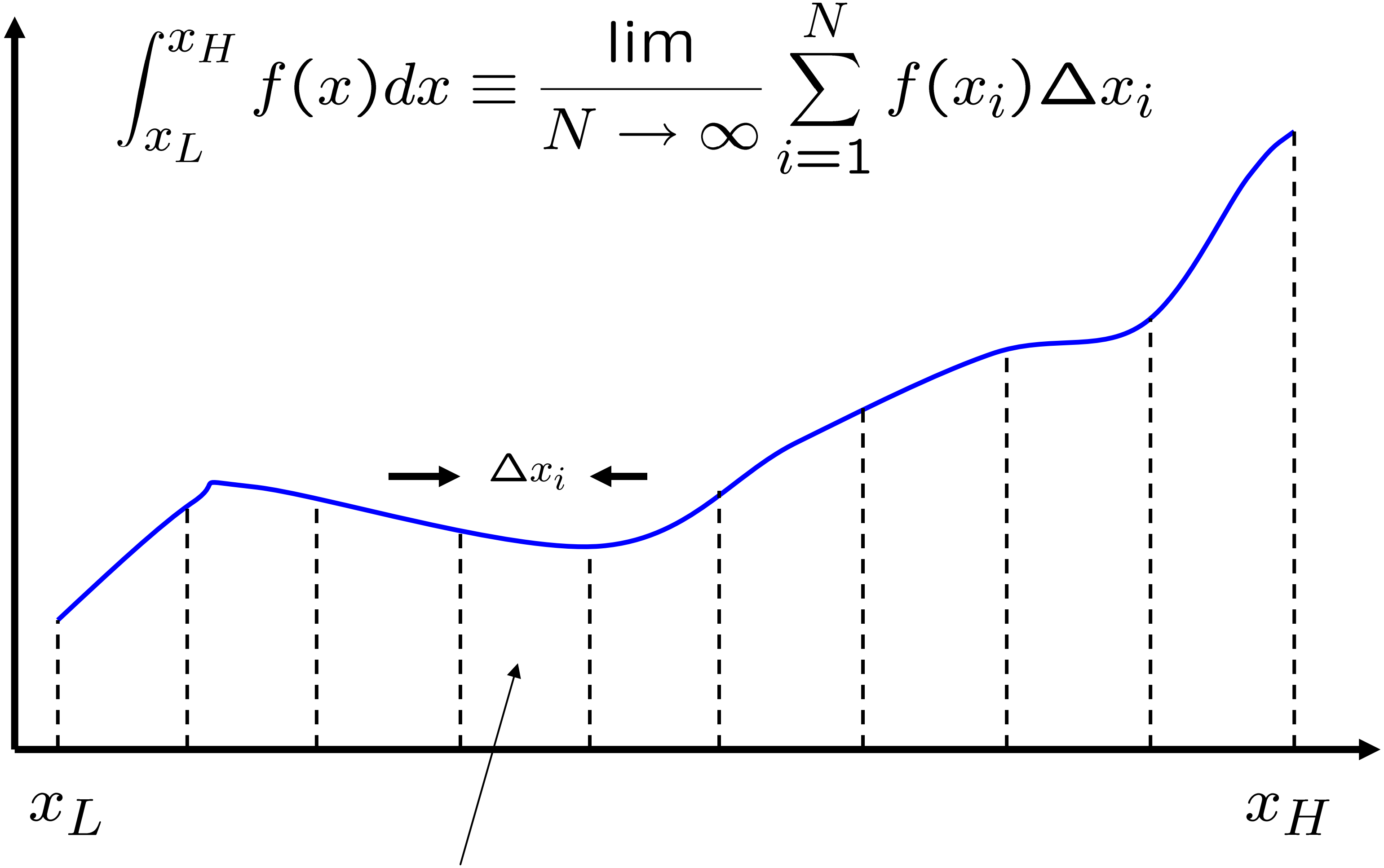
Goals for This Lecture:

- Continue with the subject of numerical integration
- Understand how to convergence test your answer

$$\int_{x_L}^{x_H} f(x)dx \equiv \lim_{N \to \infty} \sum_{i=1}^{N} f(x_i)\Delta x_i$$

