PHYS 410/555 Computational Physics: Solution of ODEs
(Reference *Numerical Recipes*, Chapters 16, 17)

Overview

- "Theory"
  - Casting systems of ODEs in first order form (canonical form)
  - Boundary / initial conditions
- Some Basic Numerical Techniques
  - Euler method
  - Second-order Runge-Kutta
- Using "Canned" Software
  - `ODEPACK` routine `lsoda`
- Applications
  - Quadrature (definite integrals)
  - Initial value problems (dynamics)
  - Boundary value problems

Note: There are *many* applications in virtually every sub-field of physics.

Casting Systems of ODEs in First Order Form

- Can *always* reduce systems of ODEs to set of first order DEs by introducing appropriate new (auxiliary) variables.

Example 1

$$y''(x) + q(x)y'(x) = r(x) \qquad {}' \equiv \frac{d}{dx} \tag{1}$$

- Introduce new variable $z(x) \equiv y'(x)$, then (1) becomes

$$y' = z \tag{2}$$
$$z' = r - qz \tag{3}$$

Example 2

$$y''''(x) = f(x) \tag{4}$$

- Introduce new variables

$$y_1(x) \equiv y'(x) \tag{5}$$
$$y_2(x) \equiv y''(x) \tag{6}$$
$$y_3(x) \equiv y'''(x) \tag{7}$$

then (4) becomes

$$y' = y_1 \tag{8}$$
$$y_1' = y_2 \tag{9}$$
$$y_2' = y_3 \tag{10}$$
$$y_3' = f \tag{11}$$

- Thus, the generic problem in ODEs is reduced to study of a set of N coupled, *first-order* DEs for the functions, $y_i, i = 1, 2, \ldots, N$

$$y_i'(x) \equiv \frac{dy_i}{dx}(x) = f_i(x, y_1, y_2, \cdots, y_N) \qquad i = 1, 2, \ldots N \tag{12}$$

where the $f_i(\cdots)$ are *known functions* of x and y_i

- *Equivalent forms:* $\mathbf{y} \equiv (y_1, y_2, \cdots, y_N)$

$$\mathbf{y}'(x) = \mathbf{f}(x, \mathbf{y}) \tag{13}$$
$$\dot{\mathbf{y}}(t) = \mathbf{f}(t, \mathbf{y}) \tag{14}$$

Boundary / Initial Conditions

- ODE problem not completely specified by DEs themselves
- Nature of boundary conditions is crucial aspect of problem
- Generally, BCs are *algebraic* conditions on certain values of the y_i in (12) that are to be satisfied at discrete specified points.
- Generally will need N conditions for N-th order system
- BCs divide ODE problems into 2 broad classes

1) Initial Value Problems

- All the y_i are given at some starting (initial) value, $t_{\min}$ and we wish to find the y_i at some final value, $t_{\max}$, or at some *set* of values

$$t_n, \qquad t_{\min} \le t_n \le t_{\max} \qquad n = 0, 1, 2, \cdots \tag{15}$$

2) (Two-point) Boundary Value Problems

- BCs are specified at more than one value of x. Typically some will be specified at $x = x_{\min}$, the remainder at $x = x_{\max}$.
- Have already considered some 2-pt BVPs, and their solution via finite difference techniques

We will focus on general techniques / software for solving IVPs, and some simple BVPs.

Some Basic Numerical Techniques for IVPs

We adopt the notation of *Numerical Recipes*, and illustrate the methods for the case of a scalar equation. The generalization to systems is straightforward.

1) The Euler Method

- Consider two values of x, x_n and $x_{n+1} = x_n + h$ (h is often called the "step size", and is completely analogous to the mesh spacing, h, used in our previous work on FD approximations)
- Then the (forward) Euler method is given by

$$y_{n+1} = y_n + hf(x_n, y_n) \tag{16}$$

- Note that we use this formula to "advance" solution from $x = x_n$ to $x = x_{n+1} = x_n + h$
- Can easily derive from $O(h)$ (forward) finite difference approximation

$$\frac{y_{n+1} - y_n}{h} = y'_n + O(h) \tag{17}$$

$$y' = f(x, y) \longrightarrow \frac{y_{n+1} - y_n}{h} = f(x_n, y_n) \tag{18}$$

- *Accuracy*: $O(h^2)$ *per step*. For fixed final $x = x_f$, number of steps scales as h^{-1}, so *global* accuracy is $O(h)$
- OK for demonstration purposes, but should *never* be used in practice—not very accurate, not very *stable*!

