ChE 2410

Mathematical Methods in Chemical Engineering

MIDTERM EXAM

Oct. 13th, 2015

Please show your intermediate steps and explain your logic, as grading will be very strict. And be neat! *Partial credit is always lost by sloppy work and presentation.* Clearly write the entire solution at the end of each problem for full credit

NAME: ____

Problem	**Possible Points**	**Points Awarded**
1	10	
2	10	
3	10	
4	15	
5	15	
Bonus Question	5	
Total:	60*	
* The maximum score is 65/60 (108%)		

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FORMULAS, EQUATIONS, AND IDENTITIES

You may (or may not) find some of these useful during your exam:

Trigonometric identities

$$e^{\pm ix} = \cos(x) \pm i\sin(x)$$

$$\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$$

$$\sin(x) = \frac{e^{ix} - e^{-ix}}{2i}$$

$$\sin^2(x) + \cos^2(x) = 1$$

$$A\sin(x) + B\cos(x) = R\sin(x + \alpha)$$
$$R = \sqrt{A^2 + B^2}, \qquad \alpha = \tan^{-1} B/A$$

$$\sqrt{a^2 - a^2\sin^2\theta} = a\cos\theta$$

Integration

$$\int u dv = uv - \int v du$$

$$\int \frac{1}{ax + b} dx = \frac{1}{a}\ln|ax + b| + C$$

Taylor series expansion

$$f(x) = f(a) + \frac{f'(a)}{1!}(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \frac{f'''(a)}{3!}(x - a)^3 + \cdots$$

1. (10 pts) Classify the following differential equations by (i) their order, as (ii) linear/nonlinear, (iii) homogenous/inhomogeneous (if applicable), as (iv) partial or ordinary, as (v) parabolic, elliptic, or hyperbolic (if applicable). You do not need to show work for this question.

(a) $y''(t) + p(t)y'(t) + q(t) = g(t)$

i) 2^{nd} order, ii) linear, iii) inhomogeneous, iv) ordinary, v) n/a

(b) $f_t = xf_x$

i) 1^{st} order, ii) linear, iii) homogeneous, iv) partial, v) parabolic (or n/a is fine)

(c) $(y')^2 = y$

i) 1^{st} order, ii) non-linear, iii) n/a iv) ordinary, v) n/a

(d) $\frac{\partial f(x,y)}{\partial x} + yf(x,y) = x^2 + y^2$

i) 1^{st} order, ii) linear, iii) inhomogeneous, iv) ordinary, v) n/a

(e) $4\frac{\partial^2 f}{\partial x^2} - \frac{\partial^2 f}{\partial x \partial y} - \frac{\partial^2 f}{\partial y^2} = 0$

i) 2^{nd} order, ii) linear, iii) homogeneous, iv) partial, v) hyperbolic

2. (10 pts) Solve the following differential equation.
(*Hint: You can use the integrating factor method*)

$$f' + \frac{2}{x}f = x - 1 + \frac{1}{x}, \qquad f(1) = 2$$

(brief summary of solution)

Using integrating factor method:

$$p(x) = e^{\int \frac{2}{x}dx} = e^{2\ln(x)} = x^2$$

Therefore:

$$f(x) = \frac{1}{x^2}\int \left(x^2\left(x - 1 + \frac{1}{x}\right)dx\right)$$
$$= \frac{1}{4}x^2 - \frac{1}{3}x + \frac{1}{2} + \frac{C}{x^2}$$

Substituting $f(1) = 2$ gives:

$$C = \frac{19}{12}$$

So that:

$$\boxed{f(x) = \frac{1}{4}x^2 - \frac{1}{3}x + \frac{1}{2} + \frac{19}{12x^2}}$$

3. (10 pts) Convert the following differential equations into difference equations. You do **<u>not</u>** need to solve the equations. Make sure your notation is clear.

(a) $f_t = f(1 - f_x) + x$

(use forward differencing in time and central differencing in space)

Very important to use <u>clear</u> and <u>precise</u> notation for this question.

Here *n* is the index for time and *j* is the index for space.

