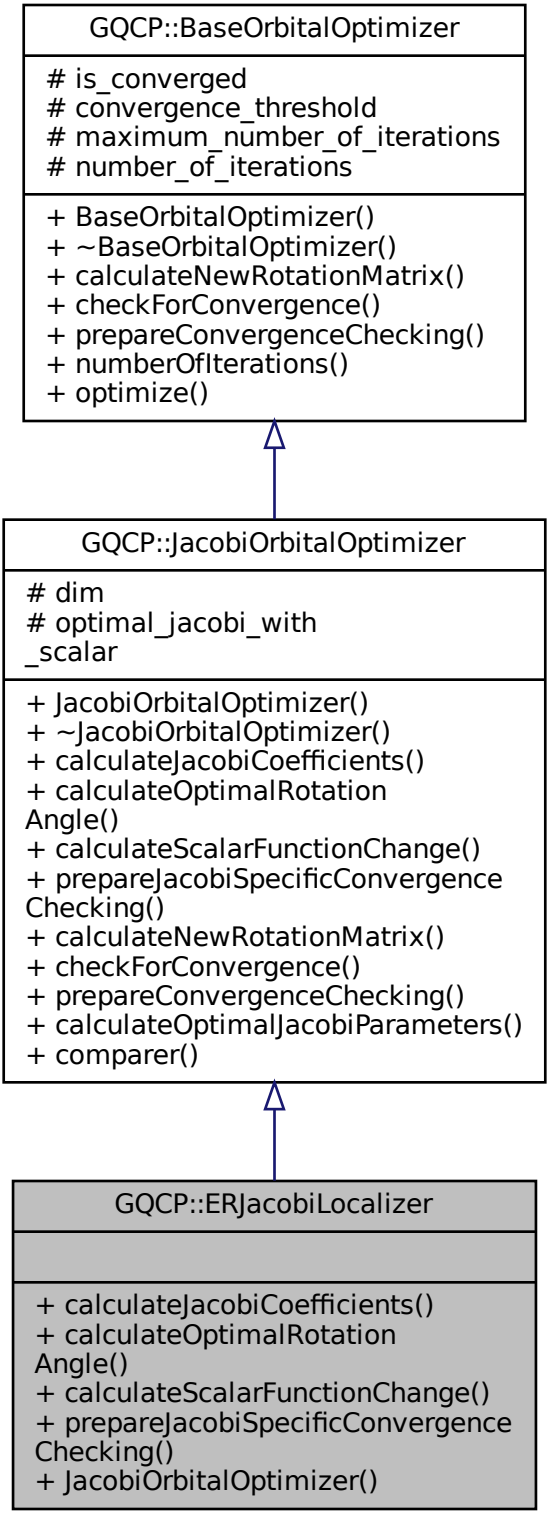
GQCP::BaseOrbitalOptimizer
is_converged
convergence_threshold
maximum_number_of_iterations
number_of_iterations
+ BaseOrbitalOptimizer()
+ ~BaseOrbitalOptimizer()
+ calculateNewRotationMatrix()
+ checkForConvergence()
+ prepareConvergenceChecking()
+ numberOfIterations()
+ optimize()
GQCP::JacobiOrbitalOptimizer
dim
optimal_jacobi_with
_scalar
+ JacobiOrbitalOptimizer()
+ ~JacobiOrbitalOptimizer()
+ calculateJacobiCoefficients()
+ calculateOptimalRotation
Angle()
+ calculateScalarFunctionChange()
+ prepareJacobiSpecificConvergence
Checking()
+ calculateNewRotationMatrix()
+ checkForConvergence()
+ prepareConvergenceChecking()
+ calculateOptimalJacobiParameters()
+ comparer()
GQCP::ERJacobiLocalizer
+ calculateJacobiCoefficients()
+ calculateOptimalRotation
Angle()
+ calculateScalarFunctionChange()
+ prepareJacobiSpecificConvergence
Checking()
+ JacobiOrbitalOptimizer()