SuperComputing Applications and Innovation

Scientific and Technical Computing in C

Day 2

Stefano Tagliaventi   Isabella Baccarelli

CINECA Roma - SCAI Department

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Outline

struct


```
struct vect3D {
  double x, y, z;
};

struct vect3D va, vb;

// REMINDER: I have to make vcross() more efficient!
struct vect3d vcross(struct vect3D u, struct vect3D v) {
  struct vect3D c;

  c.x = u.y*v.z - u.z*v.y;
  c.y = u.z*v.x - u.x*v.z;
  c.z = u.x*v.y - u.y*v.x;

  return c;
}

//...
  vc = vcross(va, vb);
```

- Aggregates a single type from named, typed components (a.k.a. members)
- The `vect3D` *tag* must be unique among structure tags
- `struct` components can be independently accessed using the `.` binary operator

`structs` Are Flexible


```
struct ion {
  struct vect3D r; // position
  struct vect3D v; // velocity
  enum element an; // atomic number
  int q;           // in units of elementary charges
};

struct ion a;
//...
  a.r.x += dt*a.v.x; // very low order in time...
```

- `struct` components can be inhomogeneous
- And they can also be `struct`s, of course
  - To access nested `struct` components, chain `.` expressions
- Best practice: order components by decreasing size
  - You'll get better performances
  - To know, you can use `sizeof()` operator on any type

`structs`: a Concrete Example

- `structs` are widely used in C Standard Library
- Like in `struct tm`, below, defined in `time.h`
  - Used to convert from/to internal time representation `time_t`

```
struct tm {
  int tm_sec; // seconds after the minute [0, 60]
  int tm_min; // minutes after the hour [0, 59]
  int tm_hour; // hours since midnight [0, 23]
  int tm_mday; // day of the month [1, 31]
  int tm_mon; // months since January [0, 11]
  int tm_year; // years since 1900
  int tm_wday; // days since Sunday [0, 6]
  int tm_yday; // days since January 1 [0, 365]
  int tm_isdst; // Daylight Saving Time flag
};
```

typedef


```
typedef struct vect3D position, velocity;

typedef enum element element; // let's spare keystrokes

typedef int charge;           // I'll maybe switch to short or signed char

typedef struct ion {
  position r;
  velocity v;
  element an;
  charge q;
} ion;

ion a;
```

- `typedef` turns a normal declaration into a declaration of a new type (as usual, a legal identifier)
- The new type can be used as the native ones
    - Great to save keystrokes
    - Even better to write self-documenting code
    - Shines in hiding and factoring out implementation details
- `struct` tags and type identifiers belong to separate sets

`typedef` in C Standard Library

- `typedef` is widely used in C Standard Library
- Mostly to abstract details that may differ among implementations
- E.g. `size_t` from `stddef.h`
  - Type of value returned by `sizeof()`
  - Different platforms allow for different memory sizes
  - `size_t` must be "`typedef`ed" to an integer type able to represent the maximum possible variable size allowed by the implementation
- E.g. `clock_t` from `time.h`
  - Type of value returned by `clock()`
  - Cast it to `double`, divide by `CLOCK_PER_SEC`, ...
  - and you'll know the CPU time in seconds used by your program from its beginning

Arrays

- ***some_type*** **a[*n*];**
  - declares a collection of *n* variables of type ***some_type***
  - the variables (a.k.a. elements) are laid out contiguously in memory
  - each element can be read or written using the syntax **a[***integer indexing expression***]**
  - first element is **a[0]**, second one is **a[1]**, last one is **a[*n*-1]**
- You can't work on an array as a whole
  - Use array elements (if allowed...) in expressions and assignments
- There is no bound checking!
  - Use a negative index, or an index too big, and you are accessing something else, if any
  - Compiler options to (very slowly) check every access
- A common mistake:
  - to access from **double a[1]** to **double a[*n*]**
  - Fortran programmers beware!

Arrays of(Arrays of(Arrays of(...)))