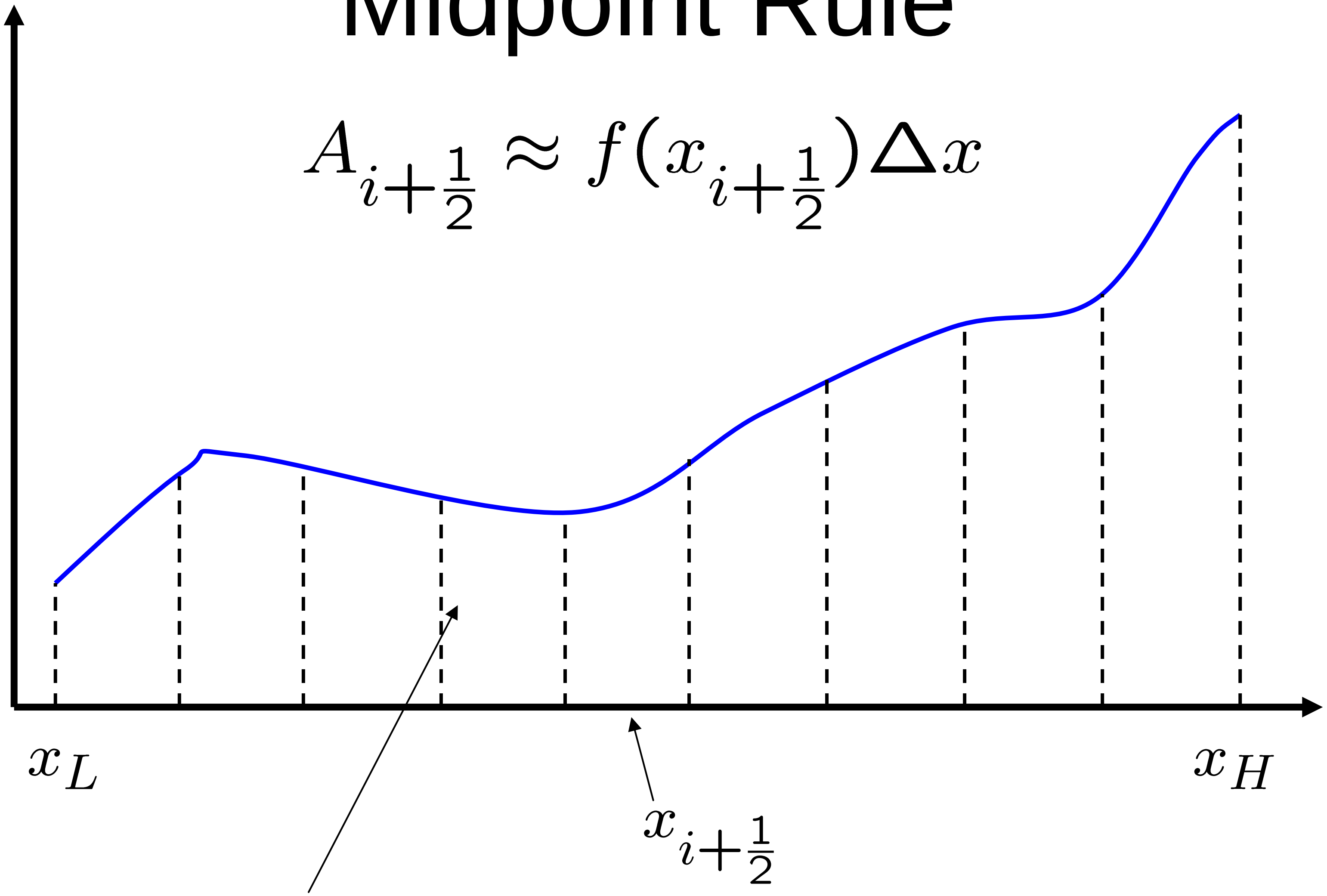


$A_i =$ Area of ith subinterval

$$\int_{x_L}^{x_H} f(x)dx \approx \sum_{i=1}^{N} A_i$$

