Figure 4.2.1. Sequential calls to the routine trapzd incorporate the information from previous calls and evaluate the integrand only at those new points necessary to refine the grid. The bottom line shows the totality of function evaluations after the fourth call. The routine qsimp, by weighting the intermediate results, transforms the trapezoid rule into Simpson's rule with essentially no additional overhead.

There are also formulas of higher order for this situation, but we will refrain from giving them.

The semi-open formulas are just the obvious combinations of equations (4.1.11)–(4.1.14) with (4.1.15)–(4.1.18), respectively. At the closed end of the integration, use the weights from the former equations; at the open end use the weights from the latter equations. One example should give the idea, the formula with error term decreasing as $1/N^3$ which is closed on the right and open on the left:

$$
\int_{x_1}^{x_N} f(x)dx = h \left[ \frac{23}{12} f_2 + \frac{7}{12} f_3 + f_4 + f_5 + \cdots + f_{N-2} + \frac{13}{12} f_{N-1} + \frac{5}{12} f_N \right] + O \left( \frac{1}{N^3} \right)
$$

CITED REFERENCES AND FURTHER READING:

4.2 Elementary Algorithms

Our starting point is equation (4.1.11), the extended trapezoidal rule. There are two facts about the trapezoidal rule which make it the starting point for a variety of algorithms. One fact is rather obvious, while the second is rather "deep."

The obvious fact is that, for a fixed function $f(x)$ to be integrated between fixed limits $a$ and $b$, one can double the number of intervals in the extended trapezoidal rule without losing the benefit of previous work. The coarsest implementation of the trapezoidal rule is to average the function at its endpoints $a$ and $b$. The first stage of refinement is to add to this average the value of the function at the halfway point. The second stage of refinement is to add the values at the 1/4 and 3/4 points. And so on (see Figure 4.2.1).

Without further ado we can write a routine with this kind of logic to it:
SUBROUTINE trapzd(func,a,b,s,n)
INTEGER n
REAL a,b,s,func
EXTERNAL func
This routine computes the n-th stage of refinement of an extended trapezoidal rule. func is input as the name of the function to be integrated between limits a and b, also input. When called with n=1, the routine returns as s the crudest estimate of \( \int_a^b f(x) dx \). Subsequent calls with n=2,3,... (in that sequential order) will improve the accuracy of s by adding \( 2^{n-2} \) additional interior points. s should not be modified between sequential calls.

INTEGER it,j
REAL del,sum,tnm,x
if (n.eq.1) then
   n=0.5*(b-a)*(func(a)+func(b))
else
   it=2**(n-2)
   tnm=it
del=(b-a)/tnm
   x=a+0.5*del
   sum=0.
doi: j=1,itr
      sum=sum+func(x)
      x=x+del
endo oi:
s=0.5*(s+(b-a)*sum/tnm)
endif
return
END

The above routine (trapzd) is a workhorse that can be harnessed in several ways. The simplest and crudest is to integrate a function by the extended trapezoidal rule where you know in advance (we can’t imagine how!) the number of steps you want. If you want \( 2^M + 1 \), you can accomplish this by the fragment

\[
\text{do } j=1, M+1
\text{call trapzd(func,a,b,s,j)}
\text{enddo}
\]

with the answer returned as s.

Much better, of course, is to refine the trapezoidal rule until some specified degree of accuracy has been achieved:

SUBROUTINE qtrap(func,a,b,s)
INTEGER JMAX
REAL a,b,func,s,EPS
EXTERNAL func
PARAMETER (EPS=1.e-6, JMAX=20)
C USES trapzd
Returns as s the integral of the function func from a to b. The parameters EPS can be set to the desired fractional accuracy and JMAX so that 2 to the power JMAX-1 is the maximum allowed number of steps. Integration is performed by the trapezoidal rule.

