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ASTR5900

HW3 - Numerical Integration

14 February 2024

Question 1

Write your own code(s) to carry out a numerical integration using both the Euler Method and a Runge-Kutta Method (either 2nd order or 4th order).

a

Use your code to solve the equation

$$\frac{dy}{dx} = y^2 + 1$$

and compare your answer with the exact solution $y = \tan(x)$. Also compare (and show and comment on) your results for both the Euler and Runge-Kutta methods, using the same number of steps for each.

b

At what value of x does your numerical solution start to break down, and how does that relate to the derivative of $y(x)$? Use a plot and/or table of numbers to show this breakdown.

c

Show that a decrease in step size increases your accuracy. Do you notice a difference in how much the accuracy improves for the Euler method, versus the Runge-Kutta?

d

In real problems, we usually perform a numerical integration on a function for which there is no known analytic solution. If you have no way to know the true/exact solution, you can still check your numerical result by running several cases with different step sizes. This is called a convergence study. If your solution is working, you should see the final solution asymptotically approaching some value, as the step-size decreases. If your solution is indeed converging, you can then use the differences in your last few cases (with the smallest step sizes) to estimate the uncertainty/precision of your final answer.

Pretend like you don't know the exact solution to the equation above. Do a convergence study, calculating the fractional difference between your highest-resolution (smallest step- size) case and a few other lower-resolution cases (make a range of step sizes over at least a factor of 10-100). Plot the fractional difference as a function of step size on a log-log scale. Show the Euler and Runge-Kutta methods on the same plot. The slope in this log- log plot is often referred to as the order of convergence. Comment on what you see.

e

Now consider the exact/known solution. Does your smallest fractional difference, between your two highest-resolution cases, well-represent the actual difference between your best solution and the exact solution (i.e., is this a good measure of the uncertainty in your result)?

In [1]:

```
import matplotlib.pyplot as plt
import numpy as np
```

1a

We first code our differential equation:

$$\frac{dy}{dx} = y^2 + 1 = f(x, y)$$

In [2]:

```
def dydx(x,y):
    return y**2 + 1
```

We now code our numerical integrators:

In [3]:

```python
#we code the euler method first (a.k.a RK1):
def euler_integration(function,y0,x0,xf,num_of_steps):
    '''
    inputs:
        - function: the differential equation we want to solve
        - y0: the initial, known y value corresponding to the initia
        - x0: the left boundary of our integration
        - xf: the right boundary of our integration
        - num_of_steps: the number of steps we want to take between
    outputs:
        - x_lst: list of length equal to num_of_steps with x values
                    each value is evenly spaced by the step size
        - y_lst: list of length equal to num_of_steps with y values
                    using the euler step
    '''
    #we calculate the step size from the given boundary points and
    #num. of steps
    step_size = float((xf - x0)/num_of_steps)
    #we initialize our xi and yi to be the initial x and y given
    xi,yi = x0,y0
    #initialize the x and y list that we will write the values of ea
    #iteration into
    x_lst,y_lst = [xi],[yi]
    #we will integrate up to our end boundary
    for i in range(1,num_of_steps+1):
        #our increment is evaluated by multiplying the iteration num
        increment = i * step_size
        #update the y value using the euler step
        y_next = yi + (step_size * function(xi,yi))
        #update the x value by adding on a step size
        x_next = x0 + increment
        xi = x_next
        yi = y_next
        #write the current x and y values into our lists
        x_lst += [xi]
        y_lst += [yi]
    return x_lst,y_lst
```

In [4]:

```
#we now code RK2 (Heun's Method):
def RK2(function,y0,x0,xf,num_of_steps):
    '''
    inputs:
        - function: the differential equation we want to solve
        - y0: the initial, known y value corresponding to the initia
        - x0: the left boundary of our integration
        - xf: the right boundary of our integration
        - num_of_steps: the number of steps we want to take between 
    outputs:
        - x_lst: list of length equal to num_of_steps with x values 
                    each value is evenly spaced by the step size
        - y_lst: list of length equal to num_of_steps with y values 
                    using the RK2 step
    '''
    #we calculate the step size from the given boundary points and
    #num. of steps
    step_size = float((xf - x0)/num_of_steps)
    #we initialize our xi and yi to be the initial x and y given
    yi = y0
    xi = x0
    #initialize our stepper
    increment = 0.
    #initialize lists to write x and y values to:
    x_lst,y_lst = [x0],[y0]
    #we start our left bound and integrate up to our end boundary
    for i in range(1,num_of_steps+1):
        #we calculate the K1 and K2 values needed for the RK2 step
        k1 = function(xi,yi)
        k2 = function(xi,yi + k1*step_size)
        #we now increase our increment size
        increment = i*step_size
        #update our x value by adding the calculated increment
        x_next = x0 + increment
        #update our y value using the Rk2 step
        y_next = yi + (1/2)*(k1 + k2)*step_size
        yi = y_next
        xi = x_next
        #write the current x and y values into our lists
        x_lst += [xi]
        y_lst += [yi]
    return x_lst,y_lst
```

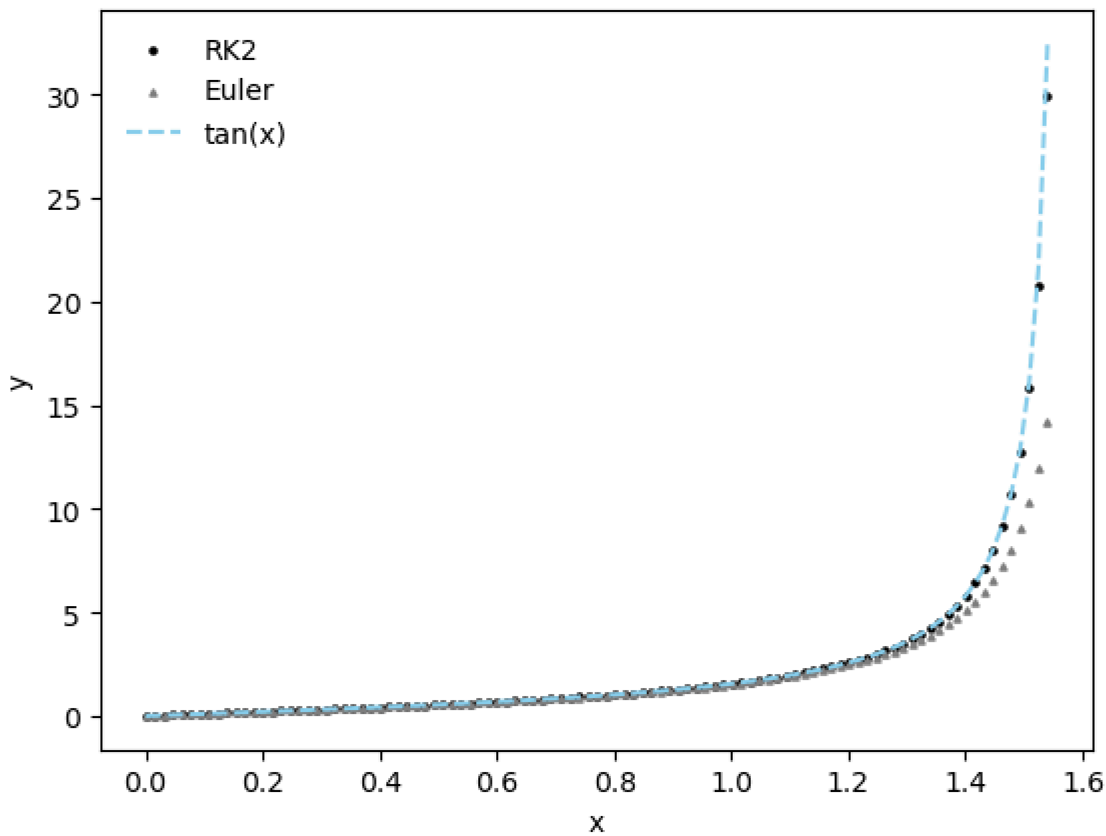
We now define a few parameters to plot the Euler and RK2 solutions against the exact solution.

