# Classical two dimensional simulator

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## 1. Equations

The system is a particle under the influence of a scalar potential that is a function only of the position of the particle in the two dimensional plane. The lagrangian for this particle is:

$$L = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\dot{y}^2 + \Phi(x, y) \tag{1}$$

Thus the movement of the particle can be solved through the Euler-Lagrange equations:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0 \tag{2}$$

$$\ddot{x} = -\frac{1}{m}\frac{\partial \Phi(x, y)}{\partial x} \tag{3}$$

$$\ddot{y} = -\frac{1}{m}\frac{\partial \Phi(x, y)}{\partial y} \tag{4}$$

## 2. Numerical resolution

First we translate the set of equations found to a form such as:

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}; t) \tag{5}$$

Where $\mathbf{y}$ and $\mathbf{f}$($\mathbf{y}$;t) are vectors for the dependent variables and their respective derivatives. In our problem we have 4 dependent variables: $x$, $y$, $\dot{x}$ and $\dot{y}$. And given the initial conditions at $t_0$, $\mathbf{y}_0$, their is determined by equations (3) and (4):

$$\frac{dx}{dt} = \dot{x} \tag{6}$$

$$\frac{dy}{dt} = \dot{y}$$

$$\frac{d\dot{x}}{dt} = \ddot{x} = -m\frac{\partial \Phi(x, y)}{\partial x}$$

$$\frac{d\dot{y}}{dt} = \ddot{y} = -m\frac{\partial\Phi(x,y)}{\partial y}$$

We can now solve this system of equations using any numerical method we prefer. Because the potential field, $\Phi(x, y)$, could vary in complexity from one point of the plane to another, I have decided that the Runge-Kutta-Fehlberg method is best suited to this problem due to its adapting time step.

## 2.1. Runge-Kutta-Fehlberg method

The Runge-Kutta Felbherg (RKF) method uses the results from two Runge-Kutta methods with order $n$ and $n + 1$ and estimates the error of the computation by taking the difference between the results. I will be using the RKF method for with order 4 and 5 (also known as RKF45) which optimizes the coefficients so only one extra calculation has to be made to estimate the error:

$$k_0 = \mathbf{f}(t_0, \mathbf{y}_0) \tag{7}$$

$$k_1 = \mathbf{f}\left(t_0 + \frac{h}{4}, \mathbf{y}_0 + \frac{h}{4}k_0\right)$$

$$k_2 = \mathbf{f}\left(t_0 + \frac{3h}{8}, \mathbf{y}_0 + \frac{3h}{32}k_0 + \frac{9h}{32}k_1\right)$$

$$k_3 = \mathbf{f}\left(t_0 + \frac{12h}{13}, \mathbf{y}_0 + \frac{1932h}{2197}k_0 - \frac{7200h}{2197}k_1 + \frac{7296h}{2197}k_2\right)$$

$$k_4 = \mathbf{f}\left(t_0 + h, \mathbf{y}_0 + \frac{439h}{216}k_0 - 8hk_1 + \frac{3680h}{513}k_2 - \frac{845h}{4104}k_3\right)$$

$$k_5 = \mathbf{f}\left(t_0 + \frac{h}{2}, \mathbf{y}_0 - \frac{8h}{27}k_0 + 2hk_1 - \frac{3544h}{2565}k_2 + \frac{1859h}{4104}k_3 - \frac{11h}{40}k_4\right)$$

$$\mathbf{y} = \mathbf{y}_0 + h\left(\frac{25}{216}k_0 + \frac{1408}{2565}k_2 + \frac{2197}{4104}k_3 - \frac{1}{5}k_4\right)$$

$$\hat{\mathbf{y}} = \mathbf{y}_0 + h\left(\frac{16}{35}k_0 + \frac{6656}{12825}k_2 + \frac{28561}{56430}k_3 - \frac{9}{50}k_4 \ + \frac{2}{55}k_5\right)$$

$$\hat{\mathbf{y}} - \mathbf{y} = h\left(\frac{1}{360}k_0 - \frac{128}{4275}k_2 - \frac{2197}{75240}k_3 + \frac{1}{50}k_4 \ + \frac{2}{55}k_5\right)$$

Where $h$ is the current step and $\hat{\mathbf{y}}$ and $\mathbf{y}$ are the values of the dependent variables after a step in the independent variable ($t$) of $h$ for the fifth and

fourth order methods respectively. A new estimation for the step size can be determined following:

$$h_{new} = h\left(\frac{h\epsilon}{|\mathbf{y} - \hat{\mathbf{y}}|}\right)^{\frac{1}{n}} \tag{8}$$

Where $n$ is the lowest order of our methods, in this case, $n = 4$ and $\epsilon$ is the error we desire in our new values. After computing the new step size we should check if it is smaller than the previous one, if it is then we compute again all the values of (7), reevaluate (8) and check again.

It is worth noting that it is not necessary to evaluate $\mathbf{y}$ nor $\hat{\mathbf{y}}$ to update the step size, the difference between the two is enough. Once the appropriate step size for the desired precision is determined we can compute $\hat{\mathbf{y}}$, which will be the next value for the dependent variables.

