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## 1) UPES

# UNIVERSITY OF PETROLEUM AND ENERGY STUDIES 

## End Semester Examination, December 2017

| Program: | B. Tech. Chemical Engg. (spl. RP); CE-RP | Semester: | V |
| :--- | :--- | :--- | :--- |
| Subject (Course): | Numerical Methods in Chemical Engineering | Max. Marks: | 100 |
| Course Code: | MATH 311 | Duration: | 3 Hrs |
| No. of page/s: | $\mathbf{0 + 3}$ |  |  |

In this OPEN BOOK and NOTES EXAM, you are allowed to have the textbook (S. K. Gupta, Numerical Methods for Engineers), all handouts provided, your own class-notes and your solutions to assignment problems

1. Show all intermediate steps of your answers (and not just the final answers) to earn marks
2. Please answer the questions in the sequence: 1, 2, 3. You can do this by assigning, $a$ priori, a few pages to each question, in the correct sequence. You may then answer the questions in whatever sequence you wish to, all parts in one place
3. No student is allowed to leave the examination hall in the first hour of the exam

## Section A: XXX <br> No questions here

## Section B: ALL THREE QUESTIONS ARE COMPULSORY [Total 100 Marks]

Q. 1 Consider the following set of coupled, non-linear ODE-BVPs with a single independent variable, $x$, and two dependent variables, $y(x)$ and $z(x)$, with $0 \leq x \leq 1,0 \leq y \leq 1,0 \leq z \leq 1$ :

$$
\begin{aligned}
& y^{\prime \prime}+3 y=3 y^{2} z \\
& z^{\prime \prime}+4 z=2 y+6 z^{2}
\end{aligned}
$$

with the following BCs:

$$
\begin{array}{ll}
y^{\prime}(0)=5 ; & y(1)=4 \\
z(0)=2 ; & z(1)=6
\end{array}
$$

(i) Use $N=2$ (i.e., $N+1=3$ ) and the FD method with expressions correct to $\mathrm{O}(\Delta x)^{2}$ to solve this problem (give the complete set of equations )

(30 Points)
Q. 2 Consider the explicit, third order Hermite ODE-IVP algorithm (given in Table 5.1):

$$
y_{n+1}=-4 y_{n}+5 y_{n-1}+h\left(4 y_{n}^{\prime}+2 y_{n-1}^{\prime}\right)+O\left(h^{3}\right)
$$

(a) Obtain the characteristic equation for this technique.
(b) Obtain $\underline{\text { all }}$ the roots, $\mu_{\mathrm{i}}$, of this equation.
(c) Identify which of these roots is the non-spurious root, $\mu_{1}$.

Hint: You may use the following expansions:

$$
\begin{aligned}
& (1+x)^{\frac{1}{2}}=1+\frac{1}{2} x-\cdots, \text { and } \\
& e^{x}=1+x \ldots
\end{aligned}
$$

(d) Now evaluate the numerical value of $\left|\mu_{1}\right|$ for $|\mathrm{h} \lambda|=0$
Q. 3 Consider a NEW quadratic spline fit for a set of given points, $\left(x_{0}, y_{0}\right),\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots$, $\left(x_{n}, y_{n}\right)$, with $n$ being an even number. You decide to fit each of the quadratic splines to three adjacent points as follows (see diagram below):

Continued...
$S_{0}(x)$ : Points $\left(x_{0}, y_{0}\right),\left(x_{1}, y_{1}\right)$ and $\left(x_{2}, y_{2}\right)$,
$S_{2}(x)$ : Points $\left(x_{2}, y_{2}\right),\left(x_{3}, y_{3}\right)$ and $\left(x_{4}, y_{4}\right), \ldots$
$S_{\mathrm{n}-2}(\mathrm{x})$ : Points $\left(x_{\mathrm{n}-2}, y_{\mathrm{n}-2}\right),\left(x_{\mathrm{n}-1}, y_{\mathrm{n}-1}\right)$ and $\left(x_{\mathrm{n}}, y_{\mathrm{n}}\right)$.


Note again that each of the spines are quadratic (not linear nor cubic) and each passes through three points as discussed above (this is a stupid thing to do, but you still do it).
(a) Write down the most convenient equations for $S_{\mathrm{i}}(x), i=0,2,4, \ldots, n-4, n-2$, involving constants, $a_{\mathrm{i}, \mathrm{j}}$.
(b) Write down all the equations for determining the constants, $a_{\mathrm{i}, \mathrm{j}}$. Since the algebra involved is quite a bit, do not solve these equations (except the ones which are extremely simple).
(c) Comment on the continuity of the values of $S_{\mathrm{i}}(x)$ and $S_{\mathrm{i}+2}(x)$ at the end-points, i.e., at $x$ $=x_{i+2}$, as well as the values of $S_{i}^{\prime}(x)$ and $S_{i}^{\prime \prime}(x)$ at these points.
(13) (35 Points)