In [5]:

```
#define our x boundaries:
xinitial,xfinal = 0,np.pi/2.04
#our initial y value is determined by the initial x value:
yinitial = np.tan(xinitial)
#define the number of steps
num_of_steps = 100
#calculate the tangent values in this range
tan_x_values = np.linspace(xinitial,xfinal,num_of_steps)
tan_y_values = np.tan(tan_x_values)
#calculate the euler and rk2 values in this range
x_lst_rk2,y_lst_rk2 = RK2(dydx,yinitial,xinitial,xfinal,num_of_steps
x_lst_euler,y_lst_euler = euler_integration(dydx,yinitial,xinitial,x
```

In [6]:

```
#plotting tan(x),rk2,and euler
plt.scatter(x_lst_rk2,y_lst_rk2,s=5,color='black',label='RK2')
plt.scatter(x_lst_euler,y_lst_euler,s=5,color='gray',marker='^',labe
plt.plot(tan_x_values,tan_y_values,linestyle='--',color='skyblue',la
plt.legend(frameon=False)
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```



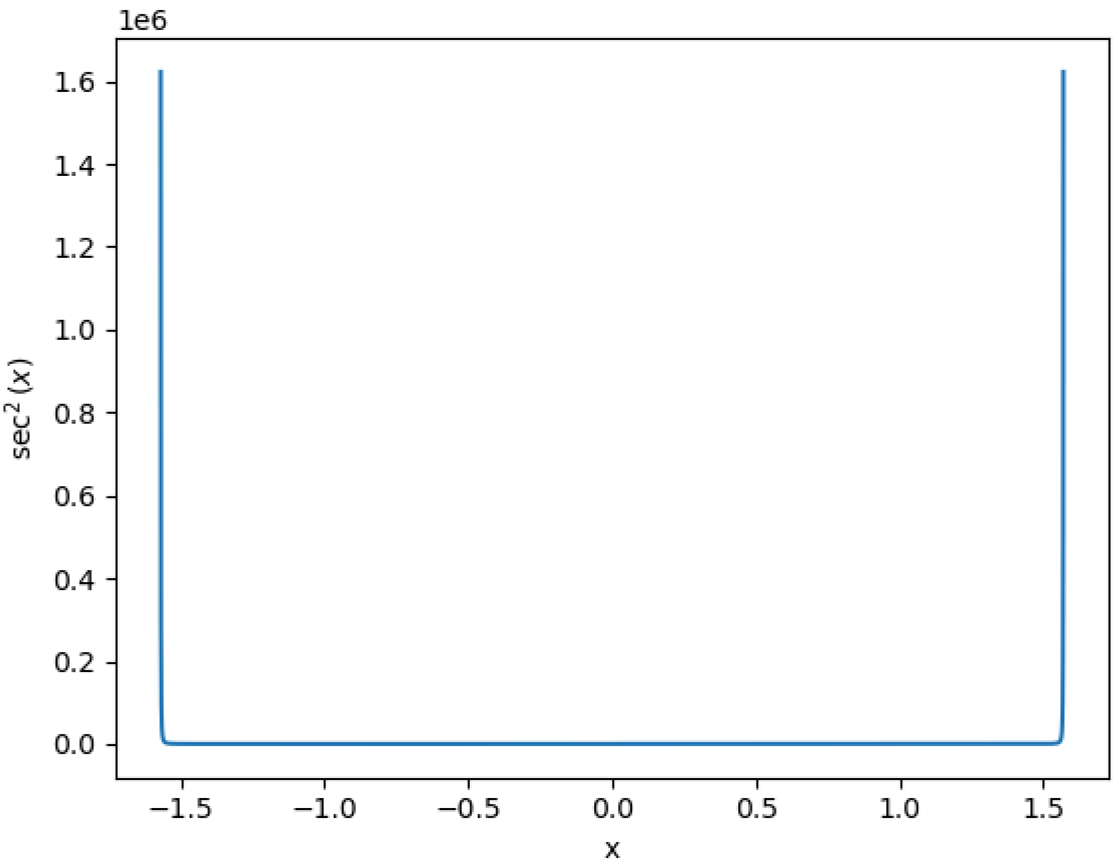
The figure above shows the exact solution to the differential equation, along with the solution obtained from the Euler and Rk2 integrators. We used 100 steps on a range of 0 to $\frac{\pi}{2.04}$. As we approach our right bound, it is clear that the Euler integrator begins to diverge from the exact solution. Meanwhile, the RK2 method is matching up with the exact solution much better in this range.

1b

The boundary for the plot above was strictly chosen so that the divergent points of tan(x) aren't reached. Specifically, tan(x) approaches positive infinity as x approaches $\frac{\pi}{2}$ from the left, which creates issues for our integrators.

To see this better, we can look at the derivative of tan(x) since the Euler and RK2 methods rely on the derivative of the solution to calculate the slope between successive points. The derivative of tan(x) is $\sec^2(x)$. Let's plot it:

In [7]:
```
sec_x_values = np.linspace(-np.pi/2.001,np.pi/2.001,100_000)
sec_y_values = 1/(np.cos(sec_x_values))
plt.plot(sec_x_values,sec_y_values**2)
plt.ylabel(r'$\sec^2(x)$')
plt.xlabel('x')
plt.show()
```



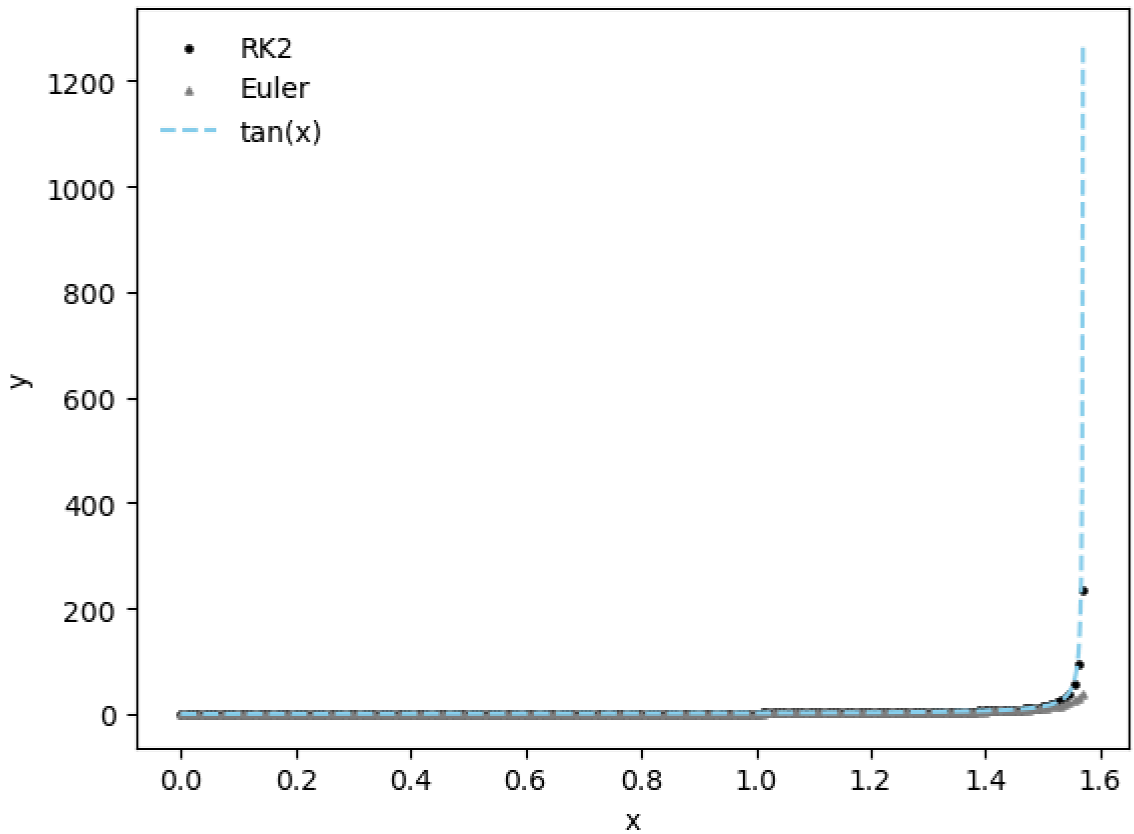
We see that $\sec^2(x)$ is growing rapidly at the boundaries of $\pm\frac{\pi}{2}$. This hints at the fact that we will have problems in our integrators at these values. Let's test it by defining a left boundary very close to $\pi/2$.

In [8]:

```
xinitial_1b,xfinal_1b = 0,np.pi/2.001
yinitial_1b = np.tan(xinitial_1b)
num_of_steps = 200

tan_x_values_1b = np.linspace(xinitial_1b,xfinal_1b,1_000)
tan_y_values_1b = np.tan(tan_x_values_1b)

x_lst_rk2_1b,y_lst_rk2_1b = RK2(dydx,yinitial_1b,xinitial_1b,xfinal_
x_lst_euler_1b,y_lst_euler_1b = euler_integration(dydx,yinitial_1b,x
```

In [9]:

```
plt.scatter(x_lst_rk2_1b,y_lst_rk2_1b,s=5,color='black',label='RK2')
plt.scatter(x_lst_euler_1b,y_lst_euler_1b,s=5,color='gray',marker='^
plt.plot(tan_x_values_1b,tan_y_values_1b,linestyle='--',color='skybl
plt.legend(frameon=False)
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```



tan(x) increases at a rate too rapidly for our integrators too keep up. For each step in x, the step in y gets much larger. We would need a lot more steps in RK2 to find additional values. Meanwhile, Euler integration has diverged from the solution close to $\pi/2$.

1c

To show how the step size influences the accurary, let's plot similar plots to those above but a various step sizes. We will plot them over a range of 0 to $\pi/2.2$.

In [10]:

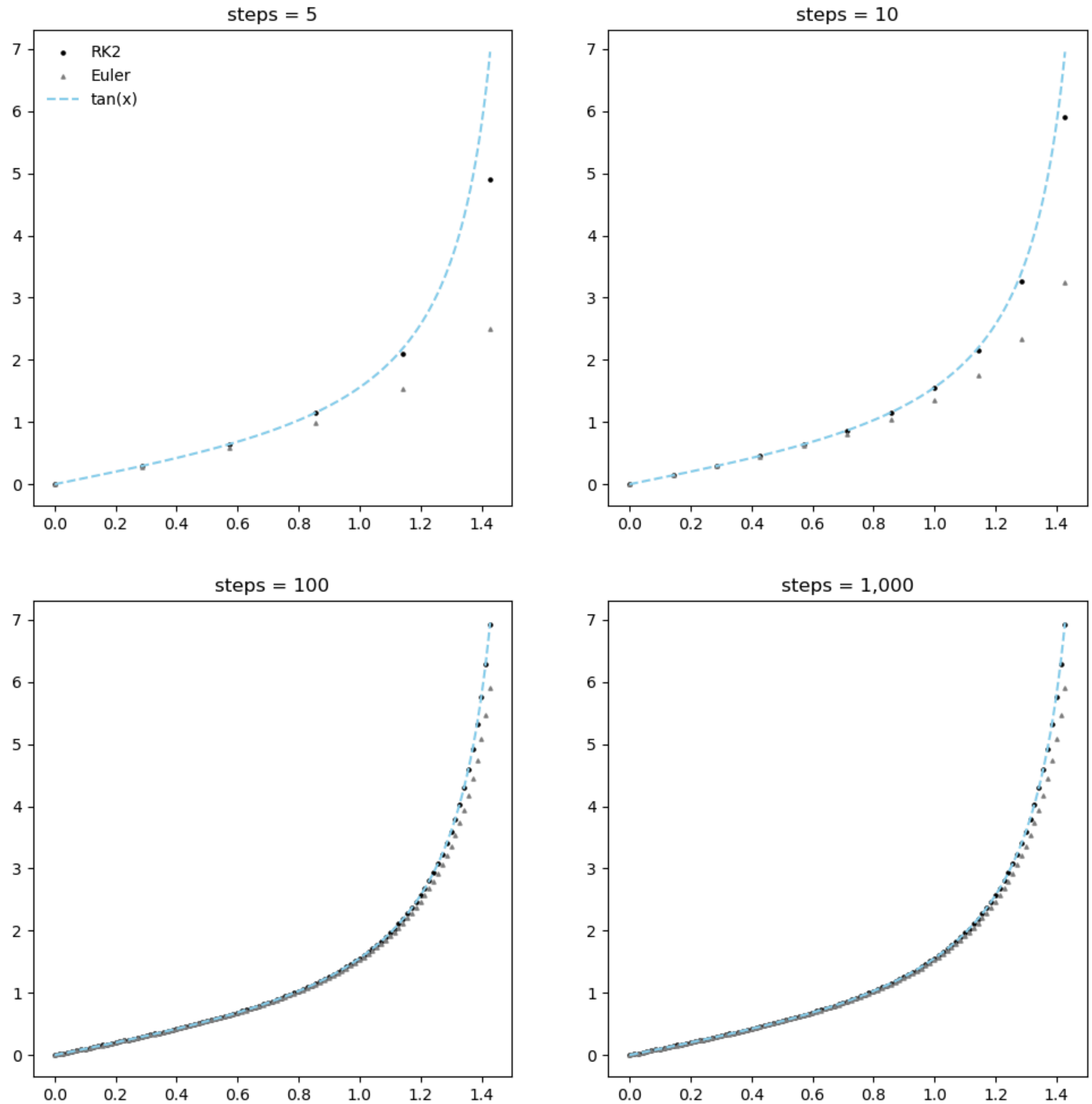
```
xinitial_1c,xfinal_1c = 0,np.pi/2.2
yinitial_1c = np.tan(xinitial_1c)
tan_x_values_1c = np.linspace(xinitial_1c,xfinal_1c,10_000)
tan_y_values_1c = np.tan(tan_x_values_1c)
```

In [11]:

```
#steps: 5
steps1 = 5
x_lst_rk2_5,y_lst_rk2_5 = RK2(dydx,yinitial_1c,xinitial_1c,xfinal_1c
x_lst_euler_5,y_lst_euler_5 = euler_integration(dydx,yinitial_1c,xin

#steps: 50
steps2 = 10
x_lst_rk2_10,y_lst_rk2_10 = RK2(dydx,yinitial,xinitial_1c,xfinal_1c,
x_lst_euler_10,y_lst_euler_10 = euler_integration(dydx,yinitial_1c,x


#steps: 100
steps3 = 100
x_lst_rk2_100,y_lst_rk2_100 = RK2(dydx,yinitial_1c,xinitial_1c,xfina
x_lst_euler_100,y_lst_euler_100 = euler_integration(dydx,yinitial_1c


#steps: 1000
steps4 = 1_000
x_lst_rk2_1000,y_lst_rk2_1000 = RK2(dydx,yinitial_1c,xinitial_1c,xfi
x_lst_euler_1000,y_lst_euler_1000 = euler_integration(dydx,yinitial_

```

In [12]:

```
#we create a four panel subplot to show the variation of convergence
#as we vary the number of steps
#steps = 5
fig, axs = plt.subplots(2,2,figsize=(12,12))
axs[0,0].scatter(x_lst_rk2_5,y_lst_rk2_5,s=5,color='black',label='RK2
axs[0,0].scatter(x_lst_euler_5,y_lst_euler_5,s=5,color='gray',marker=
axs[0,0].plot(tan_x_values_1c,tan_y_values_1c,linestyle='--',color='
axs[0,0].set_title('steps = 5')
axs[0,0].legend(frameon=False)
#steps = 10
axs[0,1].scatter(x_lst_rk2_10,y_lst_rk2_10,s=5,color='black',label='
axs[0,1].scatter(x_lst_euler_10,y_lst_euler_10,s=5,color='gray',mark
axs[0,1].plot(tan_x_values_1c,tan_y_values_1c,linestyle='--',color='
axs[0,1].set_title('steps = 10')
#steps = 100
axs[1,0].scatter(x_lst_rk2_100,y_lst_rk2_100,s=5,color='black',label=
axs[1,0].scatter(x_lst_euler_100,y_lst_euler_100,s=5,color='gray',ma
axs[1,0].plot(tan_x_values_1c,tan_y_values_1c,linestyle='--',color='
axs[1,0].set_title('steps = 100')
#steps = 1,0000
axs[1,1].scatter(x_lst_rk2_100,y_lst_rk2_100,s=5,color='black',label=
axs[1,1].scatter(x_lst_euler_100,y_lst_euler_100,s=5,color='gray',ma
axs[1,1].plot(tan_x_values_1c,tan_y_values_1c,linestyle='--',color='
axs[1,1].set_title('steps = 1,000')

plt.show()
```



Clearly, the accuracy of our integrators increases with more steps within the interval/decreasing step size. However, while RK2's accuracy increases rapidly (even from 5 steps to 10 steps), Euler's accuracy stagnates and never matches the exact solution (notice the similarities between 100 and 1,000 steps in the Euler curve).

