CITED REFERENCES AND FURTHER READING:

16.4 Richardson Extrapolation and the Bulirsch-Stoer Method

The techniques described in this section are not for differential equations containing nonsmooth functions. For example, you might have a differential equation whose right-hand side involves a function that is evaluated by table look-up and interpolation. If so, go back to Runge-Kutta with adaptive stepsize choice: That method does an excellent job of feeling its way through rocky or discontinuous terrain. It is also an excellent choice for quick-and-dirty, low-accuracy solution of a set of equations. A second warning is that the techniques in this section are not particularly good for differential equations that have singular points inside the interval of integration. A regular solution must tiptoe very carefully across such points. Runge-Kutta with adaptive stepsize can sometimes effect this; more generally, there are special techniques available for such problems, beyond our scope here.

Apart from those two caveats, we believe that the Bulirsch-Stoer method, discussed in this section, is the best known way to obtain high-accuracy solutions to ordinary differential equations with minimal computational effort. (A possible exception, infrequently encountered in practice, is discussed in §16.7.)

Three key ideas are involved. The first is Richardson’s deferred approach to the limit, which we already met in §4.3 on Romberg integration. The idea is to consider the final answer of a numerical calculation as itself being an analytic function (if a complicated one) of an adjustable parameter like the stepsize \( h \). That analytic function can be probed by performing the calculation with various values of \( h \), none of them being necessarily small enough to yield the accuracy that we desire. When we know enough about the function, we fit it to some analytic form, and then evaluate it at that mythical and golden point \( h = 0 \) (see Figure 16.4.1). Richardson extrapolation is a method for turning straw into gold! (Lead into gold for alchemist readers.)

The second idea has to do with what kind of fitting function is used. Bulirsch and Stoer first recognized the strength of rational function extrapolation in Richardson-type applications. That strength is to break the shackles of the power series and its limited radius of convergence, out only to the distance of the first pole in the complex
Figure 16.4.1. Richardson extrapolation as used in the Bulirsch-Stoer method. A large interval $H$ is spanned by different sequences of finer and finer substeps. Their results are extrapolated to an answer that is supposed to correspond to infinitely fine substeps. In the Bulirsch-Stoer method, the integrations are done by the modified midpoint method, and the extrapolation technique is rational function or polynomial extrapolation.

Rational function fits can remain good approximations to analytic functions even after the various terms in powers of $h$ all have comparable magnitudes. In other words, $h$ can be so large as to make the whole notion of the “order” of the method meaningless — and the method can still work superbly. Nevertheless, more recent experience suggests that for smooth problems straightforward polynomial extrapolation is slightly more efficient than rational function extrapolation. We will accordingly adopt polynomial extrapolation as the default, but the routine bsstep below allows easy substitution of one kind of extrapolation for the other. You might wish at this point to review §3.1–§3.2, where polynomial and rational function extrapolation were already discussed.

The third idea was discussed in the section before this one, namely to use a method whose error function is strictly even, allowing the rational function or polynomial approximation to be in terms of the variable $h^2$ instead of just $h$.

Put these ideas together and you have the Bulirsch-Stoer method [1]. A single Bulirsch-Stoer step takes us from $x$ to $x + H$, where $H$ is supposed to be quite a large — not at all infinitesimal — distance. That single step is a grand leap consisting of many (e.g., dozens to hundreds) substeps of modified midpoint method, which are then extrapolated to zero stepsize.

The sequence of separate attempts to cross the interval $H$ is made with increasing values of $n$, the number of substeps. Bulirsch and Stoer originally proposed the sequence

$$n = 2, 4, 6, 8, 12, 16, 24, 32, 48, 64, 96, \ldots, [n_j = 2n_{j-2}], \ldots$$

(16.4.1)

More recent work by Deuflhard [2,3] suggests that the sequence

$$n = 2, 4, 6, 8, 10, 12, 14, \ldots, [n_j = 2j], \ldots$$

(16.4.2)

is usually more efficient. For each step, we do not know in advance how far up this sequence we will go. After each successive $n$ is tried, a polynomial extrapolation is...
attempted. That extrapolation returns both extrapolated values and error estimates. If the errors are not satisfactory, we go higher in $n$. If they are satisfactory, we go on to the next step and begin anew with $n = 2$.