Midpoint Rule

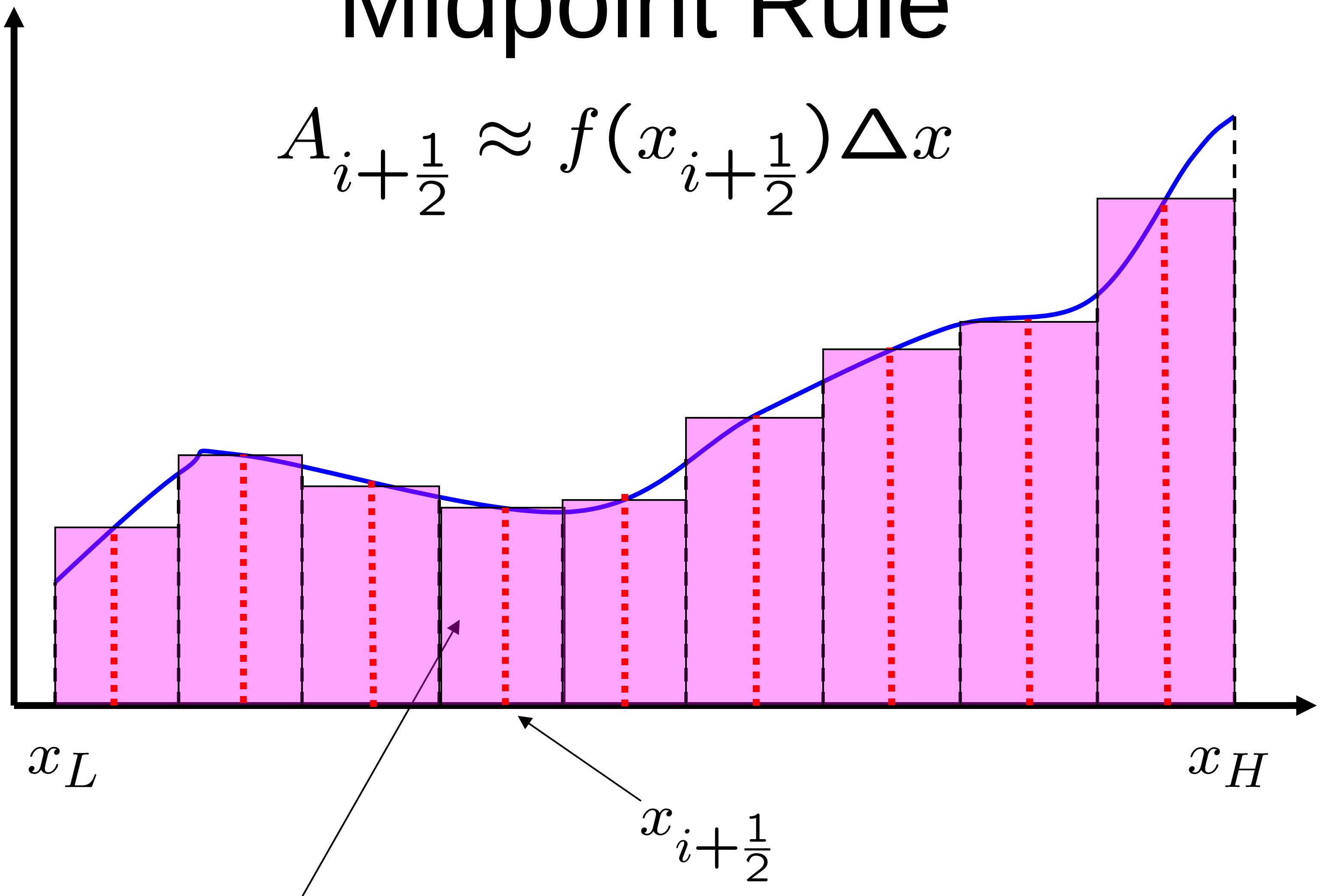
$$A_{i+\frac{1}{2}} \approx f(x_{i+\frac{1}{2}})\Delta x$$



