MQCPack

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Chapter 1

Modules Index

1.1 Modules List

Here is a list of all modules with brief descriptions:

Chapter 2

Data Type Index

2.1 Class Hierarchy

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Chapter 3

Data Type Index

3.1 Data Types List

Here are the data types with brief descriptions:

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File Index

4.1 File List

Here is a list of all files with brief descriptions:

Chapter 5

Module Documentation

5.1 mqc_algebra Module Reference

Data Types

- interface abs
- interface acos
- interface aimag
- interface asin
- interface assignment(=)
- interface atan
- interface atan2
- interface cmplx
- interface conjg
- interface contraction
- interface cos
- interface dagger
- interface dot_product
- interface matmul
- interface matrix_symm2sq
- interface mqc_cast_complex
- interface mqc_cast_real
- interface mqc_have_complex
- interface mqc_have_int
- interface mqc_have_real
- type mqc_matrix
- interface mqc_matrix_diagmatrix_put
- interface mqc_matrix_symmmatrix_put
- interface mqc_print
- type mqc_r4tensor
- type mqc_scalar
- interface mqc_set_array2vector
- type mqc_vector
- interface operator(∗)

- interface operator(**)
- interface operator(+)
- interface operator(-)
- interface operator(.dot.)
- interface operator(.eq.)
- interface operator(.ewd.)
- interface operator(.ewp.)
- interface operator(.ge.)
- interface operator(.gt.)
- interface operator(.le.)
- interface operator(.lt.)
- interface operator(.ne.)
- interface operator(.outer.)
- interface operator(.x.)
- interface operator(/)
- interface real
- interface sin
- interface sqrt
- interface tan
- interface transpose

Functions/Subroutines

- integer(kind=int64) function factorial (n)
- integer(kind=int64) function bin_coeff (N, K)
- subroutine mqc_allocate_scalar (Scalar, Data_type)

    MQC_Allocate_Scalar is used to allocate a scalar type variable of the MQC_Scalar class
- subroutine mqc_deallocate_scalar (Scalar)
- logical function mqc_scalar_isallocated (Scalar)
- subroutine mqc_input_integer_scalar (ScalarOut, ScalarIn)

    MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic scalar to an MQC_Scalar
- subroutine mqc_input_real_scalar (ScalarOut, ScalarIn)
- subroutine mqc_input_complex_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_mqcscalar_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_integer_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_real_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_complex_scalar (ScalarOut, ScalarIn)
- subroutine mqc_print_scalar_algebra1 (Scalar, IOut, Header, Blank_At_Top, Blank_At_Bottom)
- type(mqc_scalar) function mqc_scalar_cmplx (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalar_sqrt (Scalar)
- type(mqc_scalar) function mqc_scalar_sin (Scalar)
- type(mqc_scalar) function mqc_scalar_cos (Scalar)
- type(mqc_scalar) function mqc_scalar_tan (Scalar)
- type(mqc_scalar) function mqc_scalar_asin (Scalar)
- type(mqc_scalar) function mqc_scalar_acos (Scalar)
- type(mqc_scalar) function mqc_scalar_atan (Scalar)
- type(mqc_scalar) function mqc_scalar_atan2 (Scalar)
- logical function mqc_scalar_havereal (Scalar)
- logical function mqc_scalar_haveinteger (Scalar)

- logical function mqc_scalar_havecomplex (Scalar)
- real(kind=real64) function mqc_scalar_get_intrinsic_real (Scalar)
- integer(kind=int64) function mqc_scalar_get_intrinsic_integer (Scalar)
- complex(kind=real64) function mqc_scalar_get_intrinsic_complex (Scalar)
- type(mqc_scalar) function mqc_scalar_get_abs_value (Scalar)
- subroutine mqc_scalar_get_random_value (Scalar)
- type(mqc_scalar) function mqc_scalaradd (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalarsubtract (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalarmultiply (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalardivide (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalarexponent (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalarintegerexponent (Scalar, IntIn)
- type(mqc_scalar) function mqc_scalarrealexponent (Scalar, RealIn)
- type(mqc_scalar) function mqc_scalarcomplexexponent (Scalar, CompIn)
- logical function mqc_scalarne (Scalar1, Scalar2)
- logical function mqc_scalareq (Scalar1, Scalar2)
- logical function mqc_scalarlt (Scalar1, Scalar2)
- logical function mqc_realltscalar (RealIn, Scalar)
- logical function mqc_scalarltreal (Scalar, RealIn)
- logical function mqc_scalargt (Scalar1, Scalar2)
- logical function mqc_integergtscalar (IntIn, Scalar)
- logical function mqc_scalargtinteger (Scalar, IntIn)
- logical function mqc_realgtscalar (RealIn, Scalar)
- logical function mqc_scalargtreal (Scalar, RealIn)
- logical function mqc_scalarle (Scalar1, Scalar2)
- logical function mqc_reallescalar (RealIn, Scalar)
- logical function mqc_scalarlereal (Scalar, RealIn)
- logical function mqc_integerlescalar (IntIn, Scalar)
- logical function mqc_scalarleinteger (Scalar, IntIn)
- logical function mqc_scalarge (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalar_complex_conjugate (ScalarIn)
- type(mqc_scalar) function mqc_scalar_complex_realpart (ScalarIn)
- type(mqc_scalar) function mqc_scalar_complex_imagpart (ScalarIn)
- type(mqc_scalar) function mqc_integerscalarmultiply (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegermultiply (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalarmultiply (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealmultiply (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalarmultiply (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexmultiply (Scalar, ComplexIn)
- type(mqc_scalar) function mqc_integerscalardivide (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegerdivide (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalardivide (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealdivide (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalardivide (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexdivide (Scalar, ComplexIn)
- type(mqc_scalar) function mqc_integerscalaradd (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegeradd (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalaradd (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealadd (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalaradd (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexadd (Scalar, ComplexIn)

- type(mqc_scalar) function mqc_integerscalarsubtract (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegersubtract (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalarsubtract (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealsubtract (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalarsubtract (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexsubtract (Scalar, ComplexIn)
- subroutine mqc_allocate_vector (N, Vector, Data_Type)
- subroutine mqc_deallocate_vector (Vector)
- integer(kind=int64) function mqc_length_vector (Vector)
- logical function mqc_vector_havereal (Vector)
- logical function mqc_vector_haveinteger (Vector)
- logical function mqc_vector_havecomplex (Vector)
- logical function mqc_vector_iscolumn (Vector)
- subroutine mqc_vector_copy_int2real (Vector)
- subroutine mqc_vector_copy_int2complex (Vector)
- subroutine mqc_vector_copy_real2int (Vector)
- subroutine mqc_vector_copy_real2complex (Vector)
- subroutine mqc_vector_copy_complex2int (Vector)
- subroutine mqc_vector_copy_complex2real (Vector)
- type(mqc_scalar) function mqc_vector_scalar_at (Vec, I)
- type(mqc_vector) function mqc_vector_vector_at (Vec, I, J)
- subroutine mqc_set_vector2integerarray (ArrayOut, VectorIn)
- subroutine mqc_set_vector2realarray (ArrayOut, VectorIn)
- subroutine mqc_set_vector2complexarray (ArrayOut, VectorIn)
- subroutine mqc_set_array2vector_integer (VectorOut, ArrayIn)
- subroutine mqc_set_array2vector_real (VectorOut, ArrayIn)
- subroutine mqc_set_array2vector_complex (VectorOut, ArrayIn)
- subroutine mqc_set_vector2vector (VectorOut, VectorIn)
- type(mqc_vector) function mqc_vectorvectorsum (Vector1In, Vector2In)
- type(mqc_vector) function mqc_vectorvectordifference (Vector1In, Vector2In)
- type(mqc_vector) function mqc_scalarvectorsum (ScalarIn, VectorIn)
- type(mqc_vector) function mqc_scalarvectordifference (ScalarIn, VectorIn)
- type(mqc_vector) function mqc_elementvectorproduct (Vector1In, Vector2In)
- type(mqc_vector) function mqc_vector_transpose (Vector)
- type(mqc_vector) function mqc_vector_conjugate_transpose (Vector)
- type(mqc_scalar) function mqc_vectorvectordotproduct (Vector1, Vector2)
- type(mqc_matrix) function mqc_outer (VA, VB)
- type(mqc_vector) function mqc_crossproduct (Vector1In, Vector2In)
- subroutine mqc_print_vector_algebra1 (Vector, IOut, Header, Verbose, Blank_At_Top, Blank_At_Bottom)
- type(mqc_vector) function mqc_vector_cast_real (VA)
- type(mqc_vector) function mqc_vector_cast_complex (VA)
- subroutine mqc_vector_scalar_put (Vector, Scalar, I)
- subroutine mqc_vector_scalar_increment (Vector, Scalar, I)
- subroutine mqc_vector_vector_put (Vector, VectorIn, I)
- subroutine mqc_vector_initialize (Vector, Length, Scalar)
- type(mqc_vector) function mqc_scalarvectorproduct (Scalar, Vector)
- type(mqc_vector) function mqc_vectorscalarproduct (vector, scalar)
- type(mqc_vector) function mqc_vectorscalardivide (vector, scalar)
- type(mqc_vector) function mqc_realvectorproduct (RealIn, Vector)
- type(mqc_vector) function mqc_vectorrealproduct (vector, realIn)
- type(mqc_vector) function mqc_vectorrealdivide (vector, realIn)

- type(mqc_vector) function mqc_integervectorproduct (intIn, Vector)
- type(mqc_vector) function mqc_vectorintegerproduct (vector, intIn)
- type(mqc_vector) function mqc_vectorintegerdivide (vector, intIn)
- type(mqc_vector) function mqc_complexvectorproduct (CompIn, Vector)
- type(mqc_vector) function mqc_vectorcomplexproduct (vector, compIn)
- type(mqc_vector) function mqc_vectorcomplexdivide (vector, compIn)
- type(mqc_scalar) function mqc_vector_norm (vector, methodIn)
- logical function mqc_vector_isallocated (Vector)
- subroutine mqc_vector_push (Vector, Scalar)
- subroutine mqc_vector_unshift (Vector, Scalar)
- type(mqc_scalar) function mqc_vector_pop (Vector)
- type(mqc_scalar) function mqc_vector_shift (Vector)
- type(mqc_scalar) function mqc_vector_maxval (Vector)
- type(mqc_scalar) function mqc_vector_minval (Vector)
- integer function mqc_vector_maxloc (Vector)
- integer function mqc_vector_minloc (Vector)
- type(mqc_vector) function mqc_vector_argsort (Vector)
- subroutine mqc_vector_sort (Vector, idx)
- subroutine mqc_vector_sqrt (A)
- type(mqc_vector) function mqc_vector_abs (A)
- subroutine mqc_vector_power (A, P)
- type(mqc_vector) function mqc_vector_complex_realpart (A)
- type(mqc_vector) function mqc_vector_complex_imagpart (A)
- type(mqc_vector) function mqc_vector_cmplx (Vector1, Vector2)
- character(len=64) function mqc_matrix_storagetype (Matrix)
- subroutine mqc_matrix_diagonalize (A, EVals, EVecs)
- type(mqc_matrix) function mqc_matrix_cast_real (MA)
- type(mqc_matrix) function mqc_matrix_cast_complex (MA)
- type(mqc_scalar) function mqc_matrix_scalar_at (Mat, I, J)
- type(mqc_vector) function mqc_matrix_vector_at (Mat, Rows, Cols)
- recursive subroutine mqc_matrix_vector_put (Mat, VectorIn, Rows, Cols)
- type(mqc_matrix) function mqc_matrix_matrix_at (Mat, Rows, Cols)

  MQC_Matrix_Matrix_At is a function that returns a submatrix of the matrix
- subroutine mqc_matrix_diagmatrix_put_vector (diagVectorIn, mat)
- subroutine mqc_matrix_diagmatrix_put_integer (mat, diagMatrixIn)
- subroutine mqc_matrix_diagmatrix_put_real (mat, diagMatrixIn)
- subroutine mqc_matrix_diagmatrix_put_complex (mat, diagMatrixIn)
- subroutine mqc_matrix_symmmatrix_put_integer (mat, symmMatrixIn)
- subroutine mqc_matrix_symmmatrix_put_real (mat, symmMatrixIn)
- subroutine mqc_matrix_symmmatrix_put_complex (mat, symmMatrixIn)
- recursive subroutine mqc_matrix_matrix_put (Mat, MatrixIn, Rows, Cols)
- integer(kind=int64) function symindexhash (i, j, k, l)
- type(mqc_matrix) function mqc_elementmatrixproduct (A, B)
- type(mqc_matrix) function mqc_elementmatrixdivide (A, B)
- logical function mqc_matrix_test_symmetric (Matrix, Option)
- logical function mqc_matrix_test_diagonal (Matrix)
- subroutine mqc_allocate_matrix (M, N, Matrix, Data_Type, Storage)
- subroutine mqc_deallocate_matrix (Matrix)
- logical function mqc_matrix_isallocated (Matrix)
- subroutine mqc_set_integerarray2matrix (MatrixOut, ArrayIn)

- subroutine mqc_set_realarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_set_complexarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_set_matrix2integerarray (ArrayOut, MatrixIn)
- subroutine mqc_set_matrix2realarray (ArrayOut, MatrixIn)
- subroutine mqc_set_matrix2complexarray (ArrayOut, MatrixIn)
- subroutine mqc_set_matrix2matrix (MatrixOut, MatrixIn)
- subroutine mqc_print_matrix_algebra1 (Matrix, IOut, Header, Blank_At_Top, Blank_At_Bottom)
- subroutine mqc_matrix_copy_int2real (Matrix)
- subroutine mqc_matrix_copy_int2complex (Matrix)
- subroutine mqc_matrix_copy_real2int (Matrix)
- subroutine mqc_matrix_copy_real2complex (Matrix)
- subroutine mqc_matrix_copy_complex2int (Matrix)
- subroutine mqc_matrix_copy_complex2real (Matrix)
- integer(kind=int64) function mqc_matrix_rows (Matrix)
- integer(kind=int64) function mqc_matrix_columns (Matrix)
- logical function mqc_matrix_havereal (Matrix)
- logical function mqc_matrix_haveinteger (Matrix)
- logical function mqc_matrix_havecomplex (Matrix)
- logical function mqc_matrix_havefull (Matrix)
- logical function mqc_matrix_havesymmetric (Matrix)
- logical function mqc_matrix_havediagonal (Matrix)
- type(mqc_matrix) function mqc_matrix_transpose (Matrix)
- type(mqc_matrix) function mqc_matrix_conjugate_transpose (Matrix)
- type(mqc_matrix) function mqc_matrix_symmetrize (Matrix)
- subroutine mqc_matrix_full2symm (Matrix)
- subroutine mqc_matrix_symm2full (Matrix, Option)
- subroutine mqc_matrix_full2diag (Matrix)
- subroutine mqc_matrix_diag2full (Matrix)
- subroutine mqc_matrix_symm2diag (Matrix)
- subroutine mqc_matrix_diag2symm (Matrix)
- type(mqc_matrix) function mqc_matrix_symm2full_func (Matrix)
- subroutine matrix_symm2sq_integer (N, I_Symm, I_Sq)
- subroutine matrix_symm2sq_real (N, A_Symm, A_Sq)
- subroutine matrix_symm2sq_complex (N, A_Symm, A_Sq)
- type(mqc_matrix) function mqc_vector2diagmatrix (vector)
- type(mqc_matrix) function mqc_matrixmatrixsum (MA, MB)
- type(mqc_matrix) function mqc_matrixmatrixsubtract (MA, MB)
- type(mqc_matrix) function mqc_matrixmatrixproduct (MA, MB)
- type(mqc_matrix) function mqc_matrixmatrixdotproduct (MA, MB)
- type(mqc_vector) function mqc_matrixvectordotproduct (MA, VB)
- type(mqc_vector) function mqc_vectormatrixdotproduct (VA, MB)
- type(mqc_matrix) function mqc_matrixscalarproduct (Matrix, Scalar)
- type(mqc_matrix) function mqc_scalarmatrixproduct (Scalar, Matrix)
- type(mqc_scalar) function mqc_matrix_matrix_contraction (Matrix1, Matrix2)
- subroutine mqc_matrix_scalar_put (Matrix, Scalar, I, J)
- subroutine mqc_matrix_initialize (Matrix, Rows, Columns, Scalar, Storage)
- subroutine mqc_matrix_identity (matrix, n, m)
- subroutine mqc_matrix_set (matrix, scalar, storage)
- type(mqc_scalar) function mqc_matrix_norm (matrix, methodIn)
- type(mqc_scalar) function mqc_matrix_determinant (a)
- type(mqc_matrix) function mqc_matrix_inverse (a)

- type(mqc_scalar) function mqc_matrix_trace (matrix)
- subroutine mqc_matrix_generalized_eigensystem (a, bIn, eigenvals, reigenvecs, leigenvecs)
- subroutine mqc_matrix_svd (A, EVals, EUVecs, EVVecs)
- subroutine mqc_matrix_rms_max (A, rms_A, max_A)
- subroutine mqc_matrix_sqrt (A, eVals, eVecs)
- subroutine mqc_allocate_r4tensor (I, J, K, L, Tensor, Data_Type, Storage)
- subroutine mqc_deallocate_r4tensor (Tensor)
- type(mqc_scalar) function mqc_r4tensor_at (Tensor, I, J, K, L)
- subroutine mqc_r4tensor_put (Tensor, Element, I, J, K, L)
- subroutine mqc_print_r4tensor_algebra1 (Tensor, IOut, Header, blank_at_top, blank_at_bottom)
- subroutine mqc_set_array2tensor (TensorOut, ArrayIn)
- subroutine mqc_r4tensor_initialize (R4Tensor, I, J, K, L, Scalar)
- subroutine mqc_matrix_symmsymmr4tensor_put_real (r4Tensor, symmSymmMatrixIn)
- subroutine mqc_matrix_symmsymmr4tensor_put_complex (r4Tensor, symmSymmMatrixIn)
- logical function mqc_r4tensor_haveinteger (R4Tensor)
- logical function mqc_r4tensor_havereal (R4Tensor)
- logical function mqc_r4tensor_havecomplex (R4Tensor)
- type(mqc_matrix) function mqc_givens_matrix (m_size, angle, p, q)

5.1.1 Function/Subroutine Documentation

5.1.1.1 bin_coeff()

```
integer(kind=int64) function mqc_algebra::bin_coeff (
             integer(kind=int64), intent(in) N,
             integer(kind=int64), intent(in) K )
```

5.1.1.2 factorial()

```
integer(kind=int64) function mqc_algebra::factorial (
             integer(kind=int64), intent(in) n )
```

5.1.1.3 matrix_symm2sq_complex()

```
subroutine mqc_algebra::matrix_symm2sq_complex (
             integer(kind=int64), intent(in) N,
             complex(kind=real64), dimension(:), intent(in) A_Symm,
             complex(kind=real64), dimension(n,n), intent(out) A_Sq )
```

5.1.1.4 matrix_symm2sq_integer()

```
subroutine mqc_algebra::matrix_symm2sq_integer (
            integer(kind=int64), intent(in) N,
            integer(kind=int64), dimension(:), intent(in) I_Symm,
            integer(kind=int64), dimension(n,n), intent(out) I_Sq )
```

5.1.1.5 matrix_symm2sq_real()

```
subroutine mqc_algebra::matrix_symm2sq_real (
            integer(kind=int64), intent(in) N,
            real(kind=real64), dimension(:), intent(in) A_Symm,
            real(kind=real64), dimension(n,n), intent(out) A_Sq )
```

5.1.1.6 mqc_allocate_matrix()

```
subroutine mqc_algebra::mqc_allocate_matrix (
            integer(kind=int64), intent(in) M,
            integer(kind=int64), intent(in) N,
            class(mqc_matrix), intent(inout) Matrix,
            character(len=*), intent(in) Data_Type,
            character(len=*), intent(in) Storage )
```

5.1.1.7 mqc_allocate_r4tensor()

```
subroutine mqc_algebra::mqc_allocate_r4tensor (
            integer(kind=int64), intent(in) I,
            integer(kind=int64), intent(in) J,
            integer(kind=int64), intent(in) K,
            integer(kind=int64), intent(in) L,
            type(mqc_r4tensor), intent(inout) Tensor,
            character(len=*), intent(in) Data_Type,
            character(len=*), intent(in) Storage )
```

5.1.1.8 mqc_allocate_scalar()

```
subroutine mqc_algebra::mqc_allocate_scalar (
             type(mqc_scalar), intent(inout) Scalar,
             character(len=*), intent(in) Data_type )
```

MQC_Allocate_Scalar is used to allocate a scalar type variable of the MQC_Scalar class

Purpose:

```
MQC_Allocate_Scalar is a subroutine used to allocate a scalar type variable
of the MQC_Scalar class. The following options are available:

1. Data_Type = 'Real' declares the MQC_Scalar variable to be of real type.
2. Data_Type = 'Integer' declares the MQC_Scalar variable to be of integer type.
3. Data_Type = 'Complex' declares the MQC_Scalar variable to be of complex type.
```

Parameters

in,out	*Scalar*	Scalar is Type(MQC_Scalar) The name of the MQC_Scalar variable
in	*Data_Type*	Data_Type is Character(Len=*) = 'Real': the MQC_Scalar is real = 'Integer': the MQC_Scalar is integer = 'Complex': the MQC_Scalar is complex

Author

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Date

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5.1.1.9 mqc_allocate_vector()

```
subroutine mqc_algebra::mqc_allocate_vector (
             integer(kind=int64), intent(in) N,
             type(mqc_vector), intent(inout) Vector,
             character(len=*), intent(in) Data_Type )
```

5.1.1.10 mqc_complexscalaradd()

```
type(mqc_scalar) function mqc_algebra::mqc_complexscalaradd (
             complex(kind=real64), intent(in) ComplexIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.11 mqc_complexscalardivide()

```
type(mqc_scalar) function mqc_algebra::mqc_complexscalardivide (
             complex(kind=real64), intent(in) ComplexIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.12 mqc_complexscalarmultiply()

```
type(mqc_scalar) function mqc_algebra::mqc_complexscalarmultiply (
             complex(kind=real64), intent(in) ComplexIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.13 mqc_complexscalarsubtract()

```
type(mqc_scalar) function mqc_algebra::mqc_complexscalarsubtract (
             complex(kind=real64), intent(in) ComplexIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.14 mqc_complexvectorproduct()

```
type(mqc_vector) function mqc_algebra::mqc_complexvectorproduct (
             complex(kind=real64), intent(in) CompIn,
             type(mqc_vector), intent(in) Vector )
```

5.1.1.15 mqc_crossproduct()

```
type(mqc_vector) function mqc_algebra::mqc_crossproduct (
             type(mqc_vector), intent(in) Vector1In,
             type(mqc_vector), intent(in) Vector2In )
```

5.1.1.16 mqc_deallocate_matrix()

```
subroutine mqc_algebra::mqc_deallocate_matrix (
             class(mqc_matrix), intent(inout) Matrix )
```

5.1.1.17 mqc_deallocate_r4tensor()

```
subroutine mqc_algebra::mqc_deallocate_r4tensor (
             type(mqc_r4tensor), intent(inout) Tensor )
```

5.1.1.18 mqc_deallocate_scalar()

```
subroutine mqc_algebra::mqc_deallocate_scalar (
             type(mqc_scalar), intent(inout) Scalar )
```

5.1.1.19 mqc_deallocate_vector()

```
subroutine mqc_algebra::mqc_deallocate_vector (
             type(mqc_vector), intent(inout) Vector )
```

5.1.1.20 mqc_elementmatrixdivide()

```
type(mqc_matrix) function mqc_algebra::mqc_elementmatrixdivide (
             type(mqc_matrix), intent(in) A,
             type(mqc_matrix), intent(in) B )
```

5.1.1.21 mqc_elementmatrixproduct()

```
type(mqc_matrix) function mqc_algebra::mqc_elementmatrixproduct (
             type(mqc_matrix), intent(in) A,
             type(mqc_matrix), intent(in) B )
```

5.1.1.22 mqc_elementvectorproduct()

```
type(mqc_vector) function mqc_algebra::mqc_elementvectorproduct (
             type(mqc_vector), intent(in) Vector1In,
             type(mqc_vector), intent(in) Vector2In )
```

5.1.1.23 mqc_givens_matrix()

```
type(mqc_matrix) function mqc_algebra::mqc_givens_matrix (
             integer(kind=int64), intent(in) m_size,
             real(kind=real64), intent(in) angle,
             integer(kind=int64), intent(in) p,
             integer(kind=int64), intent(in) q )
```

5.1.1.24 mqc_input_complex_scalar()

```
subroutine mqc_algebra::mqc_input_complex_scalar (
             type(mqc_scalar), intent(inout) ScalarOut,
             complex(kind=real64), intent(in) ScalarIn )
```

5.1.1.25 mqc_input_integer_scalar()

```
subroutine mqc_algebra::mqc_input_integer_scalar (
             type(mqc_scalar), intent(inout) ScalarOut,
             integer(kind=int64), intent(in) ScalarIn )
```

MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic scalar to an MQC_Scalar

Purpose:

```
MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic scalar to an MQC_Scalar.
```

Parameters

in,out	*ScalarOut*	ScalarOut is Type(MQC_Scalar) The name of the output variable
in	*ScalarIn*	ScalarIn is Integer(kind=int64) The value of the input variable

Author

L. M. Thompson

Date

2016

5.1.1.26 mqc_input_real_scalar()

```
subroutine mqc_algebra::mqc_input_real_scalar (
            type(mqc_scalar), intent(inout) ScalarOut,
            real(kind=real64), intent(in) ScalarIn )
```

5.1.1.27 mqc_integergtscalar()

```
logical function mqc_algebra::mqc_integergtscalar (
            integer(kind=int64), intent(in) IntIn,
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.28 mqc_integerlescalar()

```
logical function mqc_algebra::mqc_integerlescalar (
            integer(kind=int64), intent(in) IntIn,
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.29 mqc_integerscalaradd()

```
type(mqc_scalar) function mqc_algebra::mqc_integerscalaradd (
            integer(kind=int64), intent(in) IntegerIn,
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.30 mqc_integerscalardivide()

