MQCPack

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Chapter 1

Modules Index

1.1 Modules List

Here is a list of all modules with brief descriptions:

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Data Type Index

2.1 Class Hierarchy

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

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Data Type Index

3.1 Data Types List

Here are the data types with brief descriptions:

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File Index

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Here is a list of all files with brief descriptions:

Chapter 5

Module Documentation

5.1 mqc_algebra Module Reference

Data Types

- interface abs
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- interface aimag
- interface asin
- interface assignment(=)
- interface atan
- interface atan2
- interface cmplx
- interface conjg
- interface contraction
- interface cos
- interface dagger
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- interface mqc_cast_complex
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- interface mqc_print
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- interface mqc_set_array2vector
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- interface operator(*)

- interface operator(**)
- interface operator(+)
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- 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)

  Factorial returns the factorial of an integer
- integer(kind=int64) function bin_coeff (N, K)

  Bin_Coeff returns the binomial coefficient of (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)

  MQC_Deallocate_Scalar is used to deallocate a scalar type variable of the MQC_Scalar class
- logical function mqc_scalar_isallocated (Scalar)

  MQC_Scalar_IsAllocated is used to determine the allocation status of an MQC_Scalar
- subroutine mqc_input_integer_scalar (ScalarOut, ScalarIn)

  MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic integer to an MQC_Scalar
- subroutine mqc_input_real_scalar (ScalarOut, ScalarIn)

  MQC_Input_Real_Scalar is a subroutine is used to set an intrinsic real to an MQC_Scalar
- subroutine mqc_input_complex_scalar (ScalarOut, ScalarIn)

  MQC_Input_Complex_Scalar is a subroutine is used to set an intrinsic complex to an MQC_Scalar
- subroutine mqc_output_mqcscalar_scalar (ScalarOut, ScalarIn)

  MQC_Output MQCScalar_Scalar is a subroutine used to output an MQC_scalar equal to an MQC_Scalar
- subroutine mqc_output_integer_scalar (ScalarOut, ScalarIn)

  MQC_Output_Integer_Scalar is a subroutine used to output an intrinsic integer equal to an MQC_Scalar
- subroutine mqc_output_real_scalar (ScalarOut, ScalarIn)

  MQC_Output_Real_Scalar is a subroutine used to output an intrinsic real equal to an MQC_Scalar
- subroutine mqc_output_complex_scalar (ScalarOut, ScalarIn)

  MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic complex equal to an MQC_Scalar
- subroutine mqc_print_scalar_algebra1 (Scalar, IOut, Header, Blank_At_Top, Blank_At_Bottom)

MQC_Print_Scalar_Algebra1 is a subroutine used to print an MQC_Scalar

- type(mqc_scalar) function mqc_scalar_cmplx (Scalar1, Scalar2)

  MQC_Scalar_Cmplx is a function used to set a complex MQC_Scalar type variable from two other MQC_scalars
- type(mqc_scalar) function mqc_scalar_sqrt (Scalar)

  MQC_Scalar_Sqrt is a function used to return the square root of an MQC_scalar
- type(mqc_scalar) function mqc_scalar_sin (Scalar)

  MQC_Scalar_Sin is a function used to return the sine of an MQC_scalar
- type(mqc_scalar) function mqc_scalar_cos (Scalar)

  MQC_Scalar_Cos is a function used to return the cosine of an MQC_scalar
- type(mqc_scalar) function mqc_scalar_tan (Scalar)

  MQC_Scalar_Tan is a function used to return the tangent of an MQC_scalar
- type(mqc_scalar) function mqc_scalar_asin (Scalar)

  MQC_Scalar_ASin is a function used to return the arcsin of an MQC_scalar
- type(mqc_scalar) function mqc_scalar_acos (Scalar)

  MQC_Scalar_ACos is a function used to return the arccosine of an MQC_scalar
- type(mqc_scalar) function mqc_scalar_atan (Scalar)

  MQC_Scalar_ATan is a function used to return the arctangent of an MQC_scalar
- type(mqc_scalar) function mqc_scalar_atan2 (Scalar)

  MQC_Scalar_ATan2 is a function used to return the arctangent of an MQC_scalar accounting for quadrant of Argand diagram
- logical function mqc_scalar_havereal (Scalar)

  MQC_Scalar_HaveReal is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type real
- logical function mqc_scalar_haveinteger (Scalar)

  MQC_Scalar_HaveInteger is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type integer
- logical function mqc_scalar_havecomplex (Scalar)

  MQC_Scalar_HaveComplex is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type complex
- real(kind=real64) function mqc_scalar_get_intrinsic_real (Scalar)

  MQC_Scalar_Get_Intrinsic_Real is a function that returns the MQC_scalar value as an intrinsic real
- integer(kind=int64) function mqc_scalar_get_intrinsic_integer (Scalar)

  MQC_Scalar_Get_Intrinsic_Integer is a function that returns the MQC_scalar value as an intrinsic integer
- complex(kind=real64) function mqc_scalar_get_intrinsic_complex (Scalar)

  MQC_Scalar_Get_Intrinsic_Complex is a function that returns the MQC_scalar value as an intrinsic complex
- type(mqc_scalar) function mqc_scalar_get_abs_value (Scalar)

  MQC_Scalar_Get_ABS_Value is a function that returns the absolute value of MQC_scalar variable
- subroutine mqc_scalar_get_random_value (Scalar)

  MQC_Scalar_Get_Random_Value is a function that returns a random real value from a uniform distribution between zero and one
- type(mqc_scalar) function mqc_scalaradd (Scalar1, Scalar2)

  MQC_ScalarAdd is a function that sums two MQC_Scalar objects
- type(mqc_scalar) function mqc_scalarsubtract (Scalar1, Scalar2)

  MQC_ScalarSubtract is a function that subtracts two MQC_Scalar objects
- type(mqc_scalar) function mqc_scalarmultiply (Scalar1, Scalar2)

  MQC_ScalarMultiply is a function that multiplies two MQC_Scalar objects
- type(mqc_scalar) function mqc_scalardivide (Scalar1, Scalar2)

  MQC_ScalarDivide is a function that divides two MQC_Scalar objects

- type(mqc_scalar) function mqc_scalarexponent (Scalar1, Scalar2)

  MQC_ScalarExponent is a function that raises one MQC_Scalar to the power of another MQC_Scalar
- type(mqc_scalar) function mqc_scalarintegerexponent (Scalar, IntIn)