$A_{i+\frac{1}{2}} =$ Area of i+1/2 th subinterval

Midpoint Rule

$$A_{i+\frac{1}{2}} \approx f(x_{i+\frac{1}{2}})\Delta x$$

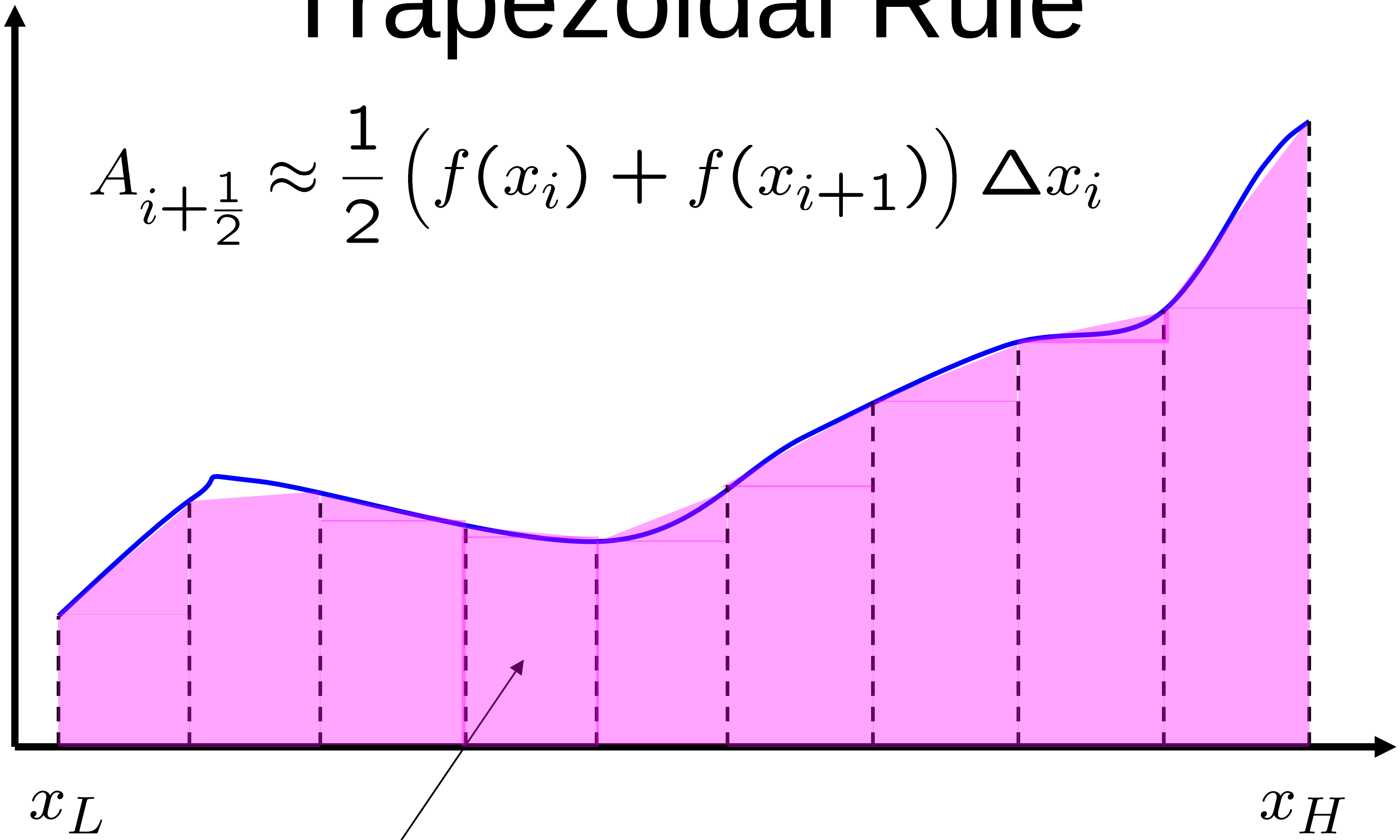


$$A_{i+\frac{1}{2}} =$$ Area of i+1/2 th subinterval

Midpoint Rule Program

```
! Purpose:  Integrate x^2 from 1.0 to 2.0 via midpoint rule
! Author:    F. Douglas Swesty
! Date:       9/28/2005
program midpoint
implicit none      ! Turn off implicit typing
Integer, parameter :: n=100   ! Number of subintervals
integer :: i            ! Loop index
real :: xlow=1.0, xhi=2.0  ! Bounds of integral
real :: dx             ! Variable to hold width of subinterval
real :: sum            ! Variable to hold sum
real :: xi             ! Variable to hold location of ith subinterval
real :: fi             ! Variable to value of function at ith subinterval

dx = (xhi-xlow)/(1.0*n)  ! Calculate with of subinterval

sum = 0.0                         ! Initialize sum
xi = xlow+0.5*dx               ! Initialize value of xi
do i = 1,n,1          ! Initiate loop
  fi = xi**2                        ! Evaluate function at ith point
  sum = sum+fi*dx                ! Accumulate sum
  xi = xi+dx                        ! Increment location of ith point
enddo                ! Terminate loop

write(*,*) ' sum = ',sum
stop                              ! Stop execution of the program
end program midpoint
```

