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.

1. \[ U_n(x) = \sqrt{\frac{2}{\pi}} \sin(n\pi x) \quad n = 1, 2, 3, \ldots \]
   expand \[ X = \sum_{n=1}^{\infty} a_n U_n(x) \]
   \[ a_n = \langle U_n | \hat{f} \rangle = \int_{0}^{1} \hat{f}(x) \sin(n\pi x) \, dx \]
   \[ = \sqrt{\frac{2}{\pi}} \left[ \frac{1}{n\pi} x - \frac{1}{(n\pi)^2} \cos(n\pi x) \right] \bigg|_{0}^{1} \]
   \[ = \sqrt{\frac{2}{\pi}} \left( \frac{1}{n\pi} - \frac{1}{(n\pi)^2} \right) = \frac{(-1)^{n+1}}{n\pi} \]
   so \[ X = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n\pi} U_n(x) = \frac{(-1)^{n+1}}{n\pi} \sin(n\pi x) \]

2. It satisfies the necessary rules: \[ \langle f | g \rangle = \langle g | f \rangle \]
   \[ \langle f | g \rangle = \langle g | f \rangle = \langle g + \lambda f | f \rangle = \langle g \rangle + \lambda \langle f \rangle \quad (\text{trivial proof}) \]

3. \[ \hat{\Omega} = \frac{d^4}{dx^4} \]
\[ \sum_{mn} = \langle U_m | \hat{\Omega} | U_n \rangle = \int_{0}^{1} U_m^*(x) \frac{d^4}{dx^4} U_n(x) \, dx \]
\[ = (\pi)^4 \langle U_m | U_n \rangle = (\pi)^4 \delta_{mn} \]
\[ \Omega = \pi^4 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \]

5. Say only are stored in \[ s_n, g = 0 \ldots n-1 \]
for \[ j \text{ in } 1, 2, \ldots, n-2 \] (inclusive)
\[ c_s = \frac{s_{i+1} - s_i}{2h} \quad c_s \text{ approx to } \hat{s}_i(x_j) \]
Errors: \[ c_s = \frac{\left( \frac{3}{2} s(x_j) + h^3 s''(x_j) + \frac{3}{4} h^4 s'''(x_j) + \frac{3}{8} h^5 s^{(4)}(x_j) + \ldots \right)}{2h} \]
\[ = \frac{1}{2h} \hat{s}_i(x_j) + O(h^3) \quad \text{error is } O(h^4) \]
(5) Each needs \( a < \frac{2}{\text{max eigen value}} \)

Approximate the eigenvalue: \( A = \begin{pmatrix} 99 & 1 \\ 1 & 99 \end{pmatrix} \)

\[ \begin{vmatrix} 99 \lambda - 1 & -1 \\ -1 & 99 \lambda - 1 \end{vmatrix} = 0 = (\lambda + 1)(198 - \lambda) + 99(198) \]

\[ 0 = (\lambda + 1)(\lambda - 199) + 99(198) \]

\[ 0 = \lambda^2 - 101\lambda - 19802 + 19600 \]

\[ 0 = \lambda^2 - 101\lambda + 100 \]

\[ \lambda = 5, 20 \]

Need \( a < \frac{2}{100} = 0.02 \) \[ \underline{\text{a} \approx 0.02} \]

To go \( t = 0 \) to \( t = 1000 \), would take at least \( \frac{1000}{0.02} = 50000 \) steps.

This is a somewhat stiff problem. Better to use a more stable algorithm such as \( \text{CG} \).

(6) \[ E = -J \sum \frac{2}{d^3} \sum_i \sum_j (s_{ij}^t - s_{ij}^r)^2 (s_{ij}^t + s_{ij}^r + s_{ij}^r + s_{ij}^r) \]

Initialize array \( s \) with every \( E \) \& \( t \) initial

Do many sweeps.

\[ \text{Run over } n^2 \text{ steps:} \]

\[ \text{Pick site } (i,j) \text{ at random.} \]

\[ \text{Calculate } \Delta = -2 \cdot (E + d_k \text{ change}) = -2 \cdot (s_{ij}^t \text{ change}) \]

\[ \text{If } \Delta \geq 0 : \text{ Flip } s_{ij} = -s_{ij}, E = E + \Delta \]

\[ \text{If } \Delta > 0 : \text{ Calculate } \text{random } w \in (0, 1) \]

\[ \text{If } e^{-\Delta / kT} \leq w , \text{ Flip } s_{ij} = -s_{ij} , E = E + \Delta \]

Repeat

Store energy at end of sweep.
The type of quantity you calculate is an average, e.g., $E_{ave} = \frac{\text{energy of all but 1st chunk of sweeps}}{\sqrt{\text{# sweeps over which you average}}}$

The entry goes as $\sqrt{\text{# sweeps}}$ over which you average and also depends on $T_{eq}$, which is higher near $T_{c}$.

\[
\frac{dx}{dt} = -7 \cos x - 3 \frac{dx}{dt} \sin (3x^2)
\]
\[
x(0) = 1 \quad \frac{dx}{dt} = 2
\]

Put $v(t) = \frac{dx}{dt}$ and $y = \left(\frac{x}{v}\right)$

Then $\frac{dy}{dt} = \left(\frac{dv}{dt}\right) = \left(\frac{d^2x}{dt^2}\right) = \left(-7 \cos x - 3v \sin (3x^2)\right)$

\[
\text{ode} \quad \text{so} \quad \frac{dy}{dt} = f(y)
\]

def rhs(y):
    x, v = y[0], y[1]
    a = -7 \cos x - 3v \sin (3x^2)
    return (v, a)

def rk4(t, y0, t):
    set up array $y = 2 \times \#$ steps in $t$
    $y[0] = y0$
    for $n$ in 0, 1, ..., 2en(t) - 1
        $h1 = y[1, n1]
        h2 = y[1, n2]
        h3 = y[1, n3]
        y[0, n+1] = y[0, n] + h1 + h2 + h3

# Main code
set up $b = 0, 0.2, 0.4, \ldots$
$y0$ = (1, 2.1)
$y = \text{rk4}(\text{rhs}, y0, t)$
plot