  MQC_ScalarIntegerExponent is a function that raises an MQC_Scalar to the power of an intrinsic integer
- type(mqc_scalar) function mqc_scalarrealexponent (Scalar, RealIn)

  MQC_ScalarRealExponent is a function that raises an MQC_Scalar to the power of an intrinsic real
- type(mqc_scalar) function mqc_scalarcomplexexponent (Scalar, CompIn)

  MQC_ScalarComplexExponent is a function that raises an MQC_Scalar to the power of an intrinsic complex
- logical function mqc_scalarne (Scalar1, Scalar2)

  MQC_ScalarNE is a function that returns TRUE if two MQC_Scalar variables are not equal
- logical function mqc_scalareq (Scalar1, Scalar2)

  MQC_ScalarEQ is a function that returns TRUE if two MQC_Scalar variables are equal
- logical function mqc_scalarlt (Scalar1, Scalar2)

  MQC_ScalarLT is a function that returns TRUE if the left MQC_Scalar is less than the right MQC_Scalar
- logical function mqc_realltscalar (RealIn, Scalar)

  MQC_RealLTScalar is a function that returns TRUE if an intrinsic real is less than a MQC_Scalar
- logical function mqc_scalarltreal (Scalar, RealIn)

  MQC_ScalarLTReal is a function that returns TRUE if a MQC_Scalar is less than an intrinsic real
- logical function mqc_scalargt (Scalar1, Scalar2)

  MQC_ScalarGT is a function that returns TRUE if the left MQC_Scalar is greater than the right MQC_Scalar
- logical function mqc_integergtscalar (IntIn, Scalar)

  MQC_IntegerGTScalar is a function that returns TRUE if an intrinsic integer is greater than a MQC_Scalar
- logical function mqc_scalargtinteger (Scalar, IntIn)

  MQC_ScalarGTInteger is a function that returns TRUE if a MQC_Scalar is greater than an intrinsic integer
- 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)
- type(mqc_matrix) function mqc_givens_matrix (m_size, angle, p, q)
- 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)

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 )
```

Bin_Coeff returns the binomial coefficient of (n,k)

Purpose:

```
Bin_Coeff is a function that returns the binomial coefficient given input
integer N and input integer K corresponding to N choose K.
```

Parameters

in	*N*	N is Integer(kind=int64) The number of objects
in	*K*	K is Integer(kind=int64) The number of permutations

Author

L. M. Thompson

Date

2016

5.1.1.2 factorial()

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

Factorial returns the factorial of an integer

Purpose:

Factorial is a function that returns the factorial of an integer.

Parameters

in	N	N is Integer(kind=int64) The argument of the factorial function

Author

L. M. Thompson

Date

2016

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

L. M. Thompson

Date

2016

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 )
```

MQC_Deallocate_Scalar is used to deallocate a scalar type variable of the MQC_Scalar class

Purpose:

MQC_Deallocate_Scalar is a subroutine used to deallocate a scalar type variable of the MQC_Scalar class.

Parameters

in,out	*Scalar*	Scalar is Type(MQC_Scalar) The name of the MQC_Scalar variable to deallocate

Author

L. M. Thompson

Date

2016

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 )
```

MQC_Input_Complex_Scalar is a subroutine is used to set an intrinsic complex to an MQC_Scalar

Purpose:

MQC_Input_Complex_Scalar is a subroutine is used to set an intrinsic complex to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Type(MQC_Scalar) The name of the output variable
in	*ScalarIn*	ScalarIn is Complex(kind=real64) The value of the input variable

Author

L. M. Thompson

Date

2017

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 integer to an MQC_Scalar

Purpose:

MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic integer 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 )
```

MQC_Input_Real_Scalar is a subroutine is used to set an intrinsic real to an MQC_Scalar

Purpose:

MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic real to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Type(MQC_Scalar) The name of the output variable
in	*ScalarIn*	ScalarIn is Real(kind=real64) The value of the input variable

Author

L. M. Thompson

Date

2016

5.1.1.27 mqc_integergtscalar()

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

MQC_IntegerGTScalar is a function that returns TRUE if an intrinsic integer is greater than a MQC_Scalar

Purpose:

MQC_IntegerGTScalar is a function that returns TRUE if an intrinsic integer is greater than a MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the intrinsic integer is greater than the real part of the MQC_Scalar and FALSE if the intrinsic integer is less than the real part of the MQC_Scalar. If the intrinsic integer is equal to the real part of the MQC_Scalar, the function returns TRUE if the imaginary part of MQC_Scalar is less than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*IntIn*	IntIn is Integer(kind=int64) The intrinsic integer that will be tested.
in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2019

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

2017

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 )
```

MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic complex equal to an MQC_Scalar

Purpose:

MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic complex equal to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Complex(kind=real64) The name of the output variable
in	*ScalarIn*	ScalarIn is Type(MQC_Scalar) The value of the input variable

Author

L. M. Thompson

Date

2017

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 )
```

MQC_Output_Integer_Scalar is a subroutine used to output an intrinsic integer equal to an MQC_Scalar

Purpose:

MQC_Output_Integer_Scalar is a subroutine used to output an intrinsic integer equal to an MQC_Scalar.

Parameters

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

Author

L. M. Thompson

Date

2016

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 )
```

MQC_Output MQCScalar_Scalar is a subroutine used to output an MQC_scalar equal to an MQC_Scalar

Purpose:

MQC_Output_MQCScalar_Scalar is a subroutine used to output an MQC_scalar equal to an MQC_Scalar.

Parameters

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

Author

L. M. Thompson

Date

2016

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 )
```

MQC_Output_Real_Scalar is a subroutine used to output an intrinsic real equal to an MQC_Scalar

Purpose:

MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic real equal to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Real(kind=real64) The name of the output variable
in	*ScalarIn*	ScalarIn is Type(MQC_Scalar) The value of the input variable

