Neutral Atom Solver

Arturo Hernandez Zeledon

1 November 2023

1 Units

This code uses Hartree units where $\frac{\hbar^2}{m_e} = e = 4\pi\epsilon_0 = 1$. m_e is the mass of the electron

2 Grids

2.1 Uniform Grid

2.2 Exponential Grid

3 Second Order Differential Equation Solver

This section focus on solving two differential equations: Schrödinger's equation for one dimensional systems (including radial potentials for DFT atomic calculations), and Poisson's equation, we are then interested on numerically solving equations of the form: be written as:

$$\frac{d^2y}{dx^2} = f(x)y + g(x) \tag{1}$$

The first step to numerically solving this equation is by rewriting it as a system of linear differential equations such that $y(x) \to y^0(x)$, $\frac{dy(x)}{dx} \to y^1(x)$ such that equations 1 became:

$$\begin{cases} \frac{dy^0}{dx} = y^1(x) \\ \frac{dy^1}{dx} = f(x)y^0(x) + g(x) \end{cases} \tag{2}$$

This system of equations can be solved with method like Runge-Kutta order 4 and/or predictor corrector Adams-Moulton order 4.
To numerically solve the equations 2 the system must be translated into discrete sets of values. First by discretizing the space, into a grid of N values such that x_i is the value of the grid at position "i". The functions are also discrete $f_i \to f(x_i)$ stands by evaluating a function f on the "i" position of the grid. And "h" stands for the delta between to consecutive points on the grid $h = x_{i+1} - x_i$, the grid points are not necessarily uniformly distributed. The objective is to find the N values of y over the grid, for a numerical solution the values of $y(x_1)$ and $y(x_2)$ must be known.

Runge-Kutta order 4

This subsection describes how a function (RK4) utilizes the Runge-Kutta order 4 method to produce the values $y^0(x_{i+1})$, and $y^1(x_{i+1})$.

$h \leftarrow (x_{i+1} - x_i)$
$y^0 \leftarrow y^0(x_i)$
$y^1 \leftarrow y^1(x_i)$
$\bar{f} \leftarrow [f(x_i), f(x_{i+1})]$
$\bar{g} \leftarrow [g(x_i), g(x_{i+1})]$
$k_{01} = h * y^1$
$k_{11} = h * (\bar{f}[1] * y^0 + \bar{g}[1])$
$k_{02} = h * (y^1 + 0.5 * k_{11})$
$k_{12} = h[*0.5 * (\bar{f}[1] + \bar{f}[2]) * (y^0 + 0.5 * k_{01}) + 0.5 * (\bar{g}[1] + \bar{g}[2])]$
$k_{03} = h * (y^1 + 0.5 * k_{12})$
$k_{13} = h[*0.5 * (\bar{f}[1] + \bar{f}[2]) * (y^0 + 0.5 * k_{02}) + 0.5 * (\bar{g}[1] + \bar{g}[2])]$
$k_{04} = h * (y^1 + k_{13})$
$k_{14} = h[\bar{f}[2] * (y^0 + k_{03}) + \bar{g}[2]]$
$y^0(x_{i+1}) = y^0 + \frac{1}{6} * (k_{01} + 2 * k_{02} + 2 * k_{03} + k_{04})$
$y^1(x_{i+1}) = y^1 + \frac{1}{6} * (k_{11} + 2 * k_{12} + 2 * k_{13} + k_{14})$
return $[y^0(x_{i+1}), y^1(x_{i+1})]$

Predictor Corrector Method Adams-Moulton Orders 4 and 5

Description of the predictor corrector Adasm-Moulton (PCAM4) function implementation, the PCAM4 the integration routine produces $y^0(x_i), y^1(x_i)$

$h \leftarrow (x_i - x_{i-1})$
$\bar{y}^0 \leftarrow [y^0(x_{i-4}), y^0(x_{i-3}), y^0(x_{i-2}), y^0(x_{i-1})]$
$\bar{y}^1 \leftarrow [y^1(x_{i-4}), y^1(x_{i-3}), y^1(x_{i-2}), y^1(x_{i-1})]$
$\bar{f} \leftarrow [f(x_{i-3}), f(x_{i-2}), f(x_{i-1}), f(x_i)]$
$\bar{g} \leftarrow [g(x_{i-3}), g(x_{i-2}), g(x_{i-1}), g(x_i)]$
$y^0_{prediction} = \bar{y}^0[4] + \frac{h}{24} * (55 * \bar{y}^1[4] - 59 * \bar{y}^1[3] + 37 * \bar{y}^1[2] - 9 * \bar{y}^1[1])$
$y^1_{prediction} = \bar{y}^1[4] + \frac{h}{24} * (55 * (\bar{y}^0[4] * f[4] + g[4]) - 59 * (\bar{y}^0[3] * f[3] + g[3]) + 37 * (\bar{y}^0[2] * f[2] + g[2]) - 9 * (\bar{y}^0[1] * f[1] + g[1]))$
$y^0_{corrector} = \bar{y}^0[4] + \frac{h}{24} * (9 * y^1_{prediction} + 19 * \bar{y}^1[3] - 5 * \bar{y}^1[2] + 1 * \bar{y}^1[1])$
$y^1_{corrector} = \bar{y}^1[4] + \frac{h}{24} * (9 * (y^0_{prediction} * f[4] + g[4]) + 19 * (\bar{y}^0[3] * f[3] + g[3]) - 5 * (\bar{y}^0[2] * f[2] + g[2]) + 1 * (\bar{y}^0[1] * f[1] + g[1]))$

3.1 Schrödinger's equation

The time independent Schrödinger equation:

$$\frac{-1}{2}\nabla^2\Psi(\vec{r}) + V(r)\Psi(\vec{r}) = E\Psi(\vec{r}) \tag{3}$$

Assuming a solution of the form:

$$\Psi(\vec{r}) = \frac{u(r)Y^l_m}{r} \tag{4}$$

Where Y^l_m are the spherical harmonics such that after substituting equation 4 into equation 3, we get a radial Schrödinger equation of the form:

$$\frac{-1}{2}\frac{d^2u(r)}{dr^2} + \frac{l(l+1)u(r)}{2r^2} + V(r)u(r) = Eu(r) \tag{5}$$

Now introduce an effective potential that contains external potential, exchange, correlation, hartree, and angular

$$V_{effe} = V_{angu}(l, r) + V_{ext}(*paramters, r) + V_{hart}(\rho, r) + V_{exch}(\rho, r) + V_{corr}(\rho, r) \tag{6}$$

Rearranging terms equation 5 became:

$$\frac{d^2u(r)}{dr^2} = 2(V_{effe} - E)u(r) \tag{7}$$

And equation 7 has the form of equation 1 with $f = 2(V_{effe} - E)$, $g = 0$, and $y = u$