg_system_mod::prg_translateandfoldtobox (coords, lattice_vectors, origin, verbose)

  Translate and fold to box.
- subroutine, public prg_system_mod::prg_centeratbox (coords, lattice_vectors, verbose)

  Translate geometric center to the center of the box.
- subroutine, public prg_system_mod::prg_wraparound (coords, lattice_vectors, index, verbose)

  Wrap around atom i using pbc.
- subroutine, public prg_system_mod::prg_translatetogeomcandfoldtobox (coords, lattice_vectors, origin)

  Translate to geometric center.
- subroutine, public prg_system_mod::prg_replicate (coords, symbols, lattice_vectors, nx, ny, nz)

  Extend/replicate system along lattice vectors.
- subroutine, public prg_system_mod::prg_get_recip_vects (lattice_vectors, recip_vectors, volr, volk)

  Get the volume of the cell and the reciprocal vectors: This soubroutine 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, nrnnstruct, 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, nrnnstruct, bml_type, factor, gcov_bml, mdimin, verbose)
- subroutine, public prg_system_mod::prg_get_covgraph_h (sy, nnStructMindist, nnStruct, nrnnstruct, 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, nrnnstruct, hetatm, 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)

11.33 /home/christian/qmd-progress/src/prg_timer_mod.F90 File Reference

Data Types

- type prg_timer_mod::timer_status_t

  Timer status type.

Modules

- module prg_timer_mod

  The timer module.

Functions/Subroutines

- subroutine, public prg_timer_mod::timer_prg_init ()

  Initialize timers.
- subroutine prg_timer_mod::prg_timer_getid ()

  Get timer id.
- subroutine, public prg_timer_mod::prg_timer_shutdown ()

  Done with timers.
- subroutine, public prg_timer_mod::prg_timer_start (itimer, tag)

  Start Timing.
- subroutine, public prg_timer_mod::prg_timer_stop (itimer, verbose)

  Stop timing.
- subroutine, public prg_timer_mod::prg_timer_collect ()
- subroutine, public prg_timer_mod::prg_timer_results ()
- real(8) function, public prg_timer_mod::time2milliseconds ()
- subroutine, public prg_timer_mod::prg_print_date_and_time (tag)
- character(2) function, private prg_timer_mod::int2char (ival)

Variables

- integer, parameter prg_timer_mod::dp = kind(1.0d0)
- integer, public prg_timer_mod::loop_timer
- integer, public prg_timer_mod::sp2_timer
- integer, public prg_timer_mod::genx_timer
- integer, public prg_timer_mod::part_timer
- integer, public prg_timer_mod::subgraph_timer
- integer, public prg_timer_mod::deortho_timer
- integer, public prg_timer_mod::ortho_timer
- integer, public prg_timer_mod::zdiag_timer
- integer, public prg_timer_mod::graphsp2_timer
- integer, public prg_timer_mod::subind_timer
- integer, public prg_timer_mod::subext_timer
- integer, public prg_timer_mod::subsp2_timer
- integer, public prg_timer_mod::suball_timer
- integer, public prg_timer_mod::bmult_timer
- integer, public prg_timer_mod::badd_timer
- integer, public prg_timer_mod::dyn_timer
- integer, public prg_timer_mod::mdloop_timer
- integer, public prg_timer_mod::buildz_timer
- integer, public prg_timer_mod::realcoul_timer
- integer, public prg_timer_mod::recipcoul_timer
- integer, public prg_timer_mod::pairpot_timer
- integer, public prg_timer_mod::halfverlet_timer
- integer, public prg_timer_mod::pos_timer
- integer, public prg_timer_mod::nlist_timer
- integer prg_timer_mod::tstart_clock
- integer prg_timer_mod::tstop_clock
- integer prg_timer_mod::tclock_rate
- integer prg_timer_mod::tclock_max
- integer prg_timer_mod::num_timers
- type(timer_status_t), dimension(:), allocatable prg_timer_mod::ptimer

11.34 /home/christian/qmd-progress/src/prg_xlbo_mod.F90 File Reference

Data Types

- type prg_xlbo_mod::xlbo_type

  General xlbo solver type.