Author

L. M. Thompson

Date

2016

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 )
```

MQC_Print_Scalar_Algebra1 is a subroutine used to print an MQC_Scalar

Purpose:

MQC_Print_Scalar_Algebra1 is a subroutine used to print an MQC_Scalar. Blank_At_Top and Blank_At_Bottom are optional logical arguments to print blank lines before or after output.

Parameters

in	*Scalar*	Scalar is Class(MQC_Scalar) The variable to be printed
in	*IOut*	IOut is Integer(kind=int64) The Fortran file number to print to
in	*Header*	Header is Character(Len=*) The title to print along with Scalar
in	*Blank_At_Top*	Blank_At_Top is Logical,Optional = .True.: print blank line above output = .False.: do not print blank line above output
in	*Blank_At_Bottom*	Blank_At_Bottom is Logical,Optional = .True.: print blank line below output = .False.: do not print blank line below output

Author

L. M. Thompson

Date

2016

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 )
```

MQC_RealLTScalar is a function that returns TRUE if an intrinsic real is less than a MQC_Scalar

Purpose:

MQC_RealLTScalar is a function that returns TRUE if an intrinsic real is less than a MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the intrinsic real is less than the real part of the MQC_Scalar and FALSE if the intrinsic real is greater than the real part of the MQC_Scalar. If the intrinsic real is equal to the real part of the MQC_Scalar, the function returns TRUE if the imaginary part of MQC_Scalar is greater than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*RealIn*	RealIn is Real(kind=real64) The intrinsic real that will be tested.
in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2019

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 )
```

MQC_Scalar_ACos is a function used to return the arccosine of an MQC_scalar

Purpose:

MQC_Scalar_ACos is a function used to return the arccosine of an MQC_scalar.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

5.1.1.123 mqc_scalar_asin()

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

MQC_Scalar_ASin is a function used to return the arcsin of an MQC_scalar

Purpose:

MQC_Scalar_ASin is a function used to return the arcsin of an MQC_scalar.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

5.1.1.124 mqc_scalar_atan()

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

MQC_Scalar_ATan is a function used to return the arctangent of an MQC_scalar

Purpose:

MQC_Scalar_ATan is a function used to return the arctangent of an MQC_scalar.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

5.1.1.125 mqc_scalar_atan2()

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

MQC_Scalar_ATan2 is a function used to return the arctangent of an MQC_scalar accounting for quadrant of Argand diagram

Purpose:

MQC_Scalar_ATan2 is a function used to return the arctangent of an MQC_scalar accounting for quadrant of Argand diagram.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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 )
```

MQC_Scalar_Cmplx is a function used to set a complex MQC_Scalar type variable from two other MQC_scalars

Purpose:

```
MQC_Scalar_Cmplx is a function used to set a complex MQC_Scalar type variable
from two other MQC_Scalar variables.
```

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The real part of MQC_Scalar_Cmplx
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The imaginary part of MQC_Scalar_Cmplx

Author

L. M. Thompson

Date

2019

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 )
```

MQC_Scalar_Cos is a function used to return the cosine of an MQC_scalar

Purpose:

MQC_Scalar_Cos is a function used to return the cosine of an MQC_scalar.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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 )
```

MQC_Scalar_Get_ABS_Value is a function that returns the absolute value of MQC_scalar variable

Purpose:

```
MQC_Scalar_Get_ABS_Value is a function that returns the absolute value
of MQC_scalar variable.
```

Parameters

in	*Scalar*	Scalar is Class(MQC_Scalar) The MQC_Scalar to be tested

Author

A. Mahler

Date

2018

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 )
```

MQC_Scalar_Get_Intrinsic_Complex is a function that returns the MQC_scalar value as an intrinsic complex

Purpose:

```
MQC_Scalar_Get_Intrinsic_Complex is a function that returns the MQC_scalar
value as an intrinsic complex.
```

Parameters

in	*Scalar*	Scalar is Class(MQC_Scalar) The MQC_Scalar to be tested

Author

L. M. Thompson

Date

2017

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 )
```

MQC_Scalar_Get_Intrinsic_Integer is a function that returns the MQC_scalar value as an intrinsic integer

Purpose:

```
MQC_Scalar_Get_Intrinsic_Integer is a function that returns the MQC_scalar
value as an intrinsic integer.
```

Parameters

in	*Scalar*	Scalar is Class(MQC_Scalar) The MQC_Scalar to be tested

Author

L. M. Thompson

Date

2017

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 )
```

MQC_Scalar_Get_Intrinsic_Real is a function that returns the MQC_scalar value as an intrinsic real

Purpose:

```
MQC_Scalar_Get_Intrinsic_Real is a function that returns the MQC_scalar
value as an intrinsic real.
```

Parameters

in	*Scalar*	Scalar is Class(MQC_Scalar) The MQC_Scalar to be tested

Author

L. M. Thompson

Date

2017

5.1.1.135 mqc_scalar_get_random_value()

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

MQC_Scalar_Get_Random_Value is a function that returns a random real value from a uniform distribution between zero and one

Purpose:

```
MQC_Scalar_Get_Random_Value is a function that returns a random real
value from a uniform distribution between zero and one.
```

Parameters

in,out	*Scalar*	Scalar is Class(MQC_Scalar) The MQC_Scalar to be filled

Author

X. Dong

Date

2019

5.1.1.136 mqc_scalar_havecomplex()

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

MQC_Scalar_HaveComplex is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type complex

Purpose:

MQC_Scalar_HaveComplex is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type complex.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar to be tested

Author

L. M. Thompson

Date

2017

5.1.1.137 mqc_scalar_haveinteger()

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

MQC_Scalar_HaveInteger is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type integer

Purpose:

MQC_Scalar_HaveInteger is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type integer.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar to be tested

Author

L. M. Thompson

Date

2017

5.1.1.138 mqc_scalar_havereal()

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

MQC_Scalar_HaveReal is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type real

Purpose:

```
MQC_Scalar_HaveReal is a function that returns TRUE or FALSE indicating
whether an MQC_scalar is of type real.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar to be tested

Author

L. M. Thompson

Date

2017

5.1.1.139 mqc_scalar_isallocated()

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

MQC_Scalar_IsAllocated is used to determine the allocation status of an MQC_Scalar

Purpose:

MQC_Scalar_IsAllocated is a subroutine used to determine the allocation status of an MQC_Scalar.