1d

We want to plot the value at some right boundary as a function of step size. We choose the right boundary to be $\frac{\pi}{2.1}$.

In [13]:

```
print('the x value we will approach: ',np.pi/2.1)
print('the y value we will approach: ',np.tan(np.pi/2.1))
```

```
the x value we will approach:  1.4959965017094252
the y value we will approach:  13.344072639597687
```

In [14]:

```
#we initialize our initial and final x values and our initial y valu
xinitial_1d,xfinal_1d = 0,np.pi/2.1
yinitial_1d = np.tan(xinitial_1d)
```

In [15]:

```
#we define an array of number of steps from 10^(1) to 10^(6)
num_of_steps_arr = [round(value) for value in np.logspace(1,6,50)]

#initialize a few lists to which we will append values into
step_size = []
euler_answer,rk2_answer = [],[]
rk2_xlst,e_xlst = [],[]
#now we will run RK2 and the Euler integrators
#for each value in our number of steps array
for steps in num_of_steps_arr:
    #compute the step size
    step_size += [(xfinal_1d - xinitial_1d)/steps]
    #run rk2 and euler for this step size
    rk2_xlst_1d,rk2_ylst_1d = RK2(dydx,yinitial_1d,xinitial_1d,xfina
    euler_xlst_1d,euler_ylst_1d = euler_integration(dydx,yinitial_1d
    #apend the final x and y value of the integration
    e_xlst += [euler_xlst_1d[-1]]
    rk2_xlst += [rk2_xlst_1d[-1]]
    euler_answer += [euler_ylst_1d[-1]]
    rk2_answer += [rk2_ylst_1d[-1]]
```

In [16]:

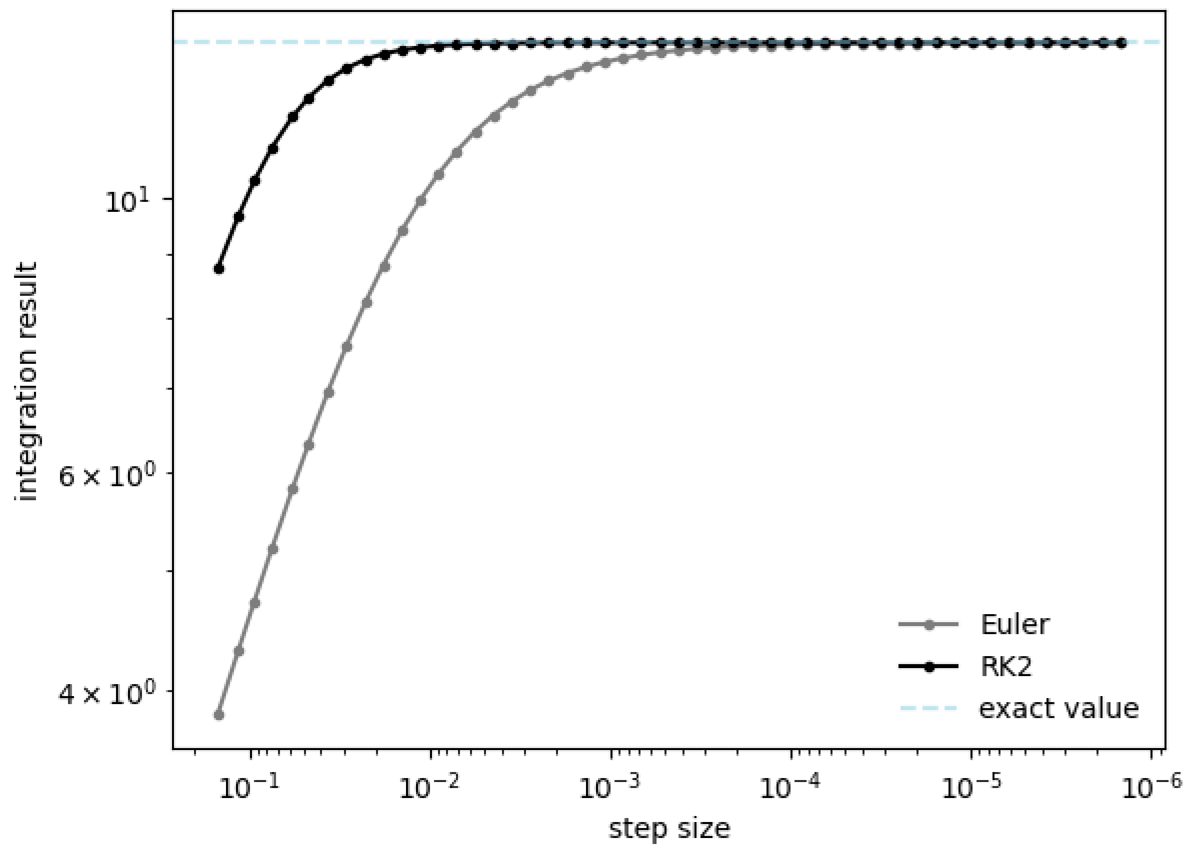
```python
print('the number of steps for each run is:')
print('\t'.join(['{:.5e}'.format(x) for x in num_of_steps_arr]))
print()
print('the step size for each run is:')
print('\t'.join(['{:.5e}'.format(x) for x in step_size]))
```

```
the number of steps for each run is:
1.00000e+01	1.30000e+01	1.60000e+01	2.00000e+01	2.60000
e+01	3.20000e+01	4.10000e+01	5.20000e+01	6.60000e+01
8.30000e+01	1.05000e+02	1.33000e+02	1.68000e+02	2.12000
e+02	2.68000e+02	3.39000e+02	4.29000e+02	5.43000e+02
6.87000e+02	8.69000e+02	1.09900e+03	1.38900e+03	1.75800
e+03	2.22300e+03	2.81200e+03	3.55600e+03	4.49800e+03
5.69000e+03	7.19700e+03	9.10300e+03	1.15140e+04	1.45630
e+04	1.84210e+04	2.33000e+04	2.94710e+04	3.72760e+04
4.71490e+04	5.96360e+04	7.54310e+04	9.54100e+04	1.20679
e+05	1.52642e+05	1.93070e+05	2.44205e+05	3.08884e+05
3.90694e+05	4.94171e+05	6.25055e+05	7.90604e+05	1.00000
e+06

the step size for each run is:
1.49600e-01	1.15077e-01	9.34998e-02	7.47998e-02	5.75383
e-02	4.67499e-02	3.64877e-02	2.87692e-02	2.26666e-02
1.80241e-02	1.42476e-02	1.12481e-02	8.90474e-03	7.05659
e-03	5.58208e-03	4.41297e-03	3.48717e-03	2.75506e-03
2.17758e-03	1.72151e-03	1.36123e-03	1.07703e-03	8.50965
e-04	6.72963e-04	5.32004e-04	4.20696e-04	3.32591e-04
2.62917e-04	2.07864e-04	1.64341e-04	1.29928e-04	1.02726
e-04	8.12115e-05	6.42059e-05	5.07616e-05	4.01330e-05
3.17291e-05	2.50855e-05	1.98326e-05	1.56797e-05	1.23965
e-05	9.80069e-06	7.74847e-06	6.12599e-06	4.84323e-06
3.82907e-06	3.02729e-06	2.39338e-06	1.89222e-06	1.49600
e-06
```

Let's visualize our results now. We will plot the result of the integration as a function of step size. We expect that our answers approach the exact value (tan($\frac{\pi}{2.1}$) ≈ 13.34) as we decrease our step size (take more steps).