```
type(mqc_scalar) function mqc_algebra::mqc_integerscalardivide (
             integer(kind=int64), intent(in) IntegerIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.31 mqc_integerscalarmultiply()

```
type(mqc_scalar) function mqc_algebra::mqc_integerscalarmultiply (
             integer(kind=int64), intent(in) IntegerIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.32 mqc_integerscalarsubtract()

```
type(mqc_scalar) function mqc_algebra::mqc_integerscalarsubtract (
             integer(kind=int64), intent(in) IntegerIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.33 mqc_integervectorproduct()

```
type(mqc_vector) function mqc_algebra::mqc_integervectorproduct (
             integer(kind=int64), intent(in) intIn,
             type(mqc_vector), intent(in) Vector )
```

5.1.1.34 mqc_length_vector()

```
integer(kind=int64) function mqc_algebra::mqc_length_vector (
             class(mqc_vector) Vector )
```

5.1.1.35 mqc_matrix_cast_complex()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_cast_complex (
             type(mqc_matrix), intent(in) MA )
```

5.1.1.36 mqc_matrix_cast_real()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_cast_real (
             type(mqc_matrix), intent(in) MA )
```

5.1.1.37 mqc_matrix_columns()

```
integer(kind=int64) function mqc_algebra::mqc_matrix_columns (
             type(mqc_matrix), intent(in) Matrix )
```

5.1.1.38 mqc_matrix_conjugate_transpose()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_conjugate_transpose (
             class(mqc_matrix), intent(in) Matrix )
```

5.1.1.39 mqc_matrix_copy_complex2int()

```
subroutine mqc_algebra::mqc_matrix_copy_complex2int (
             type(mqc_matrix) Matrix )
```

5.1.1.40 mqc_matrix_copy_complex2real()

```
subroutine mqc_algebra::mqc_matrix_copy_complex2real (
             type(mqc_matrix) Matrix )
```

5.1.1.41 mqc_matrix_copy_int2complex()

```
subroutine mqc_algebra::mqc_matrix_copy_int2complex (
             type(mqc_matrix) Matrix )
```

5.1.1.42 mqc_matrix_copy_int2real()

```
subroutine mqc_algebra::mqc_matrix_copy_int2real (
            type(mqc_matrix) Matrix )
```

5.1.1.43 mqc_matrix_copy_real2complex()

```
subroutine mqc_algebra::mqc_matrix_copy_real2complex (
            type(mqc_matrix) Matrix )
```

5.1.1.44 mqc_matrix_copy_real2int()

```
subroutine mqc_algebra::mqc_matrix_copy_real2int (
            type(mqc_matrix) Matrix )
```

5.1.1.45 mqc_matrix_determinant()

```
type(mqc_scalar) function mqc_algebra::mqc_matrix_determinant (
            class(mqc_matrix) a )
```

5.1.1.46 mqc_matrix_diag2full()

```
subroutine mqc_algebra::mqc_matrix_diag2full (
            type(mqc_matrix), intent(inout) Matrix )
```

5.1.1.47 mqc_matrix_diag2symm()

```
subroutine mqc_algebra::mqc_matrix_diag2symm (
            type(mqc_matrix), intent(inout) Matrix )
```

5.1.1.48 mqc_matrix_diagmatrix_put_complex()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put_complex (
             class(mqc_matrix), intent(inout) mat,
             complex(kind=real64), dimension(:), intent(in) diagMatrixIn )
```

5.1.1.49 mqc_matrix_diagmatrix_put_integer()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put_integer (
             class(mqc_matrix), intent(inout) mat,
             integer(kind=int64), dimension(:), intent(in) diagMatrixIn )
```

5.1.1.50 mqc_matrix_diagmatrix_put_real()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put_real (
             class(mqc_matrix), intent(inout) mat,
             real(kind=real64), dimension(:), intent(in) diagMatrixIn )
```

5.1.1.51 mqc_matrix_diagmatrix_put_vector()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put_vector (
             class(mqc_vector), intent(in) diagVectorIn,
             class(mqc_matrix), intent(inout) mat )
```

5.1.1.52 mqc_matrix_diagonalize()

```
subroutine mqc_algebra::mqc_matrix_diagonalize (
             class(mqc_matrix), intent(in) A,
             type(mqc_vector), intent(inout), optional EVals,
             type(mqc_matrix), intent(inout), optional EVecs )
```

5.1.1.53 mqc_matrix_full2diag()

```
subroutine mqc_algebra::mqc_matrix_full2diag (
             type(mqc_matrix), intent(inout) Matrix )
```

5.1.1.54 mqc_matrix_full2symm()

```
subroutine mqc_algebra::mqc_matrix_full2symm (
            type(mqc_matrix), intent(inout) Matrix )
```

5.1.1.55 mqc_matrix_generalized_eigensystem()

```
subroutine mqc_algebra::mqc_matrix_generalized_eigensystem (
            class(mqc_matrix), intent(inout) a,
            type(mqc_matrix), intent(inout), optional bIn,
            type(mqc_vector), intent(out), optional eigenvals,
            type(mqc_matrix), intent(out), optional reigenvecs,
            type(mqc_matrix), intent(out), optional leigenvecs )
```

5.1.1.56 mqc_matrix_havecomplex()

```
logical function mqc_algebra::mqc_matrix_havecomplex (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.57 mqc_matrix_havediagonal()

```
logical function mqc_algebra::mqc_matrix_havediagonal (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.58 mqc_matrix_havefull()

```
logical function mqc_algebra::mqc_matrix_havefull (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.59 mqc_matrix_haveinteger()

```
logical function mqc_algebra::mqc_matrix_haveinteger (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.60 mqc_matrix_havereal()

```
logical function mqc_algebra::mqc_matrix_havereal (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.61 mqc_matrix_havesymmetric()

```
logical function mqc_algebra::mqc_matrix_havesymmetric (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.62 mqc_matrix_identity()

```
subroutine mqc_algebra::mqc_matrix_identity (
            class(mqc_matrix), intent(inout) matrix,
            integer(kind=int64) n,
            integer(kind=int64) m )
```

5.1.1.63 mqc_matrix_initialize()

```
subroutine mqc_algebra::mqc_matrix_initialize (
            class(mqc_matrix), intent(inout) Matrix,
            integer(kind=int64), intent(in) Rows,
            integer(kind=int64), intent(in) Columns,
            class(*), optional Scalar,
            character(len=*), intent(in), optional Storage )
```

5.1.1.64 mqc_matrix_inverse()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_inverse (
            class(mqc_matrix) a )
```

5.1.1.65 mqc_matrix_isallocated()

```
logical function mqc_algebra::mqc_matrix_isallocated (
            class(mqc_matrix), intent(inout) Matrix )
```

5.1.1.66 mqc_matrix_matrix_at()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_matrix_at (
            class(mqc_matrix), intent(in) Mat,
            integer(kind=int64), dimension(:), intent(in) Rows,
            integer(kind=int64), dimension(:), intent(in) Cols )
```

MQC_Matrix_Matrix_At is a function that returns a submatrix of the matrix

Parameters

in	*Mat*	Mat is Class(MQC_Matrix) Name of the input matrix variable
in	*rows*	Rows is Integer(kind=int64),Dimension(:) If = [A,B]: output is submatrix of rows A to B If (A,B)>0 row count is from first index If (A,B)<0 row count is from last index If = [0]: submatrix of rows equivalent to [1,-1]
in	*Cols*	Cols is Integer(kind=int64),Dimension(:) If = [A,B]: output is submatrix of columns A to B If (A,B)>0 column count is from first index If (A,B)<0 column count is from last index If = [0]: submatrix of columns equivalent to [1,-1]

Author

L. M. Thompson

Date

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5.1.1.67 mqc_matrix_matrix_contraction()

```
type(mqc_scalar) function mqc_algebra::mqc_matrix_matrix_contraction (
             type(mqc_matrix), intent(in) Matrix1,
             type(mqc_matrix), intent(in) Matrix2 )
```

5.1.1.68 mqc_matrix_matrix_put()

```
recursive subroutine mqc_algebra::mqc_matrix_matrix_put (
             class(mqc_matrix), intent(inout) Mat,
             type(mqc_matrix), intent(in) MatrixIn,
             integer(kind=int64), dimension(:), intent(in) Rows,
             integer(kind=int64), dimension(:), intent(in) Cols )
```

5.1.1.69 mqc_matrix_norm()

```
type(mqc_scalar) function mqc_algebra::mqc_matrix_norm (
             class(mqc_matrix), intent(inout) matrix,
             character(len=1), intent(in), optional methodIn )
```

5.1.1.70 mqc_matrix_rms_max()

```
subroutine mqc_algebra::mqc_matrix_rms_max (
             class(mqc_matrix), intent(inout) A,
             type(mqc_scalar), intent(out) rms_A,
             type(mqc_scalar), intent(out) max_A )
```

5.1.1.71 mqc_matrix_rows()

```
integer(kind=int64) function mqc_algebra::mqc_matrix_rows (
             type(mqc_matrix), intent(in) Matrix )
```

5.1.1.72 mqc_matrix_scalar_at()

```
type(mqc_scalar) function mqc_algebra::mqc_matrix_scalar_at (
             class(mqc_matrix), intent(in) Mat,
             integer(kind=int64), intent(in) I,
             integer(kind=int64), intent(in) J )
```

5.1.1.73 mqc_matrix_scalar_put()

```
subroutine mqc_algebra::mqc_matrix_scalar_put (
             class(mqc_matrix), intent(inout) Matrix,
             type(mqc_scalar), intent(in) Scalar,
             integer(kind=int64), intent(in) I,
             integer(kind=int64), intent(in) J )
```

5.1.1.74 mqc_matrix_set()

```
subroutine mqc_algebra::mqc_matrix_set (
             class(mqc_matrix), intent(inout) matrix,
             class(*), optional scalar,
             character(len=*), intent(in), optional storage )
```

5.1.1.75 mqc_matrix_sqrt()

```
subroutine mqc_algebra::mqc_matrix_sqrt (
             class(mqc_matrix), intent(inout) A,
             type(mqc_vector), intent(inout), optional eVals,
             type(mqc_matrix), intent(inout), optional eVecs )
```

5.1.1.76 mqc_matrix_storagetype()

```
character(len=64) function mqc_algebra::mqc_matrix_storagetype (
             class(mqc_matrix), intent(in) Matrix )
```

5.1.1.77 mqc_matrix_svd()

```
subroutine mqc_algebra::mqc_matrix_svd (
             class(mqc_matrix), intent(inout) A,
             type(mqc_vector), intent(inout), optional EVals,
             type(mqc_matrix), intent(inout), optional EUVecs,
             type(mqc_matrix), intent(inout), optional EVVecs )
```

5.1.1.78 mqc_matrix_symm2diag()

```
subroutine mqc_algebra::mqc_matrix_symm2diag (
             type(mqc_matrix), intent(inout) Matrix )
```

5.1.1.79 mqc_matrix_symm2full()

```
subroutine mqc_algebra::mqc_matrix_symm2full (
            type(mqc_matrix), intent(inout) Matrix,
            character(len=*), intent(in), optional Option )
```

5.1.1.80 mqc_matrix_symm2full_func()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_symm2full_func (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.81 mqc_matrix_symmetrize()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_symmetrize (
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.82 mqc_matrix_symmmatrix_put_complex()

```
subroutine mqc_algebra::mqc_matrix_symmmatrix_put_complex (
            class(mqc_matrix), intent(inout) mat,
            complex(kind=real64), dimension(:), intent(in) symmMatrixIn )
```

5.1.1.83 mqc_matrix_symmmatrix_put_integer()

```
subroutine mqc_algebra::mqc_matrix_symmmatrix_put_integer (
            class(mqc_matrix), intent(inout) mat,
            integer(kind=int64), dimension(:), intent(in) symmMatrixIn )
```

5.1.1.84 mqc_matrix_symmmatrix_put_real()

```
subroutine mqc_algebra::mqc_matrix_symmmatrix_put_real (
            class(mqc_matrix), intent(inout) mat,
            real(kind=real64), dimension(:), intent(in) symmMatrixIn )
```

5.1.1.85 mqc_matrix_symmsymmr4tensor_put_complex()

```
subroutine mqc_algebra::mqc_matrix_symmsymmr4tensor_put_complex (
            class(mqc_r4tensor), intent(inout) r4Tensor,
            complex(kind=real64), dimension(:), intent(in) symmSymmMatrixIn )
```

5.1.1.86 mqc_matrix_symmsymmr4tensor_put_real()

```
subroutine mqc_algebra::mqc_matrix_symmsymmr4tensor_put_real (
            class(mqc_r4tensor), intent(inout) r4Tensor,
            real(kind=real64), dimension(:), intent(in) symmSymmMatrixIn )
```

5.1.1.87 mqc_matrix_test_diagonal()

```
logical function mqc_algebra::mqc_matrix_test_diagonal (
            class(mqc_matrix), intent(in) Matrix )
```

5.1.1.88 mqc_matrix_test_symmetric()

```
logical function mqc_algebra::mqc_matrix_test_symmetric (
            class(mqc_matrix), intent(in) Matrix,
            character(len=*), intent(in), optional Option )
```

5.1.1.89 mqc_matrix_trace()

```
type(mqc_scalar) function mqc_algebra::mqc_matrix_trace (
            class(mqc_matrix), intent(in) matrix )
```

5.1.1.90 mqc_matrix_transpose()

```
type(mqc_matrix) function mqc_algebra::mqc_matrix_transpose (
            class(mqc_matrix), intent(in) Matrix )
```

5.1.1.91 mqc_matrix_vector_at()

```
type(mqc_vector) function mqc_algebra::mqc_matrix_vector_at (
             class(mqc_matrix), intent(in) Mat,
             integer(kind=int64), dimension(:), intent(in) Rows,
             integer(kind=int64), dimension(:), intent(in) Cols )
```

5.1.1.92 mqc_matrix_vector_put()

```
recursive subroutine mqc_algebra::mqc_matrix_vector_put (
             class(mqc_matrix), intent(inout) Mat,
             type(mqc_vector), intent(in) VectorIn,
             integer(kind=int64), dimension(:), intent(in) Rows,
             integer(kind=int64), dimension(:), intent(in) Cols )
```

5.1.1.93 mqc_matrixmatrixdotproduct()

```
type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixdotproduct (
             type(mqc_matrix), intent(in) MA,
             type(mqc_matrix), intent(in) MB )
```

5.1.1.94 mqc_matrixmatrixproduct()

```
type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixproduct (
             type(mqc_matrix), intent(in) MA,
             type(mqc_matrix), intent(in) MB )
```

5.1.1.95 mqc_matrixmatrixsubtract()

```
type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixsubtract (
             type(mqc_matrix), intent(in) MA,
             type(mqc_matrix), intent(in) MB )
```

5.1.1.96 mqc_matrixmatrixsum()

```
type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixsum (
            type(mqc_matrix), intent(in) MA,
            type(mqc_matrix), intent(in) MB )
```

5.1.1.97 mqc_matrixscalarproduct()

```
type(mqc_matrix) function mqc_algebra::mqc_matrixscalarproduct (
            type(mqc_matrix), intent(in) Matrix,
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.98 mqc_matrixvectordotproduct()

```
type(mqc_vector) function mqc_algebra::mqc_matrixvectordotproduct (
            type(mqc_matrix), intent(in) MA,
            type(mqc_vector), intent(in) VB )
```

5.1.1.99 mqc_outer()

```
type(mqc_matrix) function mqc_algebra::mqc_outer (
            type(mqc_vector), intent(in) VA,
            type(mqc_vector), intent(in) VB )
```

5.1.1.100 mqc_output_complex_scalar()

```
subroutine mqc_algebra::mqc_output_complex_scalar (
            complex(kind=real64), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

5.1.1.101 mqc_output_integer_scalar()

```
subroutine mqc_algebra::mqc_output_integer_scalar (
            integer(kind=int64), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

5.1.1.102 mqc_output_mqcscalar_scalar()

```
subroutine mqc_algebra::mqc_output_mqcscalar_scalar (
            type(mqc_scalar), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

5.1.1.103 mqc_output_real_scalar()

```
subroutine mqc_algebra::mqc_output_real_scalar (
            real(kind=real64), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

5.1.1.104 mqc_print_matrix_algebra1()

```
subroutine mqc_algebra::mqc_print_matrix_algebra1 (
            class(mqc_matrix), intent(in) Matrix,
            integer(kind=int64), intent(in) IOut,
            character(len=*), intent(in) Header,
            logical, intent(in), optional Blank_At_Top,
            logical, intent(in), optional Blank_At_Bottom )
```

5.1.1.105 mqc_print_r4tensor_algebra1()

```
subroutine mqc_algebra::mqc_print_r4tensor_algebra1 (
            class(mqc_r4tensor), intent(in) Tensor,
            integer(kind=int64), intent(in) IOut,
            character(len=*), intent(in), optional Header,
            logical, optional blank_at_top,
            logical, optional blank_at_bottom )
```

5.1.1.106 mqc_print_scalar_algebra1()

```
subroutine mqc_algebra::mqc_print_scalar_algebra1 (
            class(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IOut,
            character(len=*), intent(in) Header,
            logical, intent(in), optional Blank_At_Top,
            logical, intent(in), optional Blank_At_Bottom )
```

5.1.1.107 mqc_print_vector_algebra1()

```
subroutine mqc_algebra::mqc_print_vector_algebra1 (
             class(mqc_vector), intent(in) Vector,
             integer(kind=int64), intent(in) IOut,
             character(len=*), intent(in) Header,
             logical, intent(in), optional Verbose,
             logical, intent(in), optional Blank_At_Top,
             logical, intent(in), optional Blank_At_Bottom )
```

5.1.1.108 mqc_r4tensor_at()

```
type(mqc_scalar) function mqc_algebra::mqc_r4tensor_at (
             class(mqc_r4tensor), intent(in) Tensor,
             integer(kind=int64), intent(in) I,
             integer(kind=int64), intent(in) J,
             integer(kind=int64), intent(in) K,
             integer(kind=int64), intent(in) L )
```

5.1.1.109 mqc_r4tensor_havecomplex()

```
logical function mqc_algebra::mqc_r4tensor_havecomplex (
             type(mqc_r4tensor), intent(in) R4Tensor )
```

5.1.1.110 mqc_r4tensor_haveinteger()

```
logical function mqc_algebra::mqc_r4tensor_haveinteger (
             type(mqc_r4tensor), intent(in) R4Tensor )
```

5.1.1.111 mqc_r4tensor_havereal()

```
logical function mqc_algebra::mqc_r4tensor_havereal (
             type(mqc_r4tensor), intent(in) R4Tensor )
```

5.1.1.112 mqc_r4tensor_initialize()

```
subroutine mqc_algebra::mqc_r4tensor_initialize (
             class(mqc_r4tensor), intent(inout) R4Tensor,
             integer(kind=int64), intent(in) I,
             integer(kind=int64), intent(in) J,
             integer(kind=int64), intent(in) K,
             integer(kind=int64), intent(in) L,
             class(*), optional Scalar )
```

5.1.1.113 mqc_r4tensor_put()

```
subroutine mqc_algebra::mqc_r4tensor_put (
             class(mqc_r4tensor), intent(inout) Tensor,
             type(mqc_scalar), intent(in) Element,
             integer(kind=int64), intent(in) I,
             integer(kind=int64), intent(in) J,
             integer(kind=int64), intent(in) K,
             integer(kind=int64), intent(in) L )
```

5.1.1.114 mqc_realgtscalar()

```
logical function mqc_algebra::mqc_realgtscalar (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.115 mqc_reallescalar()

```
logical function mqc_algebra::mqc_reallescalar (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.116 mqc_realltscalar()

```
logical function mqc_algebra::mqc_realltscalar (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.117 mqc_realscalaradd()

```
type(mqc_scalar) function mqc_algebra::mqc_realscalaradd (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.118 mqc_realscalardivide()

```
type(mqc_scalar) function mqc_algebra::mqc_realscalardivide (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.119 mqc_realscalarmultiply()

```
type(mqc_scalar) function mqc_algebra::mqc_realscalarmultiply (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.120 mqc_realscalarsubtract()

```
type(mqc_scalar) function mqc_algebra::mqc_realscalarsubtract (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.121 mqc_realvectorproduct()

```
type(mqc_vector) function mqc_algebra::mqc_realvectorproduct (
             real(kind=real64), intent(in) RealIn,
             type(mqc_vector), intent(in) Vector )
```

5.1.1.122 mqc_scalar_acos()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_acos (
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.123 mqc_scalar_asin()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_asin (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.124 mqc_scalar_atan()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_atan (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.125 mqc_scalar_atan2()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_atan2 (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.126 mqc_scalar_cmplx()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_cmplx (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.127 mqc_scalar_complex_conjugate()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_complex_conjugate (
            type(mqc_scalar), intent(in) ScalarIn )
```

5.1.1.128 mqc_scalar_complex_imagpart()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_complex_imagpart (
            type(mqc_scalar), intent(in) ScalarIn )
```

5.1.1.129 mqc_scalar_complex_realpart()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_complex_realpart (
            type(mqc_scalar), intent(in) ScalarIn )
```

5.1.1.130 mqc_scalar_cos()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_cos (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.131 mqc_scalar_get_abs_value()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_get_abs_value (
            class(mqc_scalar), intent(in) Scalar )
```

5.1.1.132 mqc_scalar_get_intrinsic_complex()

```
complex(kind=real64) function mqc_algebra::mqc_scalar_get_intrinsic_complex (
            class(mqc_scalar), intent(in) Scalar )
```

5.1.1.133 mqc_scalar_get_intrinsic_integer()

```
integer(kind=int64) function mqc_algebra::mqc_scalar_get_intrinsic_integer (
            class(mqc_scalar), intent(in) Scalar )
```

5.1.1.134 mqc_scalar_get_intrinsic_real()

```
real(kind=real64) function mqc_algebra::mqc_scalar_get_intrinsic_real (
            class(mqc_scalar), intent(in) Scalar )
```

5.1.1.135 mqc_scalar_get_random_value()

```
subroutine mqc_algebra::mqc_scalar_get_random_value (
            class(mqc_scalar) Scalar )
```

5.1.1.136 mqc_scalar_havecomplex()

```
logical function mqc_algebra::mqc_scalar_havecomplex (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.137 mqc_scalar_haveinteger()

```
logical function mqc_algebra::mqc_scalar_haveinteger (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.138 mqc_scalar_havereal()

```
logical function mqc_algebra::mqc_scalar_havereal (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.139 mqc_scalar_isallocated()

```
logical function mqc_algebra::mqc_scalar_isallocated (
            type(mqc_scalar), intent(inout) Scalar )
```

5.1.1.140 mqc_scalar_sin()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_sin (
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.141 mqc_scalar_sqrt()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_sqrt (
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.142 mqc_scalar_tan()

```
type(mqc_scalar) function mqc_algebra::mqc_scalar_tan (
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.143 mqc_scalaradd()

```
type(mqc_scalar) function mqc_algebra::mqc_scalaradd (
             type(mqc_scalar), intent(in) Scalar1,
             type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.144 mqc_scalarcomplexadd()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexadd (
             type(mqc_scalar), intent(in) Scalar,
             complex(kind=real64), intent(in) ComplexIn )
```

5.1.1.145 mqc_scalarcomplexdivide()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexdivide (
             type(mqc_scalar), intent(in) Scalar,
             complex(kind=real64), intent(in) ComplexIn )
```

5.1.1.146 mqc_scalarcomplexexponent()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexexponent (
             type(mqc_scalar), intent(in) Scalar,
             complex(kind=real64), intent(in) CompIn )
```

5.1.1.147 mqc_scalarcomplexmultiply()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexmultiply (
            type(mqc_scalar), intent(in) Scalar,
            complex(kind=real64), intent(in) ComplexIn )
```

5.1.1.148 mqc_scalarcomplexsubtract()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexsubtract (
            type(mqc_scalar), intent(in) Scalar,
            complex(kind=real64), intent(in) ComplexIn )
```

5.1.1.149 mqc_scalardivide()

```
type(mqc_scalar) function mqc_algebra::mqc_scalardivide (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.150 mqc_scalareq()

```
logical function mqc_algebra::mqc_scalareq (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.151 mqc_scalarexponent()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarexponent (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.152 mqc_scalarge()

```
logical function mqc_algebra::mqc_scalarge (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.153 mqc_scalargt()

```
logical function mqc_algebra::mqc_scalargt (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.154 mqc_scalargtinteger()

```
logical function mqc_algebra::mqc_scalargtinteger (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntIn )
```

5.1.1.155 mqc_scalargtreal()

```
logical function mqc_algebra::mqc_scalargtreal (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.156 mqc_scalarintegeradd()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarintegeradd (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntegerIn )
```

5.1.1.157 mqc_scalarintegerdivide()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarintegerdivide (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntegerIn )
```

5.1.1.158 mqc_scalarintegerexponent()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarintegerexponent (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntIn )
```

5.1.1.159 mqc_scalarintegermultiply()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarintegermultiply (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntegerIn )
```

5.1.1.160 mqc_scalarintegersubtract()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarintegersubtract (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntegerIn )
```

5.1.1.161 mqc_scalarle()

```
logical function mqc_algebra::mqc_scalarle (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.162 mqc_scalarleinteger()

```
logical function mqc_algebra::mqc_scalarleinteger (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntIn )
```

5.1.1.163 mqc_scalarlereal()

```
logical function mqc_algebra::mqc_scalarlereal (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.164 mqc_scalarlt()

```
logical function mqc_algebra::mqc_scalarlt (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.165 mqc_scalarltreal()

```
logical function mqc_algebra::mqc_scalarltreal (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.166 mqc_scalarmatrixproduct()

```
type(mqc_matrix) function mqc_algebra::mqc_scalarmatrixproduct (
            type(mqc_scalar), intent(in) Scalar,
            type(mqc_matrix), intent(in) Matrix )
```

5.1.1.167 mqc_scalarmultiply()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarmultiply (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.168 mqc_scalarne()

```
logical function mqc_algebra::mqc_scalarne (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.169 mqc_scalarrealadd()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarrealadd (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.170 mqc_scalarrealdivide()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarrealdivide (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.171 mqc_scalarrealexponent()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarrealexponent (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.172 mqc_scalarrealmultiply()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarrealmultiply (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.173 mqc_scalarrealsubtract()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarrealsubtract (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

5.1.1.174 mqc_scalarsubtract()

```
type(mqc_scalar) function mqc_algebra::mqc_scalarsubtract (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

5.1.1.175 mqc_scalarvectordifference()

