mpc2w1.tex
Week 1. 12.10.2011

MPC2 MATHEMATICS FOR CHEMISTS

Professor N. H. BINGHAM, Autumn 2011

Huxley 6M47; 020-7594 2085; n.bingham@ic.ac.uk; Office hour Fri 9-10am

Lectures: 9-11am Wed, beginning 12 October;
Tutorials: Mon 5-6, Blackett 741 (except 14 Nov.), beginning 17 October.
Course website: My homepage, link to MPC2.

SYLLABUS

I. Inhomogeneous ordinary differential equations (ODEs) [Weeks 1,2]
II. Complex numbers [Weeks 2-3]
III Partial differential equations (PDEs) [Weeks 3-5]
IV. Linear algebra [Weeks 5-7]
V. Fourier analysis [Weeks 7-9]
VI. Field theory: Vector calculus [Weeks 9-10]
Dramatis Personae: Who did what when [Week 10]
Recommended Texts.

There are innumerable books possible. It doesn't really matter which one you choose – but I strongly recommend you to find a book that suits you and use it, otherwise you rely entirely on lectures. For guidance: any book covering the six topics in the syllabus above, and with a reputable publisher (e.g. Cambridge UP, Oxford UP, Springer, Academic Press) is probably OK.

Where I have used a book, I have often relied on an enduring classic:
H. MARGENAU and G. M. MURPHY: *The mathematics of physics and chemistry*, Van Nostrand, 1943, Volume 1 (Volume 2 is also good but more advanced).

One alternative for everything except Ch. VI is another enduring classic,
H. S. W. MASSEY and H. KESTELMAN, *Ancillary mathematics*, Pitman, 1959.
There is a good treatment of Ch. VI in
H. M. SCHEY: *div, grad, curl and all that: an informal text on vector calculus*, 3rd ed., W. W. Norton.

I. INHOMOGENEOUS ORDINARY DIFFERENTIAL EQUATIONS (ODEs)

The subject dates back to, e.g., Leonhard EULER (1707-1783) and the Bernoullis. Recall: a *differential equation* (DE) is an equation involving a function ($y(x)$, say) and its derivatives, y', y'' etc., to be solved for y. The DE is *ordinary* (an ODE) if there is only one independent variable, x say (if there is more than one, the DE is *partial* – a PDE; see Ch. III).

The DE is *linear* if y and its derivatives appear only to the first power (e.g., no square terms y^2, cross terms yy', etc.). We confine attention to linear equations here (non-linear equations are very important, but much harder).

A (linear) equation is *homogeneous* if $y = 0$ is a solution – or, with all terms involving y , y', ... on the LHS, the RHS is 0. With a general RHS, $g(x) say$, the DE is *non-homogeneous.*

Differential notation. We write

$$\frac{dy}{dx}, \quad \text{or} \quad dy/dx,$$

as y' or Dy. So D, or d/dx, or .' ("prime"), denotes the operator of differentiation, or *differential operator.* Similarly, the second derivative, or

$$\frac{d^2y}{dx^2}, \quad \text{or} \quad d^2y/dx^2, = \Big(\frac{d}{dx}\Big)^2 y,$$

is written D^2y, or y'', etc. We write this also as

$$dy = y'dx.$$

NB. Read dx, dy etc. as *one symbol.* So dx^2 above means $(dx)^2$.

When the independent variable is *time*, t, it is customary to write $df(t)/dt$ as $\dot{f}$ rather than f', and the second derivative as $\ddot{f}$ rather than f''. This is the one surviving feature of Newton's notation for calculus (or fluxions, as he called it – Sir Isaac NEWTON (1645-1723), *Principia* in 1687); the other notation we use comes from Leibniz (G. LEIBNIZ (1646-1716)), including the integral sign $\int$, an elongated S for Summe (German for sum: integrals are limits of sums).

General solutions. In a (linear) DE, the *degree* is the order of the highest derivative of y – n, say. The simplest case is $n = 1$, a *first-order* DE. The usual case in Physics, and Chemistry, is $n = 2$, *second-order* DE.

To solve an nth order DE, we must integrate n times. Each integration introduces an arbitrary constant (of integration), giving n arbitrary constants (ACs) in all. To determine these, we need to be given conditions:
$n = 1$. $y(x_0) = y_0$ (*initial condition*, IC).
$n = 2$. $y(x_0) = y_0$, $y'(x_0) = y_0'$ or y_1 (ICs), or
$y(x_0) = y_0$, $y(x_1) = y_1$ (*boundary conditions*, BCs).

