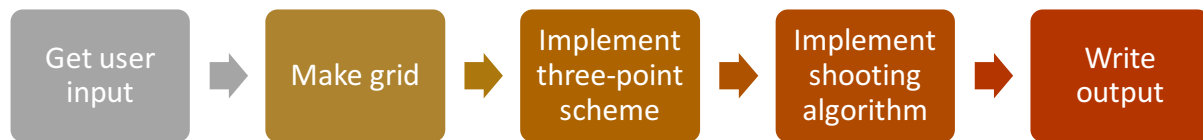


DESIGN PLAN



Get user input:

- subroutine ReadInput: reads in the number of gridpoints, the interval of the function and optionally which potential function is used.

Make grid:

- subroutine MakeGrid: set up an equidistant grid and store it in a datatype Grid
 - datatype Grid: array of the points, number of points, interval

Implement three-point scheme:

- subroutine ThreePointScheme: solves the differential equation using the three-point scheme
 - subroutine Diagonalization: diagonalizes matrices (the diagonalization routine from the Hückel exercise can be used).

Implement shooting algorithm:

- ADT ShootingAlgorithm: uses shooting algorithm to solve the differential equation
 - use ThreePointScheme subroutine to get the trial eigenvalues
 - loop over the following steps
 - integrate the differential equations from left and right
 - normalize the solutions (optionally: write a subroutine that normalizes)
 - calculate the correction to the trial eigenvalue
 - use numerical evaluation for the derivatives
 - use numerical integration routines to evaluate the integrals
 - stop the loop when a fixed point of the sequence of trial eigenvalues is found
 - construct the final eigenstate and normalize the eigenstate

Write output:

- subroutine OutputWriter: prints out the eigenstates
 - optionally: let the program plot the eigenstates

DATATYPES

Grid

ShootingAlgorithm