```
type(mqc_vector) function mqc_algebra::mqc_scalarvectordifference (
            type(mqc_scalar), intent(in) ScalarIn,
            type(mqc_vector), intent(in) VectorIn )
```

5.1.1.176 mqc_scalarvectorproduct()

```
type(mqc_vector) function mqc_algebra::mqc_scalarvectorproduct (
            type(mqc_scalar), intent(in) Scalar,
            type(mqc_vector), intent(in) Vector )
```

5.1.1.177 mqc_scalarvectorsum()

```
type(mqc_vector) function mqc_algebra::mqc_scalarvectorsum (
             type(mqc_scalar), intent(in) ScalarIn,
             type(mqc_vector), intent(in) VectorIn )
```

5.1.1.178 mqc_set_array2tensor()

```
subroutine mqc_algebra::mqc_set_array2tensor (
             type(mqc_r4tensor), intent(inout) TensorOut,
             class(*), dimension(:,:,:,:), intent(in) ArrayIn )
```

5.1.1.179 mqc_set_array2vector_complex()

```
subroutine mqc_algebra::mqc_set_array2vector_complex (
             type(mqc_vector), intent(inout) VectorOut,
             complex(kind=real64), dimension(:), intent(in) ArrayIn )
```

5.1.1.180 mqc_set_array2vector_integer()

```
subroutine mqc_algebra::mqc_set_array2vector_integer (
             type(mqc_vector), intent(inout) VectorOut,
             integer(kind=int64), dimension(:), intent(in) ArrayIn )
```

5.1.1.181 mqc_set_array2vector_real()

```
subroutine mqc_algebra::mqc_set_array2vector_real (
             type(mqc_vector), intent(inout) VectorOut,
             real(kind=real64), dimension(:), intent(in) ArrayIn )
```

5.1.1.182 mqc_set_complexarray2matrix()

```
subroutine mqc_algebra::mqc_set_complexarray2matrix (
             type(mqc_matrix), intent(inout) MatrixOut,
             complex(kind=real64), dimension(:,:), intent(in) ArrayIn )
```

5.1.1.183 mqc_set_integerarray2matrix()

```
subroutine mqc_algebra::mqc_set_integerarray2matrix (
             type(mqc_matrix), intent(inout) MatrixOut,
             integer(kind=int64), dimension(:,:), intent(in) ArrayIn )
```

5.1.1.184 mqc_set_matrix2complexarray()

```
subroutine mqc_algebra::mqc_set_matrix2complexarray (
             complex(kind=real64), dimension(:,:), intent(inout), allocatable ArrayOut,
             type(mqc_matrix), intent(in) MatrixIn )
```

5.1.1.185 mqc_set_matrix2integerarray()

```
subroutine mqc_algebra::mqc_set_matrix2integerarray (
             integer(kind=int64), dimension(:,:), intent(inout), allocatable ArrayOut,
             type(mqc_matrix), intent(in) MatrixIn )
```

5.1.1.186 mqc_set_matrix2matrix()

```
subroutine mqc_algebra::mqc_set_matrix2matrix (
             class(mqc_matrix), intent(inout) MatrixOut,
             class(mqc_matrix), intent(in) MatrixIn )
```

5.1.1.187 mqc_set_matrix2realarray()

```
subroutine mqc_algebra::mqc_set_matrix2realarray (
             real(kind=real64), dimension(:,:), intent(inout), allocatable ArrayOut,
             type(mqc_matrix), intent(in) MatrixIn )
```

5.1.1.188 mqc_set_realarray2matrix()

```
subroutine mqc_algebra::mqc_set_realarray2matrix (
             type(mqc_matrix), intent(inout) MatrixOut,
             real(kind=real64), dimension(:,:), intent(in) ArrayIn )
```

5.1.1.189 mqc_set_vector2complexarray()

```
subroutine mqc_algebra::mqc_set_vector2complexarray (
             complex(kind=real64), dimension(:), intent(inout), allocatable ArrayOut,
             type(mqc_vector), intent(in) VectorIn )
```

5.1.1.190 mqc_set_vector2integerarray()

```
subroutine mqc_algebra::mqc_set_vector2integerarray (
             integer(kind=int64), dimension(:), intent(inout), allocatable ArrayOut,
             type(mqc_vector), intent(in) VectorIn )
```

5.1.1.191 mqc_set_vector2realarray()

```
subroutine mqc_algebra::mqc_set_vector2realarray (
             real(kind=real64), dimension(:), intent(inout), allocatable ArrayOut,
             type(mqc_vector), intent(in) VectorIn )
```

5.1.1.192 mqc_set_vector2vector()

```
subroutine mqc_algebra::mqc_set_vector2vector (
             class(mqc_vector), intent(inout) VectorOut,
             class(mqc_vector), intent(in) VectorIn )
```

5.1.1.193 mqc_vector2diagmatrix()

```
type(mqc_matrix) function mqc_algebra::mqc_vector2diagmatrix (
             type(mqc_vector), intent(in) vector )
```

5.1.1.194 mqc_vector_abs()

```
type(mqc_vector) function mqc_algebra::mqc_vector_abs (
             class(mqc_vector), intent(in) A )
```

5.1.1.195 mqc_vector_argsort()

```
type(mqc_vector) function mqc_algebra::mqc_vector_argsort (
            class(mqc_vector), intent(in) Vector )
```

5.1.1.196 mqc_vector_cast_complex()

```
type(mqc_vector) function mqc_algebra::mqc_vector_cast_complex (
            type(mqc_vector), intent(in) VA )
```

5.1.1.197 mqc_vector_cast_real()

```
type(mqc_vector) function mqc_algebra::mqc_vector_cast_real (
            type(mqc_vector), intent(in) VA )
```

5.1.1.198 mqc_vector_cmplx()

```
type(mqc_vector) function mqc_algebra::mqc_vector_cmplx (
            type(mqc_vector), intent(in) Vector1,
            type(mqc_vector), intent(in) Vector2 )
```

5.1.1.199 mqc_vector_complex_imagpart()

```
type(mqc_vector) function mqc_algebra::mqc_vector_complex_imagpart (
            class(mqc_vector), intent(in) A )
```

5.1.1.200 mqc_vector_complex_realpart()

```
type(mqc_vector) function mqc_algebra::mqc_vector_complex_realpart (
            class(mqc_vector), intent(in) A )
```

5.1.1.201 mqc_vector_conjugate_transpose()

```
type(mqc_vector) function mqc_algebra::mqc_vector_conjugate_transpose (
             class(mqc_vector), intent(in) Vector )
```

5.1.1.202 mqc_vector_copy_complex2int()

```
subroutine mqc_algebra::mqc_vector_copy_complex2int (
             type(mqc_vector) Vector )
```

5.1.1.203 mqc_vector_copy_complex2real()

```
subroutine mqc_algebra::mqc_vector_copy_complex2real (
             type(mqc_vector) Vector )
```

5.1.1.204 mqc_vector_copy_int2complex()

```
subroutine mqc_algebra::mqc_vector_copy_int2complex (
             type(mqc_vector) Vector )
```

5.1.1.205 mqc_vector_copy_int2real()

```
subroutine mqc_algebra::mqc_vector_copy_int2real (
             type(mqc_vector) Vector )
```

5.1.1.206 mqc_vector_copy_real2complex()

```
subroutine mqc_algebra::mqc_vector_copy_real2complex (
             type(mqc_vector) Vector )
```

5.1.1.207 mqc_vector_copy_real2int()

```
subroutine mqc_algebra::mqc_vector_copy_real2int (
            type(mqc_vector) Vector )
```

5.1.1.208 mqc_vector_havecomplex()

```
logical function mqc_algebra::mqc_vector_havecomplex (
            type(mqc_vector), intent(in) Vector )
```

5.1.1.209 mqc_vector_haveinteger()

```
logical function mqc_algebra::mqc_vector_haveinteger (
            type(mqc_vector), intent(in) Vector )
```

5.1.1.210 mqc_vector_havereal()

```
logical function mqc_algebra::mqc_vector_havereal (
            type(mqc_vector), intent(in) Vector )
```

5.1.1.211 mqc_vector_initialize()

```
subroutine mqc_algebra::mqc_vector_initialize (
            class(mqc_vector), intent(inout) Vector,
            integer(kind=int64), intent(in) Length,
            class(*), optional Scalar )
```

5.1.1.212 mqc_vector_isallocated()

```
logical function mqc_algebra::mqc_vector_isallocated (
            class(mqc_vector), intent(inout) Vector )
```

5.1.1.213 mqc_vector_iscolumn()

```
logical function mqc_algebra::mqc_vector_iscolumn (
             type(mqc_vector), intent(in) Vector )
```

5.1.1.214 mqc_vector_maxloc()

```
integer function mqc_algebra::mqc_vector_maxloc (
             class(mqc_vector), intent(in) Vector )
```

5.1.1.215 mqc_vector_maxval()

```
type(mqc_scalar) function mqc_algebra::mqc_vector_maxval (
             class(mqc_vector), intent(in) Vector )
```

5.1.1.216 mqc_vector_minloc()

```
integer function mqc_algebra::mqc_vector_minloc (
             class(mqc_vector), intent(in) Vector )
```

5.1.1.217 mqc_vector_minval()

```
type(mqc_scalar) function mqc_algebra::mqc_vector_minval (
             class(mqc_vector), intent(in) Vector )
```

5.1.1.218 mqc_vector_norm()

```
type(mqc_scalar) function mqc_algebra::mqc_vector_norm (
             class(mqc_vector), intent(inout) vector,
             character(len=1), intent(in), optional methodIn )
```

5.1.1.219 mqc_vector_pop()

```
type(mqc_scalar) function mqc_algebra::mqc_vector_pop (
             class(mqc_vector), intent(inout) Vector )
```

5.1.1.220 mqc_vector_power()

```
subroutine mqc_algebra::mqc_vector_power (
             class(mqc_vector), intent(inout) A,
             class(*) P )
```

5.1.1.221 mqc_vector_push()

```
subroutine mqc_algebra::mqc_vector_push (
             class(mqc_vector), intent(inout) Vector,
             type(mqc_scalar), intent(in) Scalar )
```

5.1.1.222 mqc_vector_scalar_at()

```
type(mqc_scalar) function mqc_algebra::mqc_vector_scalar_at (
             class(mqc_vector) Vec,
             integer(kind=int64), intent(in) I )
```

5.1.1.223 mqc_vector_scalar_increment()

```
subroutine mqc_algebra::mqc_vector_scalar_increment (
             class(mqc_vector), intent(inout) Vector,
             type(mqc_scalar), intent(in) Scalar,
             integer(kind=int64), intent(in) I )
```

5.1.1.224 mqc_vector_scalar_put()

```
subroutine mqc_algebra::mqc_vector_scalar_put (
             class(mqc_vector), intent(inout) Vector,
             type(mqc_scalar), intent(in) Scalar,
             integer(kind=int64), intent(in) I )
```

5.1.1.225 mqc_vector_shift()

```
type(mqc_scalar) function mqc_algebra::mqc_vector_shift (
            class(mqc_vector), intent(inout) Vector )
```

5.1.1.226 mqc_vector_sort()

```
subroutine mqc_algebra::mqc_vector_sort (
            class(mqc_vector), intent(inout) Vector,
            type(mqc_vector), intent(in), optional idx )
```

5.1.1.227 mqc_vector_sqrt()

```
subroutine mqc_algebra::mqc_vector_sqrt (
            class(mqc_vector), intent(inout) A )
```

5.1.1.228 mqc_vector_transpose()

```
type(mqc_vector) function mqc_algebra::mqc_vector_transpose (
            class(mqc_vector), intent(in) Vector )
```

5.1.1.229 mqc_vector_unshift()

```
subroutine mqc_algebra::mqc_vector_unshift (
            class(mqc_vector), intent(inout) Vector,
            type(mqc_scalar), intent(in) Scalar )
```

5.1.1.230 mqc_vector_vector_at()

```
type(mqc_vector) function mqc_algebra::mqc_vector_vector_at (
            class(mqc_vector) Vec,
            integer(kind=int64), intent(in) I,
            integer(kind=int64), intent(in), optional J )
```

5.1.1.231 mqc_vector_vector_put()

```
subroutine mqc_algebra::mqc_vector_vector_put (
            class(mqc_vector), intent(inout) Vector,
            type(mqc_vector), intent(in) VectorIn,
            integer(kind=int64), intent(in), optional I )
```

5.1.1.232 mqc_vectorcomplexdivide()

```
type(mqc_vector) function mqc_algebra::mqc_vectorcomplexdivide (
            type(mqc_vector), intent(in) vector,
            complex(kind=real64), intent(in) compIn )
```

5.1.1.233 mqc_vectorcomplexproduct()

```
type(mqc_vector) function mqc_algebra::mqc_vectorcomplexproduct (
            type(mqc_vector), intent(in) vector,
            complex(kind=real64), intent(in) compIn )
```

5.1.1.234 mqc_vectorintegerdivide()

```
type(mqc_vector) function mqc_algebra::mqc_vectorintegerdivide (
            type(mqc_vector), intent(in) vector,
            integer(kind=int64), intent(in) intIn )
```

5.1.1.235 mqc_vectorintegerproduct()

```
type(mqc_vector) function mqc_algebra::mqc_vectorintegerproduct (
            type(mqc_vector), intent(in) vector,
            integer(kind=int64), intent(in) intIn )
```

5.1.1.236 mqc_vectormatrixdotproduct()

```
type(mqc_vector) function mqc_algebra::mqc_vectormatrixdotproduct (
            type(mqc_vector), intent(in) VA,
            type(mqc_matrix), intent(in) MB )
```

5.1.1.237 mqc_vectorrealdivide()

```
type(mqc_vector) function mqc_algebra::mqc_vectorrealdivide (
             type(mqc_vector), intent(in) vector,
             real(kind=real64), intent(in) realIn )
```

5.1.1.238 mqc_vectorrealproduct()

```
type(mqc_vector) function mqc_algebra::mqc_vectorrealproduct (
             type(mqc_vector), intent(in) vector,
             real(kind=real64), intent(in) realIn )
```

5.1.1.239 mqc_vectorscalardivide()

```
type(mqc_vector) function mqc_algebra::mqc_vectorscalardivide (
             type(mqc_vector), intent(in) vector,
             type(mqc_scalar), intent(in) scalar )
```

5.1.1.240 mqc_vectorscalarproduct()

```
type(mqc_vector) function mqc_algebra::mqc_vectorscalarproduct (
             type(mqc_vector), intent(in) vector,
             type(mqc_scalar), intent(in) scalar )
```

5.1.1.241 mqc_vectorvectordifference()

```
type(mqc_vector) function mqc_algebra::mqc_vectorvectordifference (
             type(mqc_vector), intent(in) Vector1In,
             type(mqc_vector), intent(in) Vector2In )
```

5.1.1.242 mqc_vectorvectordotproduct()

```
type(mqc_scalar) function mqc_algebra::mqc_vectorvectordotproduct (
             type(mqc_vector), intent(in) Vector1,
             type(mqc_vector), intent(in) Vector2 )
```

5.1.1.243 mqc_vectorvectorsum()

```
type(mqc_vector) function mqc_algebra::mqc_vectorvectorsum (
            type(mqc_vector), intent(in) Vector1In,
            type(mqc_vector), intent(in) Vector2In )
```

5.1.1.244 symindexhash()

```
integer(kind=int64) function mqc_algebra::symindexhash (
            integer(kind=int64), intent(in) i,
            integer(kind=int64), intent(in) j,
            integer(kind=int64), intent(in), optional k,
            integer(kind=int64), intent(in), optional l )
```

5.2 mqc_est Module Reference

Data Types

- interface assignment(=)
- interface contraction
- interface dagger
- interface dot_product
- interface matmul
- type mqc_determinant
- type mqc_determinant_string
- interface mqc_matrix_undospinblockghf
- interface mqc_print
- type mqc_pscf_wavefunction
- type mqc_scf_eigenvalues
- type mqc_scf_integral
- type mqc_twoeris
- type mqc_wavefunction
- interface operator(∗)
- interface operator(+)
- interface operator(-)
- interface transpose

Functions/Subroutines

- subroutine mqc_print_wavefunction (wavefunction, iOut, label)
- subroutine mqc_print_integral (integral, iOut, header, blank_at_top, blank_at_bottom)
- subroutine mqc_print_eigenvalues (eigenvalues, iOut, header, blank_at_top, blank_at_bottom)
- subroutine mqc_print_twoeris (twoERIs, iOut, header, blank_at_top, blank_at_bottom)
- logical function mqc_integral_isallocated (Integral)
- logical function mqc_eigenvalues_isallocated (Eigenvalues)
- logical function mqc_integral_has_alpha (integral)
- logical function mqc_integral_has_beta (integral)
- logical function mqc_integral_has_alphabeta (integral)
- logical function mqc_integral_has_betaalpha (integral)
- logical function mqc_eigenvalues_has_alpha (eigenvalues)
- logical function mqc_eigenvalues_has_beta (eigenvalues)
- character(len=64) function mqc_integral_array_type (integral)
- character(len=64) function mqc_eigenvalues_array_type (eigenvalues)
- character(len=64) function mqc_integral_array_name (integral)
- character(len=64) function mqc_eigenvalues_array_name (eigenvalues)
- subroutine mqc_integral_add_name (integral, arrayName)
- subroutine mqc_eigenvalues_add_name (eigenvalues, arrayName)
- integer(kind=int64) function mqc_integral_dimension (integral, label, axis)
- integer(kind=int64) function mqc_eigenvalues_dimension (eigenvalues, label)
- subroutine mqc_twoeris_allocate (twoERIs, storageType, integralType, alpha, beta, alphaBeta, betaAlpha)
- subroutine mqc_integral_allocate (integral, arrayName, arrayType, alpha, beta, alphaBeta, betaAlpha)
- subroutine mqc_eigenvalues_allocate (eigenvalues, arrayName, arrayType, alpha, beta)
- subroutine mqc_integral_identity (integral, nAlpha, nBeta, label, nAlpha2, nBeta2)
- subroutine mqc_integral_initialize (integral, nAlpha, nBeta, scalar, label, nAlpha2, nBeta2)
- type(mqc_matrix) function mqc_integral_output_block (integral, blockName)
- type(mqc_scf_integral) function mqc_integral_output_orbitals (integral, orbString, alphaOrbsIn, betaOrbsIn, axis)
- type(mqc_scf_integral) function mqc_integral_swap_orbitals (integral, alphaOrbsIn, betaOrbsIn, axis)
- type(mqc_vector) function mqc_eigenvalues_output_block (eigenvalues, blockName)
- subroutine mqc_integral_output_array (matrixOut, integralIn)
- subroutine mqc_eigenvalues_output_array (vectorOut, eigenvaluesIn)
- type(mqc_scf_integral) function mqc_integral_matrix_multiply (integralA, matrixB, label)
- type(mqc_scf_integral) function mqc_matrix_integral_multiply (matrixA, integralB, label)
- type(mqc_scf_integral) function mqc_integral_sum (integralA, integralB)
- type(mqc_scf_integral) function mqc_integral_difference (integralA, integralB)
- type(mqc_scf_integral) function mqc_integral_integral_multiply (integralA, integralB, label)
- type(mqc_scf_integral) function mqc_scalar_integral_multiply (scalar, integral)
- type(mqc_scf_integral) function mqc_integral_scalar_multiply (integral, scalar)
- type(mqc_scf_integral) function mqc_integral_eigenvalues_multiply (integralA, eigenvaluesB, label)
- type(mqc_scf_integral) function mqc_eigenvalues_integral_multiply (eigenvaluesA, integralB, label)
- type(mqc_scf_eigenvalues) function mqc_eigenvalues_eigenvalues_multiply (eigenvaluesA, eigenvaluesB, label)
- type(mqc_scalar) function mqc_eigenvalue_eigenvalue_dotproduct (eigenvalueA, eigenvalueB)
- type(mqc_scf_integral) function mqc_integral_transpose (integral, label)
- type(mqc_scf_integral) function mqc_integral_conjugate_transpose (integral, label)
- type(mqc_scalar) function mqc_integral_norm (integral, methodIn)
- subroutine mqc_matrix_spinblockghf (array, nelec, multi, elist)
- subroutine mqc_matrix_undospinblockghf_eigenvalues (eigenvaluesIn, vectorOut)
- subroutine mqc_matrix_undospinblockghf_integral (integralIn, matrixOut)
- type(mqc_scalar) function mqc_scf_integral_contraction (integral1, integral2)

- type(mqc_scf_integral) function mqc_eri_integral_contraction (eris, integral, label)
- subroutine mqc_scf_integral_generalized_eigensystem (integralA, integralB, eVals, rEVecs, lEVecs)
- subroutine mqc_scf_integral_diagonalize (integral, eVals, eVecs)
- type(mqc_scf_integral) function mqc_scf_integral_inverse (integral)
- type(mqc_scalar) function mqc_scf_integral_trace (integral)
- type(mqc_scalar) function mqc_scf_integral_determinant (integral)
- subroutine mqc_integral_set_energy_list (integral, elist)
- integer(kind=int64) function, dimension(:), allocatable mqc_integral_get_energy_list (integral)
- subroutine mqc_integral_delete_energy_list (integral)
- subroutine mqc_scf_eigenvalues_power (eigenvalues, power)
- type(mqc_scalar) function mqc_twoeris_at (twoERIs, i, j, k, l, spinBlock)
- type(mqc_scalar) function mqc_integral_at (integral, i, j, spinBlock)
- type(mqc_scalar) function mqc_eigenvalues_at (eigenvalues, i, spinBlock)
- subroutine mqc_scf_transformation_matrix (overlap, transform_matrix, nBasUse)
- subroutine gen_det_str (IOut, IPrint, NBasisIn, NAlphaIn, NBetaIn, Determinants, NCoreIn)
- type(mqc_scalar) function slater_condon (IOut, IPrint, NBasisIn, Determinants, L_A_String, L_B_String, R_A_↩String, R_B_String, Core_Hamiltonian, ERIs, UHF)
- subroutine twoeri_trans (IOut, IPrint, MO_Coeff, ERIs, MO_ERIs, UHF)
- subroutine mqc_build_ci_hamiltonian (IOut, IPrint, NBasis, Determinants, MO_Core_Ham, MO_ERIs, UHF, CI↩_Hamiltonian)
- type(mqc_matrix) function get_one_gamma_matrix (iOut, iPrint, nBasisIn, nState, determinants, ci_amplitudes, nCoreIn, nOrbsIn)

5.2.1 Function/Subroutine Documentation

5.2.1.1 gen_det_str()

```
subroutine mqc_est::gen_det_str (
            integer(kind=int64) IOut,
            integer(kind=int64) IPrint,
            type(mqc_scalar) NBasisIn,
            type(mqc_scalar) NAlphaIn,
            type(mqc_scalar) NBetaIn,
            type(mqc_determinant) Determinants,
            type(mqc_scalar), optional NCoreIn )
```

5.2.1.2 get_one_gamma_matrix()

```
type(mqc_matrix) function mqc_est::get_one_gamma_matrix (
            integer(kind=int64), intent(in) iOut,
            integer(kind=int64), intent(in) iPrint,
            type(mqc_scalar), intent(in) nBasisIn,
            integer(kind=int64), intent(in) nState,
            type(mqc_determinant), intent(in) determinants,
            type(mqc_matrix), intent(in) ci_amplitudes,
            integer(kind=int64), intent(in), optional nCoreIn,
            integer(kind=int64), intent(in), optional nOrbsIn )
```

5.2.1.3 mqc_build_ci_hamiltonian()

```
subroutine mqc_est::mqc_build_ci_hamiltonian (
             integer(kind=int64), intent(in) IOut,
             integer(kind=int64), intent(in) IPrint,
             type(mqc_scalar), intent(in) NBasis,
             type(mqc_determinant), intent(in) Determinants,
             type(mqc_scf_integral), intent(in) MO_Core_Ham,
             type(mqc_twoeris), intent(in) MO_ERIs,
             logical, intent(in) UHF,
             type(mqc_matrix), intent(out) CI_Hamiltonian )
```

5.2.1.4 mqc_eigenvalue_eigenvalue_dotproduct()

```
type(mqc_scalar) function mqc_est::mqc_eigenvalue_eigenvalue_dotproduct (
             type(mqc_scf_eigenvalues), intent(in) eigenvalueA,
             type(mqc_scf_eigenvalues), intent(in) eigenvalueB )
```

5.2.1.5 mqc_eigenvalues_add_name()

```
subroutine mqc_est::mqc_eigenvalues_add_name (
             class(mqc_scf_eigenvalues) eigenvalues,
             character(len=*) arrayName )
```

5.2.1.6 mqc_eigenvalues_allocate()

```
subroutine mqc_est::mqc_eigenvalues_allocate (
             class(mqc_scf_eigenvalues) eigenvalues,
             character(len=*) arrayName,
             character(len=*) arrayType,
             type(mqc_vector), optional alpha,
             type(mqc_vector), optional beta )
```

5.2.1.7 mqc_eigenvalues_array_name()

```
character(len=64) function mqc_est::mqc_eigenvalues_array_name (
             class(mqc_scf_eigenvalues) eigenvalues )
```

5.2.1.8 mqc_eigenvalues_array_type()

```
character(len=64) function mqc_est::mqc_eigenvalues_array_type (
            class(mqc_scf_eigenvalues) eigenvalues )
```

5.2.1.9 mqc_eigenvalues_at()

```
type(mqc_scalar) function mqc_est::mqc_eigenvalues_at (
            class(mqc_scf_eigenvalues) eigenvalues,
            integer(kind=int64) i,
            character(len=64), optional spinBlock )
```

5.2.1.10 mqc_eigenvalues_dimension()

```
integer(kind=int64) function mqc_est::mqc_eigenvalues_dimension (
            class(mqc_scf_eigenvalues), intent(in) eigenvalues,
            character(len=*), intent(in) label )
```

5.2.1.11 mqc_eigenvalues_eigenvalues_multiply()

```
type(mqc_scf_eigenvalues) function mqc_est::mqc_eigenvalues_eigenvalues_multiply (
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesA,
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesB,
            character(len=*), intent(in), optional label )
```

5.2.1.12 mqc_eigenvalues_has_alpha()