Linear differential operators. A typical linear ODE will have the form

$$a_0 y + a_1 y' + a_2 y'' = g(x).$$

The a_i on the LHS may be functions $a_i(x)$, or constants. The LHS is

$$(a_0 + a_1 \frac{d}{dx} + a_2 \frac{d^2}{dx^2})y, \quad \text{or} \quad (a_0 + a_1 D + a_2 D^2)y, \quad \text{or} \quad Ly,$$

where

$$L = a_0 + a_1 \frac{d}{dx} + a_2 \frac{d^2}{dx^2}, \quad \text{or} \quad a_0 + a_1 D + a_2 D^2$$

is a *linear differential operator* (often, not always, with constant coefficients).
Homogeneous DE:

$$Ly = 0. \qquad (H).$$

Non-homogeneous DE:

$$Ly = g. \qquad (N).$$

For a DE (H) of degree n, we say that (H) has *general solution* (GS) y_1 if
(i) $Ly_1 = 0$,
(ii) y_1 contains n arbitrary constants.
If y_2 is ANY solution of (N) – a *particular integral* (PI) – then
(i)

$$\begin{aligned} L(y_1 + y_2) &= Ly_1 + Ly_2 && \text{(linearity of } L) \\ &= 0 + g = g && \text{(by } (H) \text{ and } (N)), \end{aligned}$$

i.e. $y_1 + y_2$ satisfies (N),
(ii) $y_1 + y_2$ contains n arbitrary constants (as y_1 does). So $y_1 + y_2$ is the general solution of (N):

$$\text{GS of } (N) = \text{GS of } (H) + \text{PI of } (N).$$

Principle of Superposition. If L is a linear DO and y_1, y_2 satisfy (H), i.e.$Ly = 0$, then also $y_1 + y_2$ satisfies (H), as by linearity of L

$$L(y_1 + y_2) = Ly_1 + Ly_2 = 0 + 0 = 0.$$

Similarly, any linear combination $c_1 y_1 + c_2 y_2$ (c_i constants) is a solution:

$$L(c_1 y_1 + c_2 y_2) = c_1 Ly_1 + c_2 Ly_2 = 0 + 0 = 0.$$

Physically, one can see the Principle of Superposition at work with, e.g., water waves. The wave equation is linear (see Ch. III below); when the wakes of two ships meet, they pass through each other and continue undisturbed.
Variation of Parameters (or of Constants).

This is a method of starting with a GS of (H) and finding a GS of (N).
$n = 1$. E.g.,

$$y' - \frac{1}{x}y = x^3. \qquad (N)$$

The corresponding (H) is

$$y' - \frac{1}{x}y = 0; \quad \frac{y'}{y} = \frac{1}{x}; \quad D(\log y) = D(\log x); \quad \log y = \log x + const, \quad y = cx. \qquad (H)$$

Now allow *the constant to vary*: $c = u = u(x)$, say:

$$y = ux, \qquad y' = u'x + u, frac1xy = u.$$

Combining,

$$y' - \frac{1}{x}y = u'x.$$

So

$$u'x = x^3; \quad u' = x^2; \quad u = x^3/3 + c.$$

So

$$y = ux = x^4/3 + cx,$$

the GS of (N).
Check: $y' = 4x^3/3 + c$, $y' - y/x = 4x^3/3 + c - x^3/3 + c = x^3$. So y *is* a solution, and contains an arbitrary constant, so is the GS. Always check in this way!
$n = 2$.

$$Ly = a(x)y'' + b(x)y' +_c (x)y = f(x). \qquad (N)$$

Suppose we know two independent solutions y_1, y_2 of $Ly = 0$ (H). Take

$$y = u_1 y_1 + u_2 y_2 \qquad (u_i = u_i(x)).$$

Then

$$y' = u_1 y_1' + u_2 y_2' + (u_1' y_1 + u_2' y_2).$$

Take

$$u_1' y_1 + u_2' y_2 = 0. \tag{1}$$

Then

$$y' = u_1 y_1' + u_2 y_2'. \tag{$*$}$$

So

$$y'' = u_1' y_1' + u_2' y_2' + u_1 y_1'' + u_2 y_2''.$$

So

$$Ly = ay'' + by' + cy = (ay_1'' + by_1' + c)u_1 + (ay_2'' + by_2' + c)u_2 + au_1' y_1' + au_2' y_2'.$$