In [17]:

```
#lets visuallize our results:
plt.loglog(step_size,euler_answer,color='gray',label='Euler',marker=
plt.loglog(step_size,rk2_answer,color='black',label='RK2',marker='.'
plt.axhline(np.tan(np.pi/2.1),color='skyblue',linestyle='--',alpha=0
plt.legend(frameon=False)
plt.ylabel('integration result')
plt.xlabel('step size')
plt.gca().invert_xaxis()
plt.show()
```



In [18]:

```
print('the final Euler value for each run is:')
print('\t'.join(['{:.5e}'.format(x) for x in euler_answer]))
print()
print('the final RK2 value for each run is:')
print('\t'.join(['{:.5e}'.format(x) for x in rk2_answer]))
print()
euler_diff = abs(euler_answer[-2] - euler_answer[-1])
print('The final two values of the Euler Integration differ by {:e}'
rk2_diff = abs(rk2_answer[-2] - rk2_answer[-1])
print('The final two values of the RK2 Integration differ by {:e}'.f
```

```
the final Euler value for each run is:
3.81460e+00     4.29554e+00     4.71391e+00     5.19940e+00     5.81362
e+00    6.32789e+00     6.96573e+00     7.59127e+00     8.21976e+00
8.81256e+00     9.39699e+00     9.94936e+00     1.04520e+01     1.09039
e+01    1.13076e+01     1.16599e+01     1.19624e+01     1.22182e+01
1.24315e+01     1.26077e+01     1.27521e+01     1.28694e+01     1.29650
e+01    1.30417e+01     1.31034e+01     1.31527e+01     1.31921e+01
1.32235e+01     1.32485e+01     1.32684e+01     1.32841e+01     1.32966
e+01    1.33065e+01     1.33143e+01     1.33206e+01     1.33255e+01
1.33294e+01     1.33324e+01     1.33349e+01     1.33368e+01     1.33383
e+01    1.33395e+01     1.33405e+01     1.33412e+01     1.33418e+01
1.33423e+01     1.33427e+01     1.33430e+01     1.33432e+01     1.33434
e+01

the final RK2 value for each run is:
8.75396e+00     9.64921e+00     1.03166e+01     1.09678e+01     1.16223
e+01    1.20461e+01     1.24445e+01     1.27277e+01     1.29315e+01
1.30683e+01     1.31641e+01     1.32282e+01     1.32696e+01     1.32965
e+01    1.33139e+01     1.33250e+01     1.33321e+01     1.33365e+01
1.33393e+01     1.33411e+01     1.33422e+01     1.33429e+01     1.33433
e+01    1.33436e+01     1.33438e+01     1.33439e+01     1.33440e+01
1.33440e+01     1.33440e+01     1.33440e+01     1.33441e+01     1.33441
e+01    1.33441e+01     1.33441e+01     1.33441e+01     1.33441e+01
1.33441e+01     1.33441e+01     1.33441e+01     1.33441e+01     1.33441
e+01    1.33441e+01     1.33441e+01     1.33441e+01     1.33441e+01
1.33441e+01     1.33441e+01     1.33441e+01     1.33441e+01     1.33441
e+01

The final two values of the Euler Integration differ by 1.840024e-04
The final two values of the RK2 Integration differ by 1.361247e-09
```

We see that both the Euler and RK2 methods converge to the exact solution as we decrease step size (decreasing to the right in the plot above). RK2 converges much faster, and we can calculate exactly how much faster by constructing a convergence plot. We do this below.

We first calculate fractional difference between successive points:

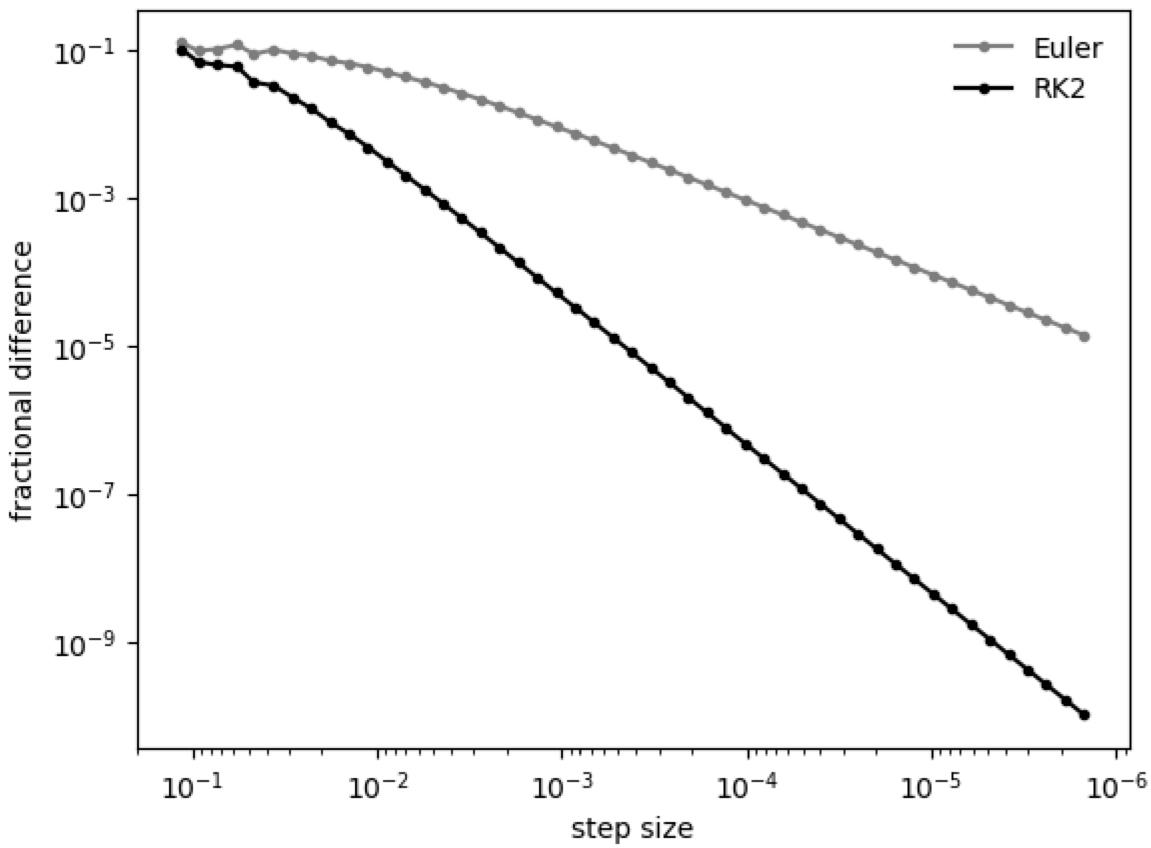
In [19]:

```
frac_diff_euler = []
frac_diff_rk2 = []
for i in range(1,len(num_of_steps_arr)):
    frac_diff_euler += [abs(euler_answer[i] - euler_answer[i-1])/eul
    frac_diff_rk2 += [abs(rk2_answer[i] - rk2_answer[i-1])/rk2_answe

```

We plot fractional difference as a function of step size:

In [20]:

```
#lets visuallize our results:
plt.loglog(step_size[1:],frac_diff_euler,color='gray',label='Euler',
plt.loglog(step_size[1:],frac_diff_rk2,color='black',label='RK2',mar
plt.legend(frameon=False)
plt.ylabel('fractional difference')
plt.xlabel('step size')
plt.gca().invert_xaxis()
plt.show()
```