```
logical function mqc_est::mqc_eigenvalues_has_alpha (
            class(mqc_scf_eigenvalues) eigenvalues )
```

5.2.1.13 mqc_eigenvalues_has_beta()

```
logical function mqc_est::mqc_eigenvalues_has_beta (
            class(mqc_scf_eigenvalues) eigenvalues )
```

5.2.1.14 mqc_eigenvalues_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::mqc_eigenvalues_integral_multiply (
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesA,
            type(mqc_scf_integral), intent(in) integralB,
            character(len=*), intent(in), optional label )
```

5.2.1.15 mqc_eigenvalues_isallocated()

```
logical function mqc_est::mqc_eigenvalues_isallocated (
            class(mqc_scf_eigenvalues), intent(inout) Eigenvalues )
```

5.2.1.16 mqc_eigenvalues_output_array()

```
subroutine mqc_est::mqc_eigenvalues_output_array (
            type(mqc_vector), intent(inout) vectorOut,
            class(mqc_scf_eigenvalues), intent(in) eigenvaluesIn )
```

5.2.1.17 mqc_eigenvalues_output_block()

```
type(mqc_vector) function mqc_est::mqc_eigenvalues_output_block (
            class(mqc_scf_eigenvalues) eigenvalues,
            character(len=*), optional blockName )
```

5.2.1.18 mqc_eri_integral_contraction()

```
type(mqc_scf_integral) function mqc_est::mqc_eri_integral_contraction (
            type(mqc_twoeris), intent(in) eris,
            type(mqc_scf_integral), intent(in) integral,
            character(len=*), optional label )
```

5.2.1.19 mqc_integral_add_name()

```
subroutine mqc_est::mqc_integral_add_name (
            class(mqc_scf_integral) integral,
            character(len=*) arrayName )
```

5.2.1.20 mqc_integral_allocate()

```
subroutine mqc_est::mqc_integral_allocate (
            class(mqc_scf_integral) integral,
            character(len=*) arrayName,
            character(len=*) arrayType,
            type(mqc_matrix), optional alpha,
            type(mqc_matrix), optional beta,
            type(mqc_matrix), optional alphaBeta,
            type(mqc_matrix), optional betaAlpha )
```

5.2.1.21 mqc_integral_array_name()

```
character(len=64) function mqc_est::mqc_integral_array_name (
            class(mqc_scf_integral) integral )
```

5.2.1.22 mqc_integral_array_type()

```
character(len=64) function mqc_est::mqc_integral_array_type (
            class(mqc_scf_integral) integral )
```

5.2.1.23 mqc_integral_at()

```
type(mqc_scalar) function mqc_est::mqc_integral_at (
            class(mqc_scf_integral) integral,
            integer(kind=int64) i,
            integer(kind=int64) j,
            character(len=64), optional spinBlock )
```

5.2.1.24 mqc_integral_conjugate_transpose()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_conjugate_transpose (
            type(mqc_scf_integral), intent(in) integral,
            character(len=*), intent(in), optional label )
```

5.2.1.25 mqc_integral_delete_energy_list()

```
subroutine mqc_est::mqc_integral_delete_energy_list (
             class(mqc_scf_integral) integral )
```

5.2.1.26 mqc_integral_difference()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_difference (
             type(mqc_scf_integral), intent(in) integralA,
             type(mqc_scf_integral), intent(in) integralB )
```

5.2.1.27 mqc_integral_dimension()

```
integer(kind=int64) function mqc_est::mqc_integral_dimension (
             class(mqc_scf_integral), intent(in) integral,
             character(len=*), intent(in) label,
             integer(kind=int64), intent(in), optional axis )
```

5.2.1.28 mqc_integral_eigenvalues_multiply()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_eigenvalues_multiply (
             type(mqc_scf_integral), intent(in) integralA,
             type(mqc_scf_eigenvalues), intent(in) eigenvaluesB,
             character(len=*), intent(in), optional label )
```

5.2.1.29 mqc_integral_get_energy_list()

```
integer(kind=int64) function, dimension(:), allocatable mqc_est::mqc_integral_get_energy_list (
             class(mqc_scf_integral) integral )
```

5.2.1.30 mqc_integral_has_alpha()

```
logical function mqc_est::mqc_integral_has_alpha (
             class(mqc_scf_integral) integral )
```

5.2.1.31 mqc_integral_has_alphabeta()

```
logical function mqc_est::mqc_integral_has_alphabeta (
            class(mqc_scf_integral) integral )
```

5.2.1.32 mqc_integral_has_beta()

```
logical function mqc_est::mqc_integral_has_beta (
            class(mqc_scf_integral) integral )
```

5.2.1.33 mqc_integral_has_betaalpha()

```
logical function mqc_est::mqc_integral_has_betaalpha (
            class(mqc_scf_integral) integral )
```

5.2.1.34 mqc_integral_identity()

```
subroutine mqc_est::mqc_integral_identity (
            class(mqc_scf_integral), intent(inout) integral,
            integer, intent(in) nAlpha,
            integer, intent(in) nBeta,
            character(len=*), intent(in), optional label,
            integer, intent(in), optional nAlpha2,
            integer, intent(in), optional nBeta2 )
```

5.2.1.35 mqc_integral_initialize()

```
subroutine mqc_est::mqc_integral_initialize (
            class(mqc_scf_integral), intent(inout) integral,
            integer, intent(in) nAlpha,
            integer, intent(in) nBeta,
            class(*), intent(in), optional scalar,
            character(len=*), intent(in), optional label,
            integer, intent(in), optional nAlpha2,
            integer, intent(in), optional nBeta2 )
```

5.2.1.36 mqc_integral_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_integral_multiply (
            type(mqc_scf_integral), intent(in) integralA,
            type(mqc_scf_integral), intent(in) integralB,
            character(len=*), intent(in), optional label )
```

5.2.1.37 mqc_integral_isallocated()

```
logical function mqc_est::mqc_integral_isallocated (
            class(mqc_scf_integral), intent(inout) Integral )
```

5.2.1.38 mqc_integral_matrix_multiply()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_matrix_multiply (
            type(mqc_scf_integral), intent(in) integralA,
            type(mqc_matrix), intent(in) matrixB,
            character(len=*), intent(in), optional label )
```

5.2.1.39 mqc_integral_norm()

```
type(mqc_scalar) function mqc_est::mqc_integral_norm (
            class(mqc_scf_integral), intent(in) integral,
            character(len=1), intent(in), optional methodIn )
```

5.2.1.40 mqc_integral_output_array()

```
subroutine mqc_est::mqc_integral_output_array (
            type(mqc_matrix), intent(inout) matrixOut,
            class(mqc_scf_integral), intent(in) integralIn )
```

5.2.1.41 mqc_integral_output_block()

```
type(mqc_matrix) function mqc_est::mqc_integral_output_block (
            class(mqc_scf_integral) integral,
            character(len=*), optional blockName )
```

5.2.1.42 mqc_integral_output_orbitals()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_output_orbitals (
             class(mqc_scf_integral), intent(in) integral,
             character(len=*), optional orbString,
             integer(kind=int64), dimension(:), optional alphaOrbsIn,
             integer(kind=int64), dimension(:), optional betaOrbsIn,
             integer(kind=int64), intent(in), optional axis )
```

5.2.1.43 mqc_integral_scalar_multiply()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_scalar_multiply (
             type(mqc_scf_integral), intent(in) integral,
             type(mqc_scalar), intent(in) scalar )
```

5.2.1.44 mqc_integral_set_energy_list()

```
subroutine mqc_est::mqc_integral_set_energy_list (
             class(mqc_scf_integral) integral,
             integer(kind=int64), dimension(:), allocatable elist )
```

5.2.1.45 mqc_integral_sum()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_sum (
             type(mqc_scf_integral), intent(in) integralA,
             type(mqc_scf_integral), intent(in) integralB )
```

5.2.1.46 mqc_integral_swap_orbitals()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_swap_orbitals (
             class(mqc_scf_integral), intent(in) integral,
             integer(kind=int64), dimension(2), optional alphaOrbsIn,
             integer(kind=int64), dimension(2), optional betaOrbsIn,
             integer(kind=int64), intent(in), optional axis )
```

5.2.1.47 mqc_integral_transpose()

```
type(mqc_scf_integral) function mqc_est::mqc_integral_transpose (
            type(mqc_scf_integral), intent(in) integral,
            character(len=*), intent(in), optional label )
```

5.2.1.48 mqc_matrix_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::mqc_matrix_integral_multiply (
            type(mqc_matrix), intent(in) matrixA,
            type(mqc_scf_integral), intent(in) integralB,
            character(len=*), intent(in), optional label )
```

5.2.1.49 mqc_matrix_spinblockghf()

```
subroutine mqc_est::mqc_matrix_spinblockghf (
            class(*), intent(inout) array,
            integer(kind=int64), optional nelec,
            integer(kind=int64), optional multi,
            integer(kind=int64), dimension(:), optional, allocatable elist )
```

5.2.1.50 mqc_matrix_undospinblockghf_eigenvalues()

```
subroutine mqc_est::mqc_matrix_undospinblockghf_eigenvalues (
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesIn,
            type(mqc_vector), intent(out) vectorOut )
```

5.2.1.51 mqc_matrix_undospinblockghf_integral()

```
subroutine mqc_est::mqc_matrix_undospinblockghf_integral (
            type(mqc_scf_integral), intent(in) integralIn,
            type(mqc_matrix), intent(out) matrixOut )
```

5.2.1.52 mqc_print_eigenvalues()

```
subroutine mqc_est::mqc_print_eigenvalues (
             class(mqc_scf_eigenvalues) eigenvalues,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in) header,
             logical, intent(in), optional blank_at_top,
             logical, intent(in), optional blank_at_bottom )
```

5.2.1.53 mqc_print_integral()

```
subroutine mqc_est::mqc_print_integral (
             class(mqc_scf_integral) integral,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in) header,
             logical, intent(in), optional blank_at_top,
             logical, intent(in), optional blank_at_bottom )
```

5.2.1.54 mqc_print_twoeris()

```
subroutine mqc_est::mqc_print_twoeris (
             class(mqc_twoeris) twoERIs,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in) header,
             logical, intent(in), optional blank_at_top,
             logical, intent(in), optional blank_at_bottom )
```

5.2.1.55 mqc_print_wavefunction()

```
subroutine mqc_est::mqc_print_wavefunction (
             class(mqc_wavefunction) wavefunction,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in), optional label )
```

5.2.1.56 mqc_scalar_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::mqc_scalar_integral_multiply (
             type(mqc_scalar), intent(in) scalar,
             type(mqc_scf_integral), intent(in) integral )
```

5.2.1.57 mqc_scf_eigenvalues_power()

```
subroutine mqc_est::mqc_scf_eigenvalues_power (
            class(mqc_scf_eigenvalues), intent(inout) eigenvalues,
            class(*) power )
```

5.2.1.58 mqc_scf_integral_contraction()

```
type(mqc_scalar) function mqc_est::mqc_scf_integral_contraction (
            type(mqc_scf_integral), intent(in) integral1,
            type(mqc_scf_integral), intent(in) integral2 )
```

5.2.1.59 mqc_scf_integral_determinant()

```
type(mqc_scalar) function mqc_est::mqc_scf_integral_determinant (
            class(mqc_scf_integral), intent(in) integral )
```

5.2.1.60 mqc_scf_integral_diagonalize()

```
subroutine mqc_est::mqc_scf_integral_diagonalize (
            class(mqc_scf_integral), intent(in) integral,
            type(mqc_scf_eigenvalues), intent(inout), optional eVals,
            type(mqc_scf_integral), intent(inout), optional eVecs )
```

5.2.1.61 mqc_scf_integral_generalized_eigensystem()

```
subroutine mqc_est::mqc_scf_integral_generalized_eigensystem (
            class(mqc_scf_integral), intent(in) integralA,
            type(mqc_scf_integral), optional integralB,
            type(mqc_scf_eigenvalues), intent(inout), optional eVals,
            type(mqc_scf_integral), intent(inout), optional rEVecs,
            type(mqc_scf_integral), intent(inout), optional lEVecs )
```

5.2.1.62 mqc_scf_integral_inverse()

```
type(mqc_scf_integral) function mqc_est::mqc_scf_integral_inverse (
            class(mqc_scf_integral), intent(in) integral )
```

5.2.1.63 mqc_scf_integral_trace()

```
type(mqc_scalar) function mqc_est::mqc_scf_integral_trace (
            class(mqc_scf_integral), intent(in) integral )
```

5.2.1.64 mqc_scf_transformation_matrix()

```
subroutine mqc_est::mqc_scf_transformation_matrix (
            type(mqc_scf_integral), intent(in) overlap,
            type(mqc_scf_integral), intent(out) transform_matrix,
            integer(kind=int64), intent(out), optional nBasUse )
```

5.2.1.65 mqc_twoeris_allocate()

```
subroutine mqc_est::mqc_twoeris_allocate (
            class(mqc_twoeris) twoERIs,
            character(len=*) storageType,
            character(len=*) integralType,
            type(mqc_r4tensor), optional alpha,
            type(mqc_r4tensor), optional beta,
            type(mqc_r4tensor), optional alphaBeta,
            type(mqc_r4tensor), optional betaAlpha )
```

5.2.1.66 mqc_twoeris_at()

```
type(mqc_scalar) function mqc_est::mqc_twoeris_at (
            class(mqc_twoeris) twoERIs,
            integer(kind=int64), intent(in) i,
            integer(kind=int64), intent(in) j,
            integer(kind=int64), intent(in) k,
            integer(kind=int64), intent(in) l,
            character(len=64), optional spinBlock )
```

5.2.1.67 slater_condon()

```
type(mqc_scalar) function mqc_est::slater_condon (
            integer(kind=int64), intent(in) IOut,
            integer(kind=int64), intent(in) IPrint,
            type(mqc_scalar), intent(in) NBasisIn,
            type(mqc_determinant), intent(in) Determinants,
            integer(kind=int64), intent(in) L_A_String,
            integer(kind=int64), intent(in) L_B_String,
            integer(kind=int64), intent(in) R_A_String,
            integer(kind=int64), intent(in) R_B_String,
            type(mqc_scf_integral), intent(in) Core_Hamiltonian,
            type(mqc_twoeris), intent(in) ERIs,
            logical, intent(in) UHF )
```

5.2.1.68 twoeri_trans()

```
subroutine mqc_est::twoeri_trans (
            integer(kind=int64) IOut,
            integer(kind=int64) IPrint,
            type(mqc_scf_integral), intent(in) MO_Coeff,
            type(mqc_twoeris), intent(in) ERIs,
            type(mqc_twoeris), intent(out) MO_ERIs,
            logical UHF )
```

Chapter 6

Data Type Documentation

6.1 mqc_algebra::abs Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_get_abs_value (Scalar)
- type(mqc_vector) function mqc_vector_abs (A)

6.1.1 Member Function/Subroutine Documentation

6.1.1.1 mqc_scalar_get_abs_value()

```
type(mqc_scalar) function mqc_algebra::abs::mqc_scalar_get_abs_value (
            class(mqc_scalar), intent(in) Scalar )
```

6.1.1.2 mqc_vector_abs()

```
type(mqc_vector) function mqc_algebra::abs::mqc_vector_abs (
            class(mqc_vector), intent(in) A )
```

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

- src/mqc_algebra.F03

6.2 mqc_algebra::acos Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_acos (Scalar)

6.2.1 Member Function/Subroutine Documentation

6.2.1.1 mqc_scalar_acos()

```
type(mqc_scalar) function mqc_algebra::acos::mqc_scalar_acos (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.3 mqc_algebra::aimag Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_complex_imagpart (ScalarIn)
- type(mqc_vector) function mqc_vector_complex_imagpart (A)

6.3.1 Member Function/Subroutine Documentation

6.3.1.1 mqc_scalar_complex_imagpart()

```
type(mqc_scalar) function mqc_algebra::aimag::mqc_scalar_complex_imagpart (
            type(mqc_scalar), intent(in) ScalarIn )
```

6.3.1.2 mqc_vector_complex_imagpart()

```
type(mqc_vector) function mqc_algebra::aimag::mqc_vector_complex_imagpart (
            class(mqc_vector), intent(in) A )
```

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

- src/mqc_algebra.F03

6.4 mqc_algebra::asin Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_asin (Scalar)

6.4.1 Member Function/Subroutine Documentation

6.4.1.1 mqc_scalar_asin()

```
type(mqc_scalar) function mqc_algebra::asin::mqc_scalar_asin (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.5 mqc_algebra::assignment(=) Interface Reference

Public Member Functions

- subroutine mqc_input_integer_scalar (ScalarOut, ScalarIn)

  MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic scalar to an MQC_Scalar
- subroutine mqc_input_real_scalar (ScalarOut, ScalarIn)
- subroutine mqc_input_complex_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_mqcscalar_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_integer_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_real_scalar (ScalarOut, ScalarIn)
- subroutine mqc_output_complex_scalar (ScalarOut, ScalarIn)
- subroutine mqc_set_vector2vector (VectorOut, VectorIn)
- subroutine mqc_set_vector2integerarray (ArrayOut, VectorIn)

- subroutine mqc_set_vector2realarray (ArrayOut, VectorIn)
- subroutine mqc_set_vector2complexarray (ArrayOut, VectorIn)
- subroutine mqc_set_array2vector_integer (VectorOut, ArrayIn)
- subroutine mqc_set_array2vector_real (VectorOut, ArrayIn)
- subroutine mqc_set_array2vector_complex (VectorOut, ArrayIn)
- subroutine mqc_set_matrix2matrix (MatrixOut, MatrixIn)
- subroutine mqc_set_matrix2integerarray (ArrayOut, MatrixIn)
- subroutine mqc_set_matrix2realarray (ArrayOut, MatrixIn)
- subroutine mqc_set_matrix2complexarray (ArrayOut, MatrixIn)
- subroutine mqc_set_integerarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_set_realarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_set_complexarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_set_array2tensor (TensorOut, ArrayIn)

6.5.1 Member Function/Subroutine Documentation

6.5.1.1 mqc_input_complex_scalar()

```
subroutine mqc_algebra::assignment(=)::mqc_input_complex_scalar (
             type(mqc_scalar), intent(inout) ScalarOut,
             complex(kind=real64), intent(in) ScalarIn )
```

6.5.1.2 mqc_input_integer_scalar()

```
subroutine mqc_algebra::assignment(=)::mqc_input_integer_scalar (
             type(mqc_scalar), intent(inout) ScalarOut,
             integer(kind=int64), intent(in) ScalarIn )
```

MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic scalar to an MQC_Scalar

Purpose:

```
MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic scalar to an MQC_Scalar.
```

Parameters

in,out	*ScalarOut*	ScalarOut is Type(MQC_Scalar) The name of the output variable
in	*ScalarIn*	ScalarIn is Integer(kind=int64) The value of the input variable

Author

L. M. Thompson

Date

2016

6.5.1.3 mqc_input_real_scalar()

```
subroutine mqc_algebra::assignment(=)::mqc_input_real_scalar (
            type(mqc_scalar), intent(inout) ScalarOut,
            real(kind=real64), intent(in) ScalarIn )
```

6.5.1.4 mqc_output_complex_scalar()

```
subroutine mqc_algebra::assignment(=)::mqc_output_complex_scalar (
            complex(kind=real64), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

6.5.1.5 mqc_output_integer_scalar()

```
subroutine mqc_algebra::assignment(=)::mqc_output_integer_scalar (
            integer(kind=int64), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

6.5.1.6 mqc_output_mqcscalar_scalar()

```
subroutine mqc_algebra::assignment(=)::mqc_output_mqcscalar_scalar (
            type(mqc_scalar), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

6.5.1.7 mqc_output_real_scalar()

```
subroutine mqc_algebra::assignment(=)::mqc_output_real_scalar (
            real(kind=real64), intent(inout) ScalarOut,
            type(mqc_scalar), intent(in) ScalarIn )
```

6.5.1.8 mqc_set_array2tensor()

```
subroutine mqc_algebra::assignment(=)::mqc_set_array2tensor (
            type(mqc_r4tensor), intent(inout) TensorOut,
            class(*), dimension(:,:,:,:), intent(in) ArrayIn )
```

6.5.1.9 mqc_set_array2vector_complex()

```
subroutine mqc_algebra::assignment(=)::mqc_set_array2vector_complex (
            type(mqc_vector), intent(inout) VectorOut,
            complex(kind=real64), dimension(:), intent(in) ArrayIn )
```

6.5.1.10 mqc_set_array2vector_integer()

```
subroutine mqc_algebra::assignment(=)::mqc_set_array2vector_integer (
            type(mqc_vector), intent(inout) VectorOut,
            integer(kind=int64), dimension(:), intent(in) ArrayIn )
```

6.5.1.11 mqc_set_array2vector_real()

```
subroutine mqc_algebra::assignment(=)::mqc_set_array2vector_real (
            type(mqc_vector), intent(inout) VectorOut,
            real(kind=real64), dimension(:), intent(in) ArrayIn )
```

6.5.1.12 mqc_set_complexarray2matrix()

```
subroutine mqc_algebra::assignment(=)::mqc_set_complexarray2matrix (
            type(mqc_matrix), intent(inout) MatrixOut,
            complex(kind=real64), dimension(:,:), intent(in) ArrayIn )
```

6.5.1.13 mqc_set_integerarray2matrix()

```
subroutine mqc_algebra::assignment(=)::mqc_set_integerarray2matrix (
            type(mqc_matrix), intent(inout) MatrixOut,
            integer(kind=int64), dimension(:,:), intent(in) ArrayIn )
```

6.5.1.14 mqc_set_matrix2complexarray()

```
subroutine mqc_algebra::assignment(=)::mqc_set_matrix2complexarray (
            complex(kind=real64), dimension(:,:), intent(inout), allocatable ArrayOut,
            type(mqc_matrix), intent(in) MatrixIn )
```

6.5.1.15 mqc_set_matrix2integerarray()

```
subroutine mqc_algebra::assignment(=)::mqc_set_matrix2integerarray (
            integer(kind=int64), dimension(:,:), intent(inout), allocatable ArrayOut,
            type(mqc_matrix), intent(in) MatrixIn )
```

6.5.1.16 mqc_set_matrix2matrix()

```
subroutine mqc_algebra::assignment(=)::mqc_set_matrix2matrix (
            class(mqc_matrix), intent(inout) MatrixOut,
            class(mqc_matrix), intent(in) MatrixIn )
```

6.5.1.17 mqc_set_matrix2realarray()

```
subroutine mqc_algebra::assignment(=)::mqc_set_matrix2realarray (
            real(kind=real64), dimension(:,:), intent(inout), allocatable ArrayOut,
            type(mqc_matrix), intent(in) MatrixIn )
```

6.5.1.18 mqc_set_realarray2matrix()

```
subroutine mqc_algebra::assignment(=)::mqc_set_realarray2matrix (
            type(mqc_matrix), intent(inout) MatrixOut,
            real(kind=real64), dimension(:,:), intent(in) ArrayIn )
```

6.5.1.19 mqc_set_vector2complexarray()

```
subroutine mqc_algebra::assignment(=)::mqc_set_vector2complexarray (
            complex(kind=real64), dimension(:), intent(inout), allocatable ArrayOut,
            type(mqc_vector), intent(in) VectorIn )
```

6.5.1.20 mqc_set_vector2integerarray()

```
subroutine mqc_algebra::assignment(=)::mqc_set_vector2integerarray (
            integer(kind=int64), dimension(:), intent(inout), allocatable ArrayOut,
            type(mqc_vector), intent(in) VectorIn )
```

6.5.1.21 mqc_set_vector2realarray()

```
subroutine mqc_algebra::assignment(=)::mqc_set_vector2realarray (
            real(kind=real64), dimension(:), intent(inout), allocatable ArrayOut,
            type(mqc_vector), intent(in) VectorIn )
```

6.5.1.22 mqc_set_vector2vector()

```
subroutine mqc_algebra::assignment(=)::mqc_set_vector2vector (
            class(mqc_vector), intent(inout) VectorOut,
            class(mqc_vector), intent(in) VectorIn )
```

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

- src/mqc_algebra.F03

6.6 mqc_est::assignment(=) Interface Reference

Public Member Functions

- subroutine mqc_integral_output_array (matrixOut, integralIn)
- subroutine mqc_eigenvalues_output_array (vectorOut, eigenvaluesIn)

6.6.1 Member Function/Subroutine Documentation

6.6.1.1 mqc_eigenvalues_output_array()

```
subroutine mqc_est::assignment(=)::mqc_eigenvalues_output_array (
            type(mqc_vector), intent(inout) vectorOut,
            class(mqc_scf_eigenvalues), intent(in) eigenvaluesIn )
```

6.6.1.2 mqc_integral_output_array()

```
subroutine mqc_est::assignment(=)::mqc_integral_output_array (
            type(mqc_matrix), intent(inout) matrixOut,
            class(mqc_scf_integral), intent(in) integralIn )
```

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

- src/mqc_est.F03

6.7 mqc_algebra::atan Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_atan (Scalar)

6.7.1 Member Function/Subroutine Documentation

6.7.1.1 mqc_scalar_atan()

```
type(mqc_scalar) function mqc_algebra::atan::mqc_scalar_atan (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.8 mqc_algebra::atan2 Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_atan2 (Scalar)

6.8.1 Member Function/Subroutine Documentation

6.8.1.1 mqc_scalar_atan2()

```
type(mqc_scalar) function mqc_algebra::atan2::mqc_scalar_atan2 (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.9 mqc_algebra::cmplx Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_cmplx (Scalar1, Scalar2)
- type(mqc_vector) function mqc_vector_cmplx (Vector1, Vector2)

6.9.1 Member Function/Subroutine Documentation

6.9.1.1 mqc_scalar_cmplx()

```
type(mqc_scalar) function mqc_algebra::cmplx::mqc_scalar_cmplx (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

6.9.1.2 mqc_vector_cmplx()

```
type(mqc_vector) function mqc_algebra::cmplx::mqc_vector_cmplx (
            type(mqc_vector), intent(in) Vector1,
            type(mqc_vector), intent(in) Vector2 )
```

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

- src/mqc_algebra.F03

6.10 mqc_algebra::conjg Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_complex_conjugate (ScalarIn)

6.10.1 Member Function/Subroutine Documentation

6.10.1.1 mqc_scalar_complex_conjugate()

