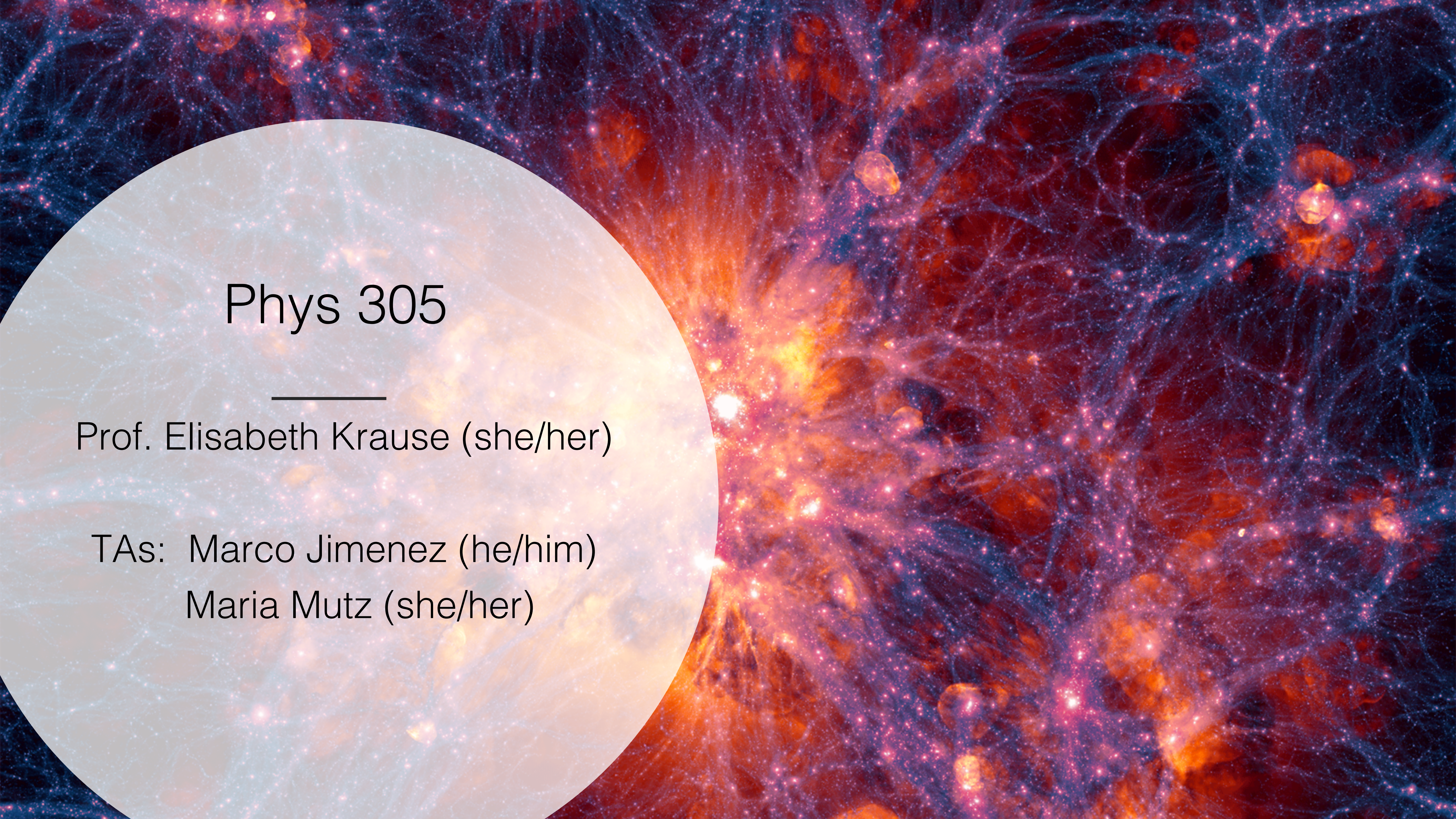

Phys 305

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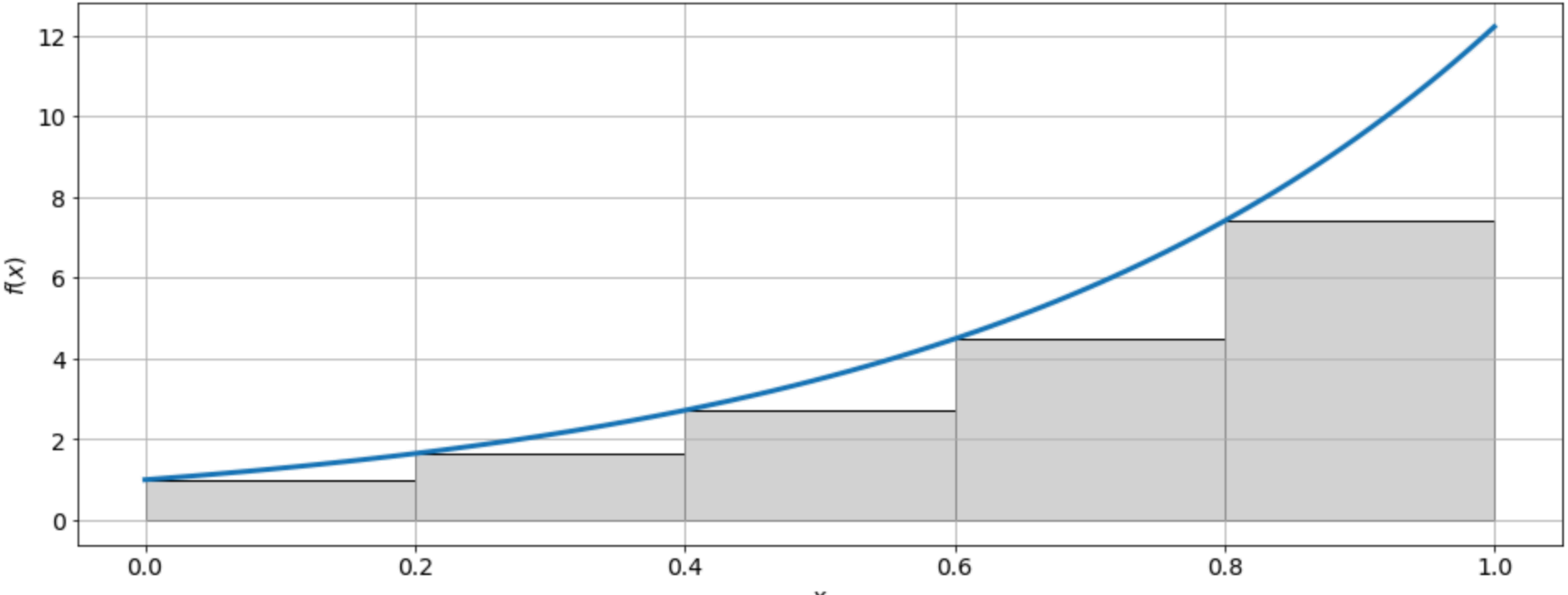
Today's Lecture

- Announcements
  - **Updated homework due date:** Mondays, at 5:00 pm (on D2L)
  - Solutions to Problem Set 1 posted on D2L (->Course Content)
  - **Problem Set 2** due 9/14/2020 at 5:00 pm (on D2L)
    - Note: Submitting zip (instead of tar.gz) folder will not result any point deductions!
- Today's lecture: more on numerical integration (Romberg, Monte Carlo)
- Outlook: Gaussian Quadrature integration, intro to term projects on Friday
  - Next week: numerical differentiation

Numerical Integration

Numerical integration: approximate area under the integrand by functions that are easy to integrate

