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Set 1 - OpenMP, Diffusion and Air Resistance

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Question 1: OpenMP recap

a) Posterior calculation

In uncertainty quantification, we are often interested in the so called *posterior distributions*:

$$f(\beta \mid x) = \frac{f(X \mid \beta) f(\beta)}{\int_{\Omega_\beta} f(X \mid \beta) f(\beta) \mathrm{d}\beta}. \tag{1}$$

We want to obtain a good estimate of the distribution of β. We start with a *prior* distribution $f(\beta)$. Our observations of β come indirectly through X. Based on this observations, we obtain a better estimate of the distribution $f(\beta \mid x)$.

Your task is to implement two integration methods, to be used for the denominator.

You will test it on two different functions:

- $f(x) = -(x-1)(x+1)^2, x \in [-1, 1]$
- $f(x) = -\exp(-x), x \in [0, \infty]$

We will do this using trapezoidal integration and Monte Carlo integration.

i) Trapezoidal integration We will rely on a simple integration scheme:

$$\int_a^b f(x) x = h\left(\frac{1}{2} f(x_0) + f(x_1) + \ldots + f(x_{N-1}) + \frac{1}{2} f(x_N)\right), \tag{2}$$

$$h = \frac{b-a}{N}, x_i = a + ih, i = 0 \ldots N, \tag{3}$$

where N is the number of intervals we divide the (b, a) into.

Tasks:

1) Implement the serial version of the method,
2) Verify your solutions, compare them with the the analytical solutions.
3) Parallelize using OpenMP: Report the speedup.

ii) Monte Carlo integration

Instead of implementing a grid based approach, we use the following idea: suppose $X \sim Unif(a, b)$. Then:

$$\mu_f = \mathbb{E}[f] = \frac{1}{b-a} \int_a^b f(x) \mathrm{d}x \to \int_a^b f(x) \mathrm{d}x = (b-a)\mu_f \tag{4}$$

An unbiased estimator for the mean is:

$$\hat{\mu}_f = \frac{1}{N}\sum_{i=1}^{n} f(x_i) \to \int_a^b f(x)\mathrm{d}x \approx (b-a)\hat{\mu}_f, \tag{5}$$

where $\{x_i\}$ are independent realizations of the random variable X.

1) Is the estimator of the integral unbiased?
2) What is the variance of the integral estimator?
3) Implement a serial version of the code and verify it. Compare error convergence with the trapezoidal method for different values of N.
4) Parallelize using OpenMP. Do you need to use barriers? Why or why not? Report the speedup.
5) Bonus: can you exploit the knowledge that our integral is of the form $\int a(x)b(x)\mathrm{d}x$?

b) 1-D diffusion equation

The 1-D diffusion equation on $\Omega = [a,b]^2$ takes the following form:

diffusion equation:	$\frac{\partial}{\partial t}f(x,t) = D\frac{\partial^2}{\partial x^2}f(x,t), f:[a,b]^2 \times [0,T] \mapsto \mathbb{R}$
initial conditions:	$f(x,0) = f_0(x),\ f_0(\cdot):\mathbb{R}\mapsto\mathbb{R}$
(Dirichlet) boundary conditions:	$f(a,t) = g_a, f(b,t) = g_b,$
compatibility conditions:	$g_a = f_0(a), g_b = f_0(b).$

where D is called the *diffusion coefficient*. The compatibility conditions limit the choices of initial conditions given a certain boundary.

In uncertainty quantification, one uses the diffusion equation to calculate the probability density function of a stochastic process as a function of time. This is done using the Fokker-Plank equations. We will not go deeper into this, but only ask you to implement a Euler-forward, central differences method for solving the diffusion equation:

$$f(x_i,t_{k+1}) \approx f(x_i,t_k) + D\frac{\delta t}{h^2}\left(f(x_{i+1},t_k) - 2f(x_i,t_k) + f(x_{i-1},t_k)\right),$$

where $h = 1/N_x, \delta t = T/N_t$, and N_x is the number of spatial intervals we choose and N_t the number of temporal intervals. $x_i = ih, t_k = k\delta t, i = 0\ldots N_x, k = 0\ldots N_t$.

1. What is the order of the method, in time and space?
2. Is the method unconditionally stable? If not, give conditions for when it is.
3. Implement a serial version of the method.
4. Implement a parallel version using OpenMP. Do you need to use barriers? When? Report the speedup.
5. Bonus: Modify the method such that synchronization is not required. Report the speedup now.

For our implementation, we take $a = 0, b = 1, g_a = 1, g_b = 0, D = 0.1, T = 0.1$, and $g(x) = -(x-1)(x+1)\mathbb{1}_{0\le x\le 1}(x)$.

Question 2: Uncertainty Quantification for Air Resistance Coefficient

Consider the mathematical model of a falling object with mass m, acceleration of gravity g and air resistance force $F_{res} = -m\alpha v^2$, where α is the air resistance coefficient. Using Newton's law, the equation of motion of the falling object is:

$$m\frac{\mathrm{d}v}{\mathrm{d}t} = mg - m\alpha v^2 \tag{6}$$

The solution for the velocity obtained from the nonlinear differential equation (6) is:

$$v(t) = v_\infty \tanh\left(\frac{g(t-t_0)}{v_\infty}\right), \tag{7}$$

where $v_\infty = \sqrt{g/\alpha}$ and t_0 is the initial time. Integrating the velocity $v(t)$ with respect to time, the solution for the vertical displacement x of the falling object is finally obtained as

$$x(t) = \frac{1}{\alpha}\ln\cosh\left(\sqrt{g\alpha}(t-t_0)\right). \tag{8}$$

Measurements for the position of the falling object are obtained by a digital camera making snapshots with an interval of Δt sec. Given the observation data $D = \{\hat{X}_1, ..., \hat{X}_N\}$ of the location of the falling object at time instances $t = \{\Delta t, ..., N\Delta t\}$, respectively, we are interested in estimating the uncertainty of the parameter α of the system given the value of the variance σ^2. Note that the measurements and the model predictions satisfy the model error equation

$$\hat{X}_k = x(k\Delta t) + E_k, \tag{9}$$

where the measurement error terms E_k are independent identically distributed (i.i.d.) and follow the zero-mean Gaussian distribution $\mathcal{N}(0, \sigma^2)$.

Assume a uniform prior for α and derive the expressions for the

1) Posterior PDF (probablity density function) $p(\alpha|D, \sigma)$,
2) The negative log-likelihood function $L(\alpha) = -\ln p(\alpha|D, \sigma)$,
3) Consider a simple case of two measurements $\hat{X}_1 = 1\,[m], \hat{X}_2 = 2\,[m]$ taken 1 s and 2 s after the beginning of the fall, respectively. Assuming $g = 9.8\,[m/s^2]$, show that $\hat{\alpha} = 8.96\,[1/m]$ is the most probable value of the air resistance coefficient (the value which maximizes the posterior PDF).
4) Given the Taylor series expansion of the negative log-likelihood about the most probable value $L(\alpha) = 0.0012 + 0.014(\alpha - \hat{\alpha})^2$, derive the Gaussian asymptotic approximation for the posterior PDF.