```
type(mqc_scalar) function mqc_algebra::conjg::mqc_scalar_complex_conjugate (
             type(mqc_scalar), intent(in) ScalarIn )
```

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

- src/mqc_algebra.F03

6.11 mqc_algebra::contraction Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_matrix_matrix_contraction (Matrix1, Matrix2)

6.11.1 Member Function/Subroutine Documentation

6.11.1.1 mqc_matrix_matrix_contraction()

```
type(mqc_scalar) function mqc_algebra::contraction::mqc_matrix_matrix_contraction (
             type(mqc_matrix), intent(in) Matrix1,
             type(mqc_matrix), intent(in) Matrix2 )
```

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

- src/mqc_algebra.F03

6.12 mqc_est::contraction Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scf_integral_contraction (integral1, integral2)
- type(mqc_scf_integral) function mqc_eri_integral_contraction (eris, integral, label)

6.12.1 Member Function/Subroutine Documentation

6.12.1.1 mqc_eri_integral_contraction()

```
type(mqc_scf_integral) function mqc_est::contraction::mqc_eri_integral_contraction (
             type(mqc_twoeris), intent(in) eris,
             type(mqc_scf_integral), intent(in) integral,
             character(len=*), optional label )
```

6.12.1.2 mqc_scf_integral_contraction()

```
type(mqc_scalar) function mqc_est::contraction::mqc_scf_integral_contraction (
             type(mqc_scf_integral), intent(in) integral1,
             type(mqc_scf_integral), intent(in) integral2 )
```

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

- src/mqc_est.F03

6.13 mqc_algebra::cos Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_cos (Scalar)

6.13.1 Member Function/Subroutine Documentation

6.13.1.1 mqc_scalar_cos()

```
type(mqc_scalar) function mqc_algebra::cos::mqc_scalar_cos (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.14 mqc_algebra::dagger Interface Reference

Public Member Functions

- type(mqc_vector) function mqc_vector_conjugate_transpose (Vector)
- type(mqc_matrix) function mqc_matrix_conjugate_transpose (Matrix)

6.14.1 Member Function/Subroutine Documentation

6.14.1.1 mqc_matrix_conjugate_transpose()

```
type(mqc_matrix) function mqc_algebra::dagger::mqc_matrix_conjugate_transpose (
            class(mqc_matrix), intent(in) Matrix )
```

6.14.1.2 mqc_vector_conjugate_transpose()

```
type(mqc_vector) function mqc_algebra::dagger::mqc_vector_conjugate_transpose (
            class(mqc_vector), intent(in) Vector )
```

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

- src/mqc_algebra.F03

6.15 mqc_est::dagger Interface Reference

Public Member Functions

- type(mqc_scf_integral) function mqc_integral_conjugate_transpose (integral, label)

6.15.1 Member Function/Subroutine Documentation

6.15.1.1 mqc_integral_conjugate_transpose()

```
type(mqc_scf_integral) function mqc_est::dagger::mqc_integral_conjugate_transpose (
            type(mqc_scf_integral), intent(in) integral,
            character(len=*), intent(in), optional label )
```

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

- src/mqc_est.F03

6.16 mqc_algebra::dot_product Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_vectorvectordotproduct (Vector1, Vector2)

6.16.1 Member Function/Subroutine Documentation

6.16.1.1 mqc_vectorvectordotproduct()

```
type(mqc_scalar) function mqc_algebra::dot_product::mqc_vectorvectordotproduct (
            type(mqc_vector), intent(in) Vector1,
            type(mqc_vector), intent(in) Vector2 )
```

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

- src/mqc_algebra.F03

6.17 mqc_est::dot_product Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_eigenvalue_eigenvalue_dotproduct (eigenvalueA, eigenvalueB)

6.17.1 Member Function/Subroutine Documentation

6.17.1.1 mqc_eigenvalue_eigenvalue_dotproduct()

```
type(mqc_scalar) function mqc_est::dot_product::mqc_eigenvalue_eigenvalue_dotproduct (
            type(mqc_scf_eigenvalues), intent(in) eigenvalueA,
            type(mqc_scf_eigenvalues), intent(in) eigenvalueB )
```

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

- src/mqc_est.F03

6.18 mqc_algebra::matmul Interface Reference

Public Member Functions

- type(mqc_matrix) function mqc_matrixmatrixdotproduct (MA, MB)
- type(mqc_vector) function mqc_matrixvectordotproduct (MA, VB)
- type(mqc_vector) function mqc_vectormatrixdotproduct (VA, MB)

6.18.1 Member Function/Subroutine Documentation

6.18.1.1 mqc_matrixmatrixdotproduct()

```
type(mqc_matrix) function mqc_algebra::matmul::mqc_matrixmatrixdotproduct (
            type(mqc_matrix), intent(in) MA,
            type(mqc_matrix), intent(in) MB )
```

6.18.1.2 mqc_matrixvectordotproduct()

```
type(mqc_vector) function mqc_algebra::matmul::mqc_matrixvectordotproduct (
            type(mqc_matrix), intent(in) MA,
            type(mqc_vector), intent(in) VB )
```

6.18.1.3 mqc_vectormatrixdotproduct()

```
type(mqc_vector) function mqc_algebra::matmul::mqc_vectormatrixdotproduct (
            type(mqc_vector), intent(in) VA,
            type(mqc_matrix), intent(in) MB )
```

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

- src/mqc_algebra.F03

6.19 mqc_est::matmul Interface Reference

Public Member Functions

- type(mqc_scf_integral) function mqc_integral_matrix_multiply (integralA, matrixB, label)
- type(mqc_scf_integral) function mqc_matrix_integral_multiply (matrixA, integralB, label)
- type(mqc_scf_integral) function mqc_integral_integral_multiply (integralA, integralB, label)
- type(mqc_scf_integral) function mqc_integral_eigenvalues_multiply (integralA, eigenvaluesB, label)
- type(mqc_scf_integral) function mqc_eigenvalues_integral_multiply (eigenvaluesA, integralB, label)
- type(mqc_scf_eigenvalues) function mqc_eigenvalues_eigenvalues_multiply (eigenvaluesA, eigenvaluesB, label)

6.19.1 Member Function/Subroutine Documentation

6.19.1.1 mqc_eigenvalues_eigenvalues_multiply()

```
type(mqc_scf_eigenvalues) function mqc_est::matmul::mqc_eigenvalues_eigenvalues_multiply (
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesA,
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesB,
            character(len=*), intent(in), optional label )
```

6.19.1.2 mqc_eigenvalues_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::matmul::mqc_eigenvalues_integral_multiply (
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesA,
            type(mqc_scf_integral), intent(in) integralB,
            character(len=*), intent(in), optional label )
```

6.19.1.3 mqc_integral_eigenvalues_multiply()

```
type(mqc_scf_integral) function mqc_est::matmul::mqc_integral_eigenvalues_multiply (
             type(mqc_scf_integral), intent(in) integralA,
             type(mqc_scf_eigenvalues), intent(in) eigenvaluesB,
             character(len=*), intent(in), optional label )
```

6.19.1.4 mqc_integral_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::matmul::mqc_integral_integral_multiply (
             type(mqc_scf_integral), intent(in) integralA,
             type(mqc_scf_integral), intent(in) integralB,
             character(len=*), intent(in), optional label )
```

6.19.1.5 mqc_integral_matrix_multiply()

```
type(mqc_scf_integral) function mqc_est::matmul::mqc_integral_matrix_multiply (
             type(mqc_scf_integral), intent(in) integralA,
             type(mqc_matrix), intent(in) matrixB,
             character(len=*), intent(in), optional label )
```

6.19.1.6 mqc_matrix_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::matmul::mqc_matrix_integral_multiply (
             type(mqc_matrix), intent(in) matrixA,
             type(mqc_scf_integral), intent(in) integralB,
             character(len=*), intent(in), optional label )
```

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

- src/mqc_est.F03

6.20 mqc_algebra::matrix_symm2sq Interface Reference

Public Member Functions

- subroutine matrix_symm2sq_integer (N, I_Symm, I_Sq)
- subroutine matrix_symm2sq_real (N, A_Symm, A_Sq)
- subroutine matrix_symm2sq_complex (N, A_Symm, A_Sq)

6.20.1 Member Function/Subroutine Documentation

6.20.1.1 matrix_symm2sq_complex()

```
subroutine mqc_algebra::matrix_symm2sq::matrix_symm2sq_complex (
             integer(kind=int64), intent(in) N,
             complex(kind=real64), dimension(:), intent(in) A_Symm,
             complex(kind=real64), dimension(n,n), intent(out) A_Sq )
```

6.20.1.2 matrix_symm2sq_integer()

```
subroutine mqc_algebra::matrix_symm2sq::matrix_symm2sq_integer (
             integer(kind=int64), intent(in) N,
             integer(kind=int64), dimension(:), intent(in) I_Symm,
             integer(kind=int64), dimension(n,n), intent(out) I_Sq )
```

6.20.1.3 matrix_symm2sq_real()

```
subroutine mqc_algebra::matrix_symm2sq::matrix_symm2sq_real (
             integer(kind=int64), intent(in) N,
             real(kind=real64), dimension(:), intent(in) A_Symm,
             real(kind=real64), dimension(n,n), intent(out) A_Sq )
```

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

- src/mqc_algebra.F03

6.21 mqc_algebra::mqc_cast_complex Interface Reference

Public Member Functions

- type(mqc_vector) function mqc_vector_cast_complex (VA)
- type(mqc_matrix) function mqc_matrix_cast_complex (MA)

6.21.1 Member Function/Subroutine Documentation

6.21.1.1 mqc_matrix_cast_complex()

```
type(mqc_matrix) function mqc_algebra::mqc_cast_complex::mqc_matrix_cast_complex (
            type(mqc_matrix), intent(in) MA )
```

6.21.1.2 mqc_vector_cast_complex()

```
type(mqc_vector) function mqc_algebra::mqc_cast_complex::mqc_vector_cast_complex (
            type(mqc_vector), intent(in) VA )
```

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

- src/mqc_algebra.F03

6.22 mqc_algebra::mqc_cast_real Interface Reference

Public Member Functions

- type(mqc_vector) function mqc_vector_cast_real (VA)
- type(mqc_matrix) function mqc_matrix_cast_real (MA)

6.22.1 Member Function/Subroutine Documentation

6.22.1.1 mqc_matrix_cast_real()

```
type(mqc_matrix) function mqc_algebra::mqc_cast_real::mqc_matrix_cast_real (
            type(mqc_matrix), intent(in) MA )
```

6.22.1.2 mqc_vector_cast_real()

```
type(mqc_vector) function mqc_algebra::mqc_cast_real::mqc_vector_cast_real (
            type(mqc_vector), intent(in) VA )
```

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

- src/mqc_algebra.F03

6.23 mqc_est::mqc_determinant Type Reference

Public Attributes

- type(mqc_determinant_string) strings
- character(len=64) order
- integer(kind=int64) ndets
- integer(kind=int64) nalpstr
- integer(kind=int64) nbetstr

6.23.1 Member Data Documentation

6.23.1.1 nalpstr

```
integer(kind=int64) mqc_est::mqc_determinant::nalpstr
```

6.23.1.2 nbetstr

```
integer(kind=int64) mqc_est::mqc_determinant::nbetstr
```

6.23.1.3 ndets

```
integer(kind=int64) mqc_est::mqc_determinant::ndets
```

6.23.1.4 order

```
character(len=64) mqc_est::mqc_determinant::order
```

6.23.1.5 strings

```
type(mqc_determinant_string) mqc_est::mqc_determinant::strings
```

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

- src/mqc_est.F03

6.24 mqc_est::mqc_determinant_string Type Reference

Public Attributes

- type(mqc_matrix) alpha
- type(mqc_matrix) beta

6.24.1 Member Data Documentation

6.24.1.1 alpha

```
type(mqc_matrix) mqc_est::mqc_determinant_string::alpha
```

6.24.1.2 beta

```
type(mqc_matrix) mqc_est::mqc_determinant_string::beta
```

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

- src/mqc_est.F03

6.25 mqc_algebra::mqc_have_complex Interface Reference

Public Member Functions

- logical function mqc_vector_havecomplex (Vector)
- logical function mqc_matrix_havecomplex (Matrix)

6.25.1 Member Function/Subroutine Documentation

6.25.1.1 mqc_matrix_havecomplex()

```
logical function mqc_algebra::mqc_have_complex::mqc_matrix_havecomplex (
            type(mqc_matrix), intent(in) Matrix )
```

6.25.1.2 mqc_vector_havecomplex()

```
logical function mqc_algebra::mqc_have_complex::mqc_vector_havecomplex (
            type(mqc_vector), intent(in) Vector )
```

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

- src/mqc_algebra.F03

6.26 mqc_algebra::mqc_have_int Interface Reference

Public Member Functions

- logical function mqc_vector_haveinteger (Vector)
- logical function mqc_matrix_haveinteger (Matrix)

6.26.1 Member Function/Subroutine Documentation

6.26.1.1 mqc_matrix_haveinteger()

```
logical function mqc_algebra::mqc_have_int::mqc_matrix_haveinteger (
            type(mqc_matrix), intent(in) Matrix )
```

6.26.1.2 mqc_vector_haveinteger()

```
logical function mqc_algebra::mqc_have_int::mqc_vector_haveinteger (
            type(mqc_vector), intent(in) Vector )
```

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

- src/mqc_algebra.F03

6.27 mqc_algebra::mqc_have_real Interface Reference

Public Member Functions

- logical function mqc_vector_havereal (Vector)
- logical function mqc_matrix_havereal (Matrix)

6.27.1 Member Function/Subroutine Documentation

6.27.1.1 mqc_matrix_havereal()

```
logical function mqc_algebra::mqc_have_real::mqc_matrix_havereal (
            type(mqc_matrix), intent(in) Matrix )
```

6.27.1.2 mqc_vector_havereal()

```
logical function mqc_algebra::mqc_have_real::mqc_vector_havereal (
            type(mqc_vector), intent(in) Vector )
```

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

- src/mqc_algebra.F03

6.28 mqc_algebra::mqc_matrix Type Reference

Public Member Functions

- Procedure, public print => mqc_print_matrix_algebra1
- Procedure, public initialize => mqc_matrix_initialize
- Procedure, public init => mqc_matrix_initialize
- Procedure, public identity => mqc_matrix_identity
- Procedure, public set => mqc_matrix_set
- Procedure, public norm => mqc_matrix_norm
- Procedure, public transpose => mqc_matrix_transpose
- Procedure, public dagger => mqc_matrix_conjugate_transpose
- Procedure, public diag => mqc_matrix_diagonalize
- Procedure, public svd => mqc_matrix_svd
- Procedure, public eigensys => mqc_matrix_generalized_eigensystem
- Procedure, public inv => mqc_matrix_inverse
- Procedure, public det => mqc_matrix_determinant
- Procedure, public trace => mqc_matrix_trace
- Procedure, public rmsmax => mqc_matrix_rms_max
- Procedure, public sqrt => mqc_matrix_sqrt
- Procedure, public at => mqc_matrix_scalar_at
- Procedure, public vat => mqc_matrix_vector_at
- Procedure, public mat => mqc_matrix_matrix_at
- Procedure, public put => mqc_matrix_scalar_put
- Procedure, public vput => mqc_matrix_vector_put
- Procedure, public mput => mqc_matrix_matrix_put
- Procedure, public s_type => mqc_matrix_storagetype

Public Attributes

- real(kind=real64), dimension(:,:), allocatable matr
- integer(kind=int64), dimension(:,:), allocatable mati
- complex(kind=real64), dimension(:,:), allocatable matc

6.28.1 Member Function/Subroutine Documentation

6.28.1.1 at()

```
Procedure, public mqc_algebra::mqc_matrix::at ( )
```

6.28.1.2 dagger()

```
Procedure, public mqc_algebra::mqc_matrix::dagger ( )
```

6.28.1.3 det()

```
Procedure, public mqc_algebra::mqc_matrix::det ( )
```

6.28.1.4 diag()

```
Procedure, public mqc_algebra::mqc_matrix::diag ( )
```

6.28.1.5 eigensys()

```
Procedure, public mqc_algebra::mqc_matrix::eigensys ( )
```

6.28.1.6 identity()

```
Procedure, public mqc_algebra::mqc_matrix::identity ( )
```

6.28.1.7 init()

```
Procedure, public mqc_algebra::mqc_matrix::init ( )
```

6.28.1.8 initialize()

```
Procedure, public mqc_algebra::mqc_matrix::initialize ( )
```

6.28.1.9 inv()

```
Procedure, public mqc_algebra::mqc_matrix::inv ( )
```

6.28.1.10 mat()

```
Procedure, public mqc_algebra::mqc_matrix::mat ( )
```

6.28.1.11 mput()

```
Procedure, public mqc_algebra::mqc_matrix::mput ( )
```

6.28.1.12 norm()

```
Procedure, public mqc_algebra::mqc_matrix::norm ( )
```

6.28.1.13 print()

```
Procedure, public mqc_algebra::mqc_matrix::print ( )
```

6.28.1.14 put()

```
Procedure, public mqc_algebra::mqc_matrix::put ( )
```

6.28.1.15 rmsmax()

```
Procedure, public mqc_algebra::mqc_matrix::rmsmax ( )
```

6.28.1.16 s_type()

```
Procedure, public mqc_algebra::mqc_matrix::s_type ( )
```

6.28.1.17 set()

```
Procedure, public mqc_algebra::mqc_matrix::set ( )
```

6.28.1.18 sqrt()

```
Procedure, public mqc_algebra::mqc_matrix::sqrt ( )
```

6.28.1.19 svd()

```
Procedure, public mqc_algebra::mqc_matrix::svd ( )
```

6.28.1.20 trace()

```
Procedure, public mqc_algebra::mqc_matrix::trace ( )
```

6.28.1.21 transpose()

```
Procedure, public mqc_algebra::mqc_matrix::transpose ( )
```

6.28.1.22 vat()

```
Procedure, public mqc_algebra::mqc_matrix::vat ( )
```

6.28.1.23 vput()

```
Procedure, public mqc_algebra::mqc_matrix::vput ( )
```

6.28.2 Member Data Documentation

6.28.2.1 matc

```
complex(kind=real64), dimension(:,:), allocatable mqc_algebra::mqc_matrix::matc
```

6.28.2.2 mati

```
integer(kind=int64), dimension(:,:), allocatable mqc_algebra::mqc_matrix::mati
```

6.28.2.3 matr

```
real(kind=real64), dimension(:,:), allocatable mqc_algebra::mqc_matrix::matr
```

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

- src/mqc_algebra.F03

6.29 mqc_algebra::mqc_matrix_diagmatrix_put Interface Reference

Public Member Functions

- subroutine mqc_matrix_diagmatrix_put_integer (mat, diagMatrixIn)
- subroutine mqc_matrix_diagmatrix_put_real (mat, diagMatrixIn)
- subroutine mqc_matrix_diagmatrix_put_complex (mat, diagMatrixIn)
- subroutine mqc_matrix_diagmatrix_put_vector (diagVectorIn, mat)

6.29.1 Member Function/Subroutine Documentation

6.29.1.1 mqc_matrix_diagmatrix_put_complex()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put::mqc_matrix_diagmatrix_put_complex (
             class(mqc_matrix), intent(inout) mat,
             complex(kind=real64), dimension(:), intent(in) diagMatrixIn )
```

6.29.1.2 mqc_matrix_diagmatrix_put_integer()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put::mqc_matrix_diagmatrix_put_integer (
             class(mqc_matrix), intent(inout) mat,
             integer(kind=int64), dimension(:), intent(in) diagMatrixIn )
```

6.29.1.3 mqc_matrix_diagmatrix_put_real()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put::mqc_matrix_diagmatrix_put_real (
             class(mqc_matrix), intent(inout) mat,
             real(kind=real64), dimension(:), intent(in) diagMatrixIn )
```

6.29.1.4 mqc_matrix_diagmatrix_put_vector()

```
subroutine mqc_algebra::mqc_matrix_diagmatrix_put::mqc_matrix_diagmatrix_put_vector (
             class(mqc_vector), intent(in) diagVectorIn,
             class(mqc_matrix), intent(inout) mat )
```

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

- src/mqc_algebra.F03

6.30 mqc_algebra::mqc_matrix_symmmatrix_put Interface Reference

Public Member Functions

- subroutine mqc_matrix_symmmatrix_put_integer (mat, symmMatrixIn)
- subroutine mqc_matrix_symmmatrix_put_real (mat, symmMatrixIn)
- subroutine mqc_matrix_symmmatrix_put_complex (mat, symmMatrixIn)

6.30.1 Member Function/Subroutine Documentation

6.30.1.1 mqc_matrix_symmmatrix_put_complex()

```
subroutine mqc_algebra::mqc_matrix_symmmatrix_put::mqc_matrix_symmmatrix_put_complex (
             class(mqc_matrix), intent(inout) mat,
             complex(kind=real64), dimension(:), intent(in) symmMatrixIn )
```

6.30.1.2 mqc_matrix_symmmatrix_put_integer()

```
subroutine mqc_algebra::mqc_matrix_symmmatrix_put::mqc_matrix_symmmatrix_put_integer (
             class(mqc_matrix), intent(inout) mat,
             integer(kind=int64), dimension(:), intent(in) symmMatrixIn )
```

6.30.1.3 mqc_matrix_symmmatrix_put_real()

```
subroutine mqc_algebra::mqc_matrix_symmmatrix_put::mqc_matrix_symmmatrix_put_real (
             class(mqc_matrix), intent(inout) mat,
             real(kind=real64), dimension(:), intent(in) symmMatrixIn )
```

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

- src/mqc_algebra.F03

6.31 mqc_est::mqc_matrix_undospinblockghf Interface Reference

Public Member Functions

- subroutine mqc_matrix_undospinblockghf_eigenvalues (eigenvaluesIn, vectorOut)
- subroutine mqc_matrix_undospinblockghf_integral (integralIn, matrixOut)

6.31.1 Member Function/Subroutine Documentation

6.31.1.1 mqc_matrix_undospinblockghf_eigenvalues()

```
subroutine mqc_est::mqc_matrix_undospinblockghf::mqc_matrix_undospinblockghf_eigenvalues (
            type(mqc_scf_eigenvalues), intent(in) eigenvaluesIn,
            type(mqc_vector), intent(out) vectorOut )
```

6.31.1.2 mqc_matrix_undospinblockghf_integral()

```
subroutine mqc_est::mqc_matrix_undospinblockghf::mqc_matrix_undospinblockghf_integral (
            type(mqc_scf_integral), intent(in) integralIn,
            type(mqc_matrix), intent(out) matrixOut )
```

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

- src/mqc_est.F03

6.32 mqc_algebra::mqc_print Interface Reference

Public Member Functions

- subroutine mqc_print_scalar_algebra1 (Scalar, IOut, Header, Blank_At_Top, Blank_At_Bottom)
- subroutine mqc_print_vector_algebra1 (Vector, IOut, Header, Verbose, Blank_At_Top, Blank_At_Bottom)
- subroutine mqc_print_matrix_algebra1 (Matrix, IOut, Header, Blank_At_Top, Blank_At_Bottom)
- subroutine mqc_print_r4tensor_algebra1 (Tensor, IOut, Header, blank_at_top, blank_at_bottom)

6.32.1 Member Function/Subroutine Documentation

6.32.1.1 mqc_print_matrix_algebra1()

```
subroutine mqc_algebra::mqc_print::mqc_print_matrix_algebra1 (
             class(mqc_matrix), intent(in) Matrix,
             integer(kind=int64), intent(in) IOut,
             character(len=*), intent(in) Header,
             logical, intent(in), optional Blank_At_Top,
             logical, intent(in), optional Blank_At_Bottom )
```

6.32.1.2 mqc_print_r4tensor_algebra1()

```
subroutine mqc_algebra::mqc_print::mqc_print_r4tensor_algebra1 (
             class(mqc_r4tensor), intent(in) Tensor,
             integer(kind=int64), intent(in) IOut,
             character(len=*), intent(in), optional Header,
             logical, optional blank_at_top,
             logical, optional blank_at_bottom )
```

6.32.1.3 mqc_print_scalar_algebra1()

```
subroutine mqc_algebra::mqc_print::mqc_print_scalar_algebra1 (
             class(mqc_scalar), intent(in) Scalar,
             integer(kind=int64), intent(in) IOut,
             character(len=*), intent(in) Header,
             logical, intent(in), optional Blank_At_Top,
             logical, intent(in), optional Blank_At_Bottom )
```

6.32.1.4 mqc_print_vector_algebra1()

```
subroutine mqc_algebra::mqc_print::mqc_print_vector_algebra1 (
             class(mqc_vector), intent(in) Vector,
             integer(kind=int64), intent(in) IOut,
             character(len=*), intent(in) Header,
             logical, intent(in), optional Verbose,
             logical, intent(in), optional Blank_At_Top,
             logical, intent(in), optional Blank_At_Bottom )
```

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

- src/mqc_algebra.F03

6.33 mqc_est::mqc_print Interface Reference

Public Member Functions

- subroutine mqc_print_wavefunction (wavefunction, iOut, label)
- subroutine mqc_print_integral (integral, iOut, header, blank_at_top, blank_at_bottom)
- subroutine mqc_print_eigenvalues (eigenvalues, iOut, header, blank_at_top, blank_at_bottom)
- subroutine mqc_print_twoeris (twoERIs, iOut, header, blank_at_top, blank_at_bottom)

6.33.1 Member Function/Subroutine Documentation

6.33.1.1 mqc_print_eigenvalues()

```
subroutine mqc_est::mqc_print::mqc_print_eigenvalues (
             class(mqc_scf_eigenvalues) eigenvalues,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in) header,
             logical, intent(in), optional blank_at_top,
             logical, intent(in), optional blank_at_bottom )
```

6.33.1.2 mqc_print_integral()

```
subroutine mqc_est::mqc_print::mqc_print_integral (
             class(mqc_scf_integral) integral,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in) header,
             logical, intent(in), optional blank_at_top,
             logical, intent(in), optional blank_at_bottom )
```

6.33.1.3 mqc_print_twoeris()

```
subroutine mqc_est::mqc_print::mqc_print_twoeris (
             class(mqc_twoeris) twoERIs,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in) header,
             logical, intent(in), optional blank_at_top,
             logical, intent(in), optional blank_at_bottom )
```

6.33.1.4 mqc_print_wavefunction()