- Riemann sum: piece-wise constant approximation



Riemann Integration

- Divide integration interval into N steps, perform Riemann sum

$$x_i = a + ih, \quad i = 1, \dots, N+1, \quad h = \frac{b-a}{N} \qquad \int_a^b f(x)dx \sim \sum_{i=0}^{N} f(x_i)(x_{i+1} - x_i) = h \sum_{i=0}^{N} f_i$$

- Now on to the approximation error

$$f(x) = f(x_i) + (x - x_i) f'(x_i) + \frac{(x - x_i)^2}{2} f''(x_i) + \dots$$

$$\int_{x_i}^{x_{i+1}} f(x)dx = (x_{i+1} - x_i) f(x_i) + \frac{(x_{i+1} - x_i)^2}{2} f'(x_i) + \frac{(x_{i+1} - x_i)^3}{3!} f''(x_i) + \dots$$

$$= \boxed{h f_i} + \boxed{h^2 \frac{1}{2} f_i'} + h^3 \frac{1}{3!} f_i'' + \dots$$

Riemann sum + leading error term

Now sum up the error over whole interval

$$\epsilon = N f'(\xi) \frac{1}{2} h^2 = N f'(\xi) \frac{1}{2} h \frac{(b-a)}{n} = h(b-a) \frac{1}{2} f'(\xi) = \mathcal{O}(h)$$

Trapezoidal Rule

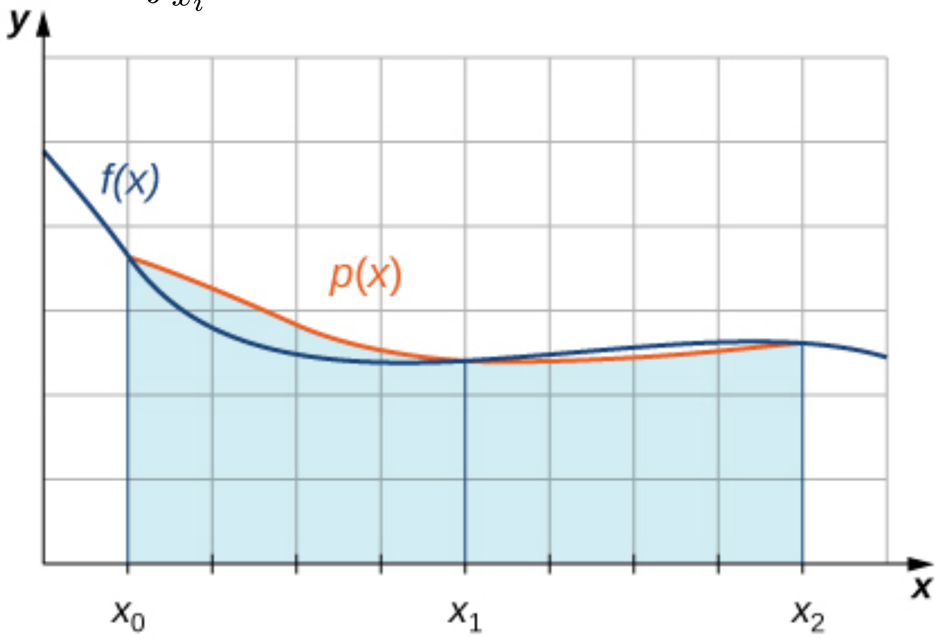
linear interpolation on sub-interval

$$f(x) \sim f_i + \frac{f_{i+1} - f_i}{h}(x - x_i)$$

$$\int_{x_i}^{x_{i+1}} f(x)dx \sim h\frac{1}{2}\left(f_{i+1} + f_i\right)$$

$$x_i = a + ih, \quad i = 1, \ldots, N+1, \quad h = \frac{b-a}{N}$$

$$\int_a^b f(x)dx \sim h\sum_{i=1}^{N}\frac{1}{2}(f(x_i) + f(x_{i+1}))$$



Error estimate: include next term, combining forward and backward interpolation

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}(f_i + f_{i+1}) + \frac{h^2}{4}(f_i' - f_{i+1}') + \frac{h^3}{12}(f_i'' + f_{i+1}'') + \ldots$$

