# Midterm Solution
PHZ 5156, Computational Physics
October 18, 2005

Some of this is just a sketch, for example problem 2. I expected more complete solutions from the class.

Midterm

10/18/05
mid p1

① $u_n(x) = \sqrt{2}\sin(n\pi x) \qquad n = 1, 2, 3, \ldots$

expand $\quad x = \sum_{n=1}^{\infty} f_n u_n(x)$

$$f_n = \langle u_n | \cancel{f} x \rangle = \sqrt{2}\int_0^1 dx\, \sin(n\pi x)\, x$$

$$= \sqrt{2}\left\{ -\frac{1}{n\pi} x\cos(n\pi x) + \frac{1}{(n\pi)^2}\sin(n\pi x)\right\}\Big|_0^1$$

$$= \sqrt{2}\left\{-\frac{1}{n\pi}\cos(n\pi)\right\} = (-1)^{n+1}\frac{\sqrt{2}}{n\pi}$$

so $\quad x = \sum_{n=1}^{\infty} (-1)^{n+1}\frac{\sqrt{2}}{n\pi} u_n(x) = \sum_{n=1}^{\infty} (-1)^{n+1}\frac{2}{n\pi}\sin(n\pi x)$

② It satisfies the necessary rules: $\langle f|g\rangle = \langle g|f\rangle^*$

and $\langle f|\alpha g + \beta h\rangle = \alpha\langle f|g\rangle + \beta\langle f|h\rangle$

(trivial proof)

③ $\hat{\Omega} = \frac{d^4}{dx^4}$

$$\Omega_{mn} = \langle u_m|\hat{\Omega}|u_n\rangle = \int_0^1 dx\, u_m^*(x)\underbrace{\frac{d^4}{dx^4}u_n(x)}_{(n\pi)^4 u_n(x)}$$

$$= (n\pi)^4\langle u_m|u_n\rangle = (n\pi)^4\delta_{mn}$$

$$\Omega = \pi^4\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2^4 & 0 \\ 0 & 0 & 3^4 \end{pmatrix}$$

④ Say entries are stored in $f_j$, $j = 0$ to $n-1$

for $j$ in $1, 2, \ldots, n-2$ : (inclusive!)

$cs = \frac{f_{j+1} - f_{j-1}}{2h} \qquad$ cs approx to $f'(x_j)$

Error: $cs = \frac{[\cancel{f(x_j)} + hf'(x_j) + \cancel{\frac{h^2}{2}f''(x_j)} + \frac{h^3}{6}f'''(x_j) + \ldots] - [1^{st} - 2^{d} + 3^{d} - 4^{th} \ldots]}{2h}$

$= f'(x_j) + O(h^2) \qquad$ error is $O(h^2)$

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mid p2

(5) Euler needs $\tau < \frac{2}{|\text{max evalue}|}$

Approximate the evalues: $A \approx \begin{pmatrix} -98 & -198 \\ 99 & 199 \end{pmatrix}$

$\begin{vmatrix} -98-\lambda & -198 \\ 99 & 199-\lambda \end{vmatrix} = 0 = -(98+\lambda)(199-\lambda) + 99(198)$

$0 = (\lambda+98)(\lambda-199) + 99(198)$

$0 = \lambda^2 - 101\lambda - 19502 + 19602$

$0 = \lambda^2 - 101\lambda + 100$

$0 = (\lambda - 100)(\lambda - 1)$ $\qquad \lambda = 1, 100$

Need $\tau <$ about $\frac{2}{100}$ $\qquad \tau \lesssim .02$

To go $t = 0$ to $1000$ would take at least $\frac{1000}{.02} = 50000$ steps.

This is a somewhat stiff problem. Better to use a more stable algorithm such as odeint.

(6) $E = -J \sum_{i,j} s_{ij}(s_{ip1,j} + s_{im1,j} + s_{i,jp1} + s_{i,jm1})$

Initialize array $s$ + energy $E$ + temp $T$

Do many sweeps

Run over $n^2$ steps:

Pick site $(i,j)$ at random

Calculate $\Delta = -2 \cdot (E$ of site$) = -2[(-J)\, s_{ij}\,(\text{above})]$

If $\Delta \leq 0$: flip $s_{ij} = -s_{ij}$, $E = E + \Delta$

If $\Delta > 0$: calculate random $w$ in $0$ to $1$

If $e^{-\Delta/k_BT}$ $w$, flip $s_{ij} = -s_{ij}$, $E = E + \Delta$

Repeat

Store energy at end of sweep.

Repeat

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p3

The type of quantity you calculate is an average, e.g. Eave = (average over all but 1st chunk of sweeps)

The error goes as $\frac{1}{\sqrt{\#\text{ sweeps over which you average}}}$ and also depends on temp — e.g. is higher near $T_c$.

(7) $\frac{d^2x}{dt^2} = -7\cos x - 3\left|\frac{dx}{dt}\right| \sin(3x^5)$

$x(0) = 1 \qquad \left.\frac{dx}{dt}\right|_0 = 2$

Put $v(t) = \frac{dx}{dt}$ and $y = \begin{pmatrix} x \\ v \end{pmatrix}$

Then $\frac{dy}{dt} = \begin{pmatrix} dx/dt \\ dv/dt \end{pmatrix} = \begin{pmatrix} v \\ d^2x/dt^2 \end{pmatrix} = \underbrace{\begin{pmatrix} v \\ -7\cos x - 3|v|\sin(3x^5) \end{pmatrix}}_{\text{make this } f(y)}$

~~step~~ so $\frac{dy}{dt} = f(y)$

```
def rhs(y):
    x,v = y(0), y(1)
    a = - 7cosx - 3|v| sin (3x^5)
    return (v, a)
def rk4(f, y0, t):
  tau = t[1] - t[0]
  set up array y = 2 x #times in t
  y[:, 0] = y0
  for n in 0, 1, ---, len(t) -1
     yn = y[:,n]
     h1 =
     h2 =
     h3 =
     h4 =
  y[:,n+1] =
```

```
#Main code
set up t=0, τ, 2τ, ..., 8.
y0 = (1., 2.)
y = rk4(rhs, y0, t)
plot
```