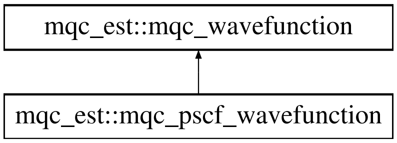
```
subroutine mqc_est::mqc_print::mqc_print_wavefunction (
            class(mqc_wavefunction) wavefunction,
            integer(kind=int64), intent(in) iOut,
            character(len=*), intent(in), optional label )
```

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

- src/mqc_est.F03

6.34 mqc_est::mqc_pscf_wavefunction Type Reference

Inheritance diagram for mqc_est::mqc_pscf_wavefunction:



Public Attributes

- integer(kind=int64) ncore
- integer(kind=int64) nval
- integer(kind=int64) nactive
- integer(kind=int64) nfrz
- type(mqc_matrix) pscf_amplitudes
- type(mqc_vector) pscf_energies

Additional Inherited Members

6.34.1 Member Data Documentation

6.34.1.1 nactive

```
integer(kind=int64) mqc_est::mqc_pscf_wavefunction::nactive
```

6.34.1.2 ncore

```
integer(kind=int64) mqc_est::mqc_pscf_wavefunction::ncore
```

6.34.1.3 nfrz

```
integer(kind=int64) mqc_est::mqc_pscf_wavefunction::nfrz
```

6.34.1.4 nval

```
integer(kind=int64) mqc_est::mqc_pscf_wavefunction::nval
```

6.34.1.5 pscf_amplitudes

```
type(mqc_matrix) mqc_est::mqc_pscf_wavefunction::pscf_amplitudes
```

6.34.1.6 pscf_energies

```
type(mqc_vector) mqc_est::mqc_pscf_wavefunction::pscf_energies
```

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

- src/mqc_est.F03

6.35 mqc_algebra::mqc_r4tensor Type Reference

Public Member Functions

- Procedure, public print => mqc_print_r4tensor_algebra1
- Procedure, public at => mqc_r4tensor_at
- Procedure, public put => mqc_r4tensor_put
- Procedure, public initialize => mqc_r4tensor_initialize
- Procedure, public init => mqc_r4tensor_initialize

6.35.1 Member Function/Subroutine Documentation

6.35.1.1 at()

```
Procedure, public mqc_algebra::mqc_r4tensor::at ( )
```

6.35.1.2 init()

```
Procedure, public mqc_algebra::mqc_r4tensor::init ( )
```

6.35.1.3 initialize()

```
Procedure, public mqc_algebra::mqc_r4tensor::initialize ( )
```

6.35.1.4 print()

```
Procedure, public mqc_algebra::mqc_r4tensor::print ( )
```

6.35.1.5 put()

```
Procedure, public mqc_algebra::mqc_r4tensor::put ( )
```

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

- src/mqc_algebra.F03

6.36 mqc_algebra::mqc_scalar Type Reference

Public Member Functions

- Procedure, public print => mqc_print_scalar_algebra1
- Procedure, public rval => mqc_scalar_get_intrinsic_real
- Procedure, public ival => mqc_scalar_get_intrinsic_integer
- Procedure, public cval => mqc_scalar_get_intrinsic_complex
- Procedure, public abs => mqc_scalar_get_abs_value
- Procedure, public random => mqc_scalar_get_random_value

6.36.1 Member Function/Subroutine Documentation

6.36.1.1 abs()

```
Procedure, public mqc_algebra::mqc_scalar::abs ( )
```

6.36.1.2 cval()

```
Procedure, public mqc_algebra::mqc_scalar::cval ( )
```

6.36.1.3 ival()

```
Procedure, public mqc_algebra::mqc_scalar::ival ( )
```

6.36.1.4 print()

```
Procedure, public mqc_algebra::mqc_scalar::print ( )
```

6.36.1.5 random()

```
Procedure, public mqc_algebra::mqc_scalar::random ( )
```

6.36.1.6 rval()

```
Procedure, public mqc_algebra::mqc_scalar::rval ( )
```

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

- src/mqc_algebra.F03

6.37 mqc_est::mqc_scf_eigenvalues Type Reference

Public Member Functions

- Procedure, public print => mqc_print_eigenvalues
- Procedure, public getlabel => mqc_eigenvalues_array_name
- Procedure, public addlabel => mqc_eigenvalues_add_name
- Procedure, public getblock => mqc_eigenvalues_output_block
- Procedure, public power => mqc_scf_eigenvalues_power
- Procedure, public at => mqc_eigenvalues_at

6.37.1 Member Function/Subroutine Documentation

6.37.1.1 addlabel()

```
Procedure, public mqc_est::mqc_scf_eigenvalues::addlabel ( )
```

6.37.1.2 at()

```
Procedure, public mqc_est::mqc_scf_eigenvalues::at ( )
```

6.37.1.3 getblock()

```
Procedure, public mqc_est::mqc_scf_eigenvalues::getblock ( )
```

6.37.1.4 getlabel()

```
Procedure, public mqc_est::mqc_scf_eigenvalues::getlabel ( )
```

6.37.1.5 power()

```
Procedure, public mqc_est::mqc_scf_eigenvalues::power ( )
```

6.37.1.6 print()

```
Procedure, public mqc_est::mqc_scf_eigenvalues::print ( )
```

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

- src/mqc_est.F03

6.38 mqc_est::mqc_scf_integral Type Reference

Public Member Functions

- Procedure, public print => mqc_print_integral
- Procedure, public getlabel => mqc_integral_array_name
- Procedure, public addlabel => mqc_integral_add_name
- Procedure, public getblock => mqc_integral_output_block
- Procedure, public identity => mqc_integral_identity
- Procedure, public init => mqc_integral_initialize
- Procedure, public diag => mqc_scf_integral_diagonalize
- Procedure, public eigensys => mqc_scf_integral_generalized_eigensystem
- Procedure, public inv => mqc_scf_integral_inverse
- Procedure, public trace => mqc_scf_integral_trace
- Procedure, public det => mqc_scf_integral_determinant
- Procedure, public norm => mqc_integral_norm
- Procedure, public setelist => mqc_integral_set_energy_list
- Procedure, public getelist => mqc_integral_get_energy_list
- Procedure, public deleteelist => mqc_integral_delete_energy_list
- Procedure, public orbitals => mqc_integral_output_orbitals
- Procedure, public swap => mqc_integral_swap_orbitals

6.38.1 Member Function/Subroutine Documentation

6.38.1.1 addlabel()

```
Procedure, public mqc_est::mqc_scf_integral::addlabel ( )
```

6.38.1.2 deleteelist()

```
Procedure, public mqc_est::mqc_scf_integral::deleteelist ( )
```

6.38.1.3 det()

```
Procedure, public mqc_est::mqc_scf_integral::det ( )
```

6.38.1.4 diag()

```
Procedure, public mqc_est::mqc_scf_integral::diag ( )
```

6.38.1.5 eigensys()

```
Procedure, public mqc_est::mqc_scf_integral::eigensys ( )
```

6.38.1.6 getblock()

```
Procedure, public mqc_est::mqc_scf_integral::getblock ( )
```

6.38.1.7 getelist()

```
Procedure, public mqc_est::mqc_scf_integral::getelist ( )
```

6.38.1.8 getlabel()

```
Procedure, public mqc_est::mqc_scf_integral::getlabel ( )
```

6.38.1.9 identity()

```
Procedure, public mqc_est::mqc_scf_integral::identity ( )
```

6.38.1.10 init()

```
Procedure, public mqc_est::mqc_scf_integral::init ( )
```

6.38.1.11 inv()

```
Procedure, public mqc_est::mqc_scf_integral::inv ( )
```

6.38.1.12 norm()

```
Procedure, public mqc_est::mqc_scf_integral::norm ( )
```

6.38.1.13 orbitals()

```
Procedure, public mqc_est::mqc_scf_integral::orbitals ( )
```

6.38.1.14 print()

```
Procedure, public mqc_est::mqc_scf_integral::print ( )
```

6.38.1.15 setelist()

```
Procedure, public mqc_est::mqc_scf_integral::setelist ( )
```

6.38.1.16 swap()

```
Procedure, public mqc_est::mqc_scf_integral::swap ( )
```

6.38.1.17 trace()

```
Procedure, public mqc_est::mqc_scf_integral::trace ( )
```

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

- src/mqc_est.F03

6.39 mqc_algebra::mqc_set_array2vector Interface Reference

Public Member Functions

- subroutine mqc_set_array2vector_integer (VectorOut, ArrayIn)
- subroutine mqc_set_array2vector_real (VectorOut, ArrayIn)
- subroutine mqc_set_array2vector_complex (VectorOut, ArrayIn)

6.39.1 Member Function/Subroutine Documentation

6.39.1.1 mqc_set_array2vector_complex()

```
subroutine mqc_algebra::mqc_set_array2vector::mqc_set_array2vector_complex (
             type(mqc_vector), intent(inout) VectorOut,
             complex(kind=real64), dimension(:), intent(in) ArrayIn )
```

6.39.1.2 mqc_set_array2vector_integer()

```
subroutine mqc_algebra::mqc_set_array2vector::mqc_set_array2vector_integer (
             type(mqc_vector), intent(inout) VectorOut,
             integer(kind=int64), dimension(:), intent(in) ArrayIn )
```

6.39.1.3 mqc_set_array2vector_real()

```
subroutine mqc_algebra::mqc_set_array2vector::mqc_set_array2vector_real (
             type(mqc_vector), intent(inout) VectorOut,
             real(kind=real64), dimension(:), intent(in) ArrayIn )
```

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

- src/mqc_algebra.F03

6.40 mqc_est::mqc_twoeris Type Reference

Public Member Functions

- procedure, public print => mqc_print_twoeris

6.40.1 Member Function/Subroutine Documentation

6.40.1.1 print()

```
procedure, public mqc_est::mqc_twoeris::print ( )
```

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

- src/mqc_est.F03

6.41 mqc_algebra::mqc_vector Type Reference

Public Member Functions

- Procedure, public print => mqc_print_vector_algebra1
- Procedure, public initialize => mqc_vector_initialize
- Procedure, public size => mqc_length_vector
- Procedure, public init => mqc_vector_initialize
- Procedure, public norm => mqc_vector_norm
- Procedure, public transpose => mqc_vector_transpose
- Procedure, public dagger => mqc_vector_conjugate_transpose
- Procedure, public at => mqc_vector_scalar_at
- Procedure, public vat => mqc_vector_vector_at
- Procedure, public put => mqc_vector_scalar_put
- Procedure, public vput => mqc_vector_vector_put
- Procedure, public push => mqc_vector_push
- Procedure, public unshift => mqc_vector_unshift
- Procedure, public pop => mqc_vector_pop
- Procedure, public shift => mqc_vector_shift
- Procedure, public maxval => mqc_vector_maxval
- Procedure, public minval => mqc_vector_minloc
- Procedure, public maxloc => mqc_vector_maxval
- Procedure, public minloc => mqc_vector_minloc
- Procedure, public argsort => mqc_vector_argsort
- Procedure, public sort => mqc_vector_sort
- Procedure, public sqrt => mqc_vector_sqrt
- Procedure, public abs => mqc_vector_abs
- Procedure, public power => mqc_vector_power
- Procedure, public diag => mqc_matrix_diagmatrix_put_vector

Public Attributes

- integer(kind=int64) length =0
- character(len=64) data_type
- real(kind=real64), dimension(:), allocatable vecr
- integer(kind=int64), dimension(:), allocatable veci
- complex(kind=real64), dimension(:), allocatable vecc

6.41.1 Member Function/Subroutine Documentation

6.41.1.1 abs()

```
Procedure, public mqc_algebra::mqc_vector::abs ( )
```

6.41.1.2 argsort()

```
Procedure, public mqc_algebra::mqc_vector::argsort ( )
```

6.41.1.3 at()

```
Procedure, public mqc_algebra::mqc_vector::at ( )
```

6.41.1.4 dagger()

```
Procedure, public mqc_algebra::mqc_vector::dagger ( )
```

6.41.1.5 diag()

```
Procedure, public mqc_algebra::mqc_vector::diag ( )
```

6.41.1.6 init()

```
Procedure, public mqc_algebra::mqc_vector::init ( )
```

6.41.1.7 initialize()

```
Procedure, public mqc_algebra::mqc_vector::initialize ( )
```

6.41.1.8 maxloc()

```
Procedure, public mqc_algebra::mqc_vector::maxloc ( )
```

6.41.1.9 maxval()

```
Procedure, public mqc_algebra::mqc_vector::maxval ( )
```

6.41.1.10 minloc()

```
Procedure, public mqc_algebra::mqc_vector::minloc ( )
```

6.41.1.11 minval()

```
Procedure, public mqc_algebra::mqc_vector::minval ( )
```

6.41.1.12 norm()

```
Procedure, public mqc_algebra::mqc_vector::norm ( )
```

6.41.1.13 pop()

```
Procedure, public mqc_algebra::mqc_vector::pop ( )
```

6.41.1.14 power()

```
Procedure, public mqc_algebra::mqc_vector::power ( )
```

6.41.1.15 print()

```
Procedure, public mqc_algebra::mqc_vector::print ( )
```

6.41.1.16 push()

```
Procedure, public mqc_algebra::mqc_vector::push ( )
```

6.41.1.17 put()

```
Procedure, public mqc_algebra::mqc_vector::put ( )
```

6.41.1.18 shift()

```
Procedure, public mqc_algebra::mqc_vector::shift ( )
```

6.41.1.19 size()

```
Procedure, public mqc_algebra::mqc_vector::size ( )
```

6.41.1.20 sort()

```
Procedure, public mqc_algebra::mqc_vector::sort ( )
```

6.41.1.21 sqrt()

```
Procedure, public mqc_algebra::mqc_vector::sqrt ( )
```

6.41.1.22 transpose()

```
Procedure, public mqc_algebra::mqc_vector::transpose ( )
```

6.41.1.23 unshift()

```
Procedure, public mqc_algebra::mqc_vector::unshift ( )
```

6.41.1.24 vat()

```
Procedure, public mqc_algebra::mqc_vector::vat ( )
```

6.41.1.25 vput()

```
Procedure, public mqc_algebra::mqc_vector::vput ( )
```

6.41.2 Member Data Documentation

6.41.2.1 data_type

```
character(len=64) mqc_algebra::mqc_vector::data_type
```

6.41.2.2 length

```
integer(kind=int64) mqc_algebra::mqc_vector::length =0
```

6.41.2.3 vecc

```
complex(kind=real64), dimension(:), allocatable mqc_algebra::mqc_vector::vecc
```

6.41.2.4 veci

```
integer(kind=int64), dimension(:), allocatable mqc_algebra::mqc_vector::veci
```

6.41.2.5 vecr

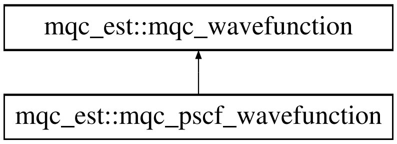
```
real(kind=real64), dimension(:), allocatable mqc_algebra::mqc_vector::vecr
```

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

- src/mqc_algebra.F03

6.42 mqc_est::mqc_wavefunction Type Reference

Inheritance diagram for mqc_est::mqc_wavefunction:



Public Member Functions

- Procedure, public print => mqc_print_wavefunction

Public Attributes

- type(mqc_scf_integral) mo_coefficients
- type(mqc_scf_eigenvalues) mo_energies
- type(mqc_scf_eigenvalues) mo_symmetries
- type(mqc_scf_integral) core_hamiltonian
- type(mqc_scf_integral) fock_matrix
- type(mqc_scf_integral) density_matrix
- type(mqc_scf_integral) scf_density_matrix
- type(mqc_scf_integral) overlap_matrix
- type(mqc_scalar) nalpha
- type(mqc_scalar) nbeta
- type(mqc_scalar) nelectrons
- type(mqc_scalar) nbasis
- type(mqc_scalar) charge
- type(mqc_scalar) multiplicity
- character(len=256) basis
- character(len=256) symmetry
- character(len=256) wf_type
- logical wf_complex

6.42.1 Member Function/Subroutine Documentation

6.42.1.1 print()

```
Procedure, public mqc_est::mqc_wavefunction::print ( )
```

6.42.2 Member Data Documentation

6.42.2.1 basis

```
character(len=256) mqc_est::mqc_wavefunction::basis
```

6.42.2.2 charge

```
type(mqc_scalar) mqc_est::mqc_wavefunction::charge
```

6.42.2.3 core_hamiltonian

```
type(mqc_scf_integral) mqc_est::mqc_wavefunction::core_hamiltonian
```

6.42.2.4 density_matrix

```
type(mqc_scf_integral) mqc_est::mqc_wavefunction::density_matrix
```

6.42.2.5 fock_matrix

```
type(mqc_scf_integral) mqc_est::mqc_wavefunction::fock_matrix
```

6.42.2.6 mo_coefficients

```
type(mqc_scf_integral) mqc_est::mqc_wavefunction::mo_coefficients
```

6.42.2.7 mo_energies

```
type(mqc_scf_eigenvalues) mqc_est::mqc_wavefunction::mo_energies
```

6.42.2.8 mo_symmetries

```
type(mqc_scf_eigenvalues) mqc_est::mqc_wavefunction::mo_symmetries
```

6.42.2.9 multiplicity

```
type(mqc_scalar) mqc_est::mqc_wavefunction::multiplicity
```

6.42.2.10 nalpha

```
type(mqc_scalar) mqc_est::mqc_wavefunction::nalpha
```

6.42.2.11 nbasis

```
type(mqc_scalar) mqc_est::mqc_wavefunction::nbasis
```

6.42.2.12 nbeta

```
type(mqc_scalar) mqc_est::mqc_wavefunction::nbeta
```

6.42.2.13 nelectrons

```
type(mqc_scalar) mqc_est::mqc_wavefunction::nelectrons
```

6.42.2.14 overlap_matrix

```
type(mqc_scf_integral) mqc_est::mqc_wavefunction::overlap_matrix
```

6.42.2.15 scf_density_matrix

```
type(mqc_scf_integral) mqc_est::mqc_wavefunction::scf_density_matrix
```

6.42.2.16 symmetry

```
character(len=256) mqc_est::mqc_wavefunction::symmetry
```

6.42.2.17 wf_complex

```
logical mqc_est::mqc_wavefunction::wf_complex
```

6.42.2.18 wf_type

```
character(len=256) mqc_est::mqc_wavefunction::wf_type
```

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

- src/mqc_est.F03

6.43 mqc_algebra::operator(*) Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalarmultiply (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_integerscalarmultiply (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegermultiply (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalarmultiply (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealmultiply (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalarmultiply (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexmultiply (Scalar, ComplexIn)
- type(mqc_vector) function mqc_scalarvectorproduct (Scalar, Vector)
- type(mqc_vector) function mqc_vectorscalarproduct (vector, scalar)
- type(mqc_matrix) function mqc_scalarmatrixproduct (Scalar, Matrix)
- type(mqc_matrix) function mqc_matrixscalarproduct (Matrix, Scalar)
- type(mqc_vector) function mqc_realvectorproduct (RealIn, Vector)
- type(mqc_vector) function mqc_vectorrealproduct (vector, realIn)
- type(mqc_vector) function mqc_integervectorproduct (intIn, Vector)
- type(mqc_vector) function mqc_vectorintegerproduct (vector, intIn)
- type(mqc_vector) function mqc_complexvectorproduct (CompIn, Vector)
- type(mqc_vector) function mqc_vectorcomplexproduct (vector, compIn)
- type(mqc_matrix) function mqc_matrixmatrixproduct (MA, MB)

6.43.1 Member Function/Subroutine Documentation

6.43.1.1 mqc_complexscalarmultiply()

```
type(mqc_scalar) function mqc_algebra::operator(*)::mqc_complexscalarmultiply (
            complex(kind=real64), intent(in) ComplexIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.43.1.2 mqc_complexvectorproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_complexvectorproduct (
            complex(kind=real64), intent(in) CompIn,
            type(mqc_vector), intent(in) Vector )
```

6.43.1.3 mqc_integerscalarmultiply()

```
type(mqc_scalar) function mqc_algebra::operator(*)::mqc_integerscalarmultiply (
            integer(kind=int64), intent(in) IntegerIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.43.1.4 mqc_integervectorproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_integervectorproduct (
            integer(kind=int64), intent(in) intIn,
            type(mqc_vector), intent(in) Vector )
```

6.43.1.5 mqc_matrixmatrixproduct()

```
type(mqc_matrix) function mqc_algebra::operator(*)::mqc_matrixmatrixproduct (
            type(mqc_matrix), intent(in) MA,
            type(mqc_matrix), intent(in) MB )
```

6.43.1.6 mqc_matrixscalarproduct()

```
type(mqc_matrix) function mqc_algebra::operator(*)::mqc_matrixscalarproduct (
            type(mqc_matrix), intent(in) Matrix,
            type(mqc_scalar), intent(in) Scalar )
```

6.43.1.7 mqc_realscalarmultiply()

```
type(mqc_scalar) function mqc_algebra::operator(*)::mqc_realscalarmultiply (
            real(kind=real64), intent(in) RealIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.43.1.8 mqc_realvectorproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_realvectorproduct (
            real(kind=real64), intent(in) RealIn,
            type(mqc_vector), intent(in) Vector )
```

6.43.1.9 mqc_scalarcomplexmultiply()

```
type(mqc_scalar) function mqc_algebra::operator(*)::mqc_scalarcomplexmultiply (
            type(mqc_scalar), intent(in) Scalar,
            complex(kind=real64), intent(in) ComplexIn )
```

6.43.1.10 mqc_scalarintegermultiply()

```
type(mqc_scalar) function mqc_algebra::operator(*)::mqc_scalarintegermultiply (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntegerIn )
```

6.43.1.11 mqc_scalarmatrixproduct()

```
type(mqc_matrix) function mqc_algebra::operator(*)::mqc_scalarmatrixproduct (
            type(mqc_scalar), intent(in) Scalar,
            type(mqc_matrix), intent(in) Matrix )
```

6.43.1.12 mqc_scalarmultiply()

```
type(mqc_scalar) function mqc_algebra::operator(*)::mqc_scalarmultiply (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

6.43.1.13 mqc_scalarrealmultiply()

```
type(mqc_scalar) function mqc_algebra::operator(*)::mqc_scalarrealmultiply (
             type(mqc_scalar), intent(in) Scalar,
             real(kind=real64), intent(in) RealIn )
```

6.43.1.14 mqc_scalarvectorproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_scalarvectorproduct (
             type(mqc_scalar), intent(in) Scalar,
             type(mqc_vector), intent(in) Vector )
```

6.43.1.15 mqc_vectorcomplexproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_vectorcomplexproduct (
             type(mqc_vector), intent(in) vector,
             complex(kind=real64), intent(in) compIn )
```

6.43.1.16 mqc_vectorintegerproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_vectorintegerproduct (
             type(mqc_vector), intent(in) vector,
             integer(kind=int64), intent(in) intIn )
```

6.43.1.17 mqc_vectorrealproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_vectorrealproduct (
             type(mqc_vector), intent(in) vector,
             real(kind=real64), intent(in) realIn )
```

6.43.1.18 mqc_vectorscalarproduct()

```
type(mqc_vector) function mqc_algebra::operator(*)::mqc_vectorscalarproduct (
             type(mqc_vector), intent(in) vector,
             type(mqc_scalar), intent(in) scalar )
```

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

- src/mqc_algebra.F03

6.44 mqc_est::operator(∗) Interface Reference

Public Member Functions

- type(mqc_scf_integral) function mqc_scalar_integral_multiply (scalar, integral)
- type(mqc_scf_integral) function mqc_integral_scalar_multiply (integral, scalar)

6.44.1 Member Function/Subroutine Documentation

6.44.1.1 mqc_integral_scalar_multiply()

```
type(mqc_scf_integral) function mqc_est::operator(*)::mqc_integral_scalar_multiply (
            type(mqc_scf_integral), intent(in) integral,
            type(mqc_scalar), intent(in) scalar )
```

6.44.1.2 mqc_scalar_integral_multiply()

```
type(mqc_scf_integral) function mqc_est::operator(*)::mqc_scalar_integral_multiply (
            type(mqc_scalar), intent(in) scalar,
            type(mqc_scf_integral), intent(in) integral )
```

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

- src/mqc_est.F03

6.45 mqc_algebra::operator(∗∗) Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalarexponent (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_scalarintegerexponent (Scalar, IntIn)
- type(mqc_scalar) function mqc_scalarrealexponent (Scalar, RealIn)
- type(mqc_scalar) function mqc_scalarcomplexexponent (Scalar, CompIn)

6.45.1 Member Function/Subroutine Documentation

6.45.1.1 mqc_scalarcomplexexponent()

```
type(mqc_scalar) function mqc_algebra::operator(**)::mqc_scalarcomplexexponent (
             type(mqc_scalar), intent(in) Scalar,
             complex(kind=real64), intent(in) CompIn )
```

6.45.1.2 mqc_scalarexponent()

```
type(mqc_scalar) function mqc_algebra::operator(**)::mqc_scalarexponent (
             type(mqc_scalar), intent(in) Scalar1,
             type(mqc_scalar), intent(in) Scalar2 )
```

6.45.1.3 mqc_scalarintegerexponent()

```
type(mqc_scalar) function mqc_algebra::operator(**)::mqc_scalarintegerexponent (
             type(mqc_scalar), intent(in) Scalar,
             integer(kind=int64), intent(in) IntIn )
```

6.45.1.4 mqc_scalarrealexponent()

```
type(mqc_scalar) function mqc_algebra::operator(**)::mqc_scalarrealexponent (
             type(mqc_scalar), intent(in) Scalar,
             real(kind=real64), intent(in) RealIn )
```

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

- src/mqc_algebra.F03

6.46 mqc_est::operator(+) Interface Reference

Public Member Functions

- type(mqc_scf_integral) function mqc_integral_sum (integralA, integralB)

6.46.1 Member Function/Subroutine Documentation

6.46.1.1 mqc_integral_sum()