Of course there must be some upper limit, beyond which we conclude that there is some obstacle in our path in the interval $H$, so that we must reduce $H$ rather than just subdivide it more finely. In the implementations below, the maximum number of $n$’s to be tried is called $\text{KMAXX}$. For reasons described below we usually take this equal to 8; the 8th value of the sequence (16.4.2) is 16, so this is the maximum number of subdivisions of $H$ that we allow.

We enforce error control, as in the Runge-Kutta method, by monitoring internal consistency, and adapting stepsize to match a prescribed bound on the local truncation error. Each new result from the sequence of modified midpoint integrations allows a tableau like that in §3.1 to be extended by one additional set of diagonals. The size of the new correction added at each stage is taken as the (conservative) error estimate. How should we use this error estimate to adjust the stepsize? The best strategy now known is due to Deuflhard [2,3]. For completeness we describe it here:

Suppose the absolute value of the error estimate returned from the $k$th column (and hence the $k + 1$st row) of the extrapolation tableau is $\epsilon_{k+1,k}$. Error control is enforced by requiring

$$
\epsilon_{k+1,k} < \epsilon
$$

(16.4.3)

as the criterion for accepting the current step, where $\epsilon$ is the required tolerance. For the even sequence (16.4.2) the order of the method is $2k + 1$:

$$
\epsilon_{k+1,k} \sim H^{2k+1}
$$

(16.4.4)

Thus a simple estimate of a new stepsize $H_k$ to obtain convergence in a fixed column $k$ would be

$$
H_k = H \left( \frac{\epsilon}{\epsilon_{k+1,k}} \right)^{1/(2k+1)}
$$

(16.4.5)

Which column $k$ should we aim to achieve convergence in? Let’s compare the work required for different $k$. Suppose $A_k$ is the work to obtain row $k$ of the extrapolation tableau, so $A_{k+1}$ is the work to obtain column $k$. We will assume the work is dominated by the cost of evaluating the functions defining the right-hand sides of the differential equations. For $n_k$ subdivisions in $H$, the number of function evaluations can be found from the recurrence

$$
A_1 = n_1 + 1
$$

$$
A_{k+1} = A_k + n_{k+1}
$$

(16.4.6)

The work per unit step to get column $k$ is $A_{k+1}/H_k$, which we nondimensionalize with a factor of $H$ and write as

$$
W_k = \frac{A_{k+1}}{H_k} H
$$

$$
= A_{k+1} \left( \frac{\epsilon_{k+1,k}}{\epsilon} \right)^{1/(2k+1)}
$$

(16.4.7)

(16.4.8)

The quantities $W_k$ can be calculated during the integration. The optimal column index $q$ is then defined by

$$
W_q = \min_{k=1,\ldots,k_f} W_k
$$

(16.4.9)

where $k_f$ is the final column, in which the error criterion (16.4.3) was satisfied. The $q$ determined from (16.4.9) defines the stepsize $H_q$ to be used as the next basic stepsize, so that we can expect to get convergence in the optimal column $q$.

Two important refinements have to be made to the strategy outlined so far:
• If the current \( H \) is “too small,” then \( k_f \) will be “too small,” and so \( q \) remains “too small.” It may be desirable to increase \( H \) and aim for convergence in a column \( q > k_f \).

• If the current \( H \) is “too big,” we may not converge at all on the current step and we will have to decrease \( H \). We would like to detect this by monitoring the quantities \( \epsilon_{k+1,k} \) for each \( k \) so we can stop the current step as soon as possible.

Deuflhard’s prescription for dealing with these two problems uses ideas from communication theory to determine the “average expected convergence behavior” of the extrapolation. His model produces certain correction factors \( \alpha(k, q) \) by which \( H_k \) is to be multiplied to try to get convergence in column \( q \). The factors \( \alpha(k, q) \) depend only on \( \epsilon \) and the sequence \( \{ n_i \} \) and so can be computed once during initialization:

\[
\alpha(k, q) = \epsilon \frac{A_{k+1} - A_{q+1}}{A_{q+1} - A_{k+1}} \quad \text{for} \quad k < q
\]

(16.4.10)

with \( \alpha(q, q) = 1 \).