$$f_{i+1}' = f_i' + hf_i'' + h^2\frac{1}{2}f_i''' + \ldots$$

$$f_{i+1}'' = f_i'' + hf_i''' + h^2\frac{1}{2}f_i^{(4)} + \ldots$$

$$\int_{x_i}^{x_{i+1}} f(x)dx = h\frac{1}{2}(f_i + f_{i+1}) - \boxed{h^3\frac{1}{12}f_i''} + \ldots$$

$$\boxed{\epsilon = -N\frac{h^3}{12}f''(\xi) = -\frac{(b-a)}{h}\frac{h^3}{12}f''(\xi) = \mathcal{O}(h^2)}$$

Improving over the Trapezoidal Rule

Richardson Extrapolation (cancellation of error terms):
Let $N_1(h)$ provide an estimate for M, with error of order h:

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots . \quad (1)$$

$$M = N_1\left(\frac{h}{2}\right) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots . \quad (2)$$

2*(2)-(1)

$$M = \underbrace{\boxed{N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right]}}_{\mathbf{N_2(h)}} + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots$$

$$M = \boxed{N_2(h)} - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots .$$

By combining estimates with different step size, we cancelled the leading order error term, and gain an order in convergence!

Improving over the Trapezoidal Rule

Romberg Integration:
Apply Richardson Extrapolation to Trapezoidal rule

$$I_n = h_n \left(\frac{1}{2} f(a) + \sum_{k=1}^{2^n - 1} f(a+kh) + \frac{1}{2} f(b) \right) \text{ with } N = 2^n \text{ and } h_n = (b-a)/2^n.$$

It can be shown that $\int_a^b f(x)dx = \sum_{i=1}^{N} \frac{1}{2} h(f_i + f_{i+1}) - \sum_{k=1}^{\lfloor 2p \rfloor} C_k h^{2k}$, apply to I_n

$$I_{n-1} = I + C_1 h_{n-1}^2 + \mathcal{O}(h^4)$$

$$I_n = I + C_1 (\frac{1}{2} h_{n-1})^2 + \mathcal{O}(h^4)$$

Now, use Richardson Extrapolation to cancel leading error term

$$I_{n,1} = \frac{4 I_{n,0} - I_{n-1,0}}{3} + \mathcal{O}(h^4)$$

$$I_{n+1,1} = \frac{4 I_{n+1,0} - I_{n,0}}{3} + \mathcal{O}(h^4)$$

$$I_{n,1} = I + C_2 (h_n)^4 + \mathcal{O}(h^6)$$

$$I_{n+1,1} = I + C_2 (\frac{1}{2} h_n)^4 + \mathcal{O}(h^6)$$

$$I_{n+1,2} = \frac{16 I_{n+1,1} - I_{n,1}}{15} + \mathcal{O}(h^6)$$

Romberg Integration

```
nextTrapezoidal(f, x_min, x_max, n):
    """
    Return the difference between the trapezoidal rule approx-
    imation for 2^n intervals and one-half the trapezoidal
    rule for 2^(n-1) intervals.
    """
    N = 2^n
    h = (x_max - x_min)/N
    I_n = 0
    for j = 1 to N/2:
        I_n = I_n + f(x_min + (2j - 1)h)

    return h I_n
```

Romberg Integration

```
romberg(f, x_min, x_max, n_max, ε):
    """
    Use Richardson extrapolation to compute the integral of f(x)
    from x_min to x_max with a relative error less than epsilon,
    using trapezoidal rules with up to 2^n_max intervals.
    """
    I_{0,0} = 1/2 (x_max − x_min)(f(x_min) + f(x_max))

    for n = 1 to n_max:
        I_{n,0} = 1/2 I_{n−1,0} + nextTrapezoidal(f, x_min, x_max, n)

        for k = 1 to n:
            q = 4^k
            I_{n,k} = (q I_{n,k−1} − I_{n−1,k−1})/(q − 1)

        if |I_{n,n} − I_{n,n−1}| < ε |I_{n,n−1}|:
            return I_{n,n}

    print "failured to converge!"
```