INTEGER j
REAL olds
olds=1.e30
Any number that is unlikely to be the average of the function at its endpoints will do here.
do j=1, JMAX
   call trapzd(func,a,b,s,j)
   if (j.gt.5) then
      Avoid spurious early convergence.
      if (abs(s-old).lt.EPS*abs(old).or.
         (s.eq.0..and.old.eq.0.)) return
   endif
   olds=s
endo j:
pause 'too many steps in qtrap'
END
Unsophisticated as it is, routine qtrap is in fact a fairly robust way of doing integrals of functions that are not very smooth. Increased sophistication will usually translate into a higher-order method whose efficiency will be greater only for sufficiently smooth integrands. qtrap is the method of choice, e.g., for an integrand which is a function of a variable that is linearly interpolated between measured data points. Be sure that you do not require too stringent an EPS, however: If qtrap takes too many steps in trying to achieve your required accuracy, accumulated roundoff errors may start increasing, and the routine may never converge. A value $10^{-6}$ is just on the edge of trouble for most 32-bit machines; it is achievable when the convergence is moderately rapid, but not otherwise.

We come now to the “deep” fact about the extended trapezoidal rule, equation (4.1.11). It is this: The error of the approximation, which begins with a term of order $1/N^2$, is in fact entirely even when expressed in powers of $1/N$. This follows directly from the Euler-Maclaurin Summation Formula,

$$\int_{x_1}^{x_N} f(x) dx = h \left[ \frac{1}{2} f_1 + f_2 + f_3 + \cdots + f_{N-1} + \frac{1}{2} f_N \right] - \frac{B_2 h^2}{2!} (f_N' - f_1') - \cdots - \frac{B_{2k} h^{2k}}{(2k)!} (f_{N-1}^{(2k-1)} - f_1^{(2k-1)}) - \cdots \quad (4.2.1)$$

Here $B_{2k}$ is a Bernoulli number, defined by the generating function

$$\frac{t}{e^t - 1} = \sum_{n=0}^{\infty} B_n \frac{t^n}{n!} \quad (4.2.2)$$

with the first few even values (odd values vanish except for $B_1 = -1/2$)

$$B_0 = 1 \quad B_2 = \frac{1}{6} \quad B_4 = -\frac{1}{30} \quad B_6 = \frac{1}{42} \quad B_8 = -\frac{1}{30} \quad B_{10} = \frac{5}{66} \quad B_{12} = -\frac{691}{2730} \quad (4.2.3)$$

Equation (4.2.1) is not a convergent expansion, but rather only an asymptotic expansion whose error when truncated at any point is always less than twice the magnitude of the first neglected term. The reason that it is not convergent is that the Bernoulli numbers become very large, e.g.,

$$B_{50} = \frac{495057205241079648212477525}{66}$$

The key point is that only even powers of $h$ occur in the error series of (4.2.1). This fact is not, in general, shared by the higher-order quadrature rules in §4.1. For example, equation (4.1.12) has an error series beginning with $O(1/N^3)$, but continuing with all subsequent powers of $N$: $1/N^4$, $1/N^5$, etc.

Suppose we evaluate (4.1.11) with $N$ steps, getting a result $S_N$, and then again with $2N$ steps, getting a result $S_{2N}$. (This is done by any two consecutive calls of
trapzd.) The leading error term in the second evaluation will be 1/4 the size of the error in the first evaluation. Therefore the combination

\[ S = \frac{4}{3} S_{2N} - \frac{1}{3} S_N \]  

(4.2.4)

will cancel out the leading order error term. But there is no error term of order \(1/N^3\), by (4.2.1). The surviving error is of order \(1/N^4\), the same as Simpson's rule. In fact, it should not take long for you to see that (4.2.4) is exactly Simpson's rule (4.1.13), alternating 2/3's, 4/3's, and all. This is the preferred method for evaluating that rule, and we can write it as a routine exactly analogous to qtrap above:

```fortran
SUBROUTINE qsimp(func,a,b,s)
INTEGER JMAX
REAL a,b,func,s,EPS
EXTERNAL func
PARAMETER (EPS=1.e-6, JMAX=20)
C USES trapzd

Returns as s the integral of the function func from a to b. The parameters EPS can be set to the desired fractional accuracy and JMAX so that 2 to the power JMAX-1 is the maximum allowed number of steps. Integration is performed by Simpson's rule.

INTEGER j
REAL os,ost,st
ost=-1.e30
os= -1.e30
do 11 j=1,JMAX
   call trapzd(func,a,b,st,j)
s=(4.*st-ost)/3.     \* Compare equation (4.2.4), above.
   if (j.gt.5) then
      if (abs(s-os).lt.EPS*abs(os).or.\*
         (s.eq.0..and.os.eq.0.)) return
   endif
   os=s
   ost=st
11 enddo

pause 'too many steps in qsimp'
END
```