- C has no concept of multidimensional arrays
- But array is a regular C type (you can even `sizeof(double[150])`)
- Thus, arrays of arrays can be declared
    - A simple, practical abstraction
    - Very annoying to Fortran or Matlab programmers
- `int a[12][31];`
    - declares an array of 12 elements
    - and each element is itself an array of 31 `int`s
- `double b[130][260][260];`
    - declares an array of 130 elements
    - and `b[37]` is itself an array of 260 elements
    - and `b[37][201]` is again an array of 260 `double`s
- By the way, you can also use `sizeof(b)`, it works

Array Memory Layout


```
int a[10];
```

a[0]	a[1]	a[2]	a[3]	a[4]	a[5]	a[6]	a[7]	a[8]	a[9]

```
int b[5][2];
```

b[0]	b[1]	b[2]	b[3]	b[4]

b[0][0]	b[0][1]	b[1][0]	b[1][1]	b[2][0]	b[2][1]	b[3][0]	b[3][1]	b[4][0]	b[4][1]

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A Very Important Digression

- Storage duration
  - To make it simple, the life time of a variable
  - Also influences the part of memory where it's allocated
- Scope
  - The region where a variable or function is accessible, a.k.a. "visible"
- Qualifiers
  - The value in a `const` variable cannot be changed
  - There are more, but we'll not discuss them
- Initializers
  - Values assigned to a variable at declaration

Storage Duration

- A variable can be
  - Automatic: it can be created when needed, and destroyed when not needed anymore
  - Static: it persists for the whole duration of the program
- Variables declared outside of any functions (i.e. at file scope) are static
- By default, are automatic:
  - all variables declared inside a compound statement
  - function parameters
- The default can be overridden using `static`
- Functions are static too, because to call them you need their code to persist in memory

Scopes

- By default, variables declared at file scope and functions are `extern`
  - i.e. visible to the linker, and to the whole program
  - Unless you declare them to be `static` only
- Variables declared at file scope and functions are visible to all blocks in the same source file
- Variables declared in a block are only visible in the block and in all scopes it encloses
  - Unless you declare them `extern`
  - But in most cases that's a symptom of bad design
- A variable declared in a block hides anything declared with the same name in enclosing scopes

Variable Initializers

- The content of an automatic variable is *uninitialized* until the variable is assigned a value
- *Uninitialized* is a polite form for ”unpredictable rubbish”
- `double f = 2.5;` is a practical shorthand for:

```
double f;
f = 2.5;
```

- Expressions can be used as initializers, as long as they can be computed at that point:

```
double pi = acos(-1.0);
double pihalf = pi/2.0;
```

is legal, while the following:

```
double pihalf = pi/2.0;
double pi = acos(-1.0);
```

obviously is not

More on Variable Initializers

- `structs` can be initialized too, as in:

```
struct vect3D V = {0.0, 1.0, 0.0};
```

- Same for arrays, as in:

```
float rot[2][2] = {{0.0, -1.0}, {1.0, 0.0}};
```

- `{0.0, 1.0, 0.0}` and `{{0.0, -1.0}, {1.0, 0.0}}` are said *compound literals*

- By default, static variables are initialized to 0
- But they can be initialized to different values
- Expressions can also be used, with some restrictions
  - For a static variable, initialization expression must be computed at compile time
  - I.e. it must be a *constant expression*, containing only constants
  - No variables, no function calls are permitted

Fast Fibonacci


```c
#include <limits.h>
#include <errno.h>
#include "fibonacci.h"

#define UINT_MAX_FIB_N 47

unsigned int FibonacciNumbers[UINT_MAX_FIB_N+1];

void fibinit(void) {
  int i;
  FibonacciNumbers[0] = 0;
  FibonacciNumbers[1] = 1;

  for (i = 2; i <= UINT_MAX_FIB_N; ++i)
    FibonacciNumbers[i] = FibonacciNumbers[i-1] + FibonacciNumbers[i-2];

}

unsigned int fib(unsigned int n) {
    if (n > UINT_MAX_FIB_N) {
    errno = ERANGE;
    return UINT_MAX;
  }
  return FibonacciNumbers[n];
}
```

Arrays

- ***`some_type name`*** **`[`** *n* **`]`**
  - declares a collection of *n* variables of type ***`some_type`***
  - the variables are laid out contiguously in memory
  - each variable can be read or written using the syntax ***`name`*** **`[`** *index* **`]`**
  - where *index* is an integer expression ranging from 0 to *n*-1

- Variables declared at *file scope*
  - Variables declared outside of any function
  - Persist for the whole program life
  - By default, they can be accessed by any function...
  - ...except where the same name is used for a parameter or local variable

- *n* can also be an expression, as long as it can be evaluated at compile time

`for (;;)`, and Some `void` Too

- `for (`*init-expr*`;` *logical-condition*`;` *incr-expr*`)`
  statement

  same as

  init-expr`;`
  `while (`*logical-condition*`)`
  `{`
    statement
    incr-expr`;`
  `}`
- But it's more compact and makes iteration bounds explicit in a single line

- What type is `void`?
  - As a return type, it tells a function returns nothing
  - As a parameter, it tells no arguments are accepted
- Why there is no `return` statement in `fibinit()`?
  - It returns nothing and completes at the closing brace