2) Second-order Runge-Kutta (Mid-point Method)

- The second-order Runge-Kutta method is given by

$$
\begin{aligned}
k_1 &= hf(x_n, y_n) && (19)\\
k_2 &= hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right) && (20)\\
y_{n+1} &= y_n + k_2 && (21)
\end{aligned}
$$

- *Global accuracy*: $O(h^2)$
- *Derivation*

$$
\frac{y_{n+1} - y_n}{h} = f(x_{n+1/2}, y_{n+1/2}) + O(h^2) \qquad (22)
$$

where $x_{n+1/2} \equiv x_n + h/2$, $y_{n+1/2} \equiv y(x_{n+1/2})$. (Exercise: Verify the above, and compute the actual form of the leading order error term.)

To retain $O(h^2)$ accuracy, need to evaluate $f(x_{n+1/2}, y_{n+1/2})$ to $O(h^2)$ (i.e. can neglect $O(h^2)$ terms), so, in turn, need to know $y_{n+1/2}$ to $O(h^2)$; proceed via Taylor series expansion

$$
\begin{aligned}
y_{n+1/2} &= y_n + \frac{1}{2}hy'_n + O(h^2)\\
&= y_n + \frac{1}{2}k_1 + O(h^2)\\
\Longrightarrow y_{n+1} &= y_n + hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right)
\end{aligned}
$$

as advertised.

Although it is "good for you" to understand some of the theory that underlies a modern ODE solver, the state of such solvers is very high, and, as with linear system solvers, can frequently be used as "black boxes"—with the important proviso that we *always* make every reasonable attempt to *validate* our results (convergence tests, independent residual tests, conserved quantities, etc.)

ODEPACK

- Public-domain collection of routines for solution of systems of ODEs (IVPs)
- We will focus on one routine, `lsoda`, which has the following header:

```
      subroutine lsoda(f, neq, y, t, tout, itol, rtol, atol, itask,
     &                 istate, iopt, rwork, lrw, iwork, liw, jac, jt)
         external    f, jac
         integer     neq, itol, itask, istate, iopt, lrw, liw, jt
         real*8      t, tout, rtol, atol
         real*8      y(neq), rwork(lrw)
         integer     iwork(liw)
```

  See source code and sample "driver" program (`tlsoda.f`) for full description of parameters and routine operation

- `f, jac`: Names of routines (subroutines) for evaluating right hand side of ODES (`f`), and Jacobian of system (`jac`). `f` is *required*, `jac` is *optional*, typically a "dummy" routine
- `neq`: number of equations / size of system (canonical first-order form)
- `y`: On input, (approximate) values of unknowns at $t = t$ `( y(i) , i = 1 , neq )`; On output, (approximate) values of unknowns at $t = t_{\rm out}$
- `t, tout`: Limits of current integration interval
- `itol, rtol, atol`: Tolerance (error-control) parameters (see `lsoda.f`, `tlsoda.f` for details)
- `itask`: Set = 1 for normal operation
- `istate`: Set = 1 intially for normal operation, thereafter set = 2 for normal operation (routine will automatically do this if integration on first interval is successful); check for negative value on return to detect abnormal completion
- `iopt`: Normally set = 0 (no optional inputs, but, again, refer to the source code for full details)
- `rwork(lrw)`: `real*8` work array of length `lrw`;
  minimum value of `lrw` is `22 + 16 * neq`
- `iwork(liw)`: `integer` work array of length `liw`;
  minimum value of `liw` is `20 + neq`
- `jt`: Set = 2 for normal operation—supply "dummy" Jacobian routine, `lsoda` will approximately compute Jacobian numerically if and when necessary

Crucial User-supplied Routine Called by `lsoda`

- `f`: Evaluates "RHS" of system of ODEs (12); *must* have header as follows

```
subroutine f(neq, t, y, ydot)
   implicit   none
   integer    neq
   real*8     t, y(neq), ydot(neq)
```