The routine qsimp will in general be more efficient than qtrap (i.e., require fewer function evaluations) when the function to be integrated has a finite 4th derivative (i.e., a continuous 3rd derivative). The combination of qsimp and its necessary workhorse trapzd is a good one for light-duty work.

CITED REFERENCES AND FURTHER READING:
4.3 Romberg Integration

We can view Romberg’s method as the natural generalization of the routine \texttt{qsimp} in the last section to integration schemes that are of higher order than Simpson’s rule. The basic idea is to use the results from \( k \) successive refinements of the extended trapezoidal rule (implemented in \texttt{trapzd}) to remove all terms in the error series up to but not including \( O(1/N^{2k}) \). The routine \texttt{qsimp} is the case of \( k = 2 \). This is one example of a very general idea that goes by the name of 

Richardson’s deferred approach to the limit: Perform some numerical algorithm for various values of a parameter \( h \), and then extrapolate the result to the continuum limit \( h = 0 \).

Equation (4.2.4), which subtracts off the leading error term, is a special case of polynomial extrapolation. In the more general Romberg case, we can use Neville’s algorithm (see §3.1) to extrapolate the successive refinements to zero stepsize. Neville’s algorithm can in fact be coded very concisely within a Romberg integration routine. For clarity of the program, however, it seems better to do the extrapolation by subroutine call to \texttt{polint}, already given in §3.1.

\begin{verbatim}
SUBROUTINE qromb(func,a,b,ss)
INTEGER JMAX,JMAXP,K,KM
REAL a,b,func,ss,EPS
EXTERNAL func
PARAMETER (EPS=1.e-6, JMAX=20, JMAXP=JMAX+1, K=5, KM=K-1)
C USES polint,trapzd

Returns as \( ss \) the integral of the function \( func \) from \( a \) to \( b \). Integration is performed by Romberg’s method of order 2\( K \), where, e.g., \( K=2 \) is Simpson’s rule. Parameters: \( EPS \) is the fractional accuracy desired, as determined by the extrapolation error estimate; \( JMAX \) limits the total number of steps; \( K \) is the number of points used in the extrapolation.

INTEGER j
REAL dss,h(JMAXP),s(JMAXP)

These store the successive trapezoidal approximations and their relative stepsizes.

\( h(1)=1. \)

\begin{verbatim}
do 11 j=1,JMAX
    call trapzd(func,a,b,s(j),j)
    if (j.ge.K) then
        call polint(h(j-KM),s(j-KM),K,0.,ss,dss)
        if (abs(dss).le.EPS*abs(ss)) return
    endif
    s(j+1)=s(j)
    h(j+1)=0.25*h(j)
\end{verbatim}

This is a key step: The factor is 0.25 even though the stepsize is decreased by only 0.5. This makes the extrapolation a polynomial in \( h^2 \) as allowed by equation (4.2.1), not just a polynomial in \( h \).

enddo

pause 'too many steps in qromb'

END
\end{verbatim}

The routine \texttt{qromb}, along with its required \texttt{trapzd} and \texttt{polint}, is quite powerful for sufficiently smooth (e.g., analytic) integrands, integrated over intervals which contain no singularities, and where the endpoints are also nonsingular. \texttt{qromb}, in such circumstances, takes many, \textit{many} fewer function evaluations than either of the routines in §4.2. For example, the integral

\[ \int_{0}^{2} x^4 \log(x + \sqrt{x^2 + 1}) \, dx \]