CHEM 555-75 **WORKSHEET 1** **Fall 2021**

Instructor: Prof. Lee M. Thompson E-mail: *lee.thompson.1@louisville.edu* Office: CB 251

1. Solve the set of simultaneous equations:

   a)

$$2x - y = 2 \tag{1}$$
$$x + y = 4 \tag{2}$$

   b)

$$2x + y = 5 \tag{3}$$
$$4x - y = 1 \tag{4}$$

   a) $x = 4 - y$
   $2(4 - y) - y = 2$
   $8 - 3y = 2$
   $y = 2,\ x = 2$

   b) $x = \frac{1}{4}(1 + y)$
   $\frac{1}{2}(1 + y) + y = 5$
   $3y = 9$
   $y = 3,\ x = 1$

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2. Solve the following using the method of Lagrange undetermined multipliers:

   a) Find the largest value of $f(x, y) = x^2 + y^2$ where $x + y = 4$.

   b) The temperature of a room is given by $T(x, y) = x^2 - 2y^2 + 2xy + 4x$. Find the temperature of the hottest point on a rod that lies along the direction $2x - y = 0$..

   a) $\Lambda = x^2 + y^2 - \lambda(x + y - 4)$
   $\frac{\partial \Lambda}{\partial x} = 2x - \lambda = 0$
   $\frac{\partial \Lambda}{\partial y} = 2y - \lambda = 0$
   $\frac{\partial \Lambda}{\partial \lambda} = -(x + y - 4) = 0$
   $x = \frac{\lambda}{2},\ y = \frac{\lambda}{2},\ \lambda = 4$
   $x = 2,\ y = 2$

   b) $\Lambda = x^2 - 2y^2 + 2xy + 4x - \lambda(2x - y)$
   $\frac{\partial \Lambda}{\partial x} = 2x + 2y + 4 - 2\lambda = 0$
   $\frac{\partial \Lambda}{\partial y} = -4y + 2x + \lambda = 0$
   $\frac{\partial \Lambda}{\partial \lambda} = -2x + y = 0$

$y = 2x$, $-4y + y = -\lambda$, $\lambda = 3y$, $y + 2y + 4 - 2(3y) = 0$, $-3y + 4 = 0$
$y = \frac{4}{3}$,$x = \frac{2}{3}$

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3. Solve the following differential equations:

   a) $\frac{dy}{dx} - xy^3 = 0$

   b) $x^2 \frac{dy}{dx} + xy^2 = 4y^2$

   c) $y(2x^2y^2 + 1)\frac{dy}{dx} + x(y^4 + 1) = 0$

   d) $\frac{dy}{dx} = -\frac{2x^2+y^2+x}{xy}$

a) $\frac{dy}{dx} - xy^3 = 0$
$\int \frac{1}{y^3} dy = \int x dx$
$-\frac{1}{2y^2} = \frac{x^2}{2} + C_1$
$y = \pm \frac{1}{\sqrt{-x^2+C}}$

b) $x^2 \frac{dy}{dx} + xy^2 = 4y^2$
$\int \frac{1}{y^2} dy = \int \frac{(4-x)}{x^2} dx$
$\int \frac{1}{y^2} dy = 4 \int \frac{1}{x^2} dx - \int \frac{1}{x} dx$
$-\frac{1}{y} = -4\frac{1}{x} - \ln(x) + C_1$

c) $y(2x^2y^2 + 1)\frac{dy}{dx} + x(y^4 + 1) = 0$
$x(y^4 + 1)dx + y(2x^2y^2 + 1)dy = 0$
$A(x, y) = xy^4 + x$, $B(x, y) = 2x^2y^3 + y$
$\frac{\partial A(x,y))}{\partial y} = 4xy^3$, $\frac{\partial B(x,y))}{\partial x} = 4xy^3$ so we have an exact differential
$f(x, y) = \int A(x, y)dx + g(y) = \int xy^4 + xdx + g(y) = \frac{x^2y^4}{2} + \frac{x^2}{2} + g(y) = C_1$
$\frac{f(x,y)}{\partial y} = 2x^2y^3 + \frac{\partial g(y)}{\partial y} = B(x, y) = 2x^2y^3 + y$
$\frac{\partial g(y)}{\partial y} = 2x^2y^3 + y - 2x^2y^3 = y$
$g(y) = \int ydy = \frac{y^2}{2} + C_2$
$f(x, y) = \frac{x^2y^4}{2} + \frac{x^2}{2} + \frac{y^2}{2} + C_2 = C_1$
$x^2y^4 + x^2 + y^2 + C = 0$