As y_1, y_2 are solutions to (H), this reduces to

$$Ly = au_1' y_1' + au_2' y_2'.$$

So (N), i.e. $Ly = g$, is

$$u_1' y_1 + u_2' y_2 = g/a. \tag{2}$$

Now (1) and (2) give us two simultaneous linear equations for two unknowns, u_1' and u_2'. We can solve these, uniquely in general, because y_1, y_2 are *independent* solutions (recall that simultaneous linear equations are uniquely solvable in general, but may have no or infinitely many solutions – see Ch. IV below). So integrating we get u_1, u_2 (involving two ACs), and hence we get $y = u_1 y_1 + u_2 y_2$.
Example.

$$y'' + y = \sec x \ (:= 1/\cos x) \tag{N}$$

(here we use := for 'is defined to be equal to'; =: is read as 'which defines'),

$$y'' + y = 0. \tag{H}$$

Independent solutions $\cos x$, $\sin x$ ($D \sin x = \cos x$, $D \cos x = -\sin x$, so $D^2 \sin = -\sin$, $D^2 \cos = -\cos$). Take $y = u_1 \cos x + u_2 \sin x$.

$$u_1' \cos x + u_2' \sin x = 0, \tag{1}$$

$$-u_1' \sin x + u_2' \cos x = 1/\cos x. \tag{2}$$

The determinant is $\cos^2 + \sin^2 = 1 \neq 0$, so a unique solution exists.
"(1) $\sin x$ + (2) $\cos x$":

$$u_2'(\sin^2 x + \cos^2 x) = 1, \qquad u_2' = 1, \qquad u_2 = x.$$

From (2),

$$u_1' = -\sin x/\cos x, \quad u_1 = -\int \sin x dx/\cos x = \int d\cos x/\cos x = \log\cos x.$$

So: GS of (N) = PI + GS of $(H) = c_1 \cos x + c_2 \sin x + \cos x \log \cos x + x \sin x$.
Example. DE $y'' + \lambda^2 y = f(x)$, ICs $y(0) = 0$, $y'(0) = 0$.

$$y'' = -\lambda^2 y, \tag{H}$$

solutions $y_1 = \cos \lambda x$, $y_2 = \sin \lambda x$.

$$y = u_1 \cos \lambda x + u_2 \sin \lambda x. \tag{N}$$

$$u_1' \cos \lambda x + u_2' \sin \lambda x = 0, \tag{1}$$

$$u_1'(-\lambda \sin \lambda x) + u_2'(\lambda \cos \lambda x) = f(x), \quad -u_1' \sin \lambda x + u_2' \cos \lambda x = f(x)/\lambda. \tag{2}$$

"(1) $\sin \lambda x$ + (2) $\cos \lambda x$":

$$u_2' = \frac{1}{\lambda} f(x) \cos \lambda x, \quad u_2 = \frac{1}{\lambda} \int_0^x f(t) \cos \lambda t dt + c_2;$$

$$u_1' = -u_2' \sin \lambda x / \cos \lambda x = -\frac{1}{\lambda} f(x) \sin \lambda x, \quad u_1 = -\frac{1}{\lambda} \int_0^x f(t) \sin \lambda t dt + c_1;$$

$$y = u_1 \cos \lambda x + u_2 \sin \lambda x = \frac{1}{\lambda} \int_0^x f(t)\{-\cos \lambda x \sin \lambda t + \sin \lambda x \cos \lambda t\} dt + c_1 \cos \lambda x + c_2 \sin \lambda x :$$

$$y = u_1 \cos \lambda x + u_2 \sin \lambda x = \frac{1}{\lambda} \int_0^x f(t) \sin \lambda(x - t) dt + c_1 \cos \lambda x + c_2 \sin \lambda x.$$

As $y(0) = 0$: $c_1 = 0$. By $(*)$,

$$y' = u_1 y_1' + u_2 y_2' = u_1(-\lambda \sin \lambda x) + u_2(\lambda \cos \lambda x).$$

As $y'(0) = 0$, $u_2(0) = 0$, $c_2 = 0$:

$$y = \frac{1}{\lambda} \int_0^x f(t) \sin \lambda(x - t) dt.$$