- *Inputs:* `neq, t, ( y(j) , j = 1 , neq )`
- *Output:* `( ydot(j) , j = 1 , neq )`

`lsoda` *Tolerance Parameters:* `itol, atol, rtol`

- `lsoda` will control step-size, order of method and type of method so that estimated local error in `y(i)` is less than

```
ewt(i) = rtol * abs(y(i)) + atol       itol .eq. 1
ewt(i) = rtol * abs(y(i)) + atol(i)    itol .eq. 2
```

  Thus, local error tests passes if, for *each* component `y(i)`, either the absolute error is less than `atol` (or `atol(i)`), or the relative error is less than `rtol`

Choosing Error Tolerances

- Can experiment, but `rtol = atol = tol` (single control parameter) often works well, particularly for y_i that exhibit significant dynamical range
- Some exceptions (of course); for example, consider 2-d motion in polar coordinates, (r, θ). If we use relative control, then for $\theta \gg 2\pi$, "acceptable local error" $\delta\theta$ will increase. Better idea to try to keep $\delta\theta$ constant via "pure absolute" control (`rtol = 0.0d0`)
- Solution eror will almost certainly grow with time, so for fixed final integration time, t_f, will need to *calibrate* error estimates, i.e. assume that

$$\left\| y_{\rm computed}(t_f) - y_{\rm exact}(t_f) \right\| \approx \kappa(t_f)\texttt{tol} \tag{23}$$

  where $\kappa(t_f)$ can be determined via calibration *if* $y_{\rm exact}$ *is known*
- However, even if $y_{\rm exact}$ is *not* known (typical case!), (23) tells us that we can expect error (at fixed time) to be *proportional* to `tol`; e.g. if `tol` goes from `1.0d-6 -> 1.0d-10`, should expect solution error to be down by about 4 orders of magnitude
- *Caveat emptor!* ("User beware!")

Checking/validating Results From ODE Integrators

1) Monitoring Conserved Quantities

- Example: For dynamical systems with a Lagrangian (Hamiltonian), total energy, $E(t)$ is conserved: $dE/dt = 0$
- Monitor variation $\delta\hat{E}(t,\epsilon)$ of computed energy $\hat{E}(t,\epsilon)$:

$$\delta\hat{E}(t,\epsilon) = \hat{E}(t,\epsilon) - \hat{E}(t_{\min},\epsilon) \tag{24}$$

  where ϵ is the error tolerance for the integrator.

- Should find that this is an $O(\epsilon)$ quantity, i.e. for ϵ sufficiently small, should have

$$\delta\hat{E}(t,\epsilon) = \epsilon f(t) + \text{higher order terms} \tag{25}$$

- Thus, e.g., if we take $\epsilon \to \epsilon/10$, should see $\delta\hat{E} \to \delta\hat{E}/10$ (approximately, so long as $\epsilon \gg \epsilon_{\text{machine}}$)

2) Independent Residual Evaluation

- *Idea*: Attempt to directly verify that approximate solution, $\hat{u}$ (u previously y!) satisfies the ODE(s) through the use of an *independent discretization* of the ODE (i.e. a discretization distinct from that used by the ODE integrator).
- *Note:* In numerical analysis, a *residual* quantity is one that should tend to 0 in some appropriate limit
- Let

$$L\left[u(t)\right] \equiv Lu(t) = 0 \tag{26}$$

  be our ODE, where L is a differential operator, and u, in general can be a *vector* of functions; will assume that L is *linear*, but technique generalizes to non-linear case

- Let $\hat{u}(t,\epsilon)$ be the solution computed by our ODE integrator for tolerance ϵ, and consider computing $\hat{u}$ on a regular mesh of output times

$$t^h \equiv t_n = t_{\min},\ t_{\min}+h,\ t_{\min}+2h,\ \cdots \tag{27}$$

  and consider, for concreteness, a second-order (in h) finite difference approximation to the ODE

$$L^h u^h = 0 \qquad L^h = L + O(h^2) \tag{28}$$

- Note that (28) *defines* u^h, and that

$$u^h(t) \neq \hat{u}\left(t^h,\epsilon\right) \tag{29}$$

- The finite difference operator L^h can be expanded as follows

$$L^h = L + h^2 E_2 + h^4 E_4 + \cdots \tag{30}$$

where, as discussed previously, E_2, E_4, etc. are higher order differential operators (involve higher order derivatives than L).

