

The goal of this assignment was to approximate the definite integral of a highly oscillatory function on an interval of the real number line through difference methods using parallel computing. Let  $K \in \{100, 101, \dots, 10000\}$  be a fixed wavenumber and  $f(K, \cdot) : [0, \pi] \subset \mathbb{R} \mapsto \mathbb{R}$ , then define

$$H(K) := \int_0^\pi f(K, x) dx \approx \sum_{i=1}^K \int_{a_i}^{b_i} f(K, x) dx \approx \sum_{i=1}^K A(K, i),$$

where  $A(K, i)$  is an approximation to the partial integral of  $f(K, \cdot)$  on  $[a_i, b_i] \subset \mathbb{R}$  of width  $\pi/K$ . Now take 101 quadrature points,  $x_{i,j}$ , on  $[a_i, b_i]$ , in order to compute  $A(K, i)$  using the midpoint method,  $A_{M,101}(K, i)$ , the trapezoid method,  $A_{T,101}(K, i)$ , and Simpson's method,  $A_{S,101}(K, i)$ , where

$$\begin{aligned} a_i &= x_{i,0} < x_{i,1} < \dots < x_{i,100} < x_{i,101} = b_i, \\ \xi_{i,j} &= \frac{x_{i,j-1} + x_{i,j}}{2}, \\ h_{i,j} &= x_{i,j} - x_{i,j-1}, \\ A_{M,101}(K, i) &:= \sum_{j=1}^{101} f(K, \xi_{i,j}) h_{i,j}, \\ A_{T,101}(K, i) &:= \sum_{j=1}^{101} \frac{1}{2} \left[ f(K, x_{i,j-1}) + f(K, x_{i,j}) \right] h_{i,j}, \\ A_{S,101}(K, i) &:= \frac{2}{3} A_{M,101}(K, i) + \frac{1}{3} A_{T,101}(K, i), \\ i &\in \{1, 2, \dots, K\}, j \in \{1, 2, \dots, 101\}. \end{aligned}$$

The above was achieved with a main file and a module written in Fortran 90 compiled with mpif90. The code is as follows:

```

module utils
contains
subroutine mts(wn, pts, qn, M, T, S)

    implicit none
    integer :: i
    integer, intent(in) :: wn, qn
    real(kind=kind(0.0d0)), dimension(0:100), intent(in) :: pts
    real(kind=kind(0.0d0)), intent(out) :: M, T, S

    M = 0; T = 0; S = 0
    do i=1, qn-1
        M = M + fn(wn, (pts(i)+pts(i-1))/2.0d0)*(pts(i)-pts(i-1))
        T = T + ((fn(wn, pts(i-1))+fn(wn, pts(i)))*(pts(i)-pts(i-1)))/2.0d0
    enddo
    S = (2.0d0/3.0d0)*M + T/3.0d0

endsubroutine mts

real(kind=kind(0.0d0)) function fn(kw, point)

    implicit none
    integer, intent(in) :: kw
    real(kind=kind(0.0d0)), intent(in) :: point

    fn = cos(100.0d0*point-kw*sin(point))

endfunction fn
endmodule utils