d) $\frac{dy}{dx} = -\frac{2x^2+y^2+x}{xy}$
$(2x^2 + y^2 + x)dx + xydy = 0$
$A(x, y) = 2x^2 + y^2 + x$, $B(x, y) = xy$
$\frac{\partial A(x,y))}{\partial y} = 2y$, $\frac{\partial B(x,y))}{\partial x} = y$ so we have an inexact differential
$\frac{1}{B(x,y)}\left(\frac{\partial A(x,y))}{\partial y} - \frac{\partial B(x,y))}{\partial x}\right) = \frac{1}{x}$ which is a function of one variable
$\mu(x) = \exp\left(\int \frac{1}{x} dx\right) = \exp(\ln(x)) = x$
$(2x^3 + xy^2 + x^2)dx + x^2ydy = 0$

$A'(x,y) = 2x^3 + xy^2 + x^2$, $B'(x,y) = x^2y$
$\frac{\partial A'(x,y))}{\partial y} = 2xy$, $\frac{\partial B'(x,y))}{\partial x} = 2xy$ so we now have an exact differential
$f(x,y) = \int A(x,y)dx + g(y) = \int (2x^3 + xy^2 + x^2)dx + g(y) = \frac{1}{2}x^4 + \frac{1}{2}x^2y^2 + \frac{1}{3}x^3 + g(y) = C_1$
$\frac{\partial}{\partial y}f(x,y) = x^2y + \frac{d}{dy}g(y) = B(x,y) = x^2y$
$\frac{d}{dy}g(y) = 0$
$g(y) = \int 0dy = C_2$
$f(x,y) = \frac{1}{2}x^4 + \frac{1}{2}x^2y^2 + \frac{1}{3}x^3 + C = 0$

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4. Consider a mass m attached to a spring. If the mass is displaced by a distance y then the spring exerts a restoring force proportional to the displacement $F(y) = -ky$, where k is the force constant determining the 'stiffness' of the spring (Hooke's law). Equally, the restoring force is proportional to the attached mass $F(y) = ma(y)$, where a is the acceleration (Newton's second law). Equating the two equations for the restoring force, we can derive a second order differential equation that governs the motion of the mass

$$-ky = m\frac{d^2y}{dt^2} \Rightarrow \frac{d^2}{dt^2}y + \omega^2 y = 0 \tag{5}$$

where $\omega^2 = \frac{k}{m}$. The expression we have just derived is the equation of motion for the simple harmonic oscillator.

For a harmonic oscillator with $\omega = 4$, determine the equation governing how the displacement of the mass varies with time, given initial ($t = 0$) displacement $y(0) = 6$ and velocity $dy(0)/dt = 32$. Using this equation, determine the amplitude, time period and frequency of oscillation for the system.

$\frac{d^2}{dt^2}y + \omega^2 y = 0$
The general solution is $y(t) = A\cos(4t) + B\sin(4t)$
Therefore, $dy(t)/dt = -4A\sin(4t) + 4B\cos(4t)$
At the initial condition ($t = 0$) $y(0) = A = 6$ and $dy(0)/dt = 4B = 32$
Therefore, $A = 6$ and $B = 8$ and the particular solution is $y(t) = 6\cos(4t) + 8\sin(4t)$
The amplitude is $a = \sqrt{A^2 + B^2} = 10$
The time period is $\frac{2\pi}{\omega} = \frac{2\pi}{4}$
The frequency is $\frac{\omega}{2\pi} = \frac{4}{2\pi}$

5. Request an account on the cardinal research cluster (CRC) which are the Universities high performance (HPC) computing facilities. Follow the steps below:

1. Go to https://ulservices.louisville.edu/jira/servicedesk/customer/portal/4/create/343 and log in.

2. Fill in the form (enter 'Lee Michael Thompson' under principle investigators name and lee.thompson.1@louisville.edu under principle investigators e-mail address) using "Access to Gaussian for completing CHEM 555 workshop" as the purpose.

3. You should receive an e-mail in a few days with information on VPN set-up (for connection from home) and an e-mail when you CRC account has been set up.

4. If you have a Mac or Linux machine, just open the terminal and type
ssh -X <ULinkID>@crc.hpc.louisville.edu

at the command prompt. If you have a windows machine, download
putty (https://www.chiark.greenend.org.uk/ sgtatham/putty/latest.html) and
xming (https://sourceforge.net/projects/xming/)
and configure to access crc.hpc.louisville.edu using your ULinkID as your username. In both cases your password is the same as your University account.