Trapezoidal Rule



$A_{i+\frac{1}{2}} =$ Area of i+1/2 th subinterval

Open & Closed Integration Rules

- The Midpoint Rule is an example of an open integration rule
  - Does not require evaluation of function at limits of integral
  - Evaluation at $x_L+\Delta x/2$ and $x_H - \Delta x/2$ instead
- The Trapezoidal rule is an example of a closed integration rule
  - Requires evaluation of function at x_L and x_H
  - Problematic if function is not defined at endpoints of integration

Trapezoidal Rule Program

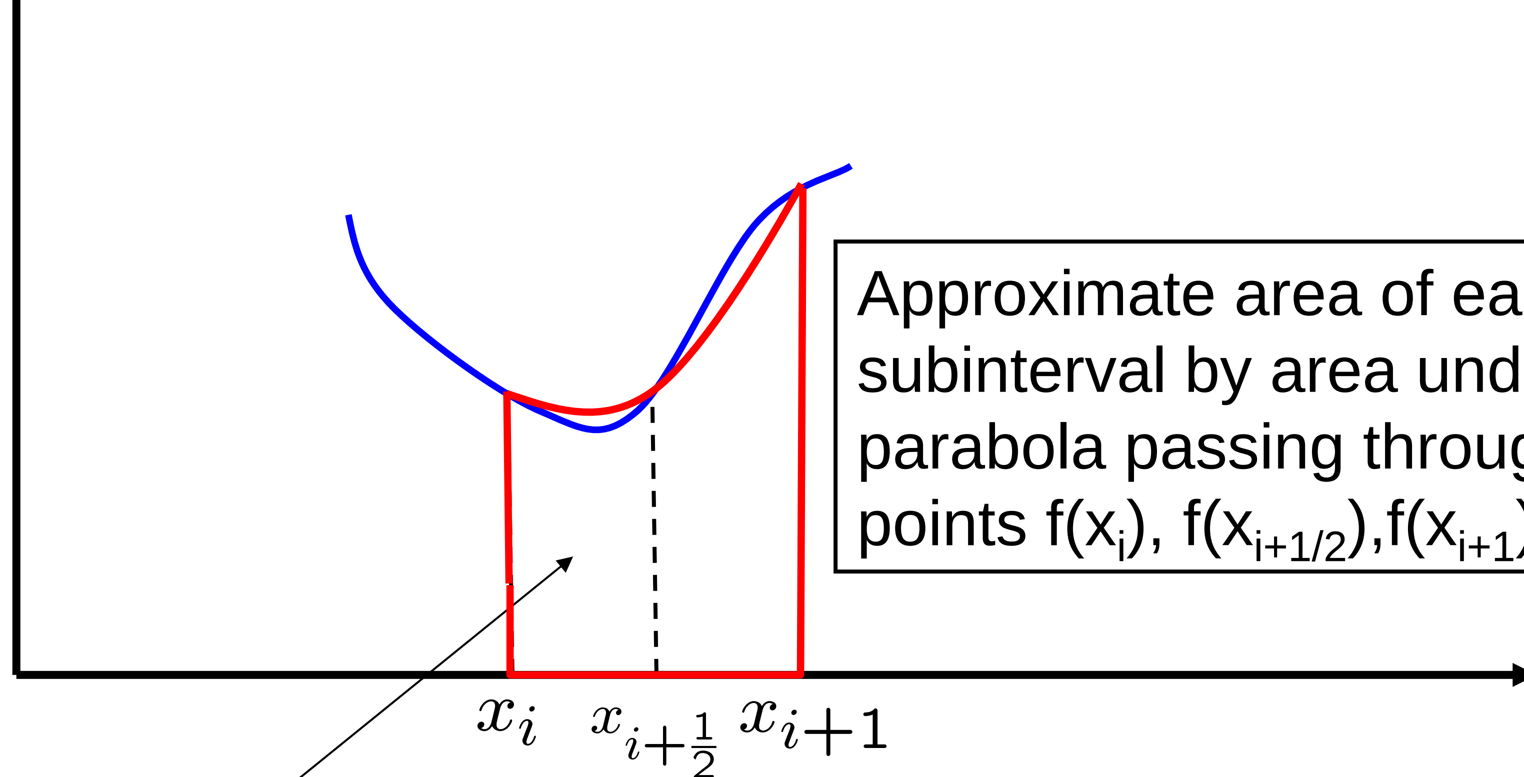
```
! Purpose:  Integrate x^2 from 1.0 to 2.0 via trapezoidal rule
! Author:    F. Douglas Swesty
! Date:       9/30/2005
program trapezoidal_rule
implicit none      ! Turn off implicit typing
Integer, parameter :: n=100   ! Number of subintervals
integer :: i            ! Loop index
real :: xlow=1.0, xhi=2.0  ! Bounds of integral
real :: dx             ! Variable to hold width of subinterval
real :: sum           ! Variable to hold sum
real :: xi             ! Variable to hold location of ith subinterval
real :: fi, fip1       ! Variable to value of function at ith subinterval

dx = (xhi-xlow)/(1.0*n)  ! Calculate with of subinterval

sum = 0.0                          ! Initialize sum
xi = xlow                         ! Initialize value of xi
do i = 1,n,1         ! Initiate loop
  fi = xi**2                           ! Evaluate function at ith point
  fip1 = (xi+deltax)**2          ! Evaluate function at i+1th point
  sum = sum+0.5*(fi+fip1)*dx   ! Accumulate sum
  xi = xi+dx                           ! Increment location of ith point
enddo                ! Terminate loop

write(*,*) ' sum = ',sum
stop                               ! Stop execution of the program
end program trapezoidal_rule
```