Now to handle the first problem, suppose convergence occurs in column \( q = k_f \). Then rather than taking \( H_q \) for the next step, we might aim to increase the stepsize to get convergence in column \( q + 1 \). Since we don’t have \( H_{q+1} \) available from the computation, we estimate it as

\[
H_{q+1} = H_q \alpha(q, q + 1)
\]

(16.4.11)

By equation (16.4.7) this replacement is efficient, i.e., reduces the work per unit step, if

\[
\frac{A_{q+1}}{H_q} > \frac{A_{q+2}}{H_{q+1}}
\]

(16.4.12)

or

\[
A_{q+1} \alpha(q, q + 1) > A_{q+2}
\]

(16.4.13)

During initialization, this inequality can be checked for \( q = 1, 2, \ldots \) to determine \( k_{\text{max}} \), the largest allowed column. Then when (16.4.12) is satisfied it will always be efficient to use \( H_{q+1} \). (In practice we limit \( k_{\text{max}} \) to 8 even when \( \epsilon \) is very small as there is very little further gain in efficiency whereas roundoff can become a problem.)

The problem of stepsize reduction is handled by computing stepsize estimates

\[
H_k = H_q \alpha(k, q), \quad k = 1, \ldots, q - 1
\]

(16.4.14)

during the current step. The \( H_k \)‘s are estimates of the stepsize to get convergence in the optimal column \( q \). If any \( H_k \) is “too small,” we abandon the current step and restart using \( H_k \). The criterion of being “too small” is taken to be

\[
H_k \alpha(k, q + 1) < H
\]

(16.4.15)

The \( \alpha \)‘s satisfy \( \alpha(k, q + 1) > \alpha(k, q) \).

During the first step, when we have no information about the solution, the stepsize reduction check is made for all \( k \). Afterwards, we test for convergence and for possible stepsize reduction only in an “order window”

\[
\max(1, q - 1) \leq k \leq \min(k_{\text{max}}, q + 1)
\]

(16.4.16)

The rationale for the order window is that if convergence appears to occur for \( k < q - 1 \) it is often spurious, resulting from some fortuitously small error estimate in the extrapolation. On the other hand, if you need to go beyond \( k = q + 1 \) to obtain convergence, your local model of the convergence behavior is obviously not very good and you need to cut the stepsize and reestablish it.

In the routine \texttt{bstep}, these various tests are actually carried out using quantities

\[
\epsilon(k) = \frac{H}{H_k} = \left( \frac{\epsilon_{k+1,k}}{\epsilon} \right)^{1/(2k+1)}
\]

(16.4.17)
called \texttt{err(k)} in the code. As usual, we include a “safety factor” in the stepsize selection. This is implemented by replacing \( \epsilon \) by 0.25\( \epsilon \). Other safety factors are explained in the program comments.

Note that while the optimal convergence column is restricted to increase by at most one on each step, a sudden drop in order is allowed by equation (16.4.9). This gives the method a degree of robustness for problems with discontinuities.
Let us remind you once again that scaling of the variables is often crucial for successful integration of differential equations. The scaling “trick” suggested in the discussion following equation (16.2.8) is a good general purpose choice, but not foolproof. Scaling by the maximum values of the variables is more robust, but requires you to have some prior information.

