```
            dy[j]=yest[j];
        }
    else {
        for (k=1;k<iest;k++)
            fx[k+1]=x[iest-k]/xest;
        for (j=1;j<=nv;j++) {           Evaluate next diagonal in tableau.
            v=d[j][1];
            d[j][1]=yy=c=yest[j];
            for (k=2;k<=iest;k++) {
                b1=fx[k]*v;
                b=b1-c;
                if (b) {
                    b=(c-v)/b;
                    ddy=c*b;
                    c=b1*b;
                } else                  Care needed to avoid division by 0.
                    ddy=v;
                if (k != iest) v=d[j][k];
                d[j][k]=ddy;
                yy += ddy;
            }
            dy[j]=ddy;
            yz[j]=yy;
        }
    }
    free_vector(fx,1,iest);
}
```

CITED REFERENCES AND FURTHER READING:

Stoer, J., and Bulirsch, R. 1980, *Introduction to Numerical Analysis* (New York: Springer-Verlag), §7.2.14. [1]

Gear, C.W. 1971, *Numerical Initial Value Problems in Ordinary Differential Equations* (Englewood Cliffs, NJ: Prentice-Hall), §6.2.

Deuflhard, P. 1983, *Numerische Mathematik*, vol. 41, pp. 399–422. [2]

Deuflhard, P. 1985, *SIAM Review*, vol. 27, pp. 505–535. [3]

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:

$$y'' = f(x, y), \qquad y(x_0) = y_0, \qquad y'(x_0) = z_0 \tag{16.5.1}$$

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

$$\begin{aligned}
&y_1 = y_0 + h[z_0 + \tfrac{1}{2}hf(x_0, y_0)] \\
&y_{k+1} - 2y_k + y_{k-1} = h^2 f(x_0 + kh, y_k), \qquad k = 1, \ldots, m-1 \\
&z_m = (y_m - y_{m-1})/h + \tfrac{1}{2}hf(x_0 + H, y_m)
\end{aligned} \tag{16.5.2}$$

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

$$\begin{aligned} \Delta_0 &= h[z_0 + \tfrac{1}{2}hf(x_0, y_0)] \\ y_1 &= y_0 + \Delta_0 \end{aligned} \tag{16.5.3}$$

Then for $k = 1, \ldots, m-1$, set

$$\begin{aligned} \Delta_k &= \Delta_{k-1} + h^2 f(x_0 + kh, y_k) \\ y_{k+1} &= y_k + \Delta_k \end{aligned} \tag{16.5.4}$$

Finally compute the derivative from

$$z_m = \Delta_{m-1}/h + \tfrac{1}{2}hf(x_0 + H, y_m) \tag{16.5.5}$$

Gragg again 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 `mmid` by the following routine `stoerm`:

```
#include "nrutil.h"

void stoerm(float y[], float d2y[], int nv, float xs, float htot, int nstep,
	float yout[], void (*derivs)(float, float [], float []))
```
Stoermer's rule for integrating $y'' = f(x,y)$ for a system of $n = \mathtt{nv}/2$ equations. On input `y[1..nv]` contains y in its first n elements and y' in its second n elements, all evaluated at `xs`. `d2y[1..nv]` contains the right-hand side function f (also evaluated at `xs`) in its first n elements. Its second n elements are not referenced. Also input is `htot`, the total step to be taken, and `nstep`, the number of substeps to be used. The output is returned as `yout[1..nv]`, with the same storage arrangement as `y`. `derivs` is the user-supplied routine that calculates f.
```
{
	int i,n,neqns,nn;
	float h,h2,halfh,x,*ytemp;

	ytemp=vector(1,nv);
	h=htot/nstep;                          Stepsize this trip.
	halfh=0.5*h;
	neqns=nv/2;                            Number of equations.
	for (i=1;i<=neqns;i++) {               First step.
		n=neqns+i;
		ytemp[i]=y[i]+(ytemp[n]=h*(y[n]+halfh*d2y[i]));
	}
	x=xs+h;
	(*derivs)(x,ytemp,yout);               Use yout for temporary storage of derivatives.
	h2=h*h;
	for (nn=2;nn<=nstep;nn++) {            General step.
		for (i=1;i<=neqns;i++)
			ytemp[i] += (ytemp[(n=neqns+i)] += h2*yout[i]);
		x += h;
		(*derivs)(x,ytemp,yout);
	}
	for (i=1;i<=neqns;i++) {               Last step.
		n=neqns+i;
		yout[n]=ytemp[n]/h+halfh*yout[i];
		yout[i]=ytemp[i];
	}
	free_vector(ytemp,1,nv);
}
```

Note that for compatibility with `bsstep` the arrays `y` and `d2y` are of length $2n$ for a system of n second-order equations. The values of y are stored in the first n elements of `y`, while the first derivatives are stored in the second n elements. The right-hand side f is stored in the first n elements of the array `d2y`; the second n elements are unused. With this storage arrangement you can use `bsstep` simply by replacing the call to `mmid` with one to `stoerm` using the same arguments; just be sure that the argument `nv` of `bsstep` is set to $2n$. You should also use the more efficient sequence of stepsizes suggested by Deuflhard:

$$n = 1, 2, 3, 4, 5, \ldots \tag{16.5.6}$$

and set `KMAXX` $= 12$ in `bsstep`.

CITED REFERENCES AND FURTHER READING:

Deuflhard, P. 1985, *SIAM Review*, vol. 27, pp. 505–535.

16.6 Stiff Sets of Equations

As soon as one deals with more than one first-order differential equation, the possibility of a *stiff* set of equations arises. Stiffness occurs in a problem where there are two or more very different scales of the independent variable on which the dependent variables are changing. For example, consider the following set of equations [1]:

$$\begin{aligned} u' &= 998u + 1998v \\ v' &= -999u - 1999v \end{aligned} \tag{16.6.1}$$

with boundary conditions

$$u(0) = 1 \qquad v(0) = 0 \tag{16.6.2}$$

By means of the transformation

$$u = 2y - z \qquad v = -y + z \tag{16.6.3}$$

we find the solution

$$\begin{aligned} u &= 2e^{-x} - e^{-1000x} \\ v &= -e^{-x} + e^{-1000x} \end{aligned} \tag{16.6.4}$$

If we integrated the system (16.6.1) with any of the methods given so far in this chapter, the presence of the e^{-1000x} term would require a stepsize $h \ll 1/1000$ for the method to be stable (the reason for this is explained below). This is so even