$$I_{0,0} = \frac{1}{2}(x_{max} - x_{min})(f(x_{min}) + f(x_{max}))$$

$$I_{n,0} = \frac{1}{2}I_{n-1,0} + \texttt{nextTrapezoidal}(f, x_{min}, x_{max}, n)$$

$$q = 4^k$$

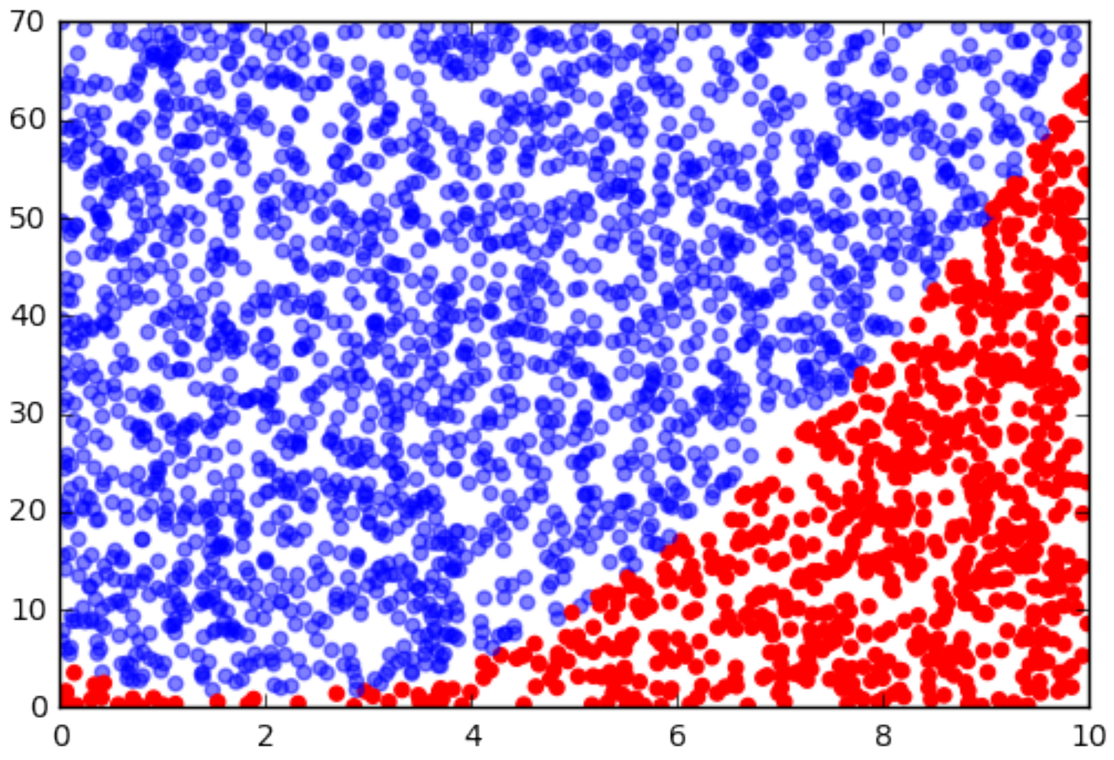
$$I_{n,k} = (qI_{n,k-1} - I_{n-1,k-1})/(q-1)$$

$$|I_{n,n} - I_{n,n-1}| < \epsilon\,|I_{n,n-1}|$$

Monte Carlo Integration

Integration by “darts”

- Define rectangular interval that encloses the integration region
- Draw random points $\{x_i, y_i\}$in this interval
- Determine fraction of points for which $f(x_i) < y_i$
- Calculate integral from fraction of point and rectangle area



Your Turn!

- Calculate the unit disk and unit ball area using Monte Carlo Integration
- Determine the convergence rate of Monte Carlo Integration in two and three dimensions