The following implementation of a Bulirsch-Stoer step has exactly the same calling sequence as the quality-controlled Runge-Kutta stepper \texttt{rkqs}. This means that the driver \texttt{odeint} in §16.2 can be used for Bulirsch-Stoer as well as Runge-Kutta: Just substitute \texttt{bsstep} for \texttt{rkqs} in \texttt{odeint}'s argument list. The routine \texttt{bsstep} calls \texttt{mmid} to take the modified midpoint sequences, and calls \texttt{pzextr}, given below, to do the polynomial extrapolation.

```fortran
SUBROUTINE bsstep(y,dydx,nv,x,htry,eps,yscal,hdid,hnext,derivs)
  INTEGER nv,NMAX,KMAXX,IMAX
  REAL eps,hdid,hnext,htry,x,dydx(nv),y(nv),yscal(nv),SAFE1,
         * SAFE2,REDMAX,REDMIN,TINY,SCALMX
  PARAMETER (NMAX=50,KMAXX=8,IMAX=KMAXX+1,SAFE1=.25,SAFE2=.7,
              * REDMAX=1.e-5,REDMIN=.7,TINY=1.e-30,SCALMX=.1)
  USES derivs,mmid,pzextr

  Bulirsch-Stoer step with monitoring of local truncation error to ensure accuracy and adjust stepsize. Input are the dependent variable vector \(y(1:nv)\) and its derivative \(dydx(1:nv)\) at the starting value of the independent variable \(x\). Also input are the stepsize to be attempted \(htry\), the required accuracy \(\epsilon\), and the vector \(\text{yscal}(1:nv)\) against which the error is scaled. On output, \(y\) and \(x\) are replaced by their new values, \(\text{hdid}\) is the stepsize that was actually accomplished, and \(\text{hnext}\) is the estimated next stepsize. \texttt{derivs} is the user-supplied subroutine that computes the right-hand side derivatives. Be sure to set \(\text{htry}\) on successive steps to the value of \(\text{hnext}\) returned from the previous step, as is the case if the routine is called by \texttt{odeint}.

  Parameters: \(NMAX\) is the maximum value of \(nv\); \(KMAXX\) is the maximum row number used in the extrapolation; \(IMAX\) is the next row number; \(SAFE1\) and \(SAFE2\) are safety factors; \(REDMAX\) is the maximum factor used when a stepsize is reduced, \(REDMIN\) the minimum; \(TINY\) prevents division by zero; \(1/\text{SCALMX}\) is the maximum factor by which a stepsize can be increased.

  INTEGER i,iq,k,kk,km,kmax,kopt,nseq(IMAX)
  REAL eps1,epsold,errmax,fact,h,red,scale,work,wrkmin,xest,
         * xnew,a(IMAX),alf(KMAXX,KMAXX),err(KMAXX),yerr(NMAX),
         * ysav(NMAX),yseq(NMAX)
  LOGICAL first,reduct
  SAVE a,alf,epsold,first,kmax,kopt,nseq,xnew
  EXTERNAL derivs
  DATA first/.true./,epsold/-1./
  DATA nseq /2,4,6,8,10,12,14,16,18/
  if(eps.ne.epsold)then
    A new tolerance, so reinitialize.
    hnext=-1.e29
    xnew=-1.e29
    eps1=SAFE1*eps
    a(1)=nseq(1)+1
    Compute work coefficients \(A_k\).
    do 11 k=1,KMAXX
      a(k+1)=a(k)+nseq(k+1)
edo 11
    do 13 iq=2,KMAXX
      Compute \(\alpha(k,q)\).
      do 12 k=1,iq-1
        alf(k,iq)=eps1**((a(k+1)-a(iq+1))/
      (a(iq+1)-a(1)+1.)*(2*k+1)))
edo 12
    enddo 13
    epsold=eps
  do 14 kopt=2,KMAXX-1
    Determine optimal row number for convergence.
    if(a(kopt+1).gt.a(kopt)*alf(kopt-1,kopt))goto 1
  enddo 14
```

