Outline

Outline

Write a program to estimate the area *C* of the unit circle using MC sampling.

$$C = \iint_{x^2+y^2 \leq 1} dxdy$$
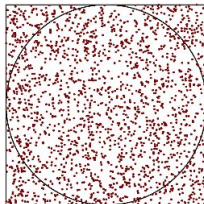
- Let's consider a quarter of the area
  $0 \leq x \leq 1$, $0 \leq y \leq 1$
- extract *N* points in there (**N**)
- count how many of them fall in (**inside**)
- 4 **inside** / **N** gives an estimate of π

hints ...

- ask user for **N**
- Repeat the following steps **N** times:
  1. assign *x* and *y* random numbers in the range $[0, 1)$
  2. If $(x^2 + y^2 \leq 1)$, increment *inside*
- print your estimate of π

- Try many different values of **N** and check MC error
- check range values for variable types to handle **N**
- Use **rand()** and **RAND_MAX** from **stdlib.h**

```
const double rand_norm = 1.0/(RAND_MAX + 1);
...
x = rand_norm * rand();
```

Outline

Write a program that implements root finding with bisection and apply it to a known function (E.g. one from `math.h`).

- Bisection method works if we are able to confine a root of $f(x)$ in an interval between a and b, so that $f(a)f(b) < 0$.
- Bisection follows an iterative search:
  1. find the middle point c of a, b
  2. evaluate $p = f(a)f(c)$
  3. if $p = 0$, you are really lucky!
     1. c is the root
  4. if $p > 0$, root is in the interval c, b
     1. set $a = c$
  5. if $p < 0$, root is in the interval a, c
     1. set $b = c$
  6. repeat from 1 until $|b - a| < \epsilon$, where ϵ is a threshold

CINECA

Use the following elements:

- **while** and **if**/**else** controls

- **fabs()**

Remember to make your program robust:

- choose appropriate ϵ to reflect the precision of the C types in use

- handle errors and exit in a controlled way

Try it with:

- a known function from **math.h**

- the **double mysteriousf(double x)** function provided in the **libmysterious.a** library, check intervals $[0, 10]$, $[10, 0]$ and $[0, 5]$

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Write a simple program that:

- asks the user for an integer number **N**
- finds and prints out all prime numbers up to **N**

A *prime number* is a natural number which has exactly *two distinct* natural number divisors: 1 and itself

program outline:

- get upper limit N from user
- for each number $2 < n < N$
  - check if an exact divisor $b < n$ of n exists
  - if no b is found, than n is prime

- Use the following elements:
  - **printf()** and **scanf()**
  - **for** construct
  - **while** construct on $b < n$ and
  - **if** construct on n

- Remember to make your program robust:
  - check for proper input from the user ($N < 0$??)
  - check type limits
  - handle errors and exit in a controlled way

Outline

Write a simple program that computes the integral from 0 to 1 of the function $f(x) = \frac{4}{(1+x^2)}$

Use the Riemann definition of an integral, that is

$$\int_a^b f(x)dx = \lim_{N \to \infty} \sum_{i=1}^{N} f(x_i)\Delta x \ , \ with \ \Delta x = \frac{b-a}{N}$$

Program outline:

- Split $[a, b]$ into N subintervals of Δx width
- compute the function $f(x)$ in the middle point x_i of each interval and multiply for Δx
- sum up all contributions
- print the result and find out if it is correct

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      Array Transformation

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Let's Build An Histogram

- Is `rand` as uniform as they say? Let's test...
- Write a program that:
  - Generates random numbers in the range 0, 1
  - Builds an histogram and computes their average
- Use `rand()` and `RAND_MAX` from `stdlib.h`
- Initialize to 0 an array of *ninterv* `int`s that holds the histogram; then, at each iteration:
  - Generate a random number
  - Find out the bin it belongs to (i.e. its index in the array)
  - Increment the corresponding array element and accumulate a sum to compute the average

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Write a program that computes the difference between each element of an array and its successive element.

$$A[x_i] \rightarrow A[x_i] - A[x_{i+1}]$$

- start with an array A[20] initialized as `A[i] = i`
- assume periodic boundary conditions
- use `%` operator in indexing expressions to implement periodic boundary conditions

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Array Smoothing

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Write a program that takes an array and applies *N* times a moving average smoothing transformation.