Parameters

in,out	*Scalar*	Scalar is Type(MQC_Scalar) The name of the MQC_Scalar variable to check allocation status

Author

L. M. Thompson

Date

2017

5.1.1.140 mqc_scalar_sin()

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

MQC_Scalar_Sin is a function used to return the sine of an MQC_scalar

Purpose:

MQC_Scalar_Sin is a function used to return the sine of an MQC_scalar.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

5.1.1.141 mqc_scalar_sqrt()

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

MQC_Scalar_Sqrt is a function used to return the square root of an MQC_scalar

Purpose:

MQC_Scalar_Sqrt is a function used to return the square root of an MQC_scalar.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2016

5.1.1.142 mqc_scalar_tan()

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

MQC_Scalar_Tan is a function used to return the tangent of an MQC_scalar

Purpose:

MQC_Scalar_Tan is a function used to return the tangent of an MQC_scalar.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarAdd is a function that sums two MQC_Scalar objects

Purpose:

MQC_ScalarAdd is a function that sums two MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar to be summed
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar to be summed

Author

L. M. Thompson

Date

2016

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 )
```

MQC_ScalarComplexExponent is a function that raises an MQC_Scalar to the power of an intrinsic complex

Purpose:

MQC_ScalarComplexExponent is a function that raises an MQC_Scalar to the power of an intrinsic complex.

Parameters

in	*Scalar*	Scalar1 is Type(MQC_Scalar) The base value
in	*CompIn*	CompIn is Complex(kind=real64) The power value

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarDivide is a function that divides two MQC_Scalar objects

Purpose:

MQC_ScalarDivide is a function that divides MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The numerator
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The denominator

Author

L. M. Thompson

Date

2016

5.1.1.150 mqc_scalareq()

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

MQC_ScalarEQ is a function that returns TRUE if two MQC_Scalar variables are equal

Purpose:

```
MQC_ScalarEQ is a function that returns TRUE if two MQC_Scalar variables
are equal.
```

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

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 )
```

MQC_ScalarExponent is a function that raises one MQC_Scalar to the power of another MQC_Scalar

Purpose:

```
MQC_ScalarExponent is a function that raises one MQC_Scalar to the power of
another MQC_Scalar.
```

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The base value
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The power value

Author

L. M. Thompson

Date

2016

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 )
```

MQC_ScalarGT is a function that returns TRUE if the left MQC_Scalar is greater than the right MQC_Scalar

Purpose:

MQC_ScalarGT is a function that returns TRUE if the left MQC_Scalar is greater than the right MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the left real part is greater than the right real part and FALSE if the left real part is less than the right real part. If the left real part is equal to the right real part, the function returns TRUE if the left imaginary part is greater than the right imaginary part and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

5.1.1.154 mqc_scalargtinteger()

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

MQC_ScalarGTInteger is a function that returns TRUE if a MQC_Scalar is greater than an intrinsic integer

Purpose:

MQC_ScalarGTInteger is a function that returns TRUE if a MQC_Scalar is greater than an intrinsic integer.

When dealing with complex numbers, the function returns TRUE if the real part of the MQC_Scalar is greater than the intrinsic integer and FALSE if the real part of the MQC_Scalar is less than the intrinsic integer. If the real part of the MQC_Scalar is equal to the intrinsic integer, the function returns TRUE if the imaginary part of MQC_Scalar is greater than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.
in	*IntIn*	IntIn is Integer(kind=int64) The intrinsic integer that will be tested.

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarIntegerExponent is a function that raises an MQC_Scalar to the power of an intrinsic integer

Purpose:

MQC_ScalarIntegerExponent is a function that raises an MQC_Scalar to the power of an intrinsic integer.

Parameters

in	*Scalar*	Scalar1 is Type(MQC_Scalar) The base value
in	*IntIn*	IntIn is Integer(kind=int64) The power value

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarLT is a function that returns TRUE if the left MQC_Scalar is less than the right MQC_Scalar

Purpose:

MQC_ScalarLT is a function that returns TRUE if the left MQC_Scalar is less than the right MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the left real part is less than the right real part and FALSE if the left real part is greater than the right real part. If the left real part is equal to the right real part, the function returns TRUE if the left imaginary part is less than the right imaginary part and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

5.1.1.165 mqc_scalarltreal()

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

MQC_ScalarLTReal is a function that returns TRUE if a MQC_Scalar is less than an intrinsic real

Purpose:

MQC_ScalarLTReal is a function that returns TRUE if a MQC_Scalar is less than an intrinsic real.

When dealing with complex numbers, the function returns TRUE if the real part of the MQC_Scalar is less than the intrinsic real and FALSE if the real part of the MQC_Scalar is greater than the intrinsic real. If the real part of the MQC_Scalar is equal to the intrinsic real, the function returns TRUE if the imaginary part of MQC_Scalar is less than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.
in	*RealIn*	RealIn is Real(kind=real64) The intrinsic real that will be tested.

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarMultiply is a function that multiplies two MQC_Scalar objects

Purpose:

MQC_ScalarMultiply is a function that multiplies two MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar to be multiplied
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar to be multiplied

Author

L. M. Thompson

Date

2016

5.1.1.168 mqc_scalarne()

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

MQC_ScalarNE is a function that returns TRUE if two MQC_Scalar variables are not equal

Purpose:

MQC_ScalarNE is a function that returns TRUE if two MQC_Scalar variables
are not equal.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

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 )
```

MQC_ScalarRealExponent is a function that raises an MQC_Scalar to the power of an intrinsic real

Purpose:

MQC_ScalarRealExponent is a function that raises an MQC_Scalar to the power of an intrinsic real.

Parameters

in	*Scalar*	Scalar1 is Type(MQC_Scalar) The base value
in	*RealIn*	RealIn is Real(kind=real64) The power value

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarSubtract is a function that subtracts two MQC_Scalar objects

Purpose:

MQC_ScalarSubtract is a function that subtracts two MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar from which Scalar2 will be subtracted
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar which will be subtracted from Scalar1

Author

L. M. Thompson

Date

2016

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)

  MQC_Scalar_Get_ABS_Value is a function that returns the absolute value of MQC_scalar variable
- 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 )
```

MQC_Scalar_Get_ABS_Value is a function that returns the absolute value of MQC_scalar variable

Purpose:

```
MQC_Scalar_Get_ABS_Value is a function that returns the absolute value
of MQC_scalar variable.
```

Parameters

in	*Scalar*	Scalar is Class(MQC_Scalar) The MQC_Scalar to be tested

Author

A. Mahler

Date

2018

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)
  MQC_Scalar_ACos is a function used to return the arccosine of an MQC_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 )
```