The following implementation of a Bulirsch-Stoer step has exactly the same calling sequence as the quality-controlled Runge-Kutta stepper \texttt{rkqs}. This means that the driver \texttt{odeint} in §16.2 can be used for Bulirsch-Stoer as well as Runge-Kutta: Just substitute \texttt{bsstep} for \texttt{rkqs} in \texttt{odeint}'s argument list. The routine \texttt{bsstep} calls \texttt{mmid} to take the modified midpoint sequences, and calls \texttt{pzextr}, given below, to do the polynomial extrapolation.

```fortran
SUBROUTINE bsstep(y,dydx,nv,x,htry,eps,yscal,hdid,hnext,derivs)
  INTEGER nv,NMAX,KMAXX,IMAX
  REAL eps,hdid,hnext,htry,x,dydx(nv),y(nv),yscal(nv),SAFE1,
         * SAFE2,REDMAX,REDMIN,TINY,SCALMX
  PARAMETER (NMAX=50,KMAXX=8,IMAX=KMAXX+1,SAFE1=.25,SAFE2=.7,
              * REDMAX=1.e-5,REDMIN=.7,TINY=1.e-30,SCALMX=.1)
  USES derivs,mmid,pzextr

  Bulirsch-Stoer step with monitoring of local truncation error to ensure accuracy and adjust stepsize. Input are the dependent variable vector \(y(1:nv)\) and its derivative \(dydx(1:nv)\) at the starting value of the independent variable \(x\). Also input are the stepsize to be attempted \(htry\), the required accuracy \(\epsilon\), and the vector \(\text{yscal}(1:nv)\) against which the error is scaled. On output, \(y\) and \(x\) are replaced by their new values, \(\text{hdid}\) is the stepsize that was actually accomplished, and \(\text{hnext}\) is the estimated next stepsize. \texttt{derivs} is the user-supplied subroutine that computes the right-hand side derivatives. Be sure to set \(\text{htry}\) on successive steps to the value of \(\text{hnext}\) returned from the previous step, as is the case if the routine is called by \texttt{odeint}.

  Parameters: \(NMAX\) is the maximum value of \(nv\); \(KMAXX\) is the maximum row number used in the extrapolation; \(IMAX\) is the next row number; \(SAFE1\) and \(SAFE2\) are safety factors; \(REDMAX\) is the maximum factor used when a stepsize is reduced, \(REDMIN\) the minimum; \(TINY\) prevents division by zero; \(1/\text{SCALMX}\) is the maximum factor by which a stepsize can be increased.

  INTEGER i,iq,k,kk,km,kmax,kopt,nseq(IMAX)
  REAL eps1,epsold,errmax,fact,h,red,scale,work,wrkmin,xest,
         * xnew,a(IMAX),alf(KMAXX,KMAXX),err(KMAXX),yerr(NMAX),
         * ysav(NMAX),yseq(NMAX)
  LOGICAL first,reduct
  SAVE a,alf,epsold,first,kmax,kopt,nseq,xnew
  EXTERNAL derivs
  DATA first/.true./,epsold/-1./
  DATA nseq /2,4,6,8,10,12,14,16,18/
  if(eps.ne.epsold)then
    A new tolerance, so reinitialize.
    hnext=-1.e29
    xnew=-1.e29
    eps1=SAFE1*eps
    a(1)=nseq(1)+1
    Compute work coefficients \(A_k\).
    do 11 k=1,KMAXX
      a(k+1)=a(k)+nseq(k+1)
edo 11
    do 13 iq=2,KMAXX
      Compute \(\alpha(k,q)\).
      do 12 k=1,iq-1
        alf(k,iq)=eps1**((a(k+1)-a(iq+1))/
      (a(iq+1)-a(1)+1.)*(2*k+1)))
edo 12
    enddo 13
    epsold=eps
  do 14 kopt=2,KMAXX-1
    Determine optimal row number for convergence.
    if(a(kopt+1).gt.a(kopt)*alf(kopt-1,kopt))goto 1
  enddo 14
```
1
kmax=kopt
endif
h=htry
do 16 i=1,nv
ysav(i)=y(i)
enddo
if(h.ne.hnext.or.x.ne.xnew)then
  first=.true.
  kopt=kmax
endif
reduct=.false.
2
do 17 k=1,kmax
  xnew=x+h
  if(xnew.eq.x)pause 'step size underflow in bsstep'
call mmid(ysav,dydx,nv,x,h,nseq(k),yseq,derivs)
xest=(h/nseq(k))**2
  errmax=errmax+abs(yerr(i)/yscal(i)))
  kopt=kmax
endif
3
red=min(red,REDMIN)
red=max(red,REDMAX)
h=h*red
reduct=.true.
goto 2
4
x=xnew
hdid=h
first=.false.
wrkmin=1.e35
16
fact=max(err(kk),SCALMX)
  work=work+fact
  scale=scale*fact
  kopt=kk+1
  wrkmin=work
  goto 18
else if(kopt.eq.kmax)then
  red=alf(km,kmax-1)*SAFE2/err(km)
goto 3
else if(alf(km,kopt).lt.err(km))then
  red=alf(km,kopt)*SAFE2/err(km)
goto 3
endif
4
x=xnew
hdid=h
first=.false.
wrkmin=1.e35
do 18 kk=1,km
  fact=max(err(kk),SCALMX)
  work=work+fact
  scale=scale*fact
  kopt=kk+1
  wrkmin=work
  goto 18
endif