```

```

program main

  use mpi
  use utils

  implicit none
  integer :: ierr, rank, num_cores, k, i, j, num2receive, tag
  real(kind=kind(0.0d0)), parameter :: pi = 4*atan(1.0d0)
  real(kind=kind(0.0d0)) :: M, T, S, PM, PT, PS, HM, HT, HS, stime, etime
  real(kind=kind(0.0d0)), dimension(:), allocatable :: mypts, allpts
  integer, dimension(mpi_status_size) :: mystatus
  integer, dimension(:), allocatable :: num2send, displs

  call mpi_init(ierr)
  call mpi_comm_rank(mpi_comm_world,rank,ierr)
  call mpi_comm_size(mpi_comm_world,num_cores,ierr)
  stime = mpi_wtime()

  open(unit=13,file="m.dat",action="write",status="replace")
  open(unit=14,file="t.dat",action="write",status="replace")
  open(unit=15,file="s.dat",action="write",status="replace")

  if (rank == 0) then
    write(*,*) "Using", num_cores, "cores."
    write(*, "(a5, a30, a30, a30)") "K", "Midpoint_H(K)", "Trapezoidal_H(K)", "Simpson's_H(K)"
  endif
  do k = 100, 10000
    allocate(allpts(0:k))
    allocate(mypts(0:k/num_cores))
    allocate(num2send(0:num_cores-1))
    allocate(displs(0:num_cores-1))

    allpts = (/j*pi/k, j=0, k)/)
    mypts = (/(-1.0, j=0, k/num_cores)/)
    displs = (/0, j=0, num_cores-1)/)
    do i=0, num_cores-1
      num2send(i) = k/num_cores
      if (i<=modulo(k,num_cores)) then
        num2send(i) = num2send(i)+1
      endif
      if (i /= 0) then
        displs(i) = displs(i-1) + num2send(i)
      endif
    enddo
    num2receive = num2send(rank)

    call mpi_scatterv(allpts,num2send,displs,mpi_double_precision,&
                     mypts,num2receive,mpi_double_precision,0,&
                     mpi_comm_world,ierr)

    PM = 0; PT = 0; PS = 0
    do i=0, size(mypts)-1
      M = 0; T = 0; S = 0
      if (mypts(i) > -1) then
        call mts(k, (/mypts(i)+j*pi/100/k, j=0, 100)/), 101, M, T, S)
        PM = PM + M
        PT = PT + T
        PS = PS + S
      endif
    enddo
    deallocate(allpts, mypts, num2send, displs)

    call mpi_barrier(mpi_comm_world, ierr)

    tag = 0
    if (rank == 0) then
      HM = PM
      HT = PT
      HS = PS
      do i = 1, num_cores-1
        call mpi_recv(PM, 1, mpi_double_precision, i, tag, mpi_comm_world, mystatus, ierr)
        call mpi_recv(PT, 1, mpi_double_precision, i, tag, mpi_comm_world, mystatus, ierr)
        call mpi_recv(PS, 1, mpi_double_precision, i, tag, mpi_comm_world, mystatus, ierr)
        HM = HM + PM
        HT = HT + PT
        HS = HS + PS
      enddo
    else
      call mpi_send(PM, 1, mpi_double_precision, 0, tag, mpi_comm_world, ierr)
      call mpi_send(PT, 1, mpi_double_precision, 0, tag, mpi_comm_world, ierr)
      call mpi_send(PS, 1, mpi_double_precision, 0, tag, mpi_comm_world, ierr)
    endif

    if (rank == 0) then
      if (modulo(k, 1000) == 0) then
        write(*, "(i5, es30.15e3, es30.15e3, es30.15e3)") k, HM, HT, HS
      endif
      write(13,*) k, HM
      write(14,*) k, HT
      write(15,*) k, HS
    endif
  enddo

  close(13); close(14); close(15)

  etime = mpi_wtime()

  if (rank == 0) then
    write(*,*) "Time taken: ", etime-stime
  endif

  call mpi_finalize(ierr)

endprogram main

```

Running the above program will compute  $H(K)$  for all  $K \in \{100, 101, \dots, 10000\}$ , writing output to the console when  $1000 \mid K$  and writing all values of  $H(K)$  to a file. Some computed values using 8 cores are as follows:

$K$	$H_{Mid}(K)$	$H_{Trap}(K)$	$H_{Simp}(K)$
1000	3.819159292450652E-002	3.819146669047201E-002	3.819155084649498E-002
2000	-4.844391641984440E-002	-4.844393643020983E-002	-4.844392308996622E-002
3000	-3.642203217829408E-002	-3.642200581893822E-002	-3.642202339184213E-002
4000	-1.417394345379661E-002	-1.417389887290094E-002	-1.417392859349807E-002
5000	1.237969805213174E-002	1.237974211425157E-002	1.237971273950503E-002
6000	2.957259450025162E-002	2.957262597415612E-002	2.957260499155312E-002
7000	2.671023841147271E-002	2.671025176115547E-002	2.671024286136696E-002
8000	6.324420119174937E-003	6.324415852441528E-003	6.324418696930464E-003
9000	-1.641023755211308E-002	-1.641025431321439E-002	-1.641024313914685E-002
10000	-2.484826969529740E-002	-2.484829140135555E-002	-2.484827693065011E-002

