

MATLAB's standard solver for ordinary differential equations (ODEs) is the function `ode45`. This function implements a Runge-Kutta method with a variable time step for efficient computation. `ode45` is designed to handle the following general problem

$$\frac{dy}{dt} = \mathbf{f}(t, \mathbf{y}) \quad \mathbf{y}(t_0) = \mathbf{y}_0 \quad [1]$$

where t is the independent variable (time, position, volume) and \mathbf{y} is a vector of dependent variables (temperature, position, concentrations) to be found. The mathematical problem is specified when the vector of functions on the right-hand side of Eq. [1], $\mathbf{f}(t, \mathbf{y})$, is set and the initial conditions, $\mathbf{y} = \mathbf{y}_0$ at time t_0 , are specified.

The notes here apply to versions of MATLAB above 5.0 and cover the basics of using the function `ode45`. For more information on this and other ODE solvers in MATLAB, see the on-line help.

Contents:

| | |
|--|----|
| Syntax for <code>ode45</code> | 2 |
| Integrating a single, first-order equation..... | 3 |
| Getting the solution at particular values of the independent variable..... | 4 |
| Integrating a set of coupled first-order equations..... | 4 |
| Integrating a second-order initial-value problem (IVP)..... | 7 |
| Integrating an N th-order initial-value problem..... | 8 |
| Changing model parameters..... | 9 |
| Integrating a second-order boundary-value problem (BVP)..... | 11 |
| Setting options in <code>ode45</code> | 12 |
| Going beyond <code>ode45</code> | 13 |

Syntax for ode45

`ode45` may be invoked from the command line via

```
[t,y] = ode45('fname', tspan, y0, opts)
```

where

fname name of the function Mfile used to evaluate the right-hand-side function in Eq. [1] at a given value of the independent variable and dependent variable(s) (string). The function definition line usually has the form

```
function dydt = fname(t,y)
```

The output variable (**dydt**) must be a vector with the same size as **y**. Note that the independent variable (**t** here) must be included in the input argument list even if it does not explicitly appear in the expressions used to generate **dydt**.

tspan 2-element vector defining the range of integration (**[t_o t_f]**) though variations are possible.

y0 vector of initial conditions for the dependent variable. There should be as many initial conditions as there are dependent variables.

opts a MATLAB structure variable that allows you to control the details of computation (if you want to). This argument is optional and, if not provided, `ode45` will use default values (see the examples below).

t Value of the independent variable at which the solution array (**y**) is calculated. Note that by default this will not be a uniformly distributed set of values.

y Values of the solution to the problem (array). Each column of **y** is a different dependent variable. The size of the array is **length(t)**-by-**length(y0)**

Specific examples of using `ode45` now follow. Mfiles for these examples are in the body of this document and should also be available in the folder that contains this document.

Integrating a single, first-order equation

The height of fluid in a tank ($h(t)$) whose outlet flow is dependent on the pressure head (height of fluid) inside the tank and whose inlet flow is a function of time may be modeled via the equation

$$\frac{dh}{dt} = \alpha(t) - \beta\sqrt{h} \quad h(0) = h_o \quad [2]$$

Find the solution, $h(t)$, for $0 < t < 30$ if the following values for the parameters are given.

$$\text{Input flow: } \alpha(t) = 10 + 4 \sin(t) \quad \beta = 2 \quad h_o = 1$$

Step 1: Identify $f(t,y)$ and write a MATLAB function Mfile to evaluate it.

In this case, we have time as the independent variable and the tank height as the (single) dependent variable. Thus, we have

$$f(t,y) \rightarrow f(t,h) = \alpha(t) - \beta\sqrt{h} \quad [3]$$

From the given information for this problem, the required Mfile, named `tankfill.m`, is

```
function dhdt = tankfill(t,h)
% RHS function for tank-fill problem

A = 10 + 4*sin(t); % alpha(t)
H = 2*sqrt(h);    % beta*sqrt(h)
dhdt = A - H;

% eof - tankfill.m
```

Step 2: Use `ode45` to solve the problem

The initial condition has the height at 1 for $t = 0$ and we want to integrate until $t = 30$. The following set of commands show explicitly how the solution is put together.

```
>> tspan = [0 30];           (integration range)
>> h0 = 1;                   (initial condition, h(0))
>> [t,h] = ode45('tankfill',tspan,h0); (solve the problem)
```

Step 3: Look at the solution

The solution can be viewed via the `plot` command as in

```
>> plot(t,h)
```

The "curve" is a little choppy though it is accurate to the default relative tolerance (0.001). Note that the places where the solution is given are not uniformly spread out. See the next section for improving appearances.