# 3. Implementation

A particle with mass $m$ and will be moving in $LxL$ box with a potential field defined by the user from different pre-made potential functions. The program will compute the trajectory of the particle until it leaves the box or a time $T$ has past since the initial instant ($t = 0$). For simplicity I have choose the box to be 200 arbitrary units.
The physical units will be determined from the units chosen for $m$, $L$ and $T$:

$$[p] = [m]\frac{[L]}{[T]} \quad [E] = [m]\frac{[L]^2}{[T]^2}$$

So for the SI ($[m] = kg$, $[L] = m$, $[T] = s$) the energy would be in Joules and the box would be 200 meters by 200 meters while in c.g.s. system ($[m] = g$, $[L] = cm$, $[T] = s$) it would be in erg and the box would be 2 meter by 2 meter.

Like previously discussed, the numerical resolution of the trajectory will be performed by the RKF45 method. While RKF45 allows for very large step sizes I have limited the biggest step size possible to make the later representation more intuitive and fluid. The (current) relevant parameters are presented next:

$$L = 200 \quad m = 1$$
$$T = 30 \quad h_{max} = 0{,}1[T] \quad n_{max} = 10 \quad \epsilon = 0{,}000001[T] = 10^{-6}[T]$$

$n_{max}$ is a parameter that limit the number of iterations that RKF45 does before fixing the final step size, it ensures that the program does not try to make the step size infinitely small in zones with discontinuities in the potential. This parameter can prevent the algorythm from acheiving the desired precision, $\epsilon$.
Also, because the potential field will not be changing with time, I can ignore all the time dependence on the set of equations (7).

## 3.1. Potentials

For defining the potential field, $\Phi(x, y)$, the users has a series of defined potentials with some parameters. The sum of the potentials at every point will make up the potential field.
For stability of the RK45 method, the functions representing these potentials should be continuous and derivable up to the first derivative.
Following is list of the implemented potentials to date with their parameters and special considerations.

1. **Woods-Saxon potential**:
   - Formula:
     - $\Phi(x,y) = -\frac{V_0}{1+e^{\frac{r-R}{a}}}, r^2 \equiv (x-x_0)^2 + (y-y_0)^2$
     - $\frac{\partial\Phi(x,y)}{\partial x} = -\frac{V_0(x-x_0)e^{\frac{r}{a}}}{ar(1+e^{\frac{r-R}{a}})}$
     - $\frac{\partial\Phi(x,y)}{\partial y} = -\frac{V_0(y-y_0)e^{\frac{r}{a}}}{ar(1+e^{\frac{r-R}{a}})}$
   - Parameters:
     - $x_0$: center $x$ position
     - $y_0$: center $y$ position
     - $V_0$: depth (if positive) or height (if negative) of the potential well/mountain
     - $R$: size of the potential well/mountain, for $r > R$ the potential rises/drops rapidly to 0
     - $a$: slope of the transition zone around $r = R$. For stability, $0{,}1 < a < 1$
   - Considerations: has an exception for $r = 0$ for the derivative. The derivative tends to 0 on $r \to 0$.

2. **Gaussian Potential**:

   - Formula:
     - $\Phi(x, y) = V_0 e^{-\frac{(x-x_0)^2+(y-y_0)^2}{2\sigma^2}}$
     - $\frac{\partial\Phi(x,y)}{\partial x} = -\frac{V_0(x-x_0)}{\sigma^2} e^{-\frac{(x-x_0)^2+(y-y_0)^2}{2\sigma^2}}$
     - $\frac{\partial\Phi(x,y)}{\partial y} = -\frac{V_0(y-y_0)}{\sigma^2} e^{-\frac{(x-x_0)^2+(y-y_0)^2}{2\sigma^2}}$
   - Parameters:
     - $x_0$: center $x$ position
     - $y_0$: center $y$ position
     - $V_0$: depth (if positive) or height (if negative) of the potential well/mountain
     - $\sigma$: controls the size of the potential well/mountain. If this potential was a normalized gaussian distribution then about 68.2 % of the values represented by the distribution would be located from 0 to $\sigma$. However, this has little to no meaning in our problem outside how wide the potential is.
   - Considerations: none

## 3.2. Testing

A series of different tests have been done on the method to see its stability and accuracy. Theoretically, the method should be accurate in all of the dependent variables according to $\epsilon$.
To show the results, 7 different plots will be shown:

- A color map of the potential field.
- The kinetic, potential and mechanical energy of the particle vs. time.
- The trajectory of the particle without time ($x$ vs. $y$).
- The trajectory of the particle for x ($x$ vs. $t$).
- The trajectory of the particle for y ($y$ vs. $t$)
- The phase space of the particle for x ($\dot{x}$ vs. $x$)

- The phase space of the particle for y ($\dot{y}$ vs. $y$)

Because the lagrangian of the particle is independent of time (see eq. 1) then on all tests the mechanical energy should be conserved (up to what $\epsilon$ allows).

Also, for initial conditions and potential fields where we expect the particle to oscillate or to make a periodic motion on either the $x$ or $y$ coordinates, a closed line should be seen on the phase space plots.

# 4. References


1. *Erwin Fehlberg*, Low-Oder classical Runge-Kutta formulas with stepsize control and their application to some heat transfer problems. NASA Technical Report 315.
   https://ntrs.nasa.gov/archive/nasa/casi.ntrs.nasa.gov/19690021375.pdf (page 18)