Is your solution accurate?

- If the integral is known analytically the error in the numerical integration can be calculated exactly.
- In general, you will not be able to do this
- The only way to understand the accuracy of your answer is convergence test your answer
- Double the number of points and look to see how much the answer changes
- Plot the result versus the number of subintervals
- Look at how much the answer changes when you double the number of subintervals

A more accurate technique: Simpson's Rule

$$A_{i+\frac{1}{2}} \approx \frac{1}{6}\left(f(x_i) + 4f(x_{i+\frac{1}{2}}) + f(x_{i+1})\right)\Delta x_i$$



Approximate area of each subinterval by area under a parabola passing through points $f(x_i)$, $f(x_{i+1/2})$,$f(x_{i+1})$

$A_{i+\frac{1}{2}} =$ Area of i+1/2th subinterval

A Derivation of Simpson's Rule

The parabolic curve $\tilde{f}(x) = Ax^2 + Bx + C$

Must pass through the two endpoints of the interval as well as the midpoint:

$$\tilde{f}(x_i) = Ax_i^2 + Bx_i + C = f(x_i)$$

$$\tilde{f}(x_{i+\frac{1}{2}}) = Ax_{i+\frac{1}{2}}^2 + Bx_{i+\frac{1}{2}} + C = f(x_{i+\frac{1}{2}})$$

$$\tilde{f}(x_{i+1}) = Ax_{i+1}^2 + Bx_{i+1} + C = f(x_{i+1})$$

Now solve for A, B, and C

Some algebra yields:

$$A = \frac{2}{(\Delta x)^2} \left\{ f(x_i) - 2f(x_{i+\frac{1}{2}}) + f(x_{i+1}) \right\}$$

$$B = -\frac{2}{(\Delta x)^2} \left\{ 2x_i(f(x_i) - 2f(x_{i+\frac{1}{2}}) + f(x_{i+1})) + \Delta x(3f(x_i) - 4f(x_{i+\frac{1}{2}}) + f(x_{i+1})) \right\}$$

$$C = \frac{2}{(\Delta x)^2} \left\{ \frac{(\Delta x)^2}{4} f(x_i) + \frac{\Delta x}{2} x_i(3f(x_i) - 4f(x_{i+\frac{1}{2}}) + f(x_{i+1})) + x_i^2(f(x_i) - 2f(x_{i+\frac{1}{2}}) + f(x_{i+1})) \right\}$$

Now integrate $\int_{x_i}^{x_{i+1}} \tilde{f}(x)dx$

to get the area under the parabola:

$$A_{i+\frac{1}{2}} = \frac{A}{3}x^3 + \frac{B}{2}x^2 + Cx$$

Substitute for A, B, and C. Do a lot of algebra to get:

$$A_{i+\frac{1}{2}} \approx \frac{1}{6}\left(f(x_i) + 4f(x_{i+\frac{1}{2}}) + f(x_{i+1})\right)\Delta x_i$$

Reading Assignment

– Read Sections 4.1,4.3