```
type(mqc_scf_integral) function mqc_est::operator(+)::mqc_integral_sum (
            type(mqc_scf_integral), intent(in) integralA,
            type(mqc_scf_integral), intent(in) integralB )
```

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

- src/mqc_est.F03

6.47 mqc_algebra::operator(+) Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalaradd (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_integerscalaradd (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegeradd (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalaradd (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealadd (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalaradd (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexadd (Scalar, ComplexIn)
- type(mqc_vector) function mqc_vectorvectorsum (Vector1In, Vector2In)
- type(mqc_vector) function mqc_scalarvectorsum (ScalarIn, VectorIn)
- type(mqc_matrix) function mqc_matrixmatrixsum (MA, MB)

6.47.1 Member Function/Subroutine Documentation

6.47.1.1 mqc_complexscalaradd()

```
type(mqc_scalar) function mqc_algebra::operator(+)::mqc_complexscalaradd (
            complex(kind=real64), intent(in) ComplexIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.47.1.2 mqc_integerscalaradd()

```
type(mqc_scalar) function mqc_algebra::operator(+)::mqc_integerscalaradd (
            integer(kind=int64), intent(in) IntegerIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.47.1.3 mqc_matrixmatrixsum()

```
type(mqc_matrix) function mqc_algebra::operator(+)::mqc_matrixmatrixsum (
             type(mqc_matrix), intent(in) MA,
             type(mqc_matrix), intent(in) MB )
```

6.47.1.4 mqc_realscalaradd()

```
type(mqc_scalar) function mqc_algebra::operator(+)::mqc_realscalaradd (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

6.47.1.5 mqc_scalaradd()

```
type(mqc_scalar) function mqc_algebra::operator(+)::mqc_scalaradd (
             type(mqc_scalar), intent(in) Scalar1,
             type(mqc_scalar), intent(in) Scalar2 )
```

6.47.1.6 mqc_scalarcomplexadd()

```
type(mqc_scalar) function mqc_algebra::operator(+)::mqc_scalarcomplexadd (
             type(mqc_scalar), intent(in) Scalar,
             complex(kind=real64), intent(in) ComplexIn )
```

6.47.1.7 mqc_scalarintegeradd()

```
type(mqc_scalar) function mqc_algebra::operator(+)::mqc_scalarintegeradd (
             type(mqc_scalar), intent(in) Scalar,
             integer(kind=int64), intent(in) IntegerIn )
```

6.47.1.8 mqc_scalarrealadd()

```
type(mqc_scalar) function mqc_algebra::operator(+)::mqc_scalarrealadd (
             type(mqc_scalar), intent(in) Scalar,
             real(kind=real64), intent(in) RealIn )
```

6.47.1.9 mqc_scalarvectorsum()

```
type(mqc_vector) function mqc_algebra::operator(+)::mqc_scalarvectorsum (
            type(mqc_scalar), intent(in) ScalarIn,
            type(mqc_vector), intent(in) VectorIn )
```

6.47.1.10 mqc_vectorvectorsum()

```
type(mqc_vector) function mqc_algebra::operator(+)::mqc_vectorvectorsum (
            type(mqc_vector), intent(in) Vector1In,
            type(mqc_vector), intent(in) Vector2In )
```

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

- src/mqc_algebra.F03

6.48 mqc_est::operator(-) Interface Reference

Public Member Functions

- type(mqc_scf_integral) function mqc_integral_difference (integralA, integralB)

6.48.1 Member Function/Subroutine Documentation

6.48.1.1 mqc_integral_difference()

```
type(mqc_scf_integral) function mqc_est::operator(-)::mqc_integral_difference (
            type(mqc_scf_integral), intent(in) integralA,
            type(mqc_scf_integral), intent(in) integralB )
```

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

- src/mqc_est.F03

6.49 mqc_algebra::operator(-) Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalarsubtract (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_integerscalarsubtract (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegersubtract (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalarsubtract (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealsubtract (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalarsubtract (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexsubtract (Scalar, ComplexIn)
- type(mqc_vector) function mqc_vectorvectordifference (Vector1In, Vector2In)
- type(mqc_vector) function mqc_scalarvectordifference (ScalarIn, VectorIn)
- type(mqc_matrix) function mqc_matrixmatrixsubtract (MA, MB)

6.49.1 Member Function/Subroutine Documentation

6.49.1.1 mqc_complexscalarsubtract()

```
type(mqc_scalar) function mqc_algebra::operator(-)::mqc_complexscalarsubtract (
             complex(kind=real64), intent(in) ComplexIn,
             type(mqc_scalar), intent(in) Scalar )
```

6.49.1.2 mqc_integerscalarsubtract()

```
type(mqc_scalar) function mqc_algebra::operator(-)::mqc_integerscalarsubtract (
             integer(kind=int64), intent(in) IntegerIn,
             type(mqc_scalar), intent(in) Scalar )
```

6.49.1.3 mqc_matrixmatrixsubtract()

```
type(mqc_matrix) function mqc_algebra::operator(-)::mqc_matrixmatrixsubtract (
             type(mqc_matrix), intent(in) MA,
             type(mqc_matrix), intent(in) MB )
```

6.49.1.4 mqc_realscalarsubtract()

```
type(mqc_scalar) function mqc_algebra::operator(-)::mqc_realscalarsubtract (
            real(kind=real64), intent(in) RealIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.49.1.5 mqc_scalarcomplexsubtract()

```
type(mqc_scalar) function mqc_algebra::operator(-)::mqc_scalarcomplexsubtract (
            type(mqc_scalar), intent(in) Scalar,
            complex(kind=real64), intent(in) ComplexIn )
```

6.49.1.6 mqc_scalarintegersubtract()

```
type(mqc_scalar) function mqc_algebra::operator(-)::mqc_scalarintegersubtract (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntegerIn )
```

6.49.1.7 mqc_scalarrealsubtract()

```
type(mqc_scalar) function mqc_algebra::operator(-)::mqc_scalarrealsubtract (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

6.49.1.8 mqc_scalarsubtract()

```
type(mqc_scalar) function mqc_algebra::operator(-)::mqc_scalarsubtract (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

6.49.1.9 mqc_scalarvectordifference()

```
type(mqc_vector) function mqc_algebra::operator(-)::mqc_scalarvectordifference (
            type(mqc_scalar), intent(in) ScalarIn,
            type(mqc_vector), intent(in) VectorIn )
```

6.49.1.10 mqc_vectorvectordifference()

```
type(mqc_vector) function mqc_algebra::operator(-)::mqc_vectorvectordifference (
            type(mqc_vector), intent(in) Vector1In,
            type(mqc_vector), intent(in) Vector2In )
```

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

- src/mqc_algebra.F03

6.50 mqc_algebra::operator(.dot.) Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_vectorvectordotproduct (Vector1, Vector2)
- type(mqc_vector) function mqc_vectormatrixdotproduct (VA, MB)
- type(mqc_vector) function mqc_matrixvectordotproduct (MA, VB)
- type(mqc_matrix) function mqc_matrixmatrixdotproduct (MA, MB)

6.50.1 Member Function/Subroutine Documentation

6.50.1.1 mqc_matrixmatrixdotproduct()

```
type(mqc_matrix) function mqc_algebra::operator(.dot.)::mqc_matrixmatrixdotproduct (
            type(mqc_matrix), intent(in) MA,
            type(mqc_matrix), intent(in) MB )
```

6.50.1.2 mqc_matrixvectordotproduct()

```
type(mqc_vector) function mqc_algebra::operator(.dot.)::mqc_matrixvectordotproduct (
            type(mqc_matrix), intent(in) MA,
            type(mqc_vector), intent(in) VB )
```

6.50.1.3 mqc_vectormatrixdotproduct()

```
type(mqc_vector) function mqc_algebra::operator(.dot.)::mqc_vectormatrixdotproduct (
            type(mqc_vector), intent(in) VA,
            type(mqc_matrix), intent(in) MB )
```

6.50.1.4 mqc_vectorvectordotproduct()

```
type(mqc_scalar) function mqc_algebra::operator(.dot.)::mqc_vectorvectordotproduct (
            type(mqc_vector), intent(in) Vector1,
            type(mqc_vector), intent(in) Vector2 )
```

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

- src/mqc_algebra.F03

6.51 mqc_algebra::operator(.eq.) Interface Reference

Public Member Functions

- logical function mqc_scalareq (Scalar1, Scalar2)

6.51.1 Member Function/Subroutine Documentation

6.51.1.1 mqc_scalareq()

```
logical function mqc_algebra::operator(.eq.)::mqc_scalareq (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

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

- src/mqc_algebra.F03

6.52 mqc_algebra::operator(.ewd.) Interface Reference

Public Member Functions

- type(mqc_matrix) function mqc_elementmatrixdivide (A, B)

6.52.1 Member Function/Subroutine Documentation

6.52.1.1 mqc_elementmatrixdivide()

```
type(mqc_matrix) function mqc_algebra::operator(.ewd.)::mqc_elementmatrixdivide (
             type(mqc_matrix), intent(in) A,
             type(mqc_matrix), intent(in) B )
```

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

- src/mqc_algebra.F03

6.53 mqc_algebra::operator(.ewp.) Interface Reference

Public Member Functions

- type(mqc_vector) function mqc_elementvectorproduct (Vector1In, Vector2In)
- type(mqc_matrix) function mqc_elementmatrixproduct (A, B)

6.53.1 Member Function/Subroutine Documentation

6.53.1.1 mqc_elementmatrixproduct()

```
type(mqc_matrix) function mqc_algebra::operator(.ewp.)::mqc_elementmatrixproduct (
             type(mqc_matrix), intent(in) A,
             type(mqc_matrix), intent(in) B )
```

6.53.1.2 mqc_elementvectorproduct()

```
type(mqc_vector) function mqc_algebra::operator(.ewp.)::mqc_elementvectorproduct (
             type(mqc_vector), intent(in) Vector1In,
             type(mqc_vector), intent(in) Vector2In )
```

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

- src/mqc_algebra.F03

6.54 mqc_algebra::operator(.ge.) Interface Reference

Public Member Functions

- logical function mqc_scalarge (Scalar1, Scalar2)

6.54.1 Member Function/Subroutine Documentation

6.54.1.1 mqc_scalarge()

```
logical function mqc_algebra::operator(.ge.)::mqc_scalarge (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

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

- src/mqc_algebra.F03

6.55 mqc_algebra::operator(.gt.) Interface Reference

Public Member Functions

- logical function mqc_scalargt (Scalar1, Scalar2)
- logical function mqc_scalargtinteger (Scalar, IntIn)
- logical function mqc_integergtscalar (IntIn, Scalar)
- logical function mqc_scalargtreal (Scalar, RealIn)
- logical function mqc_realgtscalar (RealIn, Scalar)

6.55.1 Member Function/Subroutine Documentation

6.55.1.1 mqc_integergtscalar()

```
logical function mqc_algebra::operator(.gt.)::mqc_integergtscalar (
            integer(kind=int64), intent(in) IntIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.55.1.2 mqc_realgtscalar()

```
logical function mqc_algebra::operator(.gt.)::mqc_realgtscalar (
            real(kind=real64), intent(in) RealIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.55.1.3 mqc_scalargt()

```
logical function mqc_algebra::operator(.gt.)::mqc_scalargt (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

6.55.1.4 mqc_scalargtinteger()

```
logical function mqc_algebra::operator(.gt.)::mqc_scalargtinteger (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntIn )
```

6.55.1.5 mqc_scalargtreal()

```
logical function mqc_algebra::operator(.gt.)::mqc_scalargtreal (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

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

- src/mqc_algebra.F03

6.56 mqc_algebra::operator(.le.) Interface Reference

Public Member Functions

- logical function mqc_scalarle (Scalar1, Scalar2)
- logical function mqc_scalarlereal (Scalar, RealIn)
- logical function mqc_reallescalar (RealIn, Scalar)
- logical function mqc_scalarleinteger (Scalar, IntIn)
- logical function mqc_integerlescalar (IntIn, Scalar)

6.56.1 Member Function/Subroutine Documentation

6.56.1.1 mqc_integerlescalar()

```
logical function mqc_algebra::operator(.le.)::mqc_integerlescalar (
            integer(kind=int64), intent(in) IntIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.56.1.2 mqc_reallescalar()

```
logical function mqc_algebra::operator(.le.)::mqc_reallescalar (
            real(kind=real64), intent(in) RealIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.56.1.3 mqc_scalarle()

```
logical function mqc_algebra::operator(.le.)::mqc_scalarle (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

6.56.1.4 mqc_scalarleinteger()

```
logical function mqc_algebra::operator(.le.)::mqc_scalarleinteger (
            type(mqc_scalar), intent(in) Scalar,
            integer(kind=int64), intent(in) IntIn )
```

6.56.1.5 mqc_scalarlereal()

```
logical function mqc_algebra::operator(.le.)::mqc_scalarlereal (
            type(mqc_scalar), intent(in) Scalar,
            real(kind=real64), intent(in) RealIn )
```

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

- src/mqc_algebra.F03

6.57 mqc_algebra::operator(.lt.) Interface Reference

Public Member Functions

- logical function mqc_scalarlt (Scalar1, Scalar2)
- logical function mqc_scalarltreal (Scalar, RealIn)
- logical function mqc_realltscalar (RealIn, Scalar)

6.57.1 Member Function/Subroutine Documentation

6.57.1.1 mqc_realltscalar()

```
logical function mqc_algebra::operator(.lt.)::mqc_realltscalar (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

6.57.1.2 mqc_scalarlt()

```
logical function mqc_algebra::operator(.lt.)::mqc_scalarlt (
             type(mqc_scalar), intent(in) Scalar1,
             type(mqc_scalar), intent(in) Scalar2 )
```

6.57.1.3 mqc_scalarltreal()

```
logical function mqc_algebra::operator(.lt.)::mqc_scalarltreal (
             type(mqc_scalar), intent(in) Scalar,
             real(kind=real64), intent(in) RealIn )
```

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

- src/mqc_algebra.F03

6.58 mqc_algebra::operator(.ne.) Interface Reference

Public Member Functions

- logical function mqc_scalarne (Scalar1, Scalar2)

6.58.1 Member Function/Subroutine Documentation

6.58.1.1 mqc_scalarne()

```
logical function mqc_algebra::operator(.ne.)::mqc_scalarne (
            type(mqc_scalar), intent(in) Scalar1,
            type(mqc_scalar), intent(in) Scalar2 )
```

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

- src/mqc_algebra.F03

6.59 mqc_algebra::operator(.outer.) Interface Reference

Public Member Functions

- type(mqc_matrix) function mqc_outer (VA, VB)

6.59.1 Member Function/Subroutine Documentation

6.59.1.1 mqc_outer()

```
type(mqc_matrix) function mqc_algebra::operator(.outer.)::mqc_outer (
            type(mqc_vector), intent(in) VA,
            type(mqc_vector), intent(in) VB )
```

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

- src/mqc_algebra.F03

6.60 mqc_algebra::operator(.x.) Interface Reference

Public Member Functions

- type(mqc_vector) function mqc_crossproduct (Vector1In, Vector2In)

6.60.1 Member Function/Subroutine Documentation

6.60.1.1 mqc_crossproduct()

```
type(mqc_vector) function mqc_algebra::operator(.x.)::mqc_crossproduct (
            type(mqc_vector), intent(in) Vector1In,
            type(mqc_vector), intent(in) Vector2In )
```

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

- src/mqc_algebra.F03

6.61 mqc_algebra::operator(/) Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalardivide (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_integerscalardivide (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_scalarintegerdivide (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_realscalardivide (RealIn, Scalar)
- type(mqc_scalar) function mqc_scalarrealdivide (Scalar, RealIn)
- type(mqc_scalar) function mqc_complexscalardivide (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_scalarcomplexdivide (Scalar, ComplexIn)
- type(mqc_vector) function mqc_vectorscalardivide (vector, scalar)
- type(mqc_vector) function mqc_vectorrealdivide (vector, realIn)
- type(mqc_vector) function mqc_vectorintegerdivide (vector, intIn)
- type(mqc_vector) function mqc_vectorcomplexdivide (vector, compIn)

6.61.1 Member Function/Subroutine Documentation

6.61.1.1 mqc_complexscalardivide()

```
type(mqc_scalar) function mqc_algebra::operator(/)::mqc_complexscalardivide (
            complex(kind=real64), intent(in) ComplexIn,
            type(mqc_scalar), intent(in) Scalar )
```

6.61.1.2 mqc_integerscalardivide()

```
type(mqc_scalar) function mqc_algebra::operator(/)::mqc_integerscalardivide (
             integer(kind=int64), intent(in) IntegerIn,
             type(mqc_scalar), intent(in) Scalar )
```

6.61.1.3 mqc_realscalardivide()

```
type(mqc_scalar) function mqc_algebra::operator(/)::mqc_realscalardivide (
             real(kind=real64), intent(in) RealIn,
             type(mqc_scalar), intent(in) Scalar )
```

6.61.1.4 mqc_scalarcomplexdivide()

```
type(mqc_scalar) function mqc_algebra::operator(/)::mqc_scalarcomplexdivide (
             type(mqc_scalar), intent(in) Scalar,
             complex(kind=real64), intent(in) ComplexIn )
```

6.61.1.5 mqc_scalardivide()

```
type(mqc_scalar) function mqc_algebra::operator(/)::mqc_scalardivide (
             type(mqc_scalar), intent(in) Scalar1,
             type(mqc_scalar), intent(in) Scalar2 )
```

6.61.1.6 mqc_scalarintegerdivide()

```
type(mqc_scalar) function mqc_algebra::operator(/)::mqc_scalarintegerdivide (
             type(mqc_scalar), intent(in) Scalar,
             integer(kind=int64), intent(in) IntegerIn )
```

6.61.1.7 mqc_scalarrealdivide()

```
type(mqc_scalar) function mqc_algebra::operator(/)::mqc_scalarrealdivide (
             type(mqc_scalar), intent(in) Scalar,
             real(kind=real64), intent(in) RealIn )
```

6.61.1.8 mqc_vectorcomplexdivide()

```
type(mqc_vector) function mqc_algebra::operator(/)::mqc_vectorcomplexdivide (
             type(mqc_vector), intent(in) vector,
             complex(kind=real64), intent(in) compIn )
```

6.61.1.9 mqc_vectorintegerdivide()

```
type(mqc_vector) function mqc_algebra::operator(/)::mqc_vectorintegerdivide (
             type(mqc_vector), intent(in) vector,
             integer(kind=int64), intent(in) intIn )
```

6.61.1.10 mqc_vectorrealdivide()

```
type(mqc_vector) function mqc_algebra::operator(/)::mqc_vectorrealdivide (
             type(mqc_vector), intent(in) vector,
             real(kind=real64), intent(in) realIn )
```

6.61.1.11 mqc_vectorscalardivide()

```
type(mqc_vector) function mqc_algebra::operator(/)::mqc_vectorscalardivide (
             type(mqc_vector), intent(in) vector,
             type(mqc_scalar), intent(in) scalar )
```

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

- src/mqc_algebra.F03

6.62 mqc_algebra::real Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_complex_realpart (ScalarIn)
- type(mqc_vector) function mqc_vector_complex_realpart (A)

6.62.1 Member Function/Subroutine Documentation

6.62.1.1 mqc_scalar_complex_realpart()

```
type(mqc_scalar) function mqc_algebra::real::mqc_scalar_complex_realpart (
            type(mqc_scalar), intent(in) ScalarIn )
```

6.62.1.2 mqc_vector_complex_realpart()

```
type(mqc_vector) function mqc_algebra::real::mqc_vector_complex_realpart (
            class(mqc_vector), intent(in) A )
```

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

- src/mqc_algebra.F03

6.63 mqc_algebra::sin Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_sin (Scalar)

6.63.1 Member Function/Subroutine Documentation

6.63.1.1 mqc_scalar_sin()

```
type(mqc_scalar) function mqc_algebra::sin::mqc_scalar_sin (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.64 mqc_algebra::sqrt Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_sqrt (Scalar)

6.64.1 Member Function/Subroutine Documentation

6.64.1.1 mqc_scalar_sqrt()

```
type(mqc_scalar) function mqc_algebra::sqrt::mqc_scalar_sqrt (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.65 mqc_algebra::tan Interface Reference

Public Member Functions

- type(mqc_scalar) function mqc_scalar_tan (Scalar)

6.65.1 Member Function/Subroutine Documentation

6.65.1.1 mqc_scalar_tan()

```
type(mqc_scalar) function mqc_algebra::tan::mqc_scalar_tan (
            type(mqc_scalar), intent(in) Scalar )
```

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

- src/mqc_algebra.F03

6.66 mqc_est::transpose Interface Reference

Public Member Functions

- type(mqc_scf_integral) function mqc_integral_transpose (integral, label)

6.66.1 Member Function/Subroutine Documentation

6.66.1.1 mqc_integral_transpose()

```
type(mqc_scf_integral) function mqc_est::transpose::mqc_integral_transpose (
             type(mqc_scf_integral), intent(in) integral,
             character(len=*), intent(in), optional label )
```

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

- src/mqc_est.F03

6.67 mqc_algebra::transpose Interface Reference

Public Member Functions

- type(mqc_vector) function mqc_vector_transpose (Vector)
- type(mqc_matrix) function mqc_matrix_transpose (Matrix)

6.67.1 Member Function/Subroutine Documentation

6.67.1.1 mqc_matrix_transpose()

```
type(mqc_matrix) function mqc_algebra::transpose::mqc_matrix_transpose (
             class(mqc_matrix), intent(in) Matrix )
```

6.67.1.2 mqc_vector_transpose()

