Computational and Numerical Methods Lab-09

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In [2]:
```python
import numpy as np
import matplotlib.pyplot as plt
import sympy as sp
import pandas as pd
```

In [3]:
```python
class differentiation:
    def forward_difference(self,f_exp,x,val,h=0.1):
        func = sp.lambdify(x,f_exp)
        if h == 0:
            h = 1e-7
        return (func(val+h) - func(val))/h

    def backward_difference(self,f_exp,x,val,h=0.1):
        func = sp.lambdify(x,f_exp)
        if h == 0:
            h = 1e-7
        return (func(val) - func(val-h))/h

    def central_difference(self,f_exp,x,val,h=0.1):
        func = sp.lambdify(x,f_exp)
        if h == 0:
            h = 1e-7
        return (func(val+h) - func(val-h))/(2*h)
    def true_derivative(self,f_exp,x,val):
        d_exp = sp.diff(f_exp,x)
        dfun = sp.lambdify(x,d_exp)
        return dfun(val)
```

Q1) Given a function f(x)=e^{x} , use the forward difference formula to estimate f'(1) with step sizes h=0.1 to h=0.0001. Compare your results with the analytical derivative. Plot the error with h.

Forward Difference

- The forward difference of a function f(x) is given by:

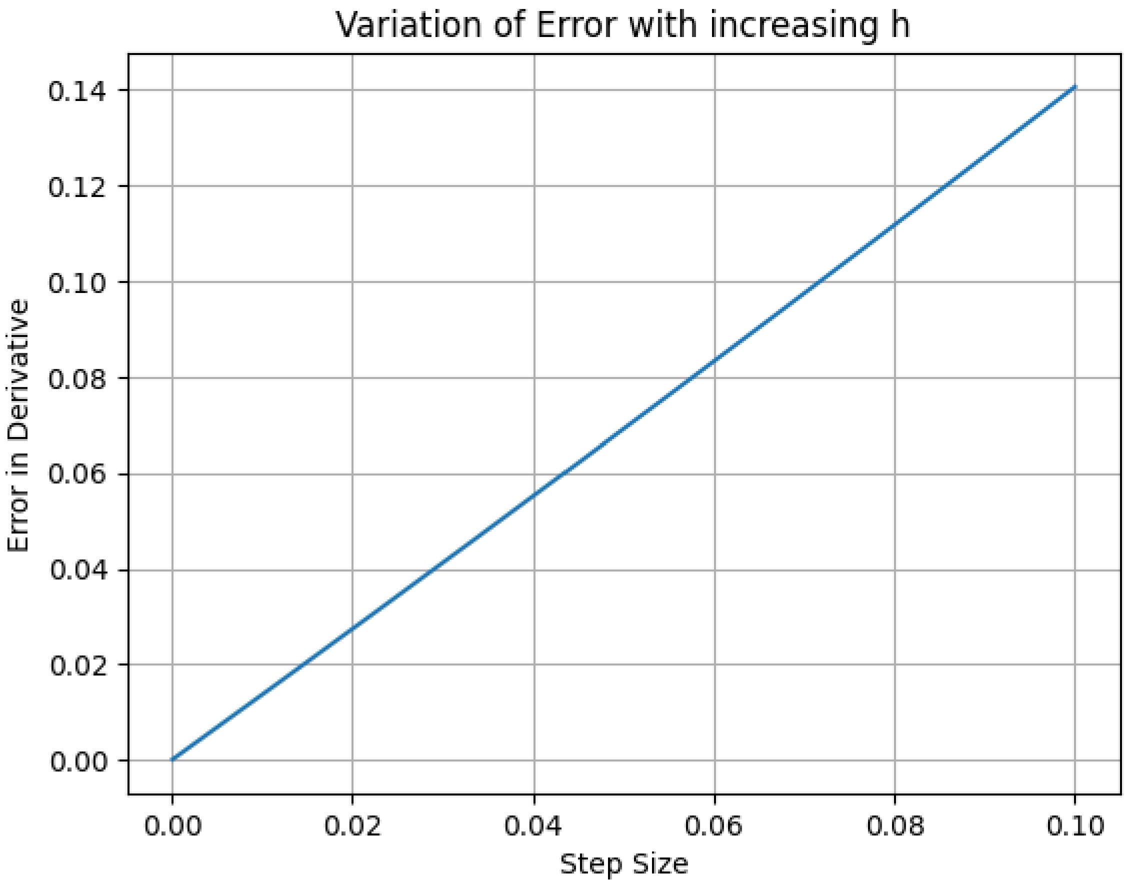
$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

