CPS 5320

Name _____

1. If the density of a fluid is $\rho(t, x, y, z)$ then if we equate the rate of change of fluid mass in an arbitrary subregion S to the rate at which it is entering/leaving, we get

   $\frac{d}{dt} \iiint_S \rho = \iint_{\partial S} \rho \mathbf{v} \bullet (-\mathbf{n})$

   where $\mathbf{v} = (\mathbf{U}, \mathbf{V}, \mathbf{W})$ is the fluid velocity and $\mathbf{n}$ is the unit outward normal, and ∂S is the boundary of S.

   a. Use the divergence theorem to derive a partial differential equation for the fluid density, and show that if the fluid is incompressible (ie, the density $\rho(t, x(t), y(t), z(t))$ of a moving piece of fluid is constant) then the fluid velocity satisfies $U_x + V_y + W_z = 0$.

   b. If the fluid is not quite incompressible, but it takes a large pressure (P) to make a small change in volume, what can the divergence equation be replaced by? This equation is the one used by the penalty method.

2. Explain why it is more efficient to distribute the columns of a matrix cyclically (0,1,2,...,NPES-1,0,1,2,...NPES-1,...) than in blocks (0,0,...0,1,1,...1,2,2,...2,...) when doing Gaussian elimination, while it doesn't matter as much when programming the Simplex method.

3. You are offered an option ("put" option) to sell an asset at price E at time T. If $V(t, s)$ is the value of the option at time t if the asset price is s at that time, V satisfies the Black-Scholes partial differential equation. What are the appropriate initial/boundary conditions for V?

4. If the MPI Fortran program below is run on NPES=3 processors, what will be output for B, on every processor?

```
      PARAMETER (N=5)
      DOUBLE PRECISION A(N),B(N)
      INCLUDE 'mpif.h'
C                     INITIALIZE MPI
      CALL MPI_INIT (IERR)
C                     NPES = NUMBER OF PROCESSORS
      CALL MPI_COMM_SIZE (MPI_COMM_WORLD,NPES,IERR)
C                     ITASK = MY PROCESSOR NUMBER
      CALL MPI_COMM_RANK (MPI_COMM_WORLD,ITASK,IERR)
      DO I=1,N
         A(I) = 10*ITASK + I
         B(I) = A(I)
      ENDDO
C
      iroot = 1
      CALL MPI_BCAST(A,N,MPI_DOUBLE_PRECISION,iroot,
     &                MPI_COMM_WORLD,IERR)
      CALL MPI_REDUCE(B,A,N,MPI_DOUBLE_PRECISION,
     &                MPI_MAX,iroot,MPI_COMM_WORLD,IERR)
      CALL MPI_ALLREDUCE(A,B,N,MPI_DOUBLE_PRECISION,
     &                MPI_SUM,MPI_COMM_WORLD,IERR)
      PRINT *, B
      CALL MPI_FINALIZE(IERR)
      STOP
      END
```

5. a. One of your homework problems was to solve the beam problem $\nabla^2(\nabla^2 u) = -\delta(x, y)$ in the unit disk. You were to calculate the boundary integral of $\frac{\partial M}{\partial n}$, where $M \equiv \nabla^2 u$ to check your answer. What should this integral be, no matter what boundary conditions were used? Show your work.

   b. What are the simply supported boundary conditions for this problem?

   c. What are the clamped boundary conditions?

   d. What are the free and unsupported boundary conditions?

6. If 99% of a program is parallelizable, about what speed-up factor should be expected when going from 1 to 16 processors? (Assume the communication time is negligible). What is the maximum speed-up possible, with many processors?

7. The Schroedinger equation is $\nabla^2\phi - V(x,y,z)\phi = -E\phi$, with $\phi = 0$ at $\rho \equiv \sqrt{x^2+y^2+z^2} = \infty$, where $V(x,y,z)$ is the potential energy of the field.

   a. In a hydrogen atom, $V(x,y,z) = -1/\rho$. Reduce the Schroedinger equation to a 1D equation, and tell which eigenvalues (if not all of them) we can find using this 1D version.

   b. In an H_2^+ molecule,

   $$V(x,y,z) = -1/\sqrt{x^2+y^2+(z+1)^2} - 1/\sqrt{x^2+y^2+(z-1)^2}.$$

   Reduce the Schroedinger equation to an axisymmetric equation and tell which eigenvalues (if not all of them) we can find using this 2D version.