In [21]:

```
print('the fractional difference between successive points in Euler 
print('\t'.join(['{:.5e}'.format(x) for x in frac_diff_euler]))
print()
print('the fractional difference between successive points in RK2 in
print('\t'.join(['{:.5e}'.format(x) for x in frac_diff_rk2]))
```

```
the fractional difference between successive points in Euler integratio
n is:
1.26077e-01     9.73979e-02     1.02990e-01     1.18133e-01     8.84597
e-02    1.00798e-01     8.98019e-02     8.27911e-02     7.21199e-02
6.63171e-02     5.87824e-02     5.05160e-02     4.32432e-02     3.70174
e-02    3.11581e-02     2.59415e-02     2.13854e-02     1.74545e-02
1.41741e-02     1.14532e-02     9.20097e-03     7.42738e-03     5.91761
e-03    4.73051e-03     3.76366e-03     2.99700e-03     2.38140e-03
1.88878e-03     1.49769e-03     1.18702e-03     9.40092e-04     7.44624
e-04    5.89271e-04     4.66299e-04     3.68919e-04     2.91866e-04
2.30842e-04     1.82582e-04     1.44395e-04     1.14179e-04     9.02909
e-05    7.13933e-05     5.64498e-05     4.46340e-05     3.52905e-05
2.79021e-05     2.20606e-05     1.74418e-05     1.37900e-05

the fractional difference between successive points in RK2 integration
is:
1.02268e-01     6.91616e-02     6.31301e-02     5.96701e-02     3.64632
e-02    3.30717e-02     2.27616e-02     1.60087e-02     1.05781e-02
7.33276e-03     4.86606e-03     3.13515e-03     2.02184e-03     1.30863
e-03    8.35896e-04     5.30648e-04     3.35180e-04     2.10662e-04
1.32356e-04     8.30778e-05     5.20340e-05     3.28265e-05     2.04783
e-05    1.28461e-05     8.03182e-06     5.03252e-06     3.14902e-06
1.96842e-06     1.23100e-06     7.69860e-07     4.81306e-07     3.01035
e-07    1.88157e-07     1.17624e-07     7.35295e-08     4.59692e-08
2.87340e-08     1.79624e-08     1.12284e-08     7.01815e-09     4.38712
e-09    2.74246e-09     1.71387e-09     1.07137e-09     6.69673e-10
4.18574e-10     2.61604e-10     1.63900e-10     1.02011e-10
```

We can now see exactly how much faster the convergence of RK2 is compared to Euler integration. The slope in log space for RK2 is 10^2. The slope in log space for Euler is 10^1. The steeper slope indicates a much faster convergence.

1e

In [22]:

```
print('The fractional difference between the two highest resolution 
print('for Euler:\t {:.5e}'.format(frac_diff_euler[-1]))
print('for RK2:\t {:.5e}'.format(frac_diff_rk2[-1]))
print()
print('The best solution obtained at a step size of {:.4e} is:\n'.fo
print('for Euler:\t {:e}'.format(euler_answer[-1]))
print('for RK2:\t {:e}'.format(rk2_answer[-1]))
print()
print('The difference between the best solution and the exact answer
print('for Euler:\t {:e}'.format(abs(euler_answer[-1]-np.tan(np.pi/2
print('for RK2:\t {:e}'.format(abs(rk2_answer[-1]-np.tan(np.pi/2.1))
```

```
The fractional difference between the two highest resolution cases is:

for Euler:	 1.37900e-05
for RK2:	 1.02011e-10

The best solution obtained at a step size of 1.4960e-06 is:

for Euler:	 1.334338e+01
for RK2:	 1.334407e+01

The difference between the best solution and the exact answer of tan(p
i/2.1)=13.34407 is:

for Euler:	 6.947930e-04
for RK2:	 2.274174e-09
```

The fractional difference does result in a good approximation of the actual difference of the best solution and the exact answer. The fractional difference is smaller by one order of magnitude to the actual difference for both cases. Thus, in scenerios where we don't have an analytical solution, a convergence plot is a great approach.

Question 2

Consider the surface of a star with a temperature of 10,000 K, where the speeds of atoms are described by a Maxwell-Boltzmann velocity distribution. Namely, the fraction $f(v)$ of particles with a speed between v and $v + dv$ is given by

$$f(v)dv = [\frac{m}{2\pi kT}]^{3/2} 4\pi v^2 \exp(-\frac{mv^2}{2kT})dv$$

a

Plot this probability density distribution of velocities for hydrogen atoms. This step is just for fun and for you to be able to double-check for bugs (e.g., check that the peak is where you expect, the numbers on the axes make sense, etc.).

b

Using your own numerical integrator, calculate what fraction of the hydrogen atoms are moving fast enough for the kinetic energy to be enough to excite the atom from the ground state (n=1)

In [23]:

```
#we define the constants first:
temp = 10_000 #surface temperature of star [K]
k_boltz = 1.38e-23 # boltzmann constant [m^2*kg/(s^2*K)]
mass_H = 1.6736e-27 #mass of hydrogen [kg]
```

In [24]:

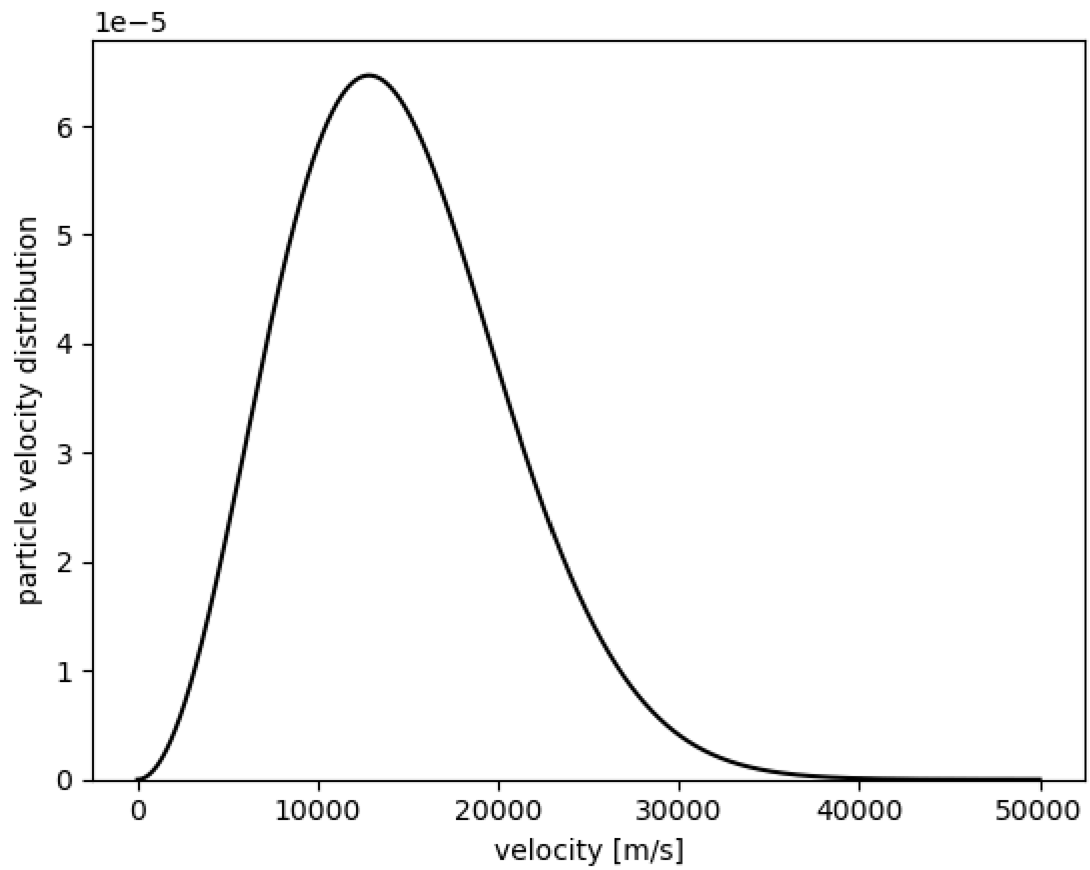
```
#we now write up the maxwell-boltzmann equation:
def maxwell_boltzmann(velocity,var1):
    term1 = (mass_H / (2.*np.pi*k_boltz*temp))**(3./2.)
    term2 = 4.*np.pi*velocity**2.
    expterm = -((mass_H * velocity**2.) / (2.*k_boltz*temp))
    return term1 * term2 *np.exp(expterm)
```

2a

Let's visually check that our function has the behavior we expect it to have.

