ChE515: Problem Set 1 (Due Date: October 4, 2007)

1. VM 1.15. Solve by finding the rank of the appropriate coefficient matrix.
2. VM 1.17.
3. VM 1.21. Verify that the sum of the eigenvalues is equal to trace (C) while their product is equal to det (C).
4. Using a suitable similarity transformation, solve the following system of ODEs.
   $$\frac{dx}{dt} = -6x - 9y + 1, \ \frac{dy}{dt} = -6x + 9y + t; \ x(0) = 4, \ y(0) = -3.$$
5. VM 1.24. Make use of the eigenvalues/eigenvectors of the coefficient matrix.
6. VM 1.37
7. Vibrating/oscillating mechanical systems are used as models in many applications ranging from quantum chemistry to structural dynamics. Consider the following system ($k > 0$):
   $$\frac{d^2x}{dt^2} = k(y - 2x)$$
   $$\frac{d^2y}{dt^2} = k(x - 2y)$$

   Represent the above system of equations in the form $\mathbf{X}'' = \mathrm{A}\,\mathbf{X}$ where $\mathbf{X} = (x, y)^t$ is the vector of unknowns and the prime denotes derivative operation. Solve the system of equations by letting $\mathbf{X} = \mathbf{U} \exp(i\omega t)$ where ω are eigenvalues to be determined.

8. Consider the following multivariate Gaussian function:
   $$f(x_1, x_2, .. x_n) = \exp\left[-\frac{1}{2}\left(a_{11}x_1^2 + 2a_{12}x_1x_2 + .. + 2a_{n-1\,n}x_{n-1}x_n + a_{nn}x_n^2\right)\right].$$

   (a). Show that f can be expressed as $\exp(-\mathbf{x}^t\mathrm{A}\mathbf{x}/2)$ where A is a symmetric matrix.

   (b). Let S denote the matrix of normalized eigenfunctions of the symmetric matrix A such that $\mathrm{S}^t \mathrm{A}\,\mathrm{S} = \mathrm{D}$, where D is the diagonal matrix of the eigenvalues of A. Note that det (S) = 1 since A is symmetric (see class notes). By using the transformation $\mathbf{x} = \mathrm{S}\,\mathbf{y}$, show that
   $$\int_{-\infty}^{\infty} .. \int_{-\infty}^{\infty} f(x_1, x_2, .. x_n)\, dx_1 dx_2 .. dx_n = \frac{(2\pi)^{n/2}}{[\det(\mathrm{A})]^{1/2}}.$$

   Hint: The suggested transformation will decouple the multiple integral into a product of n integrals of the form: $\int_{-\infty}^{\infty} \exp(-ax^2/2)\,dx = \left(\frac{2\pi}{a}\right)^{1/2}, a > 0.$

   (c). Use the above result to evaluate $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left[-\frac{1}{2}\left(3x^2 - 2xy + 3y^2\right)\right] dx\, dy$.

9. Tridiagonal matrices arise in different applications, e.g. see problem 11. Consider the tridiagonal matrix A of order $n > 2$ such that its non-zero elements are: $a_{ii} = 2$, $1 \le i \le n$; $a_{i\,i+1} = -1$, $1 \le i \le n-1$; $a_{i\,i-1} = -1$, $2 \le i \le n$. Show by direct substitution that the eigenvalues of the

above matrix are given by $\lambda_k = 2(1-\cos kh)$, $h = \pi/(n+1)$, $1 \le k \le n$, with corresponding eigenvectors $\boldsymbol{x}_k = (\sin kh, \sin 2kh, .., \sin nkh)^t$.

10. See section 1.20 VM. Cayley-Hamilton (C-H) theorem states that *every square matrix satisfies its own characteristic equation*. Show, using C-H theorem, that for a 3×3 matrix $A = \{a_{ij}\}$, $1 \le i, j \le n$, the following identity holds.

$$A^3 - (\text{trace A})A^2 + \frac{1}{2}\left[(\text{trace A})^2 - \text{trace A}^2\right]A - \det(A)I = 0.$$

11. Consider the nonlinear reaction-diffusion boundary value problem (BVP)

$$\frac{d^2y}{dx^2} - \phi^2 f(y) = 0, \quad -1 < x < 1$$
$$y(\pm 1) = 1$$

where $f(y)$ is a nonlinear function.

(i) Outline a second order accurate finite difference/Newton's iteration-based algorithm for the numerical solution of this BVP.

(ii) Use suitable LAPACK subroutines or a software package of your choice (e.g. Matlab) to solve the system of algebraic equations resulting from the finite difference approximation to obtain solutions for the following cases: (i) $f(y) = y^2$ and (ii). $f(y) = y/(1+y)$.

(iii) Examine the numerical convergence characteristics of your method. For the linear case ($f(y) = y$), plot the absolute error (with respect to the analytical solution) at $y = 0.5$ as a function of the number of x points used for $\phi = 1$ and 10.

12. Consider the following initial boundary value problem (IBVP) that represents a convection (x)-diffusion (y)-reaction problem in the domain $0 \le x^* \le L$, $0 \le y^* \le H$:

$$V\frac{\partial C^*}{\partial x^*} = D\frac{\partial^2 C^*}{\partial y^{*2}} + R(C^*),$$
$$C^*(x^* = 0, y^*) = C_0,$$
$$\frac{\partial C^*}{\partial y}(x^*, y^* = 0) = 0,$$
$$kC^*(x^*, y = H) = -D\frac{\partial C^*}{\partial y}(x^*, y^* = H)$$

where k, V and $D > 0$ and $R(C^*)$ is the reaction rate function. Define dimensionless variables $y \equiv y^*/H$, $x \equiv x^*/L$ and $C \equiv C^*/C_0$. Identify a suitable Peclet number and aspect ratio in the dimensionless equations. Construct explicit and implicit finite difference algorithms for the solution of the above IBVP.