Getting the solution at particular values of the independent variable

ode45 uses a variable-step-length algorithm to find the solution for a given ODE. Thus, **ode45** varies the size of the step of the independent variable in order to meet the accuracy you specify at any particular point along the solution. If **ode45** can take "big" steps and still meet this accuracy, it will do so and will therefore move quickly through regions where the solution does not "change" greatly. In regions where the solution changes more rapidly, **ode45** will take "smaller" steps. While this strategy is good from an efficiency or speed point of view, it means that the solution does not appear at a fixed set of values for the independent variable (as a fixed-step method would) and sometimes the solution curves look a little ragged.

The simplest way to improve on the density of solution points is to modify the input **tspan** from a 2-element vector to an N -element vector via something like

```
>> tspan = linspace(to,tf,500)';
```

and use this new version in the input list to **ode45**.

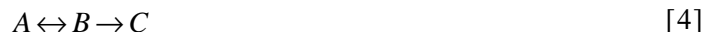
Smoother curves can also be generated by interpolation (spline interpolation usually works nicely). For example, if you wanted a smoother result from the solution for the tank-fill problem, you might do the following

```
>> ti = linspace(tspan(1),tspan(2),300); (300 points - you could use more)
>> hi = spline(t,h,ti);
>> plot(t,h,'o',ti,hi);
```

The interpolated curve smoothes out the rough edges caused by simply connecting the data points (which is what **plot** does) and so makes the graph more appealing, in a visual sense.

Integrating a set of coupled first-order equations

Chemical-kinetics problems often lead to sets of coupled, first-order ODEs. For example, consider the reaction network



Assuming a first-order reaction-rate expression for each transformation, material balances for each species lead to the following set of ODEs:

$$\begin{aligned} \frac{dA}{dt} &= -k_1A + k_2B \\ \frac{dB}{dt} &= k_1A - k_2B - k_3B \\ \frac{dC}{dt} &= k_3B \end{aligned} \quad [5]$$

with the initial conditions, $A(0) = A_o, B(0) = B_o, C(0) = C_o$. Since the equations are coupled, you cannot solve each one separately and so must solve them simultaneously.

The system in Eq. [5] can be put in the standard form for **ode45** (Eq. [1]) by defining the vectors **y**, **y_o** and **f** as

$$\mathbf{y} = \begin{bmatrix} A \\ B \\ C \end{bmatrix} \quad \mathbf{y}(0) = \mathbf{y}_o = \begin{bmatrix} A_o \\ B_o \\ C_o \end{bmatrix} \quad \mathbf{f}(t, \mathbf{y}) = \begin{bmatrix} -k_1 y_1 + k_2 y_2 \\ k_1 y_1 - (k_2 + k_3) y_2 \\ k_3 y_2 \end{bmatrix} \quad [6]$$

Solving the system represented by Eq. [6] is a simple extension of what was done for solving a single equation. We'll demonstrate the solution for the following situation

$$k_1 = 5 \quad k_2 = 2 \quad k_3 = 1 \quad A_o = 1 \quad B_o = C_o = 0$$

Step 1: Write a function Mfile to evaluate the right-hand-side expression

The primary difference here, compared to the single-equation case, is that the input variable \mathbf{y} will be a *vector*. The first element of \mathbf{y} represents the concentration of species A at a time t , and the second and third elements representing the concentrations of species B and C, respectively, at the same time, t . This ordering of variables is defined by Eq. [6]. There is no "right" order to the variables but whatever order you do choose, use it consistently. We'll call the Mfile **react.m**. It looks like this:

```
function dydt = react(t,y)
% Solve the kinetics example

dydt = zeros(size(y));

% Parameters - reaction-rate constants

k1 = 5; k2 = 2; k3 = 1;

A = y(1);           We'll be explicit about it here though you can do
B = y(2);           the calculations directly with the y-values.
C = y(3);

% Evaluate the RHS expression

dydt(1) = -k1*A + k2*B;
dydt(2) = k1*A - (k2+k3)*B;
dydt(3) = k3*B;

% eof - react.m
```

Note that the input arguments must be \mathbf{t} and \mathbf{y} (in that order) even though \mathbf{t} is not explicitly used in the function.