In [4]:
```
x = sp.symbols('x')
f_exp = sp.exp(x)
val = 1
diff = differentiation()
true_diff = diff.true_derivative(f_exp,x,1)
h = np.arange(0.0001,0.1001,0.0001)
forward_d = []
error = []
data = []
for h_val in h:
    f_diff = diff.forward_difference(f_exp,x,val,h=h_val)
    forward_d.append(f_diff)
    error.append(abs(f_diff - true_diff))
    data.append([h_val,f_diff,abs(f_diff-true_diff)])
print('True Derivative at the point x = 1 =',true_diff)
df = pd.DataFrame(data,columns = ['Step Size','Derivative Value','Error'])
display(df)
plt.plot(h,error)
plt.xlabel('Step Size')
plt.ylabel('Error in Derivative')
plt.title('Variation of Error with increasing h')
plt.grid(True)
plt.show()
```

```
True Derivative at the point x = 1 = 2.718281828459045
```

	Step Size	Derivative Value	Error
0	0.0001	2.718418	0.000136
1	0.0002	2.718554	0.000272
2	0.0003	2.718690	0.000408
3	0.0004	2.718826	0.000544
4	0.0005	2.718962	0.000680
...	...	...	...
995	0.0996	2.858261	0.139979
996	0.0997	2.858406	0.140124
997	0.0998	2.858551	0.140269
998	0.0999	2.858697	0.140415
999	0.1000	2.858842	0.140560

1000 rows × 3 columns



Q2) Using the function f(x)=sin(x), apply the backward difference method to estimate f'(1.5) for h=0.5 to h=0.000005. Compare your answer to the exact derivative. Plot the error with h.

Backward Difference

- Backward difference of a function f(x) is given by:

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

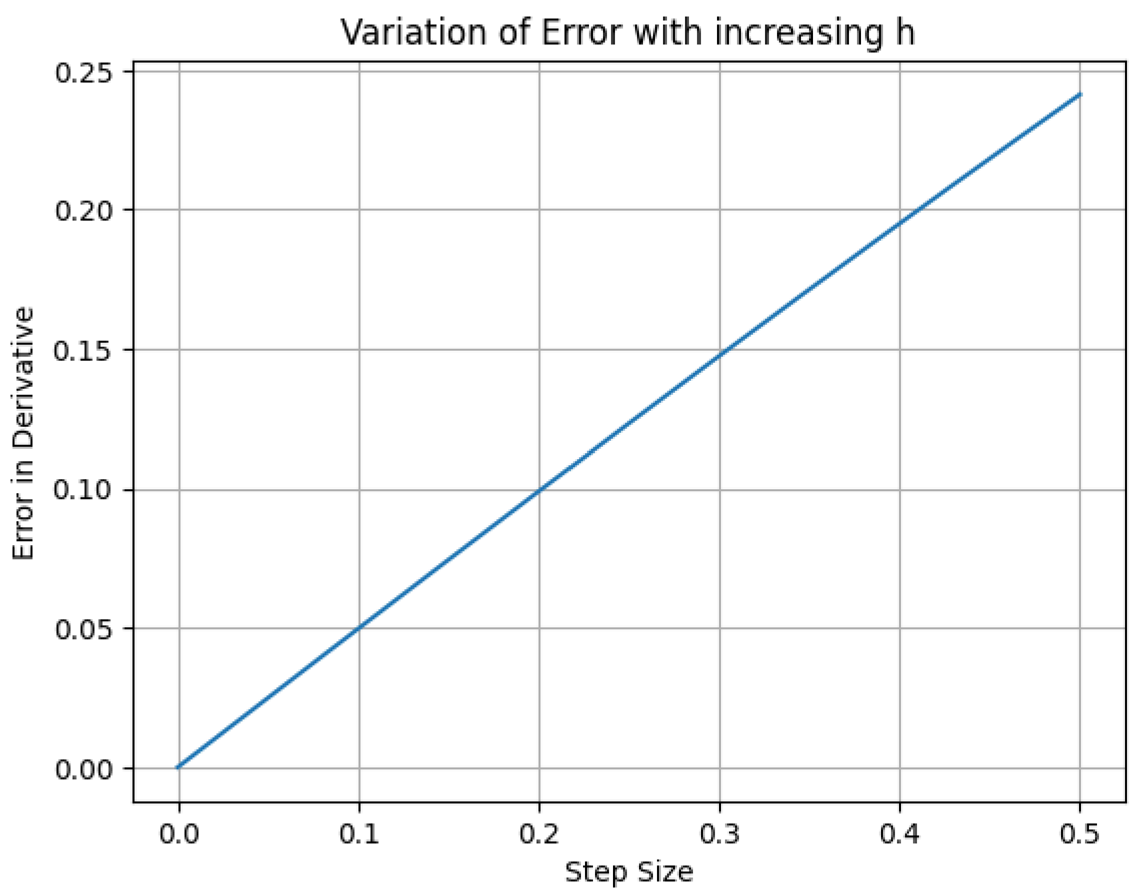
In [6]:
```
x = sp.symbols('x')
f_exp = sp.sin(x)
val = 1.5
diff = differentiation()
true_diff = diff.true_derivative(f_exp,x,val)
h = np.arange(0.000005,0.500005,0.000005)
backward_d = []
error = []
data = []
for h_val in h:
    b_diff = diff.backward_difference(f_exp,x,val,h=h_val)
    backward_d.append(b_diff)
    error.append(abs(b_diff - true_diff))
    data.append([h_val,b_diff,abs(b_diff-true_diff)])
print('True Derivative at the point x =',val,'=',true_diff)
df = pd.DataFrame(data,columns = ['Step Size','Derivative Value','Error'])
```

```python
display(df)
plt.plot(h,error)
plt.xlabel('Step Size')
plt.ylabel('Error in Derivative')
plt.title('Variation of Error with increasing h')
plt.grid(True)
plt.show()
```

```
True Derivative at the point x = 1.5 = 0.0707372016677029
```