In [39]:

```python
#construct our velocity range from 1 to 50,000 m/s with 5,000 points
velocity_arr = np.linspace(1,50_000,5_000)
#feed the array to our MB function
velocity_distribution = maxwell_boltzmann(velocity_arr,0)
#plot them against each other
plt.plot(velocity_arr,velocity_distribution,color='k')
plt.ylabel('particle velocity distribution')
plt.xlabel('velocity [m/s]')
plt.ylim(0)
plt.show()
```



2b

The energy required to ionize an electron in a Hydrogen atom is given by $\frac{13.6\text{eV}}{n^2}$ where n is the energy level the electron occupies. So the energy to excite an electron from n=1 to n=2 is given by

$$E_{1\to 2} = \frac{13.6}{1^2} - \frac{13.6}{2^2} = 13.6 - 3.4 = 10.2 \text{ eV}$$

Converting to joules, we get 1.634×10^{-18} J. Finally, we convert the joules to velocities.

$$K_E = \frac{1}{2}mv^2 \implies v = \sqrt{\frac{2 * K_E}{m}}$$

In [26]:
```
energy_threshold = 1.634e-18 #joules
velocity_threshold = np.sqrt(2 * energy_threshold / mass_H)
print('The minimum velocity to excite from n=1 to n=2 is {:.3f} m/s.
```

```
The minimum velocity to excite from n=1 to n=2 is 44189.103 m/s.
```

Now to get the fraction of hydrogen atoms with energy to excite the electron from n=1 to n=2, we need to integrate the Maxwell-Boltzmann from the velocity threshold to positive infinity. We do this below.

In [27]:
```
#set up parameters for finding number of atoms that meet excitation
x_initial,x_final = velocity_threshold, 0.1*2.99e8
y_initial = 0.0
x_lst_excite,y_lst_excite = RK2(maxwell_boltzmann,y_initial,x_initia
atoms_that_excite = y_lst_excite[-1]
```

In [28]:
```
print('The fraction of atoms that have velocities high enough to exc
```

```
The fraction of atoms that have velocities high enough to excite is 5.6
807e-05.
```

If we take into account the photoionization cross section, this number should actually be lower since a very high velocity will likely not excite/ionize the atom. But this is beyond the point of the exercise.

As a check that our integration is correct, let's integrate the entire MB curve. The answer should be one.

In [29]:
```
#set up parameters for finding total number of atoms
x_initial,x_final = 0, 3_000_000
y_initial = 0.0
x_lst_all,y_lst_all = RK2(maxwell_boltzmann,y_initial,x_initial,x_fi
total_atoms = y_lst_all[-1]
```

In [30]:
```
print('The fraction of atoms that have a velocity is {:.2f}.'.format
```

```
The fraction of atoms that have a velocity is 1.00.
```

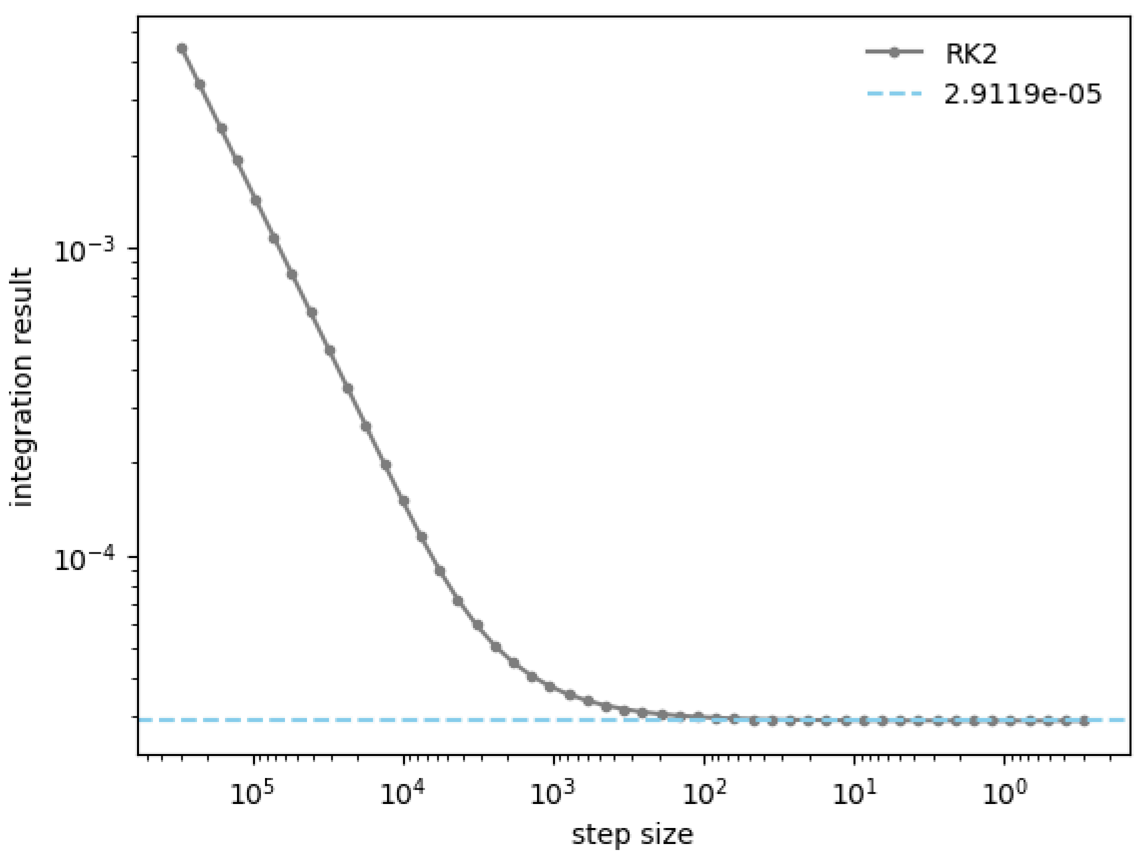
We now run convergence tests. We first plot the integration solution as a function of step size:

In [31]:

```
#set up parameters for finding total number of atoms
xinitial_2b,xfinal_2b = velocity_threshold, 3_000_000
yinitial_2b = 0.0

#we define an array of number of steps from 10^(1) to 10^(6)
num_of_steps_arr = [round(value) for value in np.logspace(1,7,50)]

#initialize a few lists to which we will append values into
step_size = []
mb_rk2_ylst,mb_rk2_xlst = [], []
#now we will run RK2
#for each value in our number of steps array
for steps in num_of_steps_arr:
    #compute the step size
    step_size += [(xfinal_2b - xinitial_2b)/steps]
    #run rk2 and euler for this step size
    rk2_xlst_2b,rk2_ylst_2b = RK2(maxwell_boltzmann,yinitial_2b,xini
    #apend the final x and y value of the integration
    mb_rk2_xlst += [rk2_xlst_2b[-1]]
    mb_rk2_ylst += [rk2_ylst_2b[-1]]
```

In [40]:

```
#lets visuallize our results:
plt.loglog(step_size,mb_rk2_ylst,color='gray',label='RK2',marker='.'
plt.axhline(mb_rk2_ylst[-1],color='skyblue',linestyle='--',label='{:
plt.ylabel('integration result')
plt.xlabel('step size')
plt.gca().invert_xaxis()
plt.legend(frameon=False)
plt.show()
```