Step 2: Use **ode45** to solve the problem

No time interval is given so we'll pick one (0 to 4) and see what the solution looks like. If a longer or shorter interval is needed, we can simply re-execute the function with a new value for the ending time. Following the outline for the single-equation problem, the call to **ode45** is,

```
>> [t,y] = ode45('react',[0 4],[1 0 0]);
```

Note that the initial condition is provided directly in the call to **ode45**. You could also have defined a variable $\mathbf{y0}$ prior to the call to **ode45** and used that variable as an input.

Take a moment to look at the outputs. The number of points at which the solution is known is

```
>> length(t)
```

Also consider the shape of the output variable **y**:

```
>> size(y)
```

Is the result as stated above (i.e., is it **length(t)**-by-**length(y0)**)?

Step 3: Look at the solution

If you want to see the time-course of all species, use the command

```
>> plot(t,y)
```

The blue line will be the first column of **y** (species A). The green and red lines will be the second and third columns of **y** (species B and C, respectively).

If you wanted to look at only one species (for example, species B), you would give the command

```
>> plot(t,y(:,2))
```

since the second column of **y** holds the information on species B.

Integrating a second-order initial-value problem (IVP)

A mass-spring-dashpot system can be modeled via the following second-order ODE

$$\ddot{y} + c\dot{y} + \omega^2 y = g(t) \quad y(0) = y_o, v(0) = \dot{y}(0) = v_o \quad [7]$$

In this model, c represents a retarding force proportional to the velocity of the mass, ω^2 is the natural frequency of the system and $g(t)$ is the forcing (or input) function. The initial conditions are the initial position (y_o) and initial velocity (v_o).

`ode45` is set up to handle only first-order equations and so a method is needed to convert this second-order equation into one (or more) first-order equations which are equivalent. The conversion is accomplished through a technique called "reduction of order". We'll illustrate the solution for the particular set of conditions

$$c = 5 \quad \omega = 2 \quad y(0) = 1 \quad v(0) = 0 \quad g(t) = \sin(t)$$

Step 1: Define the components of a vector $\mathbf{p} = [p_1 \ p_2]^T$ as follows:

$$\begin{aligned} p_1 &= y \\ p_2 &= \dot{y} \end{aligned} \quad [8]$$

Step 2: Form the first derivatives of each of the components of \mathbf{p}

Using the given differential equation, we can write a system of first-order equations as

$$\begin{aligned} \dot{p}_1 &= \dot{y} = p_2 \\ \dot{p}_2 &= \ddot{y} = g(t) - c\dot{y} - \omega^2 y \\ &= g(t) - cp_2 - \omega^2 p_1 \end{aligned} \quad [9]$$

In writing the expression for the second component, we've used the governing ODE (Eq. [7]).

Step 3: Cast the problem in the format needed to use `ode45`.

$$\dot{\mathbf{p}} = \frac{d\mathbf{p}}{dt} = \frac{d}{dt} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} p_2 \\ g(t) - cp_2 - \omega^2 p_1 \end{bmatrix} = \begin{bmatrix} f_1(t, \mathbf{p}) \\ f_2(t, \mathbf{p}) \end{bmatrix} = \mathbf{f}(t, \mathbf{p}) \quad [10]$$

Step 4: Collect the initial conditions into a single vector

$$\mathbf{p}(0) = \mathbf{p}_o = \begin{bmatrix} p_1(0) \\ p_2(0) \end{bmatrix} = \begin{bmatrix} y(0) \\ \dot{y}(0) \end{bmatrix} = \begin{bmatrix} y_o \\ v_o \end{bmatrix} \quad [11]$$

Step 5: Apply `ode45` to solve the system of equations

The Mfile for the RHS function for this problem will be called `spring.m`. Here it is:

```
function pdot = spring(t,p)
% Spring example problem
```

```

% Parameters - damping coefficient and natural frequency

c = 5; w = 2;

g = sin(t); % forcing function
pdot = zeros(size(p));
pdot(1) = p(2);
pdot(2) = g - c*p(2) - (w^2)*p(1);

% eof - spring.m

```

The call to `ode45` is, for a solution interval of 0 to 20,

```

>> p0 = [1 0]; % (initial position and velocity)
>> [t,p] = ode45('spring',[0 20],p0);

```

Step 6: Look at the results

If you wanted to look at only the displacement, you'd want to look at the first column of **p** (see the definition of **p** in the first step, Eq. [8]). Hence, you would give the command

```

>> plot(t,p(:,1))

```

An interesting plot for these sorts of problems is the phase-plane plot, a plot of the velocity of the mass versus its position. This plot is easily created from your solution via

```

>> plot(p(:,1),p(:,2))

```

Phase-plane plots are useful in analyzing general features of dynamic systems.

