Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo
Swiss Federal Institute of Technology Zurich

Prof. Petros Koumoutsakos
CSE Lab, ETH Zürich
www.cse-lab.ethz.ch

Advanced Computational Science
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Serie 2 Ausgabe: March 3, 2009 Abgabe: March 10, 2009

Guidelines

▷ Submission: Submit a written or typed report with your answers and graphics.

▷ Code: Send your source code (and makefile) to the TA of your session. Use "[ACS] Homework2" in the subject of your email.

▷ Credit: Your report should list all the contributors.

▷ Bugs: Print-outs of your source code are *not* required in your report, unless you have bugs. Help us give you partial marks.

▷ Deadline: Assignments have to be handed in at the beginning of the next exercise session.

Exercise 1 (10 points) Newton-Cotes scheme in 1D (paper and pencil)

According to the Newton-Cotes scheme, an integral of a function over a domain can be approximated as a weighted sum of function values at discrete points, i.e.

$$\int_a^b f(x)\,dx \approx \sum_{k=0}^{N} f(x_k) \int_a^b L_k(x)dx = (b-a) \sum_{k=0}^{N} C_k^N f(x_k)$$

where $L_k(x)$, the Lagrange polynomial is given by

$$L_k(x) = \frac{(x-x_0)\cdots(x-x_{k-1})(x-x_{k+1})\cdots(x-x_N)}{(x_k-x_0)\cdots(x_k-x_{k-1})(x_k-x_{k+1})\cdots(x_k-x_N)} \ .$$

Derive the Cotes numbers, C_k^N for $N = 3$.

Exercise 2 (10 points) Trapezoidal and Simpson's quadrature on a 2D domain (paper and pencil)

Show using Lagrange interpolation that the Trapezoidal and Simpson's quadrature for the integral over one sub-interval of a 2D domain

$$\int_{y_j}^{y_{j+1}} \int_{x_i}^{x_{i+1}} f(x,y)\,dx\,dy$$

is given by

▷ [Trapezoidal quadrature (**5 points**)]

$$\frac{hk}{4}[f(x_i,y_j) + f(x_i,y_{j+1}) + f(x_{i+1},y_j) + f(x_{i+1},y_{j+1})]$$

▷ [Simpson's quadrature (**5 points**)]

$$\begin{aligned}\frac{hk}{36}[f(x_i,y_j)+4f(x_i,y_{j+1/2})+f(x_i,y_{j+1})\\ +4f(x_{i+1/2},y_j)+16f(x_{i+1/2},y_{j+1/2})+4f(x_{i+1/2},y_{j+1})\\ +f(x_{i+1},y_j)+4f(x_{i+1},y_{j+1/2})+f(x_{i+1},y_{j+1})]\end{aligned}$$

where $h = x_{i+1} - x_i$ and $k = y_{j+1} - y_j$.

Exercise 3 (30 points) Trapezoidal and Simpson's quadrature on a 2D domain (programming)

In a particle accelerator experiment, a sensor array counts positrons as a function of their energy T and their angular deviation θ with respect to the collision direction. The physicists are interested in the total emission of positrons in the range $[0, T_{\text{max}}] \times [0, \theta_{\text{max}}]$

$$I(f) = \int_0^{T_{\text{max}}} \int_0^{\theta_{\text{max}}} f(T, \theta)\, dT\, d\theta$$

where $f(T, \theta)$ is the positron intensity.

There are two theoretical models for this intensity

▷ [Intensity 1] $f_1(T, \theta) = e^{(T/T_{\text{max}})+(\theta/\theta_{\text{max}})}$

▷ [Intensity 2] $f_2(T, \theta) = \sqrt{(1 - (T/T_{\text{max}})^2 - (\theta/\theta_{\text{max}})^2 + (T/T_{\text{max}})^2(\theta/\theta_{\text{max}})^2)}$.

This is a potentially challenging integration problem: it needs to be computed efficiently and the integrand can pose some problems to quadrature formulas. We take $T_{\text{max}} = 1$ and $\theta_{\text{max}} = \pi/2$.

(i) Use Trapezoidal and Simpson's quadratures to evaluate the total emissions $I(f_1)$ and $I(f_2)$ if the sensor array provides 33×33 evenly spaced data points (**10 points**) ,

(ii) For both schemes, study the behavior of the error $e = |I(f_{1,2}) - I^{\text{exact}}(f_{1,2})|$ if the array provides 17×17, 33×33, 65×65, 129×129 and 257×257 measurements (**10 points**)

(iii) Verify if the error behavior agrees with the theoretical prediction, if not discuss the reason (**10 points**).

(*Tips*: (i) Trapezoidal and Simpson's quadratures are of order 2 and 4 respectively. (ii) Plot $\log(e)$ vs. $\log h$ where h is the size of one sub-interval $(T_{i+1} - T_i)/T_{\text{max}}$. The slope of the line gives the order of the numerical method.)