	Step Size	Derivative Value	Error
0	0.000005	0.070740	0.000002
1	0.000010	0.070742	0.000005
2	0.000015	0.070745	0.000007
3	0.000020	0.070747	0.000010
4	0.000025	0.070750	0.000012
...	...	...	...
99995	0.499980	0.312039	0.241302
99996	0.499985	0.312041	0.241304
99997	0.499990	0.312043	0.241306
99998	0.499995	0.312046	0.241309
99999	0.500000	0.312048	0.241311

100000 rows × 3 columns



Q3) For f(x)=ln(x), use the central difference approximation to calculate f′(2) for h=0.1. Compare the results with the actual derivative.

Central Difference

- Central difference of a function f(x) is given by:

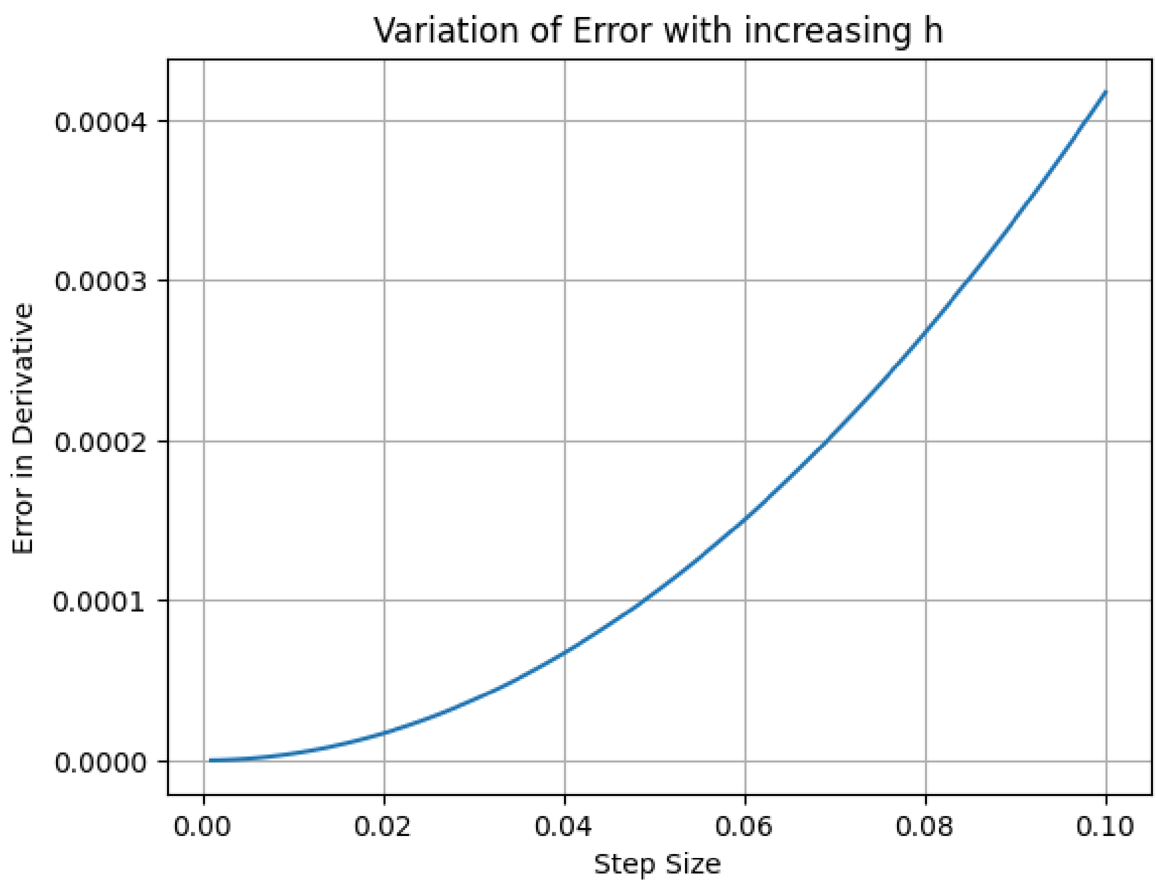
$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