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = f_j^n \left(1 - \frac{f_{j+1}^n - f_{j-1}^n}{2\Delta x}\right) + j\Delta x$$

(b) $\dfrac{\partial u}{\partial t} = \alpha \dfrac{\partial^2 u}{\partial x^2} + \beta \dfrac{\partial u}{\partial y}$

(use forward differencing in t, central differencing in x, and backward differencing in y)

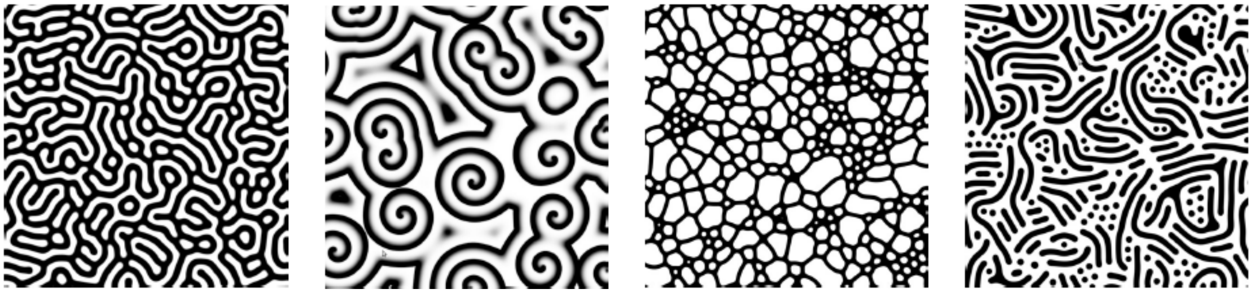
Very important to use <u>clear</u> and <u>precise</u> notation for this question.

Here *n* is the index for time and *j* is the index for *x*, and *i* is the index for *y*.

Every *u* term must have all 3 indices specified, otherwise the meaning is ambiguous.

$$\frac{u_{j,i}^{n+1} - u_{j,i}^n}{\Delta t} = \alpha \frac{u_{j+1,i}^n - 2u_{j,i}^n + u_{j-1,i}^n}{\Delta x^2} + \beta \frac{u_{j,i}^n - u_{j,i-1}^n}{\Delta y}$$

4. (15 pts)



Two chemicals reacting and diffusing on a surface have surprisingly complex behaviors!

Many fascinating phenomena are governed by the reaction-diffusion equation (see figure above). The simplest reaction-diffusion equation concerning the concentration u of a single chemical in one dimension is given by,

$$u_t = Du_{xx} + Ru(1-u)$$

where D is the diffusion coefficient, R is a reaction rate constant (with units of 1/s).

Notice that this is a *nonlinear partial differential equation*. It is prohibitively difficult to find analytical solutions, but it is possible to solve this equation numerically.

Consider the steady-state case, when $u_t = 0$, for a 5cm packed bed reactor where $D = 2\ \mathrm{cm}^2/\mathrm{s}$ and $R = 1\ \mathrm{s}^{-1}$. The concentration of u has been measured at three points:

$$u(0\mathrm{cm}) = 3\ \mathrm{mol/L}, \qquad u(1\mathrm{cm}) = 2\ \mathrm{mol/L}, \qquad u(5\mathrm{cm}) = 30\ \mathrm{mol/L}$$

The measurement at 5cm seems suspicious. You have been asked to model this reaction using the other two measurements and compare your prediction of u at $x = 5$cm to the untrustworthy measurement.

Use the central difference approximation to help solve this nonlinear differential equation. Use $\Delta x = 1$cm. Report your calculated concentration at $x = 5$cm. Was the measurement at $x = 5$cm reasonable?

(Additional space on following page for your solution)

$$0 = Du_{xx} + Ru(1-u)$$
$$= 2u_{xx} + u(1-u)$$

$$\therefore 2\frac{u_{j+1} - 2u_j + u_{j-1}}{\Delta x^2} = -u_j(1-u_j)$$

$$u_{j+1} = 2u_j - u_{j-1} - \frac{1}{2}u_j(1-u_j)$$

4. (Additional space for your solution on this page)