- Now, we can write

$$\hat{u}(t, \epsilon) = u(t) + e(t, \epsilon) \tag{31}$$

where $e(t, \epsilon)$ is the error in the solution computed using the ODE integrator

- Next, consider the action of L^h on $\hat{u}(t, \epsilon)$; suppressing explicit t-dependence, we have

$$\begin{aligned} L^h \hat{u}(\epsilon) &= \left(L + h^2 E_2 + h^4 E_4 + \cdots\right)(u + e(\epsilon)) & (32) \\ &= Lu + h^2 E_2 u + \cdots + L^h e(\epsilon) & (33) \\ &\approx h^2 E_2 [u] + L^h [e(\epsilon)] & (34) \end{aligned}$$

- Now, assume that

$$h^2 E_2 [u] \gg L^h [e(\epsilon)] \tag{35}$$

then

$$L^h \hat{u} \approx h^2 E_2 [u] = O(h^2) \tag{36}$$

- With a high-accuracy ODE solver such as `lsoda`, it is usually possible to satisfy (35), at least over *some* time interval $(t_{\min}, t_{\max})$, and as long as h is not chosen too small

- *Note:* Key idea is to show/check *correctness* of implementation; e.g. checking for errors in coding of equations.

Example:

- Consider the ODE describing simple harmonic motion, (with the gross abuse of notation, $' \equiv d/dt$!):

$$u''(t) = -u(t) \tag{37}$$

  that we will solve on $0 \le t \le t_{\rm max}$ with the initial values $u(0)$ and $u'(0)$ given

- General solution of (37) is

$$\begin{aligned} u(t) &= A\sin(t) + B\cos(t) && (38)\\ u'(t) &= A\cos(t) - B\sin(t) && (39) \end{aligned}$$

  Evaluating (39) at $t = 0$ yields

$$\begin{aligned} A &= u'(0) && (40)\\ B &= u(0) && (41) \end{aligned}$$

  So specific solution satisfying initial conditions is

$$u(t) = u'(0)\sin(t) + u(0)\cos(t) \tag{42}$$

- Cast (37) in canonical form; define

$$\begin{aligned} y_1 &\equiv u && (43)\\ y_2 &\equiv u' && (44) \end{aligned}$$

  Then (37) becomes

$$\begin{aligned} y_1' &\equiv y_2 && (45)\\ y_2' &\equiv -y_1 && (46) \end{aligned}$$

- *RHS routine called by* `lsoda`

```
c===========================================================
c     Implements differential equations:
c
c     u'' = -u
c
c     y(1) := u
c     y(2) := u'
c
c     y(1)' :=  y(2)
c     y(2)' := -y(1)
c
c     Called by ODEPACK routine LSODA.
c===========================================================
      subroutine fcn(neq,t,y,yprime)
         implicit    none

         integer     neq
         real*8      t,     y(neq),    yprime(neq)

         yprime(1) =  y(2)
         yprime(2) = -y(1)

         return
      end
```

Independent Residual Evaluator

- First, rewrite (37) in form (26)

$$u''(t) + u(t) = 0 \tag{47}$$

- Next, using e.g. `lsoda`, generate solution $\hat{u}(t^h, \epsilon)$ on a level-ℓ uniform mesh:

$$t^h_n = 0, h, 2h, \cdots t_{\max} \tag{48}$$

with

$$h = \frac{t_{\max}}{2^\ell} \tag{49}$$

- Then, apply $O(h^2)$ finite-difference discretization of (47) to $\hat{u}$ to compute *residual* R_n:

$$R_n \equiv \frac{\hat{u}_{n+1} - 2\hat{u}_n + \hat{u}_{n-1}}{h^2} + \hat{u}_n \qquad n = 1, 3, \cdots 2^\ell - 1 \tag{50}$$

- In particular, should find that RMS value (ℓ_2 norm) of R_n is an $O(h^2)$ quantity:

$$\left[\frac{\sum_n |R_n|^2}{2^\ell - 1}\right]^{\frac{1}{2}} \equiv \|\mathbf{R}\|_2 = O(h^2) \tag{51}$$

See `tlsoda.f`, `chk-tlsoda.f` for implementation.