Save the starting values.
A new stepsize or a new integration: re-establish
the order window.
Evaluate the sequence of modified midpoint
integrations.
Squared, since error series is even.
Perform extrapolation.
Compute normalized error estimate $\epsilon(k)$.
Scale error relative to tolerance.
In order window.
Converged.
Check for possible stepsize reduction.
* 
Compute optimal row for convergence and
corresponding stepsize.
The polynomial extrapolation routine is based on the same algorithm as \texttt{polint} §3.1. It is simpler in that it is always extrapolating to zero, rather than to an arbitrary value. However, it is more complicated in that it must individually extrapolate each component of a vector of quantities.

```fortran
SUBROUTINE pzextr(iest,xest,yest,yz,dy,nv)
INTEGER iest,nv,IMAX,NMAX
REAL xest,dy(nv),yest(nv),yz(nv)
PARAMETER (IMAX=13,NMAX=50)
Use polynomial extrapolation to evaluate \(nv\) functions at \(x=0\) by fitting a polynomial to a sequence of estimates with progressively smaller values \(x=xest\), and corresponding function vectors \(yest(1:nv)\). This call is number \(iest\) in the sequence of calls. Extrapolated function values are output as \(yz(1:nv)\), and their estimated error is output as \(dy(1:nv)\).
Parameters: Maximum expected value of \(iest\) is \(IMAX\); of \(nv\) is \(NMAX\).

INTEGER j,k1
REAL delta,f1,f2,q,d(NMAX),qcol(NMAX,IMAX),x(IMAX)
SAVE qcol,x
x(iest)=xest
Save current independent variable.
do      11 j=1,nv
   dy(j)=yest(j)
   yz(j)=yest(j)
enddo 11
if(iest.eq.1) then
      Store first estimate in first column.
do      12 j=1,nv
   qcol(j,1)=yest(j)
enddo 12
else
      do 13 j=1,nv
   d(j)=yest(j)
enddo 13
   do 15 k1=1,iest-1
      delta=1./(x(iest-k1)-xest)
      f1=xest*delta
      f2=x(iest-k1)*delta
      do 14 j=1,nv
         q=qcol(j,k1)
         qcol(j,k1)=dy(j)
         delta=d(j)-q
         dy(j)=f1*delta
         d(j)=f2+delta
         yz(j)=yz(j)+dy(j)
      enddo 14
   enddo 15
   do 16 j=1,nv
      qcol(j,iest)=dy(j)
enddo 16
endif
return
END
```

The polynomial extrapolation routine is based on the same algorithm as \texttt{polint} §3.1. It is simpler in that it is always extrapolating to zero, rather than to an arbitrary value. However, it is more complicated in that it must individually extrapolate each component of a vector of quantities.
Current wisdom favors polynomial extrapolation over rational function extrapolation in the Bulirsch-Stoer method. However, our feeling is that this view is guided more by the kinds of problems used for tests than by one method being actually “better.” Accordingly, we provide the optional routine \texttt{rzextr} for rational function extrapolation, an exact substitution for \texttt{pzextr} above.

```fortran
SUBROUTINE rzextr(iest,xest,yest,yz,dy,nv)
  INTEGER iest,nv,IMAX,NMAX
  REAL xest,dy(nv),yest(nv),yz(nv)
  PARAMETER (IMAX=13,NMAX=50)

  Exact substitute for \texttt{pzextr}, but uses diagonal rational function extrapolation instead of polynomial extrapolation.

  INTEGER j,k
  REAL b,b1,c,ddy,v,yy,d(NMAX,IMAX),fx(IMAX),x(IMAX)
  SAVE d,x

  x(iest)=xest
  Save current independent variable.

  if(iest.eq.1) then
    do 11 j=1,nv
      yz(j)=yest(j)
      d(j,1)=yest(j)
      dy(j)=yest(j)
    enddo 11
  else
    do 12 k=1,iest-1
      fx(k+1)=x(iest-k)/xest
    enddo 12
  endif

  do 14 j=1,nv

    yy=yest(j)
    c=yy
    d(j,1)=yy
    do 13 k=2,iest
      b1=fx(k)*v
      b=b1-c
      if(b.ne.0.) then
        b=(c-v)/b
        ddy=c*b
        c=b1*b
      else
        Care needed to avoid division by 0.
        ddy=v
      endif
      if (k.ne.iest) v=d(j,k)
      dy(j)=ddy
    enddo 14
  dy(j)=ddy
  yz(j)=yy
  if(iest.eq.1) then
    do 11 j=1,nv
      yz(j)=yest(j)
      d(j,1)=yest(j)
      dy(j)=yest(j)
    enddo 11
  else
    do 12 k=1,iest-1
      fx(k+1)=x(iest-k)/xest
    enddo 12
  endif
  return
END
```