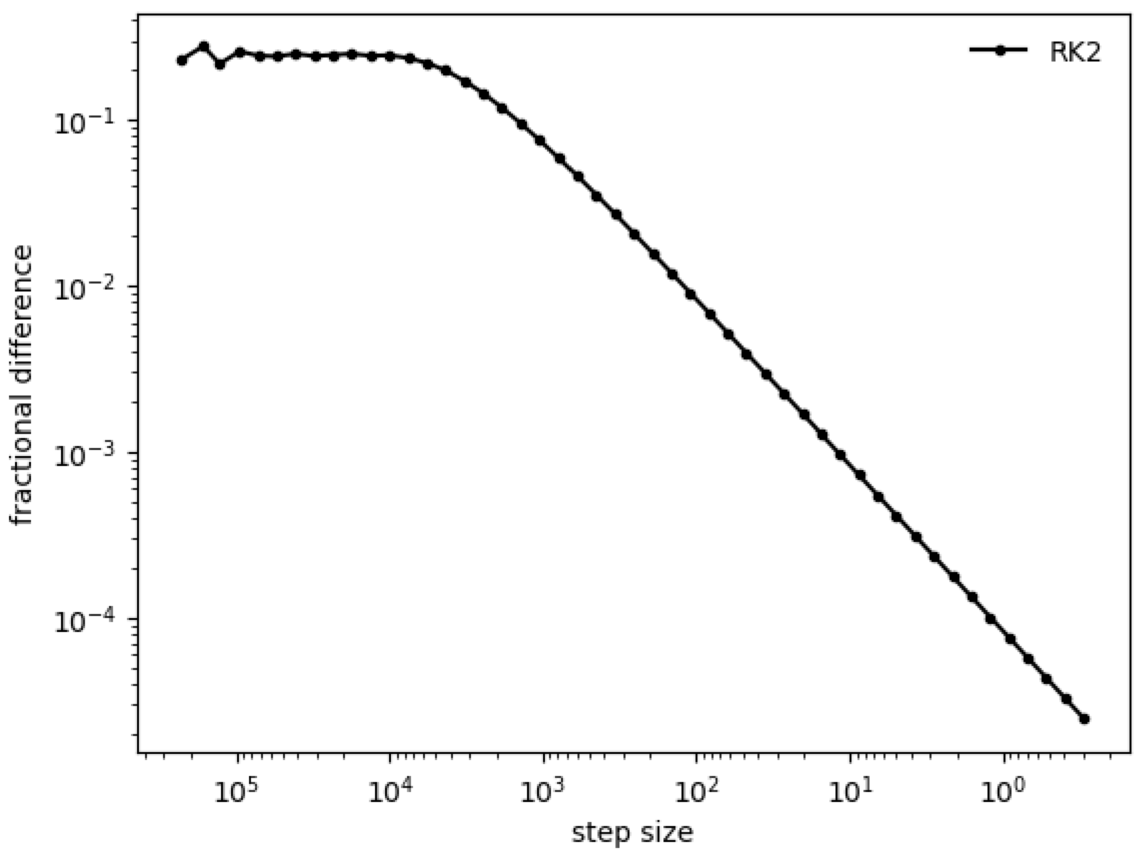
In [33]:
```
print('The best solution obtain is: {:.4e}'.format(mb_rk2_ylst[-1]))
```

```
The best solution obtain is: 2.9119e-05
```

We now plot the fractional difference of each step size iteration:

In [34]:
```
frac_diff_rk2_mb = []
for i in range(1,len(num_of_steps_arr)):
    frac_diff_rk2_mb += [abs(mb_rk2_ylst[i] - mb_rk2_ylst[i-1])/mb_rk
```

In [35]:
```
#lets visuallize our results:
plt.loglog(step_size[1:],frac_diff_rk2_mb,color='black',label='RK2',
plt.legend(frameon=False)
plt.ylabel('fractional difference')
plt.xlabel('step size')
plt.gca().invert_xaxis()
plt.show()
```



In [36]:
```
print('The fractional difference between the two highest resolution
```

```
The fractional difference between the two highest resolution cases is:
2.4789e-05
```

Thus, the fraction of atoms that can excite Hydrogen is $2.9119 \times 10^{-5} \pm 2.4789 \times 10^{-5}$. The error on this is not great, but it can be improved by increasing the number of steps (decreasing the step size). However, because it is becoming computationally taxing to do more steps, we stop here.

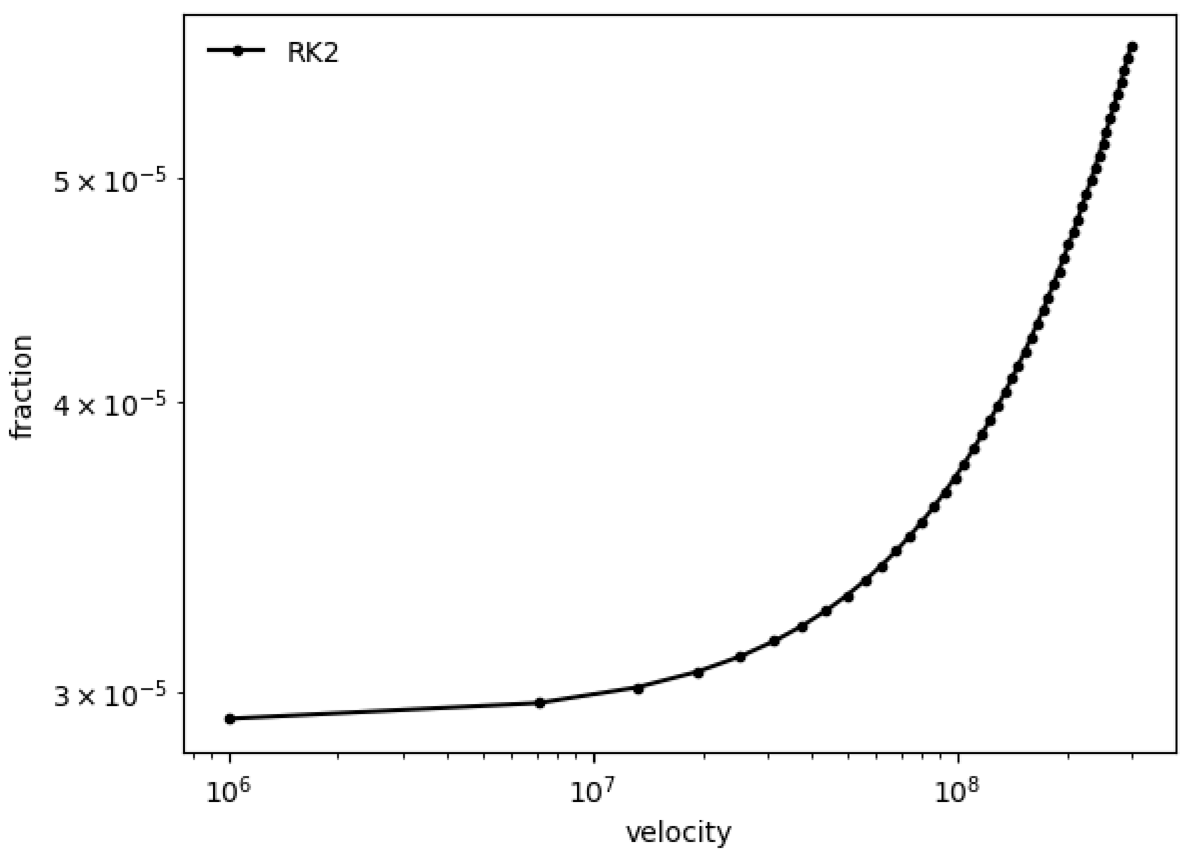
Let's now consider how our solution changes as we vary the right boundary of our solution:

In [37]:

```
velocity_range = np.linspace(1e6,3e8,50)
mb2b1_rk2_ylst,mb2b1_rk2_xlst = [], []
for velocity_right_boundary in velocity_range:
    #set up parameters for finding total number of atoms
    xinitial_2b1,xfinal_2b1 = velocity_threshold, velocity_right_bou
    yinitial_2b1 = 0.0
    rk2_xlst_2b1,rk2_ylst_2b1 = RK2(maxwell_boltzmann,yinitial_2b1,x
    #apend the final x and y value of the integration
    mb2b1_rk2_xlst += [rk2_xlst_2b1[-1]]
    mb2b1_rk2_ylst += [rk2_ylst_2b1[-1]]
```

In [38]:

```
#lets visuallize our results:
plt.loglog(velocity_range,mb2b1_rk2_ylst,color='black',label='RK2',m
plt.legend(frameon=False)
plt.ylabel('fraction')
plt.xlabel('velocity')
plt.show()
```



As we increase our velocity, the solution diverges from the "best solution" we arrived at above. This makes sense since we have kept the step size constant. So as we increase our velocity, our precision is decreasing because of increasing range. To fix this issue, we would need to also decrease step size as we increase velocity.