Note on Solution Sensitivity/Ill-conditioning

- In integrating from t to $t_{\rm out}$, `lsoda` will typically evaluate RHS of ODEs at many intermediate values t_I, $t \le t_I \le t_{\rm out}$ according to the details of the algorithm, and the user-specified tolerances; these t_I are typically "invisible" to the user

- If, as is frequently the case, one wants to tabulate the solution at many values, e.g. on a grid

$$t_n \equiv t_{\rm min},\ t_{\rm min} + h,\ \cdots t_{\rm max} - h,\ t_{\rm max} \tag{52}$$

  then will generally find that, for fixed tolerance, the computed value at $t = t_{\rm max}$, e.g., will depend on specifics of the output values of t_n requested

- If results are *highly* dependent on choice of t_n, this is a sign that problem is *sensitive* (poorly conditioned); the gravitational n-body problem is a classic example

- In such a case, will also tend to find significant dependence of results on small changes in error tolerances

BOTTOM LINE: Need to be CAREFUL in use of "black box" software!

IVP Applications

1) "Quadrature"/Definite integrals

- Suppose we wish to evaluate definite integral

$$\int_{x_1}^{x_2} f(x)dx \tag{53}$$

- Consider $I(x)$ such that

$$\frac{dI}{dx} = f(x) \tag{54}$$

  Then, we have

$$\begin{aligned} \int_{x_1}^{x_2} \frac{dI}{dx} dx &= \int_{x_1}^{x_2} f(x)dx & (55) \\ \Longrightarrow I(x_2) - I(x_1) &= \int_{x_1}^{x_2} f(x)dx & (56) \end{aligned}$$

So, with the initial condition

$$I(x_1) = 0 \tag{57}$$

we have

$$I(x_2) = \int_{x_1}^{x_2} f(x)dx \tag{58}$$

Example:

- Use above technique and `lsoda` to compute approximate value of

$$I(x; x_1, x_2) = \int_{x_1}^{x_2} e^{-x^2} dx \tag{59}$$

where, for example, $I(x, 0, \infty) = \sqrt{\pi}/2$.

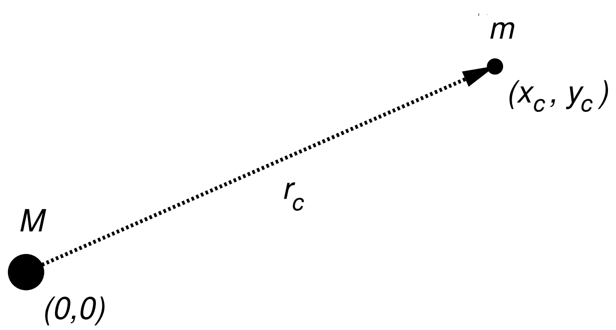
- *RHS routine called by* `lsoda`

```
subroutine fcn(neq,x,y,yprime)
   implicit    none

   integer     neq
   real*8      x,     y(neq),    yprime(neq)

   yprime(1) = exp(-x**2)
   return
end
```

- Should expect *local* tolerance to provide better estimate of *global* accuracy in this case (quadrature)—why?

2) Restricted 2-body problem

- Consider point particle with mass m, interacting with another mass, M, with $M \gg m$—treat M as *fixed*, study dynamics of m (test particle)



- *Dynamical variables:* coordinates of test particle— x_c, y_c
- *Equations of motion*

$$\sum \mathbf{F} = m\,\mathbf{a} \tag{60}$$

$$m\,\mathbf{a} = -G\,\frac{Mm}{|\mathbf{r}_c|^2}\,\hat{\mathbf{r}}_c = -G\,\frac{Mm}{{r_c}^3}\,\mathbf{r}_c \tag{61}$$