MQC_Scalar_ACos is a function used to return the arccosine of an MQC_scalar

Purpose:

```
MQC_Scalar_ACos is a function used to return the arccosine of an MQC_scalar.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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)

  MQC_Scalar_ASin is a function used to return the arcsin of an MQC_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 )
```

MQC_Scalar_ASin is a function used to return the arcsin of an MQC_scalar

Purpose:

```
MQC_Scalar_ASin is a function used to return the arcsin of an MQC_scalar.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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 integer to an MQC_Scalar
- subroutine mqc_input_real_scalar (ScalarOut, ScalarIn)

  MQC_Input_Real_Scalar is a subroutine is used to set an intrinsic real to an MQC_Scalar
- subroutine mqc_input_complex_scalar (ScalarOut, ScalarIn)

  MQC_Input_Complex_Scalar is a subroutine is used to set an intrinsic complex to an MQC_Scalar
- subroutine mqc_output_mqcscalar_scalar (ScalarOut, ScalarIn)

  MQC_Output MQCScalar_Scalar is a subroutine used to output an MQC_scalar equal to an MQC_Scalar
- subroutine mqc_output_integer_scalar (ScalarOut, ScalarIn)

  MQC_Output_Integer_Scalar is a subroutine used to output an intrinsic integer equal to an MQC_Scalar
- subroutine mqc_output_real_scalar (ScalarOut, ScalarIn)

  MQC_Output_Real_Scalar is a subroutine used to output an intrinsic real equal to an MQC_Scalar
- subroutine mqc_output_complex_scalar (ScalarOut, ScalarIn)

  MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic complex equal to an MQC_Scalar
- 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 )
```

MQC_Input_Complex_Scalar is a subroutine is used to set an intrinsic complex to an MQC_Scalar

Purpose:

MQC_Input_Complex_Scalar is a subroutine is used to set an intrinsic complex to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Type(MQC_Scalar) The name of the output variable
in	*ScalarIn*	ScalarIn is Complex(kind=real64) The value of the input variable

Author

L. M. Thompson

Date

2017

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 integer to an MQC_Scalar

Purpose:

MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic integer 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 )
```

MQC_Input_Real_Scalar is a subroutine is used to set an intrinsic real to an MQC_Scalar

Purpose:

MQC_Input_Integer_Scalar is a subroutine is used to set an intrinsic real to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Type(MQC_Scalar) The name of the output variable
in	*ScalarIn*	ScalarIn is Real(kind=real64) The value of the input variable

Author

L. M. Thompson

Date

2016

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 )
```

MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic complex equal to an MQC_Scalar

Purpose:

MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic complex equal to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Complex(kind=real64) The name of the output variable
in	*ScalarIn*	ScalarIn is Type(MQC_Scalar) The value of the input variable

Author

L. M. Thompson

Date

2017

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 )
```

MQC_Output_Integer_Scalar is a subroutine used to output an intrinsic integer equal to an MQC_Scalar

Purpose:

MQC_Output_Integer_Scalar is a subroutine used to output an intrinsic integer equal to an MQC_Scalar.

Parameters

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

Author

L. M. Thompson

Date

2016

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 )
```

MQC_Output MQCScalar_Scalar is a subroutine used to output an MQC_scalar equal to an MQC_Scalar

Purpose:

MQC_Output_MQCScalar_Scalar is a subroutine used to output an MQC_scalar equal to an MQC_Scalar.

Parameters

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

Author

L. M. Thompson

Date

2016

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 )
```

MQC_Output_Real_Scalar is a subroutine used to output an intrinsic real equal to an MQC_Scalar

Purpose:

MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic real equal to an MQC_Scalar.

Parameters

in,out	*ScalarOut*	ScalarOut is Real(kind=real64) The name of the output variable
in	*ScalarIn*	ScalarIn is Type(MQC_Scalar) The value of the input variable

Author

L. M. Thompson

Date

2016

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)
  MQC_Scalar_ATan is a function used to return the arctangent of an MQC_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 )
```

MQC_Scalar_ATan is a function used to return the arctangent of an MQC_scalar

Purpose:

```
MQC_Scalar_ATan is a function used to return the arctangent of an MQC_scalar.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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)

  MQC_Scalar_ATan2 is a function used to return the arctangent of an MQC_scalar accounting for quadrant of Argand diagram

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 )
```

MQC_Scalar_ATan2 is a function used to return the arctangent of an MQC_scalar accounting for quadrant of Argand diagram

Purpose:

```
MQC_Scalar_ATan2 is a function used to return the arctangent of an MQC_scalar
accounting for quadrant of Argand diagram.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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)

  MQC_Scalar_Cmplx is a function used to set a complex MQC_Scalar type variable from two other MQC_scalars
- 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 )
```

MQC_Scalar_Cmplx is a function used to set a complex MQC_Scalar type variable from two other MQC_scalars

Purpose:

```
MQC_Scalar_Cmplx is a function used to set a complex MQC_Scalar type variable
from two other MQC_Scalar variables.
```

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The real part of MQC_Scalar_Cmplx
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The imaginary part of MQC_Scalar_Cmplx

Author

L. M. Thompson

Date

2019

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)

  MQC_Scalar_Cos is a function used to return the cosine of an MQC_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 )
```

MQC_Scalar_Cos is a function used to return the cosine of an MQC_scalar

Purpose:

```
MQC_Scalar_Cos is a function used to return the cosine of an MQC_scalar.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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)

  MQC_Print_Scalar_Algebra1 is a subroutine used to print an MQC_Scalar
- 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 )
```

MQC_Print_Scalar_Algebra1 is a subroutine used to print an MQC_Scalar

Purpose:

MQC_Print_Scalar_Algebra1 is a subroutine used to print an MQC_Scalar. Blank_At_Top and Blank_At_Bottom are optional logical arguments to print blank lines before or after output.

Parameters

in	*Scalar*	Scalar is Class(MQC_Scalar) The variable to be printed
in	*IOut*	IOut is Integer(kind=int64) The Fortran file number to print to
in	*Header*	Header is Character(Len=*) The title to print along with Scalar
in	*Blank_At_Top*	Blank_At_Top is Logical,Optional = .True.: print blank line above output = .False.: do not print blank line above output
in	*Blank_At_Bottom*	Blank_At_Bottom is Logical,Optional = .True.: print blank line below output = .False.: do not print blank line below output

Author

L. M. Thompson

Date

2016

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()

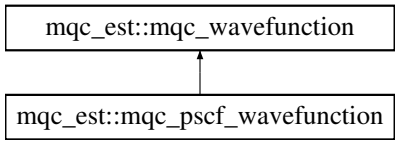
```
subroutine mqc_est::mqc_print::mqc_print_wavefunction (
             class(mqc_wavefunction) wavefunction,
             integer(kind=int64), intent(in) iOut,
             character(len=*), intent(in), optional label )
```

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

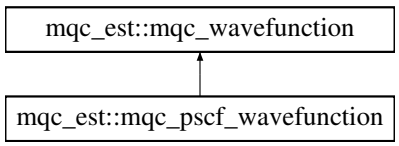
```
real(kind=real64), dimension(:), allocatable mqc_algebra::mqc_vector::vecr
```

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)

  MQC_ScalarMultiply is a function that multiplies two MQC_Scalar objects
- 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 )
```