Integrating an *N*th-order initial-value problem

To use `ode45` to integrate an *N*th-order ODE, you simply continue the process outlined in the section on integrating a 2nd-order ODE. The first element of the vector **p** is set to the dependent variable and then subsequent elements are defined as the derivatives of the dependent variable up to one less than the order of the equation. Finally, the initial conditions are collected into one vector to give the format presented in Eq. [1].

For example, the 4th-order equation

$$a \frac{d^4 y}{dx^4} + b \frac{d^3 y}{dx^3} + c \frac{d^2 y}{dx^2} + d \frac{dy}{dx} + ey = 0 \quad [12]$$

would generate the first-order system

$$\frac{d}{dt} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{bmatrix} = \begin{bmatrix} p_2 \\ p_3 \\ p_4 \\ -(bp_4 + cp_3 + dp_2 + ep_1)/a \end{bmatrix} \quad [13]$$

which, along with an appropriate set of initial conditions would complete the set-up for `ode45`.

Changing model parameters

In all the examples given above, the parameter values were given specific variables in the Mfile used to evaluate the RHS function (the model of the system). This is fine for one-shot cases and in instances where you don't anticipate a desire to change the parameters. However, this situation is not fine where you want to be able to change the parameters (e.g., change the damping coefficient in order to see the result in a phase-plane plot). One approach to changing parameters is to simply edit the file every time you want to make a change. While having the advantage of simplicity, this approach suffers from inflexibility, especially as the number of parameters and as the frequency of the changes increase. To get other parameters into the function, you need to use an expanded version of the syntax for `ode45`, one that allows "other" information to be provided to the derivative function when `ode45` uses that function. This is most easily seen by an example (and by reading the on-line help on `ode45`).

Step 1: Write the Mfile for the RHS function so that it allows more input variables. The parameter list starts after the dependent variable and after a required input called `flag`.

For this example, we will re-write `spring.m` so that `c` and `w` are given their values via the function definition line. The altered Mfile is

```
function pdot = spring2(t,p,flag,c,w)
% Spring example problem

% Parameters - c is the damping coefficient and
%              w is the natural frequency

pdot = zeros(size(p));
g = sin(t); % forcing function

pdot(1) = p(2);
pdot(2) = g - c*p(2) - (w^2)*p(1);

% eof - spring2.m
```

Step 2: Write a driver script that implements your logic and allows you to set values of the parameters for the problem.

The script created here will do the following

1. Implement a loop that
 - a. asks for values of the parameters
 - b. solves the ODE
 - c. plots the phase-plane view of the solution
2. Exits if no inputs are given

Certainly more sophisticated scripts are possible but this has the essence of the idea. The script is called `dospring.m` and it is:

```
%DOSPRING Interactive plotting of the phase-plane

while 1 % infinite loop

    C_SPRING = input('Damping coefficient [c]: ');
```

```

if isempty(C_SPRING) % how to get out
    break
end

W_SPRING = input('Natural frequency [w]: ');

[t,p] = ode45('spring2',[0 20],[1 0],[],C_SPRING,W_SPRING);

plot(p(:,1),p(:,2))
title('Phase-plane plot of results')
xlabel('position')
ylabel('velocity')

end

% eos - dospring.m

```

Note the additions to the call to `ode45`. First, a placeholder for the “options” input is inserted (an empty array) so that “default” options are used. Then, the parameters for the model are provided *in the order that they appear in the definition line* of the RHS function.

Try the script out and modify it (e.g., you could add the frequency and/or amplitude of the forcing function as something to be changed).

Integrating a second-order boundary-value problem (BVP)

`ode45` was written to solve initial-value problems (IVPs). Hence it cannot be (directly) used to solve, for example, the following problem derived from a model of heat-transfer in a rod:

$$\frac{d^2 y}{dx^2} - y = 0 \quad y(0) = 1 \quad \left. \frac{dy}{dx} \right|_{x=1} = 0 \quad [14]$$

since the value of the derivative at $x = 0$ is not specified (it is known at $x = 1$, though). Equation [14] is a boundary-value problem (BVP) and is common in models based on transport phenomena (heat transfer, mass transfer and fluid mechanics).

All is not lost because one way to solve a BVP is to pretend it is an IVP. To make up for the lack of knowledge of the derivative at the initial point, you can guess a value, do the integration and then check yourself by seeing how close you are to meeting the conditions at the other end of the interval. When you have guessed the right starting values, you have the solution to the problem. This approach is sometimes called the "shooting method" by analogy to the ballistics problem of landing an artillery shell on a target by specifying only its set-up (powder charge and angle of the barrel).