- Divide by m, and resolve into x and y components:

$$\ddot{x}_c = -\frac{GM}{{r_c}^3}\,x_c \tag{62}$$

$$\ddot{y}_c = -\frac{GM}{{r_c}^3}\,y_c \tag{63}$$

- 2 second-order ODEs $\longrightarrow$ 4 first order ODEs
- Rewrite in canonical form; define

$$y_1 = x_c \tag{64}$$

$$y_2 = y_c \tag{65}$$

$$y_3 = \dot{x}_c \tag{66}$$

$$y_4 = \dot{y}_c \tag{67}$$

Then we have

$$\dot{y}_1 = y_3 \tag{68}$$

$$\dot{y}_2 = y_4 \tag{69}$$

$$\dot{y}_3 = -\frac{GM}{{r_c}^3}\,y_1 \tag{70}$$

$$\dot{y}_4 = -\frac{GM}{{r_c}^3}\,y_2 \tag{71}$$

where

$${r_c}^3 = \left({y_1}^2 + {y_2}^2\right)^{3/2} \tag{72}$$

- Initial values:

$$y_1(0),\ y_2(0):\qquad \text{Initial position of particle} \tag{73}$$

$$y_3(0),\ y_4(0):\qquad \text{Initial velocity of particle} \tag{74}$$

- Initial conditions for circular orbit: $\mathbf{v} \perp \mathbf{r}_c$

$$|\mathbf{a}| = \frac{v^2}{r_c} = \frac{GM}{{r_c}^2} \Longrightarrow v = \left(\frac{GM}{r_c}\right)^{1/2} \tag{75}$$

Then, setting $G = M = 1$ (choice of units)

$$\Longrightarrow v = {r_c}^{-1/2} \tag{76}$$

- Typical circular orbit

$$r_c = 1, \qquad v = 1 \tag{77}$$

$$\mathbf{r}_c(0) = (1.0, 0.0) \qquad \mathbf{v}(0) = (0.0, 1.0) \tag{78}$$

- Will get elliptical orbits by changing any of $x_c(0), y_c(0), v_x(0), v_y(0)$ (If changes too drastic, may get hyperbolic or parabolic (unbound) orbits)

"Quality assessment" (calibration)

- Make use of existence of *conserved* total energy, $E_{\rm tot}$ and angular momentum (w.r.t. $(0,0)$), $J_{\rm tot}$

$$E_{\rm tot} = T + V_{\rm grav} = \frac{1}{2}mv^2 - G\,\frac{Mm}{r_c} \tag{79}$$

$$J_{\rm tot} = |\mathbf{r} \times m\,\mathbf{v}| \tag{80}$$

- Particle mass enters as arbitrary parameter (test particle limit), compute *specific* quantities, E, J:

$$E = \frac{E_{\rm tot}}{m} = \frac{1}{2}v^2 - G\,\frac{M}{r_c} \tag{81}$$

$$J = \frac{J_{\rm tot}}{m} = |\mathbf{r} \times \mathbf{v}| \tag{82}$$

Get

$$E = \frac{1}{2}\left({v_x}^2 + {v_y}^2\right) - \frac{GM}{({x_c}^2 + {y_c}^2)^{1/2}} \tag{83}$$

$$J = x v_y - y v_x \tag{84}$$

- As discussed previously, should expect

$$\Delta E(t) \equiv E(t) - E(0) \approx \epsilon\,\kappa_E(t) \tag{85}$$

$$\Delta J(t) \equiv J(t) - J(0) \approx \epsilon\,\kappa_J(t) \tag{86}$$

where ϵ is the `lsoda` tolerance; e.g. if we make the tolerance 10 times more stringent, should find roughly factor of 10 improvement in energy, angular momentum conservation

- *RHS routine called by* `lsoda`

```
      subroutine fcn(neq,t,y,yprime)
         implicit    none

c-----------------------------------------------------------
c        Problem parameters (G, M) passed in via common
c        block defined in 'fcn.inc'
c-----------------------------------------------------------
         include    'fcn.inc'

         integer     neq
         real*8      t,     y(neq),    yprime(neq)

         real*8      c1

         c1 = -G * M / (y(1)**2 + y(2)**2)**1.5d0

         yprime(1) = y(3)
         yprime(2) = y(4)
         yprime(3) = c1 * y(1)
         yprime(4) = c1 * y(2)

         return
      end
```

- *Include file defining additional parameters*

```
c-------------------------------------------------------------
c     Application specific common block for communication with
c     derivative evaluating routine 'fcn' (optional) ...
c-------------------------------------------------------------

      real*8  G,          M
      common / com_fcn /
     &        G,          M
```