In [9]:
```
x = sp.symbols('x')
f_exp = sp.log(x)
val = 2
diff = differentiation()
true_diff = diff.true_derivative(f_exp,x,val)
h = np.arange(0.001,0.101,0.001)
central_d = []
error = []
data = []
for h_val in h:
    c_diff = diff.central_difference(f_exp,x,val,h=h_val)
    central_d.append(c_diff)
    error.append(abs(c_diff - true_diff))
    data.append([h_val,c_diff,abs(c_diff-true_diff)])
print('True Derivative at the point x =',val,'=',true_diff)
print('Central Difference for h = 0.1 is :',central_d[-1])
print('Error for h = 0.1 is',abs(central_d[-1] - true_diff))
df = pd.DataFrame(data,columns = ['Step Size','Derivative Value','Error'])
display(df)
plt.plot(h,error)
plt.xlabel('Step Size')
plt.ylabel('Error in Derivative')
plt.title('Variation of Error with increasing h')
plt.grid(True)
plt.show()
```

```
True Derivative at the point x = 2 = 0.5
Central Difference for h = 0.1 is : 0.5004172927849132
Error for h = 0.1 is 0.00041729278491320354
```

	Step Size	Derivative Value	Error
0	0.001	0.500000	4.166662e-08
1	0.002	0.500000	1.666668e-07
2	0.003	0.500000	3.750005e-07
3	0.004	0.500001	6.666683e-07
4	0.005	0.500001	1.041671e-06
...	...	...	...
95	0.096	0.500385	3.845317e-04
96	0.097	0.500393	3.925959e-04
97	0.098	0.500401	4.007441e-04
98	0.099	0.500409	4.089764e-04
99	0.100	0.500417	4.172928e-04

100 rows × 3 columns



Q4) Use the method of undetermined coefficient method to estimate the second derivative of f(x)=x^3 at x=1 with h=0.1. How does the result compare to the exact second derivative?

Method of undetermined coefficient

- Consider f"(x) ≈ Af(x+h)+ Bf(x)+ Cf(x-h)

- expand f(x+h) and f(x-h) using taylor series.
- substitute those values in the above equation and compare coefficients
- Final equation:

$$f''(x) \approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}$$

In [10]:
```
import sympy as sp

x = sp.Symbol('x')
fx = x**3
f_diff = sp.diff(fx, x, 2)

exact_value = f_diff.subs(x, 1)

h = 0.1
x0 = 1

f_x_h = (x0 + h)**3
f_x_0 = x0**3
f_x_minus_h = (x0 - h)**3

# after solving on pen and paper we get the following equation for second order
estimate_value = (f_x_minus_h - 2*f_x_0 + f_x_h) / h**2

print('Estimated value of second derivative of f(x)=',estimate_value)
print('Exact value of second derivative of f(x)=',exact_value)
```

```
Estimated value of second derivative of f(x)= 6.000000000000049
Exact value of second derivative of f(x)= 6
```