Step 1: Set up the problem so that `ode45` can solve it

Using the approach of turning a second order equation into a pair of coupled first-order equations, we have

$$\frac{d}{dx} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} p_2 \\ p_1 \end{bmatrix} \quad \mathbf{p}(0) = \begin{bmatrix} 1 \\ v \end{bmatrix} \quad [15]$$

where v has been used to represent the (unknown) value of the derivative at $x = 0$. The Mfile used to evaluate the RHS is as follows

```
function dpdx = hotrod(x,p)
% Hot-rod problem illustrating the shooting method

dpdx = zeros(size(p));

dpdx(1) = p(2);
dpdx(2) = p(1);

% eof - hotrod.m
```

Step 2: Guess a value of the initial slope and integrate to $x = 1$

The problem will be iterative so it's not likely that the first guess will be right. From the physics of the problem, the end of the rod (at $x = 1$) will be colder than the place we are starting from ($x = 0$) and so we'll guess a negative value for the initial slope.

```
>> v = -1;
>> [x,p] = ode45('hotrod',[0 1],[1 v]);
```

The value of the derivative at $x = 1$ is the last value in the second column of \mathbf{p} (why?). Thus, we can check the accuracy of the first guess via

```
>> p(length(x),2)
```

which I found to be -0.3679. That's too low (it should be zero).

Step 3: Iterate until the boundary condition at $x = 1$ is met

You can use brute force here if you have only one problem or you could finesse it by hooking the whole thing up to **fzero** and have **fzero** do the guessing. Here are my brute-force results:

| <u>Value of v</u> | <u>Slope at $x = 1$</u> |
|--------------------------------|------------------------------------|
| -1.0 | -0.3679 |
| -0.5 | -0.4037 |
| -0.75 | -0.0179 |
| -0.76 | -0.0025 |

The trend is obvious and so the initial slope is around -0.76 (the exact value is $-\tanh(1) = -0.7611\dots$). Using **fzero** would be a good alternative if this problem were to be solved many times over.

Step 4: Look at the results

Even though we are guessing the initial slope to solve the problem, it is the solution, $y(x)$, that we are really interested in. This solution is in the first column of **p** and may be viewed via

```
>> plot(x,p(:,1))
```

Setting options in ode45

The input **opts** is a MATLAB structure variable that can be used to control the performance of the various ODE-solvers in MATLAB. The most common option that you'll likely want to alter is the accuracy to which solutions are computed. To make this process easy, a pair of functions are available – **odeset** for creating and changing options and **odeget** for displaying information on options. To see what the current settings are, try the command

```
>> odeset
```

Default values for any setting are denoted by the braces, **{}**.

MATLAB uses two accuracy measures for solving ODEs – the relative tolerance (**RelTol** in **opts**) and the absolute tolerance (**AbsTol** in **opts**). Each step in the integration is taken so that it satisfies the condition

$$\text{Error at step } j \leq \max_k(\text{RelTol} \cdot y_{jk}, \text{AbsTol}_k)$$

where the subscript k ranges over all the components of the solution vector at time step j . To alter the default settings, use commands such as

```
>> oldOpts = odeset;  
>> newOpts = odeset(oldOpts, 'RelTol', 1e-6)
```

Information on the settings for the other options is available in the on-line help.

Going beyond ode45

The solver **ode45** is not the be-all and end-all of ODE-solvers. While **ode45** should be your first choice for integration, there are problems that the function performs poorly on or even fails on. In such cases, there are fallback solvers that are available. All these solvers use the same syntax as **ode45** (see page 2) but have options for handling more difficult or sophisticated problems.

Here are some suggestions for handling non-standard ODE problems:

- If accuracy you desire is not obtainable via **ode45**, try the function **ode113**. This solver uses a variable order method that may be able to improve over what **ode45** does.
- If **ode45** is taking too long to compute a solution, your problem may be “stiff” (i.e., it involves a system with a wide range of time constants). Try the function **ode15s**.
- If your system of equations has the form

$$\mathbf{M} \frac{dy}{dt} = \mathbf{f}(t, \mathbf{y})$$

where **M** is a (typically non-singular) matrix, try the function **ode15s**.

You’ll find more information on these function in the on-line help and documentation. For example, try the on-line function reference (available through the command **helpdesk**) on any of the solvers noted above.