MQC_ScalarMultiply is a function that multiplies two MQC_Scalar objects

Purpose:

MQC_ScalarMultiply is a function that multiplies two MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar to be multiplied
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar to be multiplied

Author

L. M. Thompson

Date

2016

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)

  MQC_ScalarExponent is a function that raises one MQC_Scalar to the power of another MQC_Scalar
- type(mqc_scalar) function mqc_scalarintegerexponent (Scalar, IntIn)

  MQC_ScalarIntegerExponent is a function that raises an MQC_Scalar to the power of an intrinsic integer
- type(mqc_scalar) function mqc_scalarrealexponent (Scalar, RealIn)

  MQC_ScalarRealExponent is a function that raises an MQC_Scalar to the power of an intrinsic real
- type(mqc_scalar) function mqc_scalarcomplexexponent (Scalar, CompIn)

  MQC_ScalarComplexExponent is a function that raises an MQC_Scalar to the power of an intrinsic complex

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 )
```

MQC_ScalarComplexExponent is a function that raises an MQC_Scalar to the power of an intrinsic complex

Purpose:

```
MQC_ScalarComplexExponent is a function that raises an MQC_Scalar to the power of an
intrinsic complex.
```

Parameters

in	*Scalar*	Scalar1 is Type(MQC_Scalar) The base value
in	*CompIn*	CompIn is Complex(kind=real64) The power value

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarExponent is a function that raises one MQC_Scalar to the power of another MQC_Scalar

Purpose:

MQC_ScalarExponent is a function that raises one MQC_Scalar to the power of another MQC_Scalar.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The base value
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The power value

Author

L. M. Thompson

Date

2016

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 )
```

MQC_ScalarIntegerExponent is a function that raises an MQC_Scalar to the power of an intrinsic integer

Purpose:

MQC_ScalarIntegerExponent is a function that raises an MQC_Scalar to the power of an intrinsic integer.

Parameters

in	*Scalar*	Scalar1 is Type(MQC_Scalar) The base value
in	*IntIn*	IntIn is Integer(kind=int64) The power value

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarRealExponent is a function that raises an MQC_Scalar to the power of an intrinsic real

Purpose:

MQC_ScalarRealExponent is a function that raises an MQC_Scalar to the power of an intrinsic real.

Parameters

in	*Scalar*	Scalar1 is Type(MQC_Scalar) The base value
in	*RealIn*	RealIn is Real(kind=real64) The power value

Author

L. M. Thompson

Date

2019

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)

  MQC_ScalarAdd is a function that sums two MQC_Scalar objects
- 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 )
```

MQC_ScalarAdd is a function that sums two MQC_Scalar objects

Purpose:

MQC_ScalarAdd is a function that sums two MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar to be summed
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar to be summed

Author

L. M. Thompson

Date

2016

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)

  MQC_ScalarSubtract is a function that subtracts two MQC_Scalar objects
- 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 )
```

MQC_ScalarSubtract is a function that subtracts two MQC_Scalar objects

Purpose:

MQC_ScalarSubtract is a function that subtracts two MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar from which Scalar2 will be subtracted
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar which will be subtracted from Scalar1

Author

L. M. Thompson

Date

2016

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)

  MQC_ScalarEQ is a function that returns TRUE if two MQC_Scalar variables are equal

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 )
```

MQC_ScalarEQ is a function that returns TRUE if two MQC_Scalar variables are equal

Purpose:

```
MQC_ScalarEQ is a function that returns TRUE if two MQC_Scalar variables
are equal.
```

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

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)

  MQC_ScalarGT is a function that returns TRUE if the left MQC_Scalar is greater than the right MQC_Scalar
- logical function mqc_scalargtinteger (Scalar, IntIn)

  MQC_ScalarGTInteger is a function that returns TRUE if a MQC_Scalar is greater than an intrinsic integer
- logical function mqc_integergtscalar (IntIn, Scalar)

  MQC_IntegerGTScalar is a function that returns TRUE if an intrinsic integer is greater than a MQC_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 )
```

MQC_IntegerGTScalar is a function that returns TRUE if an intrinsic integer is greater than a MQC_Scalar

Purpose:

MQC_IntegerGTScalar is a function that returns TRUE if an intrinsic integer is greater than a MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the intrinsic integer is greater than the real part of the MQC_Scalar and FALSE if the intrinsic integer is less than the real part of the MQC_Scalar. If the intrinsic integer is equal to the real part of the MQC_Scalar, the function returns TRUE if the imaginary part of MQC_Scalar is less than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*IntIn*	IntIn is Integer(kind=int64) The intrinsic integer that will be tested.
in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarGT is a function that returns TRUE if the left MQC_Scalar is greater than the right MQC_Scalar

Purpose:

MQC_ScalarGT is a function that returns TRUE if the left MQC_Scalar is greater than the right MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the left real part is greater than the right real part and FALSE if the left real part is less than the right real part. If the left real part is equal to the right real part, the function returns TRUE if the left imaginary part is greater than the right imaginary part and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