In [11]:
```
def trapezoidal(f_exp,x,n,a,b):
    func = sp.lambdify(x,f_exp)
    h = (b-a)/n
    x = np.linspace(a,b,n+1)
    f = func(x)
    res = 0.5*(f[0] + f[-1])
    for i in range(1,n):
      res += f[i]
    res *= ((b-a)/n)
    return res

def simpsons(f_exp,x,n,a,b):
    func = sp.lambdify(x,f_exp)
    h = (b-a)/n
    x = np.linspace(a,b,n+1)
    f = func(x)
    res = f[0] + f[-1]
    for i in range(1,n):
        if i%2:
            res += 4*f[i]
        else:
            res += 2*f[i]
    #res += function(b) + f[n-2] + 4*f[n-1]
    res *= (b-a)/(3*n)
    return res
```

```python
def exact_integral(f_exp,x,a,b):
    return sp.integrate(f_exp, (x, a, b)).evalf()
```

Q5) Apply the trapezoidal rule to approximate the integral of f(x)=cos(x) from x=0 to x=2π using 2, 4, 6, 8, 10, 12 subintervals. Compare your result with the exact value of the integral. Plot the error with number of subintervals.

Trapezoidal Rule

- The Trapezoidal Rule is a numerical integration method that approximates the area under a curve as a trapezoid. It is useful when the function f(x) is smooth and well-behaved over the interval.
- Formula:

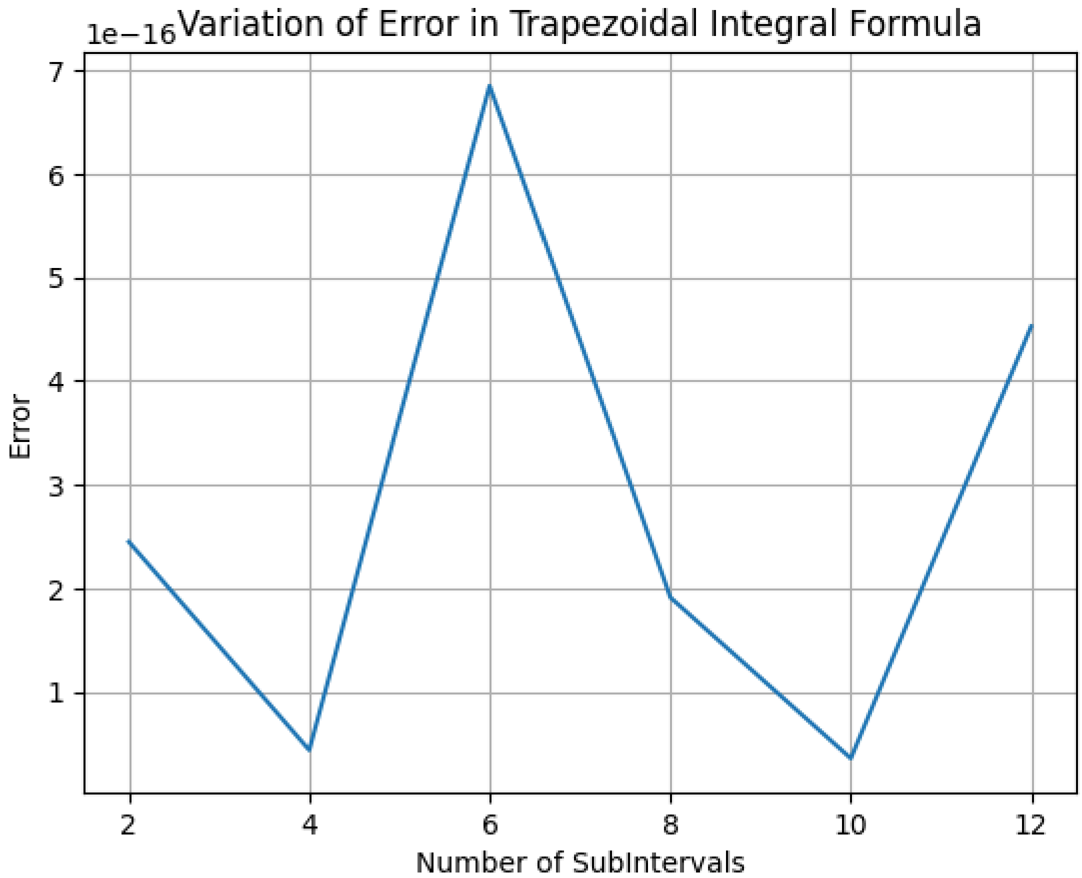
$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\left[f(a)+f(b)\right]$$