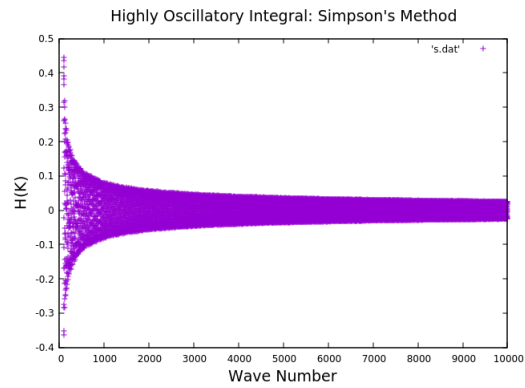
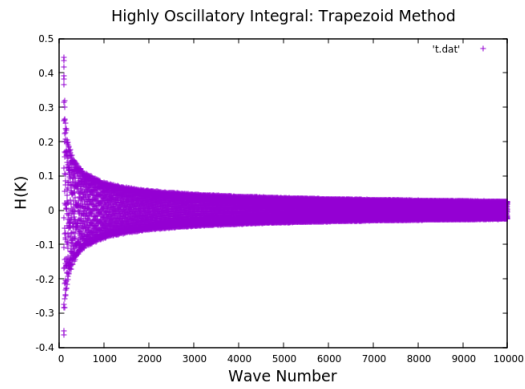
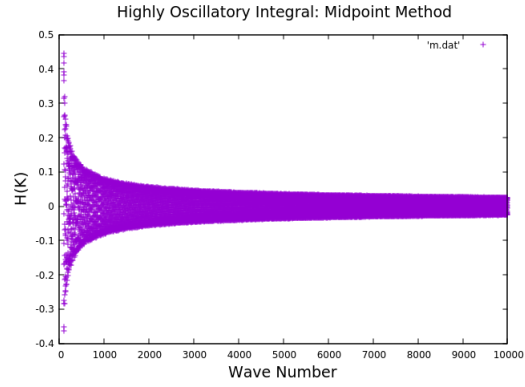
Some computed values using 16 cores are as follows:

$K$	$H_{Mid}(K)$	$H_{Trap}(K)$	$H_{Simp}(K)$
1000	3.462382957648013E-002	3.462385379110549E-002	3.462383764802190E-002
2000	-4.837051599804793E-002	-4.837054657167911E-002	-4.837052618925834E-002
3000	-3.644134234250336E-002	-3.644134045213760E-002	-3.644134171238143E-002
4000	-1.392567124702175E-002	-1.392564881449324E-002	-1.392566376951225E-002
5000	1.336853847205303E-002	1.336853524529409E-002	1.336853739646673E-002
6000	2.958710956778173E-002	2.958714345406040E-002	2.958712086320795E-002
7000	2.713810248334630E-002	2.713810085494336E-002	2.713810194054531E-002
8000	6.025862388101258E-003	6.025892103065393E-003	6.025872293089307E-003
9000	-1.674350874433848E-002	-1.674350783603062E-002	-1.674350844156919E-002
10000	-2.521455576408334E-002	-2.521453767524605E-002	-2.521454973447090E-002

Something to note is that the computed values depend on the number of cores used. This is probably not good and is because of the way the subintervals are created and scattered to the cores. In order to compute the integral, the program creates  $K$  starting points, one for each of the  $K$  subintervals,  $\left\{0, \frac{\pi}{K}, \frac{2\pi}{K}, \dots, \frac{(K-1)\pi}{K}\right\}$ . These starting points are then scattered to each of the cores in a balanced way. The cores then loop through their starting points and evaluate an integral by creating 101 quadrature points for each starting point,  $\left\{\frac{i\pi}{K}, \frac{i\pi}{K} + \frac{\pi}{100K}, \dots, \frac{(i+1)\pi}{K}\right\}$ . By running the program with different numbers of cores, the complexity of the program can be determined. Time taken by number of cores used is as follows:

Number of Cores	Time to Compute (s)
1	572.56358560398803
2	303.70187161699869
4	170.86698438599706
8	92.290132593014278
16	49.949442379001994
32	30.678848117997404

On average, doubling the amount of cores used, decreases the amount of time taken by a factor of 1.8, this suggests that the complexity for this program is linear. The values of  $H(K)$  and  $K$  for  $K \in \{100, 101, \dots, 10000\}$  were then graphed using `gnuplots`, these graphs are shown below:



We see that as  $K$  grows large the value of  $H(K)$  appears to be approaching 0. This makes sense as we are calculating the integral of  $\cos$  on  $[0, \pi]$ .