Let's refer to the x = 0cm point as $j = 1$ or x_1 with a corresponding concentration u_1

$$@x = 2\text{ cm} \rightarrow u_3 = 2u_2 - u_1 - \frac{1}{2}u_2(1 - u_2)$$
$$= 2(2) - 3 - \frac{1}{2}(2)(1 - 2) = 2$$

$$@x = 3\text{ cm} \rightarrow u_4 = 2u_3 - u_2 - \frac{1}{2}u_3(1 - u_3)$$
$$= 2(2) - 2 - \frac{1}{2}(2)(1 - 2) = 3$$

$$@x = 4\text{ cm} \rightarrow u_5 = 2u_4 - u_3 - \frac{1}{2}u_4(1 - u_4)$$
$$= 2(3) - 2 - \frac{1}{2}(3)(1 - 3) = 7$$

$$@x = 5\text{ cm} \rightarrow u_6 = 2u_5 - u_4 - \frac{1}{2}u_5(1 - u_5)$$
$$= 2(7) - 3 - \frac{1}{2}(7)(1 - 7) = 32$$

Thus the measurement of 30 mol/L at x = 5 cm was reasonable after all.

5. (15 pts) Consider the partial differential equation:

$$f_t = cf_x, \qquad c \text{ is a constant}$$

The Lax-Friedrichs scheme transforms the above differential equation into the following difference equation:

$$f_j^{n+1} = \frac{(f_{j+1}^n + f_{j-1}^n)}{2} + \frac{c\,\lambda}{2}(f_{j+1}^n - f_{j-1}^n)$$

Use von Neumann analysis to assess the stability of this scheme. Under what conditions, if any, is Lax-Friedrichs stable? Show your work.

Most students got to this point OK:

$$e^{a\Delta t} = \frac{e^{ik\Delta x} + e^{-ik\Delta x}}{2} + \frac{c\lambda}{2}(e^{ik\Delta x} - e^{-ik\Delta x})$$

Using Euler's formula and replacing $e^{a\Delta t}$ with G we get:

$$G = \cos(k\Delta x) + i\,c\lambda\sin(k\Delta x)$$

We want to see under what conditions $|G| <= 1$

$$|G| = \sqrt{\cos^2(k\Delta x) + (c\lambda)^2\sin^2(k\Delta x)} \leq 1\,?$$

$$\sqrt{\cos^2(k\Delta x) + (c\lambda)^2\sin^2(k\Delta x)} \leq 1$$
$$\cos^2(k\Delta x) + (c\lambda)^2\sin^2(k\Delta x) \leq 1$$
$$(c\lambda)^2\sin^2(k\Delta x) \leq 1 - \cos^2(k\Delta x)$$
$$(c\lambda)^2\sin^2(k\Delta x) \leq \sin^2(k\Delta x)$$
$$(c\lambda)^2 \leq 1$$

Therefore $|G| \leq 1$ when $\lambda \leq 1/c$

(Note that there

6. (5 pts, bonus question) Only attempt this question if you have finished all of the other questions and have extra time.

Convert the following differential equation into a difference equation. You do **not** need to solve. Make sure your notation is clear.

$$f_t = f_{xy}$$

(use forward differencing in t, and central differencing in both x and y)

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)$$

Let i be the index for x and j be the index for y:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right) = \frac{\partial}{\partial x} q_{i,j} \approx \frac{q_{i+1,j} - q_{i-1,j}}{2\Delta \text{x}} = \frac{\frac{\partial f}{\partial y}_{i+1,j} - \frac{\partial f}{\partial y}_{i-1,j}}{2\Delta \text{x}}$$

Which simplifies as follows:

$$\frac{\frac{\partial f}{\partial y}_{i+1,j} - \frac{\partial f}{\partial y}_{i-1,j}}{2\Delta \text{x}} = \frac{\left(\frac{f_{i,j+1} - f_{i,j-1}}{2\Delta y}\right)_{i+1,j} - \left(\frac{f_{i,j+1} - f_{i,j-1}}{2\Delta y}\right)_{i-1,j}}{2\Delta \text{x}}$$

$$= \frac{\left(\frac{f_{i+1,j+1} - f_{i+1,j-1}}{2\Delta y}\right) - \left(\frac{f_{i-1,j+1} - f_{i-1,j-1}}{2\Delta y}\right)}{2\Delta \text{x}}$$

$$= \frac{f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}}{4\Delta x \Delta y}$$

For this questions, students either received full credit (5/5) or nothing (0/5).

There were no part marks.