A moving average smoothing is a substitution:

$$A[x_i] \rightarrow \frac{1}{2k+1} \sum_{j=i-k}^{i+k} A[x_j]$$

- assume periodic boundary conditions on data
- iterate for $N = 1, 2, 5, 10$ times
- check your program with $k = 1, 2, 16$

  hints

- start with an array A[20] initialized as **A[i] = i**
- check results at each iteration printing smoothed array elements
- Use **%** operator in indexing expressions to implement periodic boundary conditions

Outline

Working with Matrices

Write functions using VLA to compute:

- matrix-vector product
- matrix-matrix product

- collect your functions in the source file
  linear_algebra_vla.c
- initialize matrix **A[i][j]=i*j, B[i][j]=i+j, V[i]=i**
- start with small squared 3x3 matrix to check results
- write **printMatrix()** and **printVector()** functions to check results
- try with a non-square matrix input too

Outline

Outline

Using Pointers to Functions

Use **qsort**, and **comparedouble** (from Module 7) to sort an array of n **double** random numbers in the range 0, 10

But **qsort** can be more powerful!
Initialize an array of **vec3d** variables with random numbers, and sort them by their first component

Using Pointers to Functions II

Write a comparison function for module of **vect3d** data types and use it to sort a big vector of **vect3d**

- group your vect3d definition and functions in **vect3d.c** source
- write a test program to sort a **vect3d A[1000]** array
- initialize each **vect3d** element with random components ranging from 0.0 to 10.0

Outline

Working with Matrices (II)

Rewrite your linear_algebra functions for matrix-vector and matrix-matrix product without VLA, using pointers to **double**

- collect your functions in **linear_algebra.c**
- remember to cast function arguments appropriately
- check results against your previous version

Outline

BLAS Library

The BLAS library (Basic Linear Algebra Subprograms) contains routines for basic vector and matrix operations.

- Quick Reference:
  http://www.netlib.org/blas/index.html

- BLAS are divided into 3 levels:
  - Level 1: vector-vector operations
  - Level 2: matrix-vector operations
  - Level 3: matrix-matrix operations

- widely used in scientific software

- Often provided as a part of architecture optimized Math Libraries:
  ACML(AMD), ESSL(IBM), GotoBLAS, MKL(Intel), Sun Performance Library, etc

BLAS C Interface

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- originally written for Fortran77
- BLAS provides a standard C interface
    - ... but include file name is not!
- function names are all lowercase and of the form:
  cblas_x*name*(...)
    - *x* denotes the data type:
      s for **float**,
      d for **double**,
      c for **float complex**,
      z for **double complex**

An Example Involving Vectors

BLAS Level 1: $op: \; y \leftarrow \alpha x + y$

   cblas_saxpy (n, α, x, incx, y, incy)

- the name says it all!
- **n** is the size of vectors **x** and **y**
- α is the vector **x** multiplyer
- **incx, incy** are increments to select vector elements

An Example With Vectors And Matrices

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BLAS Level 2: $op: y \leftarrow \alpha A x + \beta y$

cblas_dgemv (CblasRowMajor, CblasNoTrans, m, n, α, A, lda, x, incx, β, y, incy)

- this is a general matrix vector multiply and add
- **CblasRowMajor** selects memory layout of data
  enum **CBLAS_ORDER {CblasRowMajor, CblasColMajor}**
- **CblasNoTrans** is used to transpose matrix
  enum **CBLAS_TRANSPOSE {CblasNoTrans, CblasTrans, CblasConjTrans}**
- **m, n** are dimensions of matrix A
- **lda** is the leading dimension of array A
- **incx, incy** are increments to select vector elements
- Matrices and vectors are passed as pointers (cast as appropriate!)