```
type(mqc_vector) function mqc_algebra::transpose::mqc_vector_transpose (
             class(mqc_vector), intent(in) Vector )
```

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

- src/mqc_algebra.F03

Chapter 7

File Documentation

7.1 src/mqc_algebra.F03 File Reference

Data Types

- type mqc_algebra::mqc_scalar
- type mqc_algebra::mqc_vector
- type mqc_algebra::mqc_matrix
- type mqc_algebra::mqc_r4tensor
- interface mqc_algebra::mqc_print
- interface mqc_algebra::contraction
- interface mqc_algebra::conjg
- interface mqc_algebra::mqc_have_real
- interface mqc_algebra::mqc_have_int
- interface mqc_algebra::mqc_have_complex
- interface mqc_algebra::mqc_cast_real
- interface mqc_algebra::mqc_cast_complex
- interface mqc_algebra::matmul
- interface mqc_algebra::transpose
- interface mqc_algebra::dagger
- interface mqc_algebra::cmplx
- interface mqc_algebra::sqrt
- interface mqc_algebra::abs
- interface mqc_algebra::real
- interface mqc_algebra::aimag
- interface mqc_algebra::sin
- interface mqc_algebra::cos
- interface mqc_algebra::tan
- interface mqc_algebra::asin
- interface mqc_algebra::acos
- interface mqc_algebra::atan
- interface mqc_algebra::atan2
- interface mqc_algebra::mqc_set_array2vector
- interface mqc_algebra::mqc_matrix_symmmatrix_put

- interface mqc_algebra::mqc_matrix_diagmatrix_put
- interface mqc_algebra::matrix_symm2sq
- interface mqc_algebra::dot_product
- interface mqc_algebra::assignment(=)
- interface mqc_algebra::operator(+)
- interface mqc_algebra::operator(-)
- interface mqc_algebra::operator(∗)
- interface mqc_algebra::operator(/)
- interface mqc_algebra::operator(∗∗)
- interface mqc_algebra::operator(.ne.)
- interface mqc_algebra::operator(.eq.)
- interface mqc_algebra::operator(.lt.)
- interface mqc_algebra::operator(.gt.)
- interface mqc_algebra::operator(.le.)
- interface mqc_algebra::operator(.ge.)
- interface mqc_algebra::assignment(=)
- interface mqc_algebra::operator(.dot.)
- interface mqc_algebra::operator(∗)
- interface mqc_algebra::operator(/)
- interface mqc_algebra::operator(+)
- interface mqc_algebra::operator(-)
- interface mqc_algebra::operator(.ewp.)
- interface mqc_algebra::operator(.ewd.)
- interface mqc_algebra::operator(.x.)
- interface mqc_algebra::operator(.outer.)
- interface mqc_algebra::assignment(=)
- interface mqc_algebra::operator(+)
- interface mqc_algebra::operator(-)
- interface mqc_algebra::operator(∗)
- interface mqc_algebra::operator(.dot.)
- interface mqc_algebra::assignment(=)

Modules

- module mqc_algebra

Functions/Subroutines

- integer(kind=int64) function mqc_algebra::factorial (n)
- integer(kind=int64) function mqc_algebra::bin_coeff (N, K)
- subroutine mqc_algebra::mqc_allocate_scalar (Scalar, Data_type)

  MQC_Allocate_Scalar is used to allocate a scalar type variable of the MQC_Scalar class
- subroutine mqc_algebra::mqc_deallocate_scalar (Scalar)
- logical function mqc_algebra::mqc_scalar_isallocated (Scalar)
- subroutine mqc_algebra::mqc_input_integer_scalar (ScalarOut, ScalarIn)

  MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic scalar to an MQC_Scalar
- subroutine mqc_algebra::mqc_input_real_scalar (ScalarOut, ScalarIn)
- subroutine mqc_algebra::mqc_input_complex_scalar (ScalarOut, ScalarIn)

- subroutine mqc_algebra::mqc_output_mqcscalar_scalar (ScalarOut, ScalarIn)
- subroutine mqc_algebra::mqc_output_integer_scalar (ScalarOut, ScalarIn)
- subroutine mqc_algebra::mqc_output_real_scalar (ScalarOut, ScalarIn)
- subroutine mqc_algebra::mqc_output_complex_scalar (ScalarOut, ScalarIn)
- subroutine mqc_algebra::mqc_print_scalar_algebra1 (Scalar, IOut, Header, Blank_At_Top, Blank_At_Bottom)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_cmplx (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_sqrt (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_sin (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_cos (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_tan (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_asin (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_acos (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_atan (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_atan2 (Scalar)
- logical function mqc_algebra::mqc_scalar_havereal (Scalar)
- logical function mqc_algebra::mqc_scalar_haveinteger (Scalar)
- logical function mqc_algebra::mqc_scalar_havecomplex (Scalar)
- real(kind=real64) function mqc_algebra::mqc_scalar_get_intrinsic_real (Scalar)
- integer(kind=int64) function mqc_algebra::mqc_scalar_get_intrinsic_integer (Scalar)
- complex(kind=real64) function mqc_algebra::mqc_scalar_get_intrinsic_complex (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_get_abs_value (Scalar)
- subroutine mqc_algebra::mqc_scalar_get_random_value (Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalaradd (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_algebra::mqc_scalarsubtract (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_algebra::mqc_scalarmultiply (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_algebra::mqc_scalardivide (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_algebra::mqc_scalarexponent (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_algebra::mqc_scalarintegerexponent (Scalar, IntIn)
- type(mqc_scalar) function mqc_algebra::mqc_scalarrealexponent (Scalar, RealIn)
- type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexexponent (Scalar, CompIn)
- logical function mqc_algebra::mqc_scalarne (Scalar1, Scalar2)
- logical function mqc_algebra::mqc_scalareq (Scalar1, Scalar2)
- logical function mqc_algebra::mqc_scalarlt (Scalar1, Scalar2)
- logical function mqc_algebra::mqc_realltscalar (RealIn, Scalar)
- logical function mqc_algebra::mqc_scalarltreal (Scalar, RealIn)
- logical function mqc_algebra::mqc_scalargt (Scalar1, Scalar2)
- logical function mqc_algebra::mqc_integergtscalar (IntIn, Scalar)
- logical function mqc_algebra::mqc_scalargtinteger (Scalar, IntIn)
- logical function mqc_algebra::mqc_realgtscalar (RealIn, Scalar)
- logical function mqc_algebra::mqc_scalargtreal (Scalar, RealIn)
- logical function mqc_algebra::mqc_scalarle (Scalar1, Scalar2)
- logical function mqc_algebra::mqc_reallescalar (RealIn, Scalar)
- logical function mqc_algebra::mqc_scalarlereal (Scalar, RealIn)
- logical function mqc_algebra::mqc_integerlescalar (IntIn, Scalar)
- logical function mqc_algebra::mqc_scalarleinteger (Scalar, IntIn)
- logical function mqc_algebra::mqc_scalarge (Scalar1, Scalar2)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_complex_conjugate (ScalarIn)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_complex_realpart (ScalarIn)
- type(mqc_scalar) function mqc_algebra::mqc_scalar_complex_imagpart (ScalarIn)
- type(mqc_scalar) function mqc_algebra::mqc_integerscalarmultiply (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarintegermultiply (Scalar, IntegerIn)

- type(mqc_scalar) function mqc_algebra::mqc_realscalarmultiply (RealIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarrealmultiply (Scalar, RealIn)
- type(mqc_scalar) function mqc_algebra::mqc_complexscalarmultiply (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexmultiply (Scalar, ComplexIn)
- type(mqc_scalar) function mqc_algebra::mqc_integerscalardivide (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarintegerdivide (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_algebra::mqc_realscalardivide (RealIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarrealdivide (Scalar, RealIn)
- type(mqc_scalar) function mqc_algebra::mqc_complexscalardivide (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexdivide (Scalar, ComplexIn)
- type(mqc_scalar) function mqc_algebra::mqc_integerscalaradd (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarintegeradd (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_algebra::mqc_realscalaradd (RealIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarrealadd (Scalar, RealIn)
- type(mqc_scalar) function mqc_algebra::mqc_complexscalaradd (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexadd (Scalar, ComplexIn)
- type(mqc_scalar) function mqc_algebra::mqc_integerscalarsubtract (IntegerIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarintegersubtract (Scalar, IntegerIn)
- type(mqc_scalar) function mqc_algebra::mqc_realscalarsubtract (RealIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarrealsubtract (Scalar, RealIn)
- type(mqc_scalar) function mqc_algebra::mqc_complexscalarsubtract (ComplexIn, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexsubtract (Scalar, ComplexIn)
- subroutine mqc_algebra::mqc_allocate_vector (N, Vector, Data_Type)
- subroutine mqc_algebra::mqc_deallocate_vector (Vector)
- integer(kind=int64) function mqc_algebra::mqc_length_vector (Vector)
- logical function mqc_algebra::mqc_vector_havereal (Vector)
- logical function mqc_algebra::mqc_vector_haveinteger (Vector)
- logical function mqc_algebra::mqc_vector_havecomplex (Vector)
- logical function mqc_algebra::mqc_vector_iscolumn (Vector)
- subroutine mqc_algebra::mqc_vector_copy_int2real (Vector)
- subroutine mqc_algebra::mqc_vector_copy_int2complex (Vector)
- subroutine mqc_algebra::mqc_vector_copy_real2int (Vector)
- subroutine mqc_algebra::mqc_vector_copy_real2complex (Vector)
- subroutine mqc_algebra::mqc_vector_copy_complex2int (Vector)
- subroutine mqc_algebra::mqc_vector_copy_complex2real (Vector)
- type(mqc_scalar) function mqc_algebra::mqc_vector_scalar_at (Vec, I)
- type(mqc_vector) function mqc_algebra::mqc_vector_vector_at (Vec, I, J)
- subroutine mqc_algebra::mqc_set_vector2integerarray (ArrayOut, VectorIn)
- subroutine mqc_algebra::mqc_set_vector2realarray (ArrayOut, VectorIn)
- subroutine mqc_algebra::mqc_set_vector2complexarray (ArrayOut, VectorIn)
- subroutine mqc_algebra::mqc_set_array2vector_integer (VectorOut, ArrayIn)
- subroutine mqc_algebra::mqc_set_array2vector_real (VectorOut, ArrayIn)
- subroutine mqc_algebra::mqc_set_array2vector_complex (VectorOut, ArrayIn)
- subroutine mqc_algebra::mqc_set_vector2vector (VectorOut, VectorIn)
- type(mqc_vector) function mqc_algebra::mqc_vectorvectorsum (Vector1In, Vector2In)
- type(mqc_vector) function mqc_algebra::mqc_vectorvectordifference (Vector1In, Vector2In)
- type(mqc_vector) function mqc_algebra::mqc_scalarvectorsum (ScalarIn, VectorIn)
- type(mqc_vector) function mqc_algebra::mqc_scalarvectordifference (ScalarIn, VectorIn)
- type(mqc_vector) function mqc_algebra::mqc_elementvectorproduct (Vector1In, Vector2In)
- type(mqc_vector) function mqc_algebra::mqc_vector_transpose (Vector)
- type(mqc_vector) function mqc_algebra::mqc_vector_conjugate_transpose (Vector)

- type(mqc_scalar) function mqc_algebra::mqc_vectorvectordotproduct (Vector1, Vector2)
- type(mqc_matrix) function mqc_algebra::mqc_outer (VA, VB)
- type(mqc_vector) function mqc_algebra::mqc_crossproduct (Vector1In, Vector2In)
- subroutine mqc_algebra::mqc_print_vector_algebra1 (Vector, IOut, Header, Verbose, Blank_At_Top, Blank_At←_Bottom)
- type(mqc_vector) function mqc_algebra::mqc_vector_cast_real (VA)
- type(mqc_vector) function mqc_algebra::mqc_vector_cast_complex (VA)
- subroutine mqc_algebra::mqc_vector_scalar_put (Vector, Scalar, I)
- subroutine mqc_algebra::mqc_vector_scalar_increment (Vector, Scalar, I)
- subroutine mqc_algebra::mqc_vector_vector_put (Vector, VectorIn, I)
- subroutine mqc_algebra::mqc_vector_initialize (Vector, Length, Scalar)
- type(mqc_vector) function mqc_algebra::mqc_scalarvectorproduct (Scalar, Vector)
- type(mqc_vector) function mqc_algebra::mqc_vectorscalarproduct (vector, scalar)
- type(mqc_vector) function mqc_algebra::mqc_vectorscalardivide (vector, scalar)
- type(mqc_vector) function mqc_algebra::mqc_realvectorproduct (RealIn, Vector)
- type(mqc_vector) function mqc_algebra::mqc_vectorrealproduct (vector, realIn)
- type(mqc_vector) function mqc_algebra::mqc_vectorrealdivide (vector, realIn)
- type(mqc_vector) function mqc_algebra::mqc_integervectorproduct (intIn, Vector)
- type(mqc_vector) function mqc_algebra::mqc_vectorintegerproduct (vector, intIn)
- type(mqc_vector) function mqc_algebra::mqc_vectorintegerdivide (vector, intIn)
- type(mqc_vector) function mqc_algebra::mqc_complexvectorproduct (CompIn, Vector)
- type(mqc_vector) function mqc_algebra::mqc_vectorcomplexproduct (vector, compIn)
- type(mqc_vector) function mqc_algebra::mqc_vectorcomplexdivide (vector, compIn)
- type(mqc_scalar) function mqc_algebra::mqc_vector_norm (vector, methodIn)
- logical function mqc_algebra::mqc_vector_isallocated (Vector)
- subroutine mqc_algebra::mqc_vector_push (Vector, Scalar)
- subroutine mqc_algebra::mqc_vector_unshift (Vector, Scalar)
- type(mqc_scalar) function mqc_algebra::mqc_vector_pop (Vector)
- type(mqc_scalar) function mqc_algebra::mqc_vector_shift (Vector)
- type(mqc_scalar) function mqc_algebra::mqc_vector_maxval (Vector)
- type(mqc_scalar) function mqc_algebra::mqc_vector_minval (Vector)
- integer function mqc_algebra::mqc_vector_maxloc (Vector)
- integer function mqc_algebra::mqc_vector_minloc (Vector)
- type(mqc_vector) function mqc_algebra::mqc_vector_argsort (Vector)
- subroutine mqc_algebra::mqc_vector_sort (Vector, idx)
- subroutine mqc_algebra::mqc_vector_sqrt (A)
- type(mqc_vector) function mqc_algebra::mqc_vector_abs (A)
- subroutine mqc_algebra::mqc_vector_power (A, P)
- type(mqc_vector) function mqc_algebra::mqc_vector_complex_realpart (A)
- type(mqc_vector) function mqc_algebra::mqc_vector_complex_imagpart (A)
- type(mqc_vector) function mqc_algebra::mqc_vector_cmplx (Vector1, Vector2)
- character(len=64) function mqc_algebra::mqc_matrix_storagetype (Matrix)
- subroutine mqc_algebra::mqc_matrix_diagonalize (A, EVals, EVecs)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_cast_real (MA)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_cast_complex (MA)
- type(mqc_scalar) function mqc_algebra::mqc_matrix_scalar_at (Mat, I, J)
- type(mqc_vector) function mqc_algebra::mqc_matrix_vector_at (Mat, Rows, Cols)
- recursive subroutine mqc_algebra::mqc_matrix_vector_put (Mat, VectorIn, Rows, Cols)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_matrix_at (Mat, Rows, Cols)

  MQC_Matrix_Matrix_At is a function that returns a submatrix of the matrix
- subroutine mqc_algebra::mqc_matrix_diagmatrix_put_vector (diagVectorIn, mat)

- subroutine mqc_algebra::mqc_matrix_diagmatrix_put_integer (mat, diagMatrixIn)
- subroutine mqc_algebra::mqc_matrix_diagmatrix_put_real (mat, diagMatrixIn)
- subroutine mqc_algebra::mqc_matrix_diagmatrix_put_complex (mat, diagMatrixIn)
- subroutine mqc_algebra::mqc_matrix_symmmatrix_put_integer (mat, symmMatrixIn)
- subroutine mqc_algebra::mqc_matrix_symmmatrix_put_real (mat, symmMatrixIn)
- subroutine mqc_algebra::mqc_matrix_symmmatrix_put_complex (mat, symmMatrixIn)
- recursive subroutine mqc_algebra::mqc_matrix_matrix_put (Mat, MatrixIn, Rows, Cols)
- integer(kind=int64) function mqc_algebra::symindexhash (i, j, k, l)
- type(mqc_matrix) function mqc_algebra::mqc_elementmatrixproduct (A, B)
- type(mqc_matrix) function mqc_algebra::mqc_elementmatrixdivide (A, B)
- logical function mqc_algebra::mqc_matrix_test_symmetric (Matrix, Option)
- logical function mqc_algebra::mqc_matrix_test_diagonal (Matrix)
- subroutine mqc_algebra::mqc_allocate_matrix (M, N, Matrix, Data_Type, Storage)
- subroutine mqc_algebra::mqc_deallocate_matrix (Matrix)
- logical function mqc_algebra::mqc_matrix_isallocated (Matrix)
- subroutine mqc_algebra::mqc_set_integerarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_algebra::mqc_set_realarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_algebra::mqc_set_complexarray2matrix (MatrixOut, ArrayIn)
- subroutine mqc_algebra::mqc_set_matrix2integerarray (ArrayOut, MatrixIn)
- subroutine mqc_algebra::mqc_set_matrix2realarray (ArrayOut, MatrixIn)
- subroutine mqc_algebra::mqc_set_matrix2complexarray (ArrayOut, MatrixIn)
- subroutine mqc_algebra::mqc_set_matrix2matrix (MatrixOut, MatrixIn)
- subroutine mqc_algebra::mqc_print_matrix_algebra1 (Matrix, IOut, Header, Blank_At_Top, Blank_At_Bottom)
- subroutine mqc_algebra::mqc_matrix_copy_int2real (Matrix)
- subroutine mqc_algebra::mqc_matrix_copy_int2complex (Matrix)
- subroutine mqc_algebra::mqc_matrix_copy_real2int (Matrix)
- subroutine mqc_algebra::mqc_matrix_copy_real2complex (Matrix)
- subroutine mqc_algebra::mqc_matrix_copy_complex2int (Matrix)
- subroutine mqc_algebra::mqc_matrix_copy_complex2real (Matrix)
- integer(kind=int64) function mqc_algebra::mqc_matrix_rows (Matrix)
- integer(kind=int64) function mqc_algebra::mqc_matrix_columns (Matrix)
- logical function mqc_algebra::mqc_matrix_havereal (Matrix)
- logical function mqc_algebra::mqc_matrix_haveinteger (Matrix)
- logical function mqc_algebra::mqc_matrix_havecomplex (Matrix)
- logical function mqc_algebra::mqc_matrix_havefull (Matrix)
- logical function mqc_algebra::mqc_matrix_havesymmetric (Matrix)
- logical function mqc_algebra::mqc_matrix_havediagonal (Matrix)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_transpose (Matrix)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_conjugate_transpose (Matrix)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_symmetrize (Matrix)
- subroutine mqc_algebra::mqc_matrix_full2symm (Matrix)
- subroutine mqc_algebra::mqc_matrix_symm2full (Matrix, Option)
- subroutine mqc_algebra::mqc_matrix_full2diag (Matrix)
- subroutine mqc_algebra::mqc_matrix_diag2full (Matrix)
- subroutine mqc_algebra::mqc_matrix_symm2diag (Matrix)
- subroutine mqc_algebra::mqc_matrix_diag2symm (Matrix)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_symm2full_func (Matrix)
- subroutine mqc_algebra::matrix_symm2sq_integer (N, I_Symm, I_Sq)
- subroutine mqc_algebra::matrix_symm2sq_real (N, A_Symm, A_Sq)
- subroutine mqc_algebra::matrix_symm2sq_complex (N, A_Symm, A_Sq)
- type(mqc_matrix) function mqc_algebra::mqc_vector2diagmatrix (vector)

- type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixsum (MA, MB)
- type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixsubtract (MA, MB)
- type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixproduct (MA, MB)
- type(mqc_matrix) function mqc_algebra::mqc_matrixmatrixdotproduct (MA, MB)
- type(mqc_vector) function mqc_algebra::mqc_matrixvectordotproduct (MA, VB)
- type(mqc_vector) function mqc_algebra::mqc_vectormatrixdotproduct (VA, MB)
- type(mqc_matrix) function mqc_algebra::mqc_matrixscalarproduct (Matrix, Scalar)
- type(mqc_matrix) function mqc_algebra::mqc_scalarmatrixproduct (Scalar, Matrix)
- type(mqc_scalar) function mqc_algebra::mqc_matrix_matrix_contraction (Matrix1, Matrix2)
- subroutine mqc_algebra::mqc_matrix_scalar_put (Matrix, Scalar, I, J)
- subroutine mqc_algebra::mqc_matrix_initialize (Matrix, Rows, Columns, Scalar, Storage)
- subroutine mqc_algebra::mqc_matrix_identity (matrix, n, m)
- subroutine mqc_algebra::mqc_matrix_set (matrix, scalar, storage)
- type(mqc_scalar) function mqc_algebra::mqc_matrix_norm (matrix, methodIn)
- type(mqc_scalar) function mqc_algebra::mqc_matrix_determinant (a)
- type(mqc_matrix) function mqc_algebra::mqc_matrix_inverse (a)
- type(mqc_scalar) function mqc_algebra::mqc_matrix_trace (matrix)
- subroutine mqc_algebra::mqc_matrix_generalized_eigensystem (a, bIn, eigenvals, reigenvecs, leigenvecs)
- subroutine mqc_algebra::mqc_matrix_svd (A, EVals, EUVecs, EVVecs)
- subroutine mqc_algebra::mqc_matrix_rms_max (A, rms_A, max_A)
- subroutine mqc_algebra::mqc_matrix_sqrt (A, eVals, eVecs)
- subroutine mqc_algebra::mqc_allocate_r4tensor (I, J, K, L, Tensor, Data_Type, Storage)
- subroutine mqc_algebra::mqc_deallocate_r4tensor (Tensor)
- type(mqc_scalar) function mqc_algebra::mqc_r4tensor_at (Tensor, I, J, K, L)
- subroutine mqc_algebra::mqc_r4tensor_put (Tensor, Element, I, J, K, L)
- subroutine mqc_algebra::mqc_print_r4tensor_algebra1 (Tensor, IOut, Header, blank_at_top, blank_at_bottom)
- subroutine mqc_algebra::mqc_set_array2tensor (TensorOut, ArrayIn)
- subroutine mqc_algebra::mqc_r4tensor_initialize (R4Tensor, I, J, K, L, Scalar)
- subroutine mqc_algebra::mqc_matrix_symmsymmr4tensor_put_real (r4Tensor, symmSymmMatrixIn)
- subroutine mqc_algebra::mqc_matrix_symmsymmr4tensor_put_complex (r4Tensor, symmSymmMatrixIn)
- logical function mqc_algebra::mqc_r4tensor_haveinteger (R4Tensor)
- logical function mqc_algebra::mqc_r4tensor_havereal (R4Tensor)
- logical function mqc_algebra::mqc_r4tensor_havecomplex (R4Tensor)
- type(mqc_matrix) function mqc_algebra::mqc_givens_matrix (m_size, angle, p, q)

7.2 src/mqc_est.F03 File Reference

Data Types

- type mqc_est::mqc_scf_integral
- type mqc_est::mqc_scf_eigenvalues
- type mqc_est::mqc_wavefunction
- type mqc_est::mqc_pscf_wavefunction
- type mqc_est::mqc_determinant_string
- type mqc_est::mqc_determinant
- type mqc_est::mqc_twoeris
- interface mqc_est::mqc_print
- interface mqc_est::matmul

- interface mqc_est::dot_product
- interface mqc_est::transpose
- interface mqc_est::dagger
- interface mqc_est::contraction
- interface mqc_est::mqc_matrix_undospinblockghf
- interface mqc_est::assignment(=)
- interface mqc_est::operator(+)
- interface mqc_est::operator(-)
- interface mqc_est::operator(∗)

Modules

- module mqc_est

Functions/Subroutines

- subroutine mqc_est::mqc_print_wavefunction (wavefunction, iOut, label)
- subroutine mqc_est::mqc_print_integral (integral, iOut, header, blank_at_top, blank_at_bottom)
- subroutine mqc_est::mqc_print_eigenvalues (eigenvalues, iOut, header, blank_at_top, blank_at_bottom)
- subroutine mqc_est::mqc_print_twoeris (twoERIs, iOut, header, blank_at_top, blank_at_bottom)
- logical function mqc_est::mqc_integral_isallocated (Integral)
- logical function mqc_est::mqc_eigenvalues_isallocated (Eigenvalues)
- logical function mqc_est::mqc_integral_has_alpha (integral)
- logical function mqc_est::mqc_integral_has_beta (integral)
- logical function mqc_est::mqc_integral_has_alphabeta (integral)
- logical function mqc_est::mqc_integral_has_betaalpha (integral)
- logical function mqc_est::mqc_eigenvalues_has_alpha (eigenvalues)
- logical function mqc_est::mqc_eigenvalues_has_beta (eigenvalues)
- character(len=64) function mqc_est::mqc_integral_array_type (integral)
- character(len=64) function mqc_est::mqc_eigenvalues_array_type (eigenvalues)
- character(len=64) function mqc_est::mqc_integral_array_name (integral)
- character(len=64) function mqc_est::mqc_eigenvalues_array_name (eigenvalues)
- subroutine mqc_est::mqc_integral_add_name (integral, arrayName)
- subroutine mqc_est::mqc_eigenvalues_add_name (eigenvalues, arrayName)
- integer(kind=int64) function mqc_est::mqc_integral_dimension (integral, label, axis)
- integer(kind=int64) function mqc_est::mqc_eigenvalues_dimension (eigenvalues, label)
- subroutine mqc_est::mqc_twoeris_allocate (twoERIs, storageType, integralType, alpha, beta, alphaBeta, betaAlpha)
- subroutine mqc_est::mqc_integral_allocate (integral, arrayName, arrayType, alpha, beta, alphaBeta, betaAlpha)
- subroutine mqc_est::mqc_eigenvalues_allocate (eigenvalues, arrayName, arrayType, alpha, beta)
- subroutine mqc_est::mqc_integral_identity (integral, nAlpha, nBeta, label, nAlpha2, nBeta2)
- subroutine mqc_est::mqc_integral_initialize (integral, nAlpha, nBeta, scalar, label, nAlpha2, nBeta2)
- type(mqc_matrix) function mqc_est::mqc_integral_output_block (integral, blockName)
- type(mqc_scf_integral) function mqc_est::mqc_integral_output_orbitals (integral, orbString, alphaOrbsIn, betaOrbsIn, axis)
- type(mqc_scf_integral) function mqc_est::mqc_integral_swap_orbitals (integral, alphaOrbsIn, betaOrbsIn, axis)
- type(mqc_vector) function mqc_est::mqc_eigenvalues_output_block (eigenvalues, blockName)
- subroutine mqc_est::mqc_integral_output_array (matrixOut, integralIn)
- subroutine mqc_est::mqc_eigenvalues_output_array (vectorOut, eigenvaluesIn)

- type(mqc_scf_integral) function mqc_est::mqc_integral_matrix_multiply (integralA, matrixB, label)
- type(mqc_scf_integral) function mqc_est::mqc_matrix_integral_multiply (matrixA, integralB, label)
- type(mqc_scf_integral) function mqc_est::mqc_integral_sum (integralA, integralB)
- type(mqc_scf_integral) function mqc_est::mqc_integral_difference (integralA, integralB)
- type(mqc_scf_integral) function mqc_est::mqc_integral_integral_multiply (integralA, integralB, label)
- type(mqc_scf_integral) function mqc_est::mqc_scalar_integral_multiply (scalar, integral)
- type(mqc_scf_integral) function mqc_est::mqc_integral_scalar_multiply (integral, scalar)
- type(mqc_scf_integral) function mqc_est::mqc_integral_eigenvalues_multiply (integralA, eigenvaluesB, label)
- type(mqc_scf_integral) function mqc_est::mqc_eigenvalues_integral_multiply (eigenvaluesA, integralB, label)
- type(mqc_scf_eigenvalues) function mqc_est::mqc_eigenvalues_eigenvalues_multiply (eigenvaluesA, eigenvaluesB, label)
- type(mqc_scalar) function mqc_est::mqc_eigenvalue_eigenvalue_dotproduct (eigenvalueA, eigenvalueB)
- type(mqc_scf_integral) function mqc_est::mqc_integral_transpose (integral, label)
- type(mqc_scf_integral) function mqc_est::mqc_integral_conjugate_transpose (integral, label)
- type(mqc_scalar) function mqc_est::mqc_integral_norm (integral, methodIn)
- subroutine mqc_est::mqc_matrix_spinblockghf (array, nelec, multi, elist)
- subroutine mqc_est::mqc_matrix_undospinblockghf_eigenvalues (eigenvaluesIn, vectorOut)
- subroutine mqc_est::mqc_matrix_undospinblockghf_integral (integralIn, matrixOut)
- type(mqc_scalar) function mqc_est::mqc_scf_integral_contraction (integral1, integral2)
- type(mqc_scf_integral) function mqc_est::mqc_eri_integral_contraction (eris, integral, label)
- subroutine mqc_est::mqc_scf_integral_generalized_eigensystem (integralA, integralB, eVals, rEVecs, lEVecs)
- subroutine mqc_est::mqc_scf_integral_diagonalize (integral, eVals, eVecs)
- type(mqc_scf_integral) function mqc_est::mqc_scf_integral_inverse (integral)
- type(mqc_scalar) function mqc_est::mqc_scf_integral_trace (integral)
- type(mqc_scalar) function mqc_est::mqc_scf_integral_determinant (integral)
- subroutine mqc_est::mqc_integral_set_energy_list (integral, elist)
- integer(kind=int64) function, dimension(:), allocatable mqc_est::mqc_integral_get_energy_list (integral)
- subroutine mqc_est::mqc_integral_delete_energy_list (integral)
- subroutine mqc_est::mqc_scf_eigenvalues_power (eigenvalues, power)
- type(mqc_scalar) function mqc_est::mqc_twoeris_at (twoERIs, i, j, k, l, spinBlock)
- type(mqc_scalar) function mqc_est::mqc_integral_at (integral, i, j, spinBlock)
- type(mqc_scalar) function mqc_est::mqc_eigenvalues_at (eigenvalues, i, spinBlock)
- subroutine mqc_est::mqc_scf_transformation_matrix (overlap, transform_matrix, nBasUse)
- subroutine mqc_est::gen_det_str (IOut, IPrint, NBasisIn, NAlphaIn, NBetaIn, Determinants, NCoreIn)
- type(mqc_scalar) function mqc_est::slater_condon (IOut, IPrint, NBasisIn, Determinants, L_A_String, L_B_String, R_A_String, R_B_String, Core_Hamiltonian, ERIs, UHF)
- subroutine mqc_est::twoeri_trans (IOut, IPrint, MO_Coeff, ERIs, MO_ERIs, UHF)
- subroutine mqc_est::mqc_build_ci_hamiltonian (IOut, IPrint, NBasis, Determinants, MO_Core_Ham, MO_ERIs, UHF, CI_Hamiltonian)
- type(mqc_matrix) function mqc_est::get_one_gamma_matrix (iOut, iPrint, nBasisIn, nState, determinants, ci_←amplitudes, nCoreIn, nOrbsIn)

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