In [12]:
```python
x = sp.symbols('x')
f_exp = sp.cos(x)
a = 0
b = 2 * np.pi
n_val = [2,4,6,8,10,12]
true_integral = exact_integral(f_exp,x,a,b)
error = []
trap_integral = []
data = []
for n in n_val:
    trap_i = trapezoidal(f_exp,x,n,a,b)
    trap_integral.append(trap_i)
    error.append(abs(trap_i - true_integral))
    data.append([n,trap_i,abs(trap_i - true_integral)])
df = pd.DataFrame(data,columns=['Subintervals','Integral Value','Error'])
print('True Value of Integral is',true_integral)
display(df)
plt.plot(n_val,error)
plt.grid(True)
plt.xlabel('Number of SubIntervals')
plt.ylabel('Error')
plt.title('Variation of Error in Trapezoidal Integral Formula')
plt.plot()
```

```
True Value of Integral is -2.44929359829471e-16
```

	Subintervals	Integral Value	Error
0	2	0.000000e+00	2.44929359829471e-16
1	4	-2.885506e-16	4.36212442287978e-17
2	6	-9.300983e-16	6.85168906306164e-16
3	8	-4.359836e-16	1.91054202421608e-16
4	10	-2.092721e-16	3.56572499489527e-17
5	12	-6.975737e-16	4.52644339772256e-16

```
Out[12]: []
```



Q6) Approximate the integral of f(x)=1/(1+x^2) from x=0 to x=1 using Simpson's rule with 6 subintervals. Compare this with the actual value of the integral.

Simpson's Rule

- Simpson's Rule provides a higher-order approximation by fitting a quadratic (parabolic) curve through three points and calculating the area under the parabola.
- Formula:

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

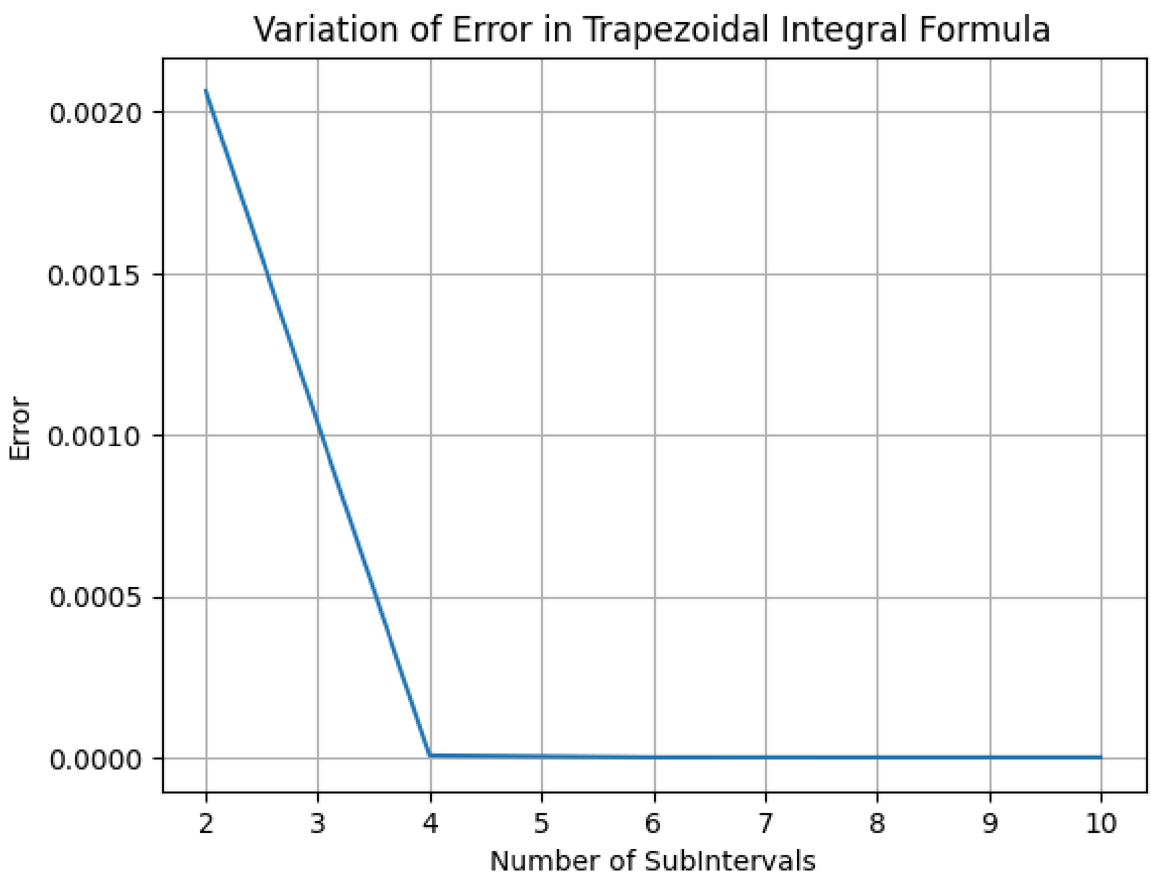
In [13]:

```
x = sp.symbols('x')
f_exp = 1/(1+x**2)
a = 0
b = 1
n_val = [2,4,6,8,10]
true_integral = exact_integral(f_exp,x,a,b)
error = []
sim_integral = []
data = []
for n in n_val:
    simpson_i = simpsons(f_exp,x,n,a,b)
    sim_integral.append(simpson_i)
    error.append(abs(simpson_i - true_integral))
    data.append([n,simpson_i,abs(simpson_i - true_integral)])
df = pd.DataFrame(data,columns=['Subintervals','Integral Value','Error'])
print('True Value of Integral is',true_integral)
print('Simspons Value of Integral is',sim_integral[0])
print('Error Value of Integral is',error[0])
display(df)
plt.plot(n_val,error)
plt.grid(True)
plt.xlabel('Number of SubIntervals')
plt.ylabel('Error')
plt.title('Variation of Error in Trapezoidal Integral Formula')
plt.plot()
```

```
True Value of Integral is 0.785398163397448
Simspons Value of Integral is 0.783333333333333
Error Value of Integral is 0.00206483006411495
```

	Subintervals	Integral Value	Error
0	2	0.783333	0.00206483006411495
1	4	0.785392	6.00653470317347e-6
2	6	0.785398	2.18163437537555e-7
3	8	0.785398	3.77827715780654e-8
4	10	0.785398	9.91264459404562e-9

Out[13]: []



Q7) Use the composite trapezoidal rule and composite Simpson's method to approximate the integral of   from x=0 to x=1 with n subintervals. Compare plot the values in one figure.

Composite Trapezoidal Rule

- The Composite Trapezoidal Rule improves the basic Trapezoidal Rule by dividing the interval [a,b] into multiple smaller subintervals and applying the trapezoidal rule to each.
- Formula:

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

  where h=(b-a)/n

Composite Simpson's Rule

- The Composite Simpson's Rule applies Simpson's Rule over multiple subintervals to improve accuracy.
- Formula:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(x_0) + 4\sum_{i=1,3,5,\dots}^{n-1} f(x_i) + 2\sum_{i=2,4,6,\dots}^{n-2} f(x_i) + f(x_n)\right]$$