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 )
```

MQC_ScalarGTInteger is a function that returns TRUE if a MQC_Scalar is greater than an intrinsic integer

Purpose:

MQC_ScalarGTInteger is a function that returns TRUE if a MQC_Scalar is greater than an intrinsic integer.

When dealing with complex numbers, the function returns TRUE if the real part of the MQC_Scalar is greater than the intrinsic integer and FALSE if the real part of the MQC_Scalar is less than the intrinsic integer. If the real part of the MQC_Scalar is equal to the intrinsic integer, the function returns TRUE if the imaginary part of MQC_Scalar is greater than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.
in	*IntIn*	IntIn is Integer(kind=int64) The intrinsic integer that will be tested.

Author

L. M. Thompson

Date

2019

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)

  MQC_ScalarLT is a function that returns TRUE if the left MQC_Scalar is less than the right MQC_Scalar
- logical function mqc_scalarltreal (Scalar, RealIn)

  MQC_ScalarLTReal is a function that returns TRUE if a MQC_Scalar is less than an intrinsic real
- logical function mqc_realltscalar (RealIn, Scalar)

  MQC_RealLTScalar is a function that returns TRUE if an intrinsic real is less than a MQC_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 )
```

MQC_RealLTScalar is a function that returns TRUE if an intrinsic real is less than a MQC_Scalar

Purpose:

MQC_RealLTScalar is a function that returns TRUE if an intrinsic real is less than a MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the intrinsic real is less than the real part of the MQC_Scalar and FALSE if the intrinsic real is greater than the real part of the MQC_Scalar. If the intrinsic real is equal to the real part of the MQC_Scalar, the function returns TRUE if the imaginary part of MQC_Scalar is greater than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*RealIn*	RealIn is Real(kind=real64) The intrinsic real that will be tested.
in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2019

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 )
```

MQC_ScalarLT is a function that returns TRUE if the left MQC_Scalar is less than the right MQC_Scalar

Purpose:

MQC_ScalarLT is a function that returns TRUE if the left MQC_Scalar is less than the right MQC_Scalar.

When dealing with complex numbers, the function returns TRUE if the left real part is less than the right real part and FALSE if the left real part is greater than the right real part. If the left real part is equal to the right real part, the function returns TRUE if the left imaginary part is less than the right imaginary part and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

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 )
```

MQC_ScalarLTReal is a function that returns TRUE if a MQC_Scalar is less than an intrinsic real

Purpose:

MQC_ScalarLTReal is a function that returns TRUE if a MQC_Scalar is less than an intrinsic real.

When dealing with complex numbers, the function returns TRUE if the real part of the MQC_Scalar is less than the intrinsic real and FALSE if the real part of the MQC_Scalar is greater than the intrinsic real. If the real part of the MQC_Scalar is equal to the intrinsic real, the function returns TRUE if the imaginary part of MQC_Scalar is less than zero and FALSE otherwise. Note that this is the same procedure used in python.

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The MQC_Scalar that will be tested.
in	*RealIn*	RealIn is Real(kind=real64) The intrinsic real that will be tested.

Author

L. M. Thompson

Date

2019

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)

  MQC_ScalarNE is a function that returns TRUE if two MQC_Scalar variables are not equal

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 )
```

MQC_ScalarNE is a function that returns TRUE if two MQC_Scalar variables are not equal

Purpose:

```
MQC_ScalarNE is a function that returns TRUE if two MQC_Scalar variables
are not equal.
```

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The first MQC_Scalar that will be tested.
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The second MQC_Scalar that will be tested.

Author

L. M. Thompson

Date

2016

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)

  MQC_ScalarDivide is a function that divides two MQC_Scalar objects
- 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 )
```

MQC_ScalarDivide is a function that divides two MQC_Scalar objects

Purpose:

MQC_ScalarDivide is a function that divides MQC_Scalar objects.

Parameters

in	*Scalar1*	Scalar1 is Type(MQC_Scalar) The numerator
in	*Scalar2*	Scalar2 is Type(MQC_Scalar) The denominator

Author

L. M. Thompson

Date

2016

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)

  MQC_Scalar_Sin is a function used to return the sine of an MQC_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 )
```

MQC_Scalar_Sin is a function used to return the sine of an MQC_scalar

Purpose:

```
MQC_Scalar_Sin is a function used to return the sine of an MQC_scalar.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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)
  MQC_Scalar_Sqrt is a function used to return the square root of an MQC_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 )
```

MQC_Scalar_Sqrt is a function used to return the square root of an MQC_scalar

Purpose:

```
MQC_Scalar_Sqrt is a function used to return the square root of an MQC_scalar.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2016

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)
  MQC_Scalar_Tan is a function used to return the tangent of an MQC_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 )
```

MQC_Scalar_Tan is a function used to return the tangent of an MQC_scalar

Purpose:

```
MQC_Scalar_Tan is a function used to return the tangent of an MQC_scalar.
```

Parameters

in	*Scalar*	Scalar is Type(MQC_Scalar) The argument of the function

Author

L. M. Thompson

Date

2019

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)

  Factorial returns the factorial of an integer
- integer(kind=int64) function mqc_algebra::bin_coeff (N, K)

  Bin_Coeff returns the binomial coefficient of (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)

  MQC_Deallocate_Scalar is used to deallocate a scalar type variable of the MQC_Scalar class
- logical function mqc_algebra::mqc_scalar_isallocated (Scalar)

  MQC_Scalar_IsAllocated is used to determine the allocation status of an MQC_Scalar

- subroutine mqc_algebra::mqc_input_integer_scalar (ScalarOut, ScalarIn)

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

  MQC_Input_Real_Scalar is a subroutine is used to set an intrinsic real to an MQC_Scalar
- subroutine mqc_algebra::mqc_input_complex_scalar (ScalarOut, ScalarIn)

  MQC_Input_Complex_Scalar is a subroutine is used to set an intrinsic complex to an MQC_Scalar
- subroutine mqc_algebra::mqc_output_mqcscalar_scalar (ScalarOut, ScalarIn)

  MQC_Output MQCScalar_Scalar is a subroutine used to output an MQC_scalar equal to an MQC_Scalar
- subroutine mqc_algebra::mqc_output_integer_scalar (ScalarOut, ScalarIn)

  MQC_Output_Integer_Scalar is a subroutine used to output an intrinsic integer equal to an MQC_Scalar
- subroutine mqc_algebra::mqc_output_real_scalar (ScalarOut, ScalarIn)

  MQC_Output_Real_Scalar is a subroutine used to output an intrinsic real equal to an MQC_Scalar
- subroutine mqc_algebra::mqc_output_complex_scalar (ScalarOut, ScalarIn)

  MQC_Output_Complex_Scalar is a subroutine used to output an intrinsic complex equal to an MQC_Scalar
- subroutine mqc_algebra::mqc_print_scalar_algebra1 (Scalar, IOut, Header, Blank_At_Top, Blank_At_Bottom)

  MQC_Print_Scalar_Algebra1 is a subroutine used to print an MQC_Scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_cmplx (Scalar1, Scalar2)

  MQC_Scalar_Cmplx is a function used to set a complex MQC_Scalar type variable from two other MQC_scalars
- type(mqc_scalar) function mqc_algebra::mqc_scalar_sqrt (Scalar)

  MQC_Scalar_Sqrt is a function used to return the square root of an MQC_scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_sin (Scalar)

  MQC_Scalar_Sin is a function used to return the sine of an MQC_scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_cos (Scalar)

  MQC_Scalar_Cos is a function used to return the cosine of an MQC_scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_tan (Scalar)

  MQC_Scalar_Tan is a function used to return the tangent of an MQC_scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_asin (Scalar)

  MQC_Scalar_ASin is a function used to return the arcsin of an MQC_scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_acos (Scalar)

  MQC_Scalar_ACos is a function used to return the arccosine of an MQC_scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_atan (Scalar)

  MQC_Scalar_ATan is a function used to return the arctangent of an MQC_scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalar_atan2 (Scalar)

  MQC_Scalar_ATan2 is a function used to return the arctangent of an MQC_scalar accounting for quadrant of Argand diagram
- logical function mqc_algebra::mqc_scalar_havereal (Scalar)

  MQC_Scalar_HaveReal is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type real
- logical function mqc_algebra::mqc_scalar_haveinteger (Scalar)

  MQC_Scalar_HaveInteger is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type integer
- logical function mqc_algebra::mqc_scalar_havecomplex (Scalar)

  MQC_Scalar_HaveComplex is a function that returns TRUE or FALSE indicating whether an MQC_scalar is of type complex
- real(kind=real64) function mqc_algebra::mqc_scalar_get_intrinsic_real (Scalar)

  MQC_Scalar_Get_Intrinsic_Real is a function that returns the MQC_scalar value as an intrinsic real
- integer(kind=int64) function mqc_algebra::mqc_scalar_get_intrinsic_integer (Scalar)

  MQC_Scalar_Get_Intrinsic_Integer is a function that returns the MQC_scalar value as an intrinsic integer

- complex(kind=real64) function mqc_algebra::mqc_scalar_get_intrinsic_complex (Scalar)

  MQC_Scalar_Get_Intrinsic_Complex is a function that returns the MQC_scalar value as an intrinsic complex
- type(mqc_scalar) function mqc_algebra::mqc_scalar_get_abs_value (Scalar)

  MQC_Scalar_Get_ABS_Value is a function that returns the absolute value of MQC_scalar variable
- subroutine mqc_algebra::mqc_scalar_get_random_value (Scalar)

  MQC_Scalar_Get_Random_Value is a function that returns a random real value from a uniform distribution between zero and one
- type(mqc_scalar) function mqc_algebra::mqc_scalaradd (Scalar1, Scalar2)

  MQC_ScalarAdd is a function that sums two MQC_Scalar objects
- type(mqc_scalar) function mqc_algebra::mqc_scalarsubtract (Scalar1, Scalar2)

  MQC_ScalarSubtract is a function that subtracts two MQC_Scalar objects
- type(mqc_scalar) function mqc_algebra::mqc_scalarmultiply (Scalar1, Scalar2)

  MQC_ScalarMultiply is a function that multiplies two MQC_Scalar objects
- type(mqc_scalar) function mqc_algebra::mqc_scalardivide (Scalar1, Scalar2)

  MQC_ScalarDivide is a function that divides two MQC_Scalar objects
- type(mqc_scalar) function mqc_algebra::mqc_scalarexponent (Scalar1, Scalar2)

  MQC_ScalarExponent is a function that raises one MQC_Scalar to the power of another MQC_Scalar
- type(mqc_scalar) function mqc_algebra::mqc_scalarintegerexponent (Scalar, IntIn)

  MQC_ScalarIntegerExponent is a function that raises an MQC_Scalar to the power of an intrinsic integer
- type(mqc_scalar) function mqc_algebra::mqc_scalarrealexponent (Scalar, RealIn)

  MQC_ScalarRealExponent is a function that raises an MQC_Scalar to the power of an intrinsic real
- type(mqc_scalar) function mqc_algebra::mqc_scalarcomplexexponent (Scalar, CompIn)

  MQC_ScalarComplexExponent is a function that raises an MQC_Scalar to the power of an intrinsic complex
- logical function mqc_algebra::mqc_scalarne (Scalar1, Scalar2)

  MQC_ScalarNE is a function that returns TRUE if two MQC_Scalar variables are not equal
- logical function mqc_algebra::mqc_scalareq (Scalar1, Scalar2)

  MQC_ScalarEQ is a function that returns TRUE if two MQC_Scalar variables are equal
- logical function mqc_algebra::mqc_scalarlt (Scalar1, Scalar2)

  MQC_ScalarLT is a function that returns TRUE if the left MQC_Scalar is less than the right MQC_Scalar
- logical function mqc_algebra::mqc_realltscalar (RealIn, Scalar)

  MQC_RealLTScalar is a function that returns TRUE if an intrinsic real is less than a MQC_Scalar
- logical function mqc_algebra::mqc_scalarltreal (Scalar, RealIn)

  MQC_ScalarLTReal is a function that returns TRUE if a MQC_Scalar is less than an intrinsic real
- logical function mqc_algebra::mqc_scalargt (Scalar1, Scalar2)

  MQC_ScalarGT is a function that returns TRUE if the left MQC_Scalar is greater than the right MQC_Scalar
- logical function mqc_algebra::mqc_integergtscalar (IntIn, Scalar)

  MQC_IntegerGTScalar is a function that returns TRUE if an intrinsic integer is greater than a MQC_Scalar
- logical function mqc_algebra::mqc_scalargtinteger (Scalar, IntIn)

  MQC_ScalarGTInteger is a function that returns TRUE if a MQC_Scalar is greater than an intrinsic integer
- 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)
- type(mqc_matrix) function mqc_algebra::mqc_givens_matrix (m_size, angle, p, q)
- 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)

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, beta↩Alpha)
- 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, beta↩ OrbsIn, 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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