Modules

- module prg_xlbo_mod

  A module to perform XLBO integration.

Functions/Subroutines

- subroutine, public prg_xlbo_mod::prg_parse_xlbo (xlbo, filename)

  The parser for XLBO parser.
- subroutine, public prg_xlbo_mod::prg_xlbo_nint (charges, n, n_0, n_1, n_2, n_3, n_4, n_5, mdstep, xl)

  This routine integrates the dynamical variable "n".
- subroutine, public prg_xlbo_mod::prg_xlbo_fcoulupdate (fcoul, charges, n)

  Adjust forces for the linearized XLBOMD functional.

Variables

- integer, parameter prg_xlbo_mod::dp = kind(1.0d0)
- real(dp), parameter prg_xlbo_mod::c0 = -6.0_dp

  Coefficients for modified Verlet integration.
- real(dp), parameter prg_xlbo_mod::c1 = 14.0_dp
- real(dp), parameter prg_xlbo_mod::c2 = -8.0_dp
- real(dp), parameter prg_xlbo_mod::c3 = -3.0_dp
- real(dp), parameter prg_xlbo_mod::c4 = 4.0_dp
- real(dp), parameter prg_xlbo_mod::c5 = -1.0_dp
- real(dp), parameter prg_xlbo_mod::kappa = 1.82_dp

  Coefficients for modified Verlet integration.
- real(dp), parameter prg_xlbo_mod::alpha = 0.018_dp
- real(dp), parameter prg_xlbo_mod::cc = 0.9_dp

11.35 /home/christian/qmd-progress/src/prg_xlkernel_mod.F90 File Reference

Data Types

- type prg_xlkernel_mod::xlk_type

Modules

- module prg_xlkernel_mod

  Add name.

Functions/Subroutines

- subroutine, public prg_xlkernel_mod::prg_parse_xlkernel (input, filename)

  The parser for the mixer routines.
- subroutine, public prg_xlkernel_mod::prg_fermi (D0, QQ, ee, gap, Fe_vec, mu0, H, Z, Nocc, T, OccErrLim, MaxIt, HDIM)
- subroutine, public prg_xlkernel_mod::prg_kernel_fermi_full (KK, JJ, D0, mu0, mu1, T, RX, RY, RZ, LBox, Hubbard_U, Element_Type, Nr_atoms, MaxIt, eps, m, HDIM, Max_Nr_Neigh, Coulomb_acc, TIMERATIO, nnRx, nnRy, nnRz, nrnnlist, 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, TIMERATIO, nnRx, nnRy, nnRz, nrnnlist, 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)

Bibliography

[1] S. M. Mniszewski, M. J. Cawkwell, M. E. Wall, J. Mohd-Yusof, N. Bock, T. C. Germann, and A. M. N. Niklasson. Efficient parallel linear scaling construction of the density matrix for born–oppenheimer molecular dynamics. *Journal of Chemical Theory and Computation*, 11(10):4644–4654, 2015. PMID: 26574255. 63, 64, 189, 190

[2] Christian F. A. Negre, Susan M. Mniszewski, Marc J. Cawkwell, Nicolas Bock, Michael E. Wall, and Anders M. N. Niklasson. Recursive factorization of the inverse overlap matrix in linear-scaling quantum molecular dynamics simulations. *Journal of Chemical Theory and Computation*, 12(7):3063–3073, 2016. PMID: 27267207. 45

[3] Anders M. N. Niklasson. A note on the pulay force at finite electronic temperatures. *The Journal of Chemical Physics*, 129(24), 2008. 117

[4] Anders M. N. Niklasson, Valéry Weber, and Matt Challacombe. Nonorthogonal density-matrix perturbation theory. *The Journal of Chemical Physics*, 123(4), 2005. 126

[5] Valéry Weber, Anders M. N. Niklasson, and Matt Challacombe. Higher-order response in o(n) by perturbed projection. *The Journal of Chemical Physics*, 123(4), 2005. 125, 127, 239

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