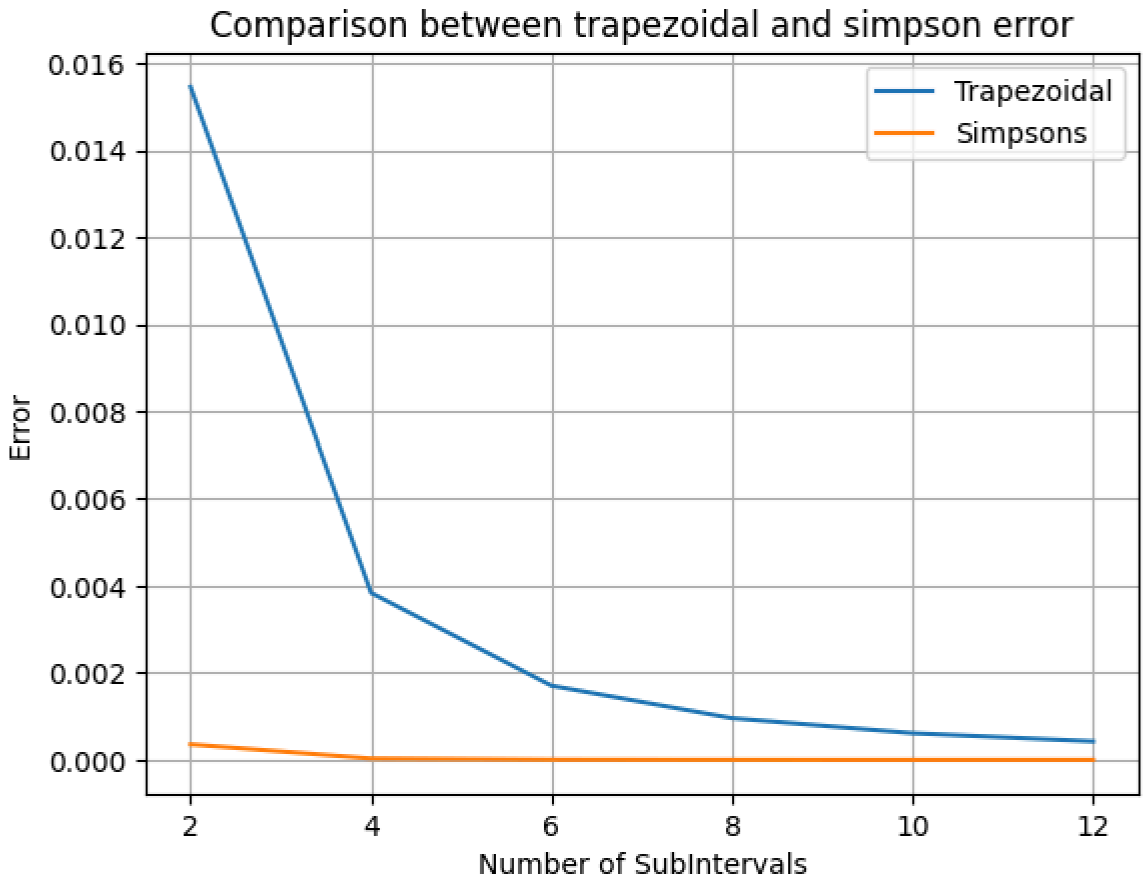
  where h=(b-a)/n

In [14]:
```
x = sp.symbols('x')
f_exp = sp.exp(-x**2)
a = 0
b = 1
n_val = [2,4,6,8,10,12]
true_integral = exact_integral(f_exp,x,a,b)
error_trap = []
error_sim = []
trap_integral = []
data = []
for n in n_val:
    trap_i = trapezoidal(f_exp,x,n,a,b)
    simpson_i = simpsons(f_exp,x,n,a,b)
    trap_integral.append(trap_i)
    error_trap.append(abs(trap_i - true_integral))
    error_sim.append(abs(simpson_i - true_integral))
    data.append([n,trap_i,abs(trap_i - true_integral),simpson_i,abs(simpson_i -
df = pd.DataFrame(data,columns=['Subintervals','Integral Value for Trapezoidal',
print('True Value of Integral is',true_integral)
display(df)
plt.plot(n_val,error_trap,label = 'Trapezoidal')
plt.plot(n_val,error_sim,label = 'Simpsons')
plt.legend()
plt.grid(True)
plt.xlabel('Number of SubIntervals')
plt.ylabel('Error')
plt.title('Comparison between trapezoidal and simpson error')
plt.plot()
```

```
True Value of Integral is 0.746824132812427
```

	Subintervals	Integral Value for Trapezoidal	Trapzoidal Error	Integral Value for Simpsons	Simpsons Error
0	2	0.731370	0.0154538809838640	0.747180	0.000356296097083320
1	4	0.742984	0.00384003501204577	0.746855	3.12469785602731e-5
2	6	0.745119	0.00170472037624769	0.746830	6.25867691794735e-6
3	8	0.745866	0.000958517966731853	0.746826	1.98771503945316e-6
4	10	0.746211	0.000613336680677534	0.746825	8.15442016577350e-7
5	12	0.746398	0.000425884918986652	0.746825	3.93566767287190e-7

Out[14]: []


Comparison between trapezoidal and simpson error
Trapezoidal
Simpsons
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
Error
2
4
6
8
10
12
Number of SubIntervals