CITED REFERENCES AND FURTHER READING:
16.5 Second-Order Conservative Equations

Usually when you have a system of high-order differential equations to solve it is best to reformulate them as a system of first-order equations, as discussed in §16.0. There is a particular class of equations that occurs quite frequently in practice where you can gain about a factor of two in efficiency by differencing the equations directly. The equations are second-order systems where the derivative does not appear on the right-hand side:

\[ y''(x) = f(x,y), \quad y(x_0) = y_0, \quad y'(x_0) = z_0 \]  

(16.5.1)

As usual, \( y \) can denote a vector of values.

Stoermer’s rule, dating back to 1907, has been a popular method for discretizing such systems. With \( h = H/m \) we have

\[ y_1 = y_0 + h[z_0 + \frac{1}{2}h f(x_0, y_0)] \]

\[ y_{k+1} - 2y_k + y_{k-1} = h^2 f(x_k + kh, y_k), \quad k = 1, \ldots, m - 1 \]  

(16.5.2)

\[ z_m = (y_m - y_{m-1})/h + \frac{1}{2}h f(x_0 + H, y_m) \]

Here \( z_m \) is \( y'(x_0 + H) \). Henrici showed how to rewrite equations (16.5.2) to reduce roundoff error by using the quantities \( \Delta_k \equiv y_{k+1} - y_k \). Start with

\[ \Delta_0 = h[z_0 + \frac{1}{2}h f(x_0, y_0)] \]

\[ y_1 = y_0 + \Delta_0 \]  

(16.5.3)

Then for \( k = 1, \ldots, m - 1 \), set

\[ \Delta_k = \Delta_{k-1} + h^2 f(x_k + kh, y_k) \]

\[ y_{k+1} = y_k + \Delta_k \]  

(16.5.4)

Finally compute the derivative from

\[ z_m = \Delta_{m-1}/h + \frac{1}{2}h f(x_0 + H, y_m) \]  

(16.5.5)

Gragg showed that the error series for equations (16.5.3)–(16.5.5) contains only even powers of \( h \), and so the method is a logical candidate for extrapolation à la Bulirsch-Stoer.

We replace \( \text{mid} \) by the following routine \text{stoerm}:

```fortran
SUBROUTINE stoerm(y,d2y,nv,xs,htot,nstep,yout,derivs)
INTEGER nstep,nv,NMAX
REAL htot,xs,d2y(nv),y(nv),yout(nv)
EXTERNAL derivs
PARAMETER (NMAX=50) Maximum value of nv.
C USES derivs
Stoermer’s rule for integrating \( y'' = f(x,y) \) for a system of \( n = nv/2 \) equations. On input \( y(1:nv) \) contains \( y \) in its first \( n \) elements and \( y' \) in its second \( n \) elements, all evaluated at \( x \). \text{d2y}(1:nv) contains the right-hand side function \( f \) (also evaluated at \( x \)) in its first \( n \) elements. Its second \( n \) elements are not referenced. Also input is \text{htot}, the total step to be taken, and \text{nstep}, the number of substeps to be used. The output is returned as \( yout(1:nv) \), with the same storage arrangement as \( y \). \text{derivs} is the user-supplied subroutine that calculates \( f \).
INTEGER i,n,neqns,nm
REAL h,h2,halfh,x,ytemp(NMAX)
h=htot/nstep
halfh=0.5*h
neqns=nv/2
do i=1,neqns
  ytemp(n)=h*(y(n)+halfh*d2y(i))
enddo
```

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