Level 2 BLAS In Action

Multiply a matrix A[20][10] by a vector x[10] and put results
into vector y[10]

```
int i, m = 20, n = 10;
double A[m][n], x[n], y[n];
double alpha = 1.0, beta = 0.0;
int lda = n, incx = incy = 1;
double dx = 0.05;

for (i=1; i<=m; i++) {
  for (j=1; j<=n; j++) {
    A[i][j] = (double) i * j + 0.5;
  }
}
for (i=0; i<n; i++) {
  x[i] = cos((double) i*dx);
}

cblas_dgemv (CblasRowMajor, CblasNoTrans,
  m, n, alpha, (double *) A, lda,
  x, incx, beta, y, incy);
```

Selecting Elements

From matrix A[20][10], Let's extract a submatrix subA[8][5],
And let's multiply it by even elements of vector x[10]

```
int i, m = 20, n = 10;
int subm = 8, subn = 5;
double A[m][n], x[n], y[subm];
double alpha = 1.0, beta = 0.0;
int lda = n, incx = 2, incy = 1;
double dx = 0.05;

for (i=1; i<=m; i++) {
  for (j=1; j<=n; j++) {
    A[i][j] = (double) i * j + 0.5;
  }
}
for (i=0; i<n; i++) {
  x[i] = cos((double) i*dx);
}

cblas_dgemv (CblasRowMajor, CblasNoTrans,
  subm, subn, alpha, (double *) A, lda,
  x, incx, beta, y, incy);
```

Yet Another BLAS Example: Matrices

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BLAS Level 3: $op: C \leftarrow \alpha AB + \beta C$

**cblas_zhemm (CblasRight, CblasUpper,
  m, n, α, A, lda, B, ldb, β, C, ldc)**

- this is an hermitian matrix matrix multiply and add
- **CblasRight** and **CblasUpper** select matrix representation in memory (half the elements is enough for hermitian ones)
- **m, n** are sizes of matrix **A**, **B**, **C**
- **lda, ldb, ldc** are leading dimensions of array **A**, **B**, and **C**
- Matrices and vectors are passed as pointers (cast as appropriate!)

Using BLAS library

Use BLAS library to compute matrix-matrix and matrix-vector product

The BLAS functions you need:

- DGEMV: Double precision GEneral Matrix-Vector product (BLAS lev2)

- DGEMM: Double precision GEneral Matrix-Matrix product (BLAS lev3)

- Use GSL (GNU Scientific Library) library **libgslcblas.a** in **lib/**

- include header file **include/gsl_cblas.h**

- do cast your arrays to proper BLAS function parameters

Timing Your Function

Use **clock()** function from **time.h** for timing your version of matrix-matrix product function against BLAS GEMM for square matrices of sizes $100, 200, 500, 1000$

- **clock_t clock(void);** returns the processor clock time used since the beginning of the program
- divide the returned value by **CLOCKS_PER_SEC** to get the number of seconds
- adapt the following code to measure your functions

```
#include <time.h>
  clock_t start, stop;
  double t = 0.0;

  // Start timer
  start = clock();
  // call your function
  // Stop timer
  stop = clock();
  t = (double) (stop-start)/CLOCKS_PER_SEC;
```

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   Parse ASCII file

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Command Line Parsing

Write a program that parses command line and:

- accepts stand alone options (on/off switch)
- accepts option with a single argument (int, double and string)
- outputs a report of what it parsed

- use `int argc, char *argv[]` parameters of `main()`
- use `switch` control
- use `strto...()`, `strcmp()`

Outline

Parsing a file

Write a function that accepts a string containing a file name as its argument, and parses the file, storing retrieved values into global variables; the file has the format:

- **keyword value**
- empty lines or starting with a # should be ignored

Use main program in **simpleparsermain.c** and the input file **param.dat** to test your function.
Recognized parameters:

- **nx** (int) number of points in the x direction;
- **ny** (int) number of points in the y direction;
- **tol** (double) some kind of tolerance or threshold;

Of course feel free to add more keys if you want! Hints:

- Use **fgets()** to retrieve input lines, and test its return value;
- Parse input lines with **sscanf()**;

Parsing a file II

After implementing and testing a very simple version:

- Find a way to check that values found in the file have the expected type and correct domain range (nx < 0 is nonsense)
- check for multiple parameter definitions
- Return an error message and exit if you find an unrecognized key;
- What if a line starts with white spaces? Did you already handle this?

Consider using **strtok()** or similar to implement more flexible and complicated parsing.

Parse a structured ASCII file

Write a program that reads protein coordinates from a .pdb
file format

- .pdb file format files are wide used in bioinformatic

- coordinates begins with **ATOM** tag

```
ATOM 1 N PRO A 1 8.316 21.206 21.530 1.00 17.44 N ATOM 2 CA PRO A 1 7.608 20.729 20.33
1.00 17.44 C ATOM 3 C PRO A 1 8.487 20.707 19.092 1.00 17.44 C ATOM 4 O PRO A 1 9.466
21.457 19.005 1.00 17.44 O
```

Seek in your file

Use seek I/O functionality to collect elements from a binary file

- open the **binaryfile.dat** file from course package
- read elements using the following steps
  - 8 bytes 128 bytes bakward from end of file, set bookmark **A** here
  - 8 bytes 32 bytes from the beginnig, set bookmark **B** here
  - 4 bytes 32 bytes from bookmark **A**
  - 16 bytes 64 bytes from bookmark **B**
- convert read elements to chars and print them

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Let's Make Comparisons

- Write a program that:
    - Initializes an array of 900000 **double**s with random numbers in the range 0, 1
    - Writes the array 10 times to an ASCII file.
    - Uses **time** and **difftime** from **time.h** to time the writing operation
- Remember to print enough decimal digits, to recover exact binary form of your data
- Try writing array elements on one line with no white spaces in between
- Try writing one element per line
- How big is your output file?

Let's Make Comparisons

- Modify your program so that it writes to a binary file with `fwrite`
- Try different solutions:
  - Write one element at a time: pointer arithmetic will help;
  - Write the array in chunks of 1000 elements;
  - Write the whole array with a single call to `fwrite`.
  - In any case, check the value returned by `fwrite`.
- What about output file dimensions?
- And what about time?

Walking Around In Our File

- Our output file now contains 10 copies of our array
- Let's read the first element of each copy in the file
- Let's print it together with its position
    - Let's use `fseek` to reach the right position
    - And `ftell` to have the current position returned
    - Remember to `fopen` the file with all the necessary modes

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Big Array Transformation

Rewrite your Array Transformation program so that the transformation is performed by a function which takes the array to be processed as an argument.

- use VLA array in your first version
- check you program with $size = 1000, 10000, 100000$
- does this work with automatic array declarations?
- after you checked, use **malloc** to dynamically allocate the array
- remember to use **free** on dynamically allocated variables

Array Transformation With Unknown Dimensions

Rewrite your array transformation program so that it reads input data from the file

- write a file containing a floating point number on each line
- let the first line contains the number of subsequent lines in the file (int)
- Once you read the first line, you can call **calloc** to allocate enough space to hold data
- Don't forget to check if **calloc** succeeded

Working with Matrices

Rewrite your linear algebra functions so to allocate your matrices with **malloc**.

- remove printing functions
- use BLAS library to check results
- cast your argument appropriately

Rights & Credits

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**Dynamic
Memory**
Memory Allocation

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