Hiding Implementation Details

- Array `FibonacciNumbers` is by default visible to the whole program
  - It could be accidentally modified or clash with another variable of the same name
  - Declaring it `static` will make it invisible to other modules
- `fibinit()` must be called in advance for `fib()` to return correct results
  - What if the call is omitted? Let's automate the process
  - Declaring it `static`, we make a function invisible to other modules
  - A variable declared in a function "disappears" when function returns, `static` will make it persist from call to call
- Best practices:
  - always hide irrelevant implementation details
  - if possible, automate initialization mechanisms

Fast Fibonacci: More Robust


```c
#include <limits.h>
#include <stdbool.h>
#include <errno.h>
#include "fibonacci.h"

#define UINT_MAX_FIB_N 47

static unsigned int FibonacciNumbers[UINT_MAX_FIB_N+1];

static void fibinit(void) {
  int i;
  FibonacciNumbers[0] = 0;
  FibonacciNumbers[1] = 1;

  for (i = 2; i <= UINT_MAX_FIB_N; ++i)
    FibonacciNumbers[i] = FibonacciNumbers[i-1] + FibonacciNumbers[i-2];

}

unsigned int fib(unsigned int n) {
  static bool doinit = true;

  if (doinit) {
    fibinit();
    doinit = false;
  }
  if (n > UINT_MAX_FIB_N) {
    errno = ERANGE;
    return UINT_MAX;
  }
  return FibonacciNumbers[n];
}
```

Arrays and Storage Classes

- Static arrays must be dimensioned with constant expressions
- Before C99, this was true for automatic arrays too
  - So to use an array in a function, you had to dimension it for the largest possible amount of work
  - A waste of memory and error prone
- C99 has a much better way
- Variable length arrays
  - Arrays whose size is unknown until run time
  - Automatic arrays can have their dimension specified by a nonconstant expression
  - Every time execution enters the block, the expression is evaluated
  - And the array size is determined, up to exit from the block

Arrays as Function Arguments

- Arrays can be huge
  - And usually are, in S&T computing
  - Passing them by value would be too costly
- Moreover, arrays cannot be used in assignments
  - Thus a function cannot return an array
- The solution
  - The address of the array is passed to a function
  - And elements can be accessed by it
  - (Later on, you'll understand how)
- This allows elements to be assigned to
  - Thus a function has a way to “return” an array result
  - A mixed blessing: allows changes to happen by mistake
- Best practice: declare an array parameter `const` if your only intent is reading its elements

Averaging, the C99 Way

- Let's write a function to average an array of **`doubles`**
- And make it generic in the array length
- Variable length array parameters come to the rescue

```
double avg(int n, const double a[n]) {
  int i;
  double sum = 0.0;

  for (i=0; i<n; ++i)
    sum += a[i];

  return sum/n;
}
```

Beware: **`double avg(double a[n], int n)`** does not work!

Averaging, the Old Way

- Before C99, there were no VLAs
- The solution was simple
  - Compiler just uses type size to find the right element
  - No bounds checking, no bound needed
- Many still write that way: it’s equivalent, but less readable

```
double avg(int n, const double a[]) {
  int i;
  double sum = 0.0;

  for (i=0; i<n; ++i)
    sum += a[i];

  return sum/n;
}
```

Calling **avg()**

- New or old style, simply pass array dimension and name
- If **`avg()`** is written using VLAs, pedantic compilers may give a warning on function call, even if it's correct: they are wrong, check with Standard document or good book

```
double mydata[N];
double mydata_avg;

// read or compute N doubles into mydata[]

mydata_avg = avg(N, mydata);
```

Averaging Arrays of Arbitrary Length

- Let's generalize the average to set of *m* numbers
- And make it generic, as usual
- Again, VLA parameters come to the rescue

```
void avg(int n, int m, const double a[n][m], double b[m]) {

  int i, j;

  for (j=0; j<m; ++j)
    b[j] = 0;

  for (i=0; i<n; ++i)
    for (j=0; j<m; ++j)
      b[j] += a[i][j];

  for (j=0; j<m; ++j)
    b[j] /= n;
}
```

Notice: this order of loops nesting gives faster execution

Calling Generic `avg()`

- Again, simply pass array dimension and name
- Using casts for arrays of doubles
- If `avg()` is written using VLAs, pedantic compilers may give a warning on function call, even if it's correct: they are wrong, check with Standard document or good book

```
double mydata1[N][12];
double mydata1_avg[12];
double mydata2[N][7];
double mydata2_avg[7];
double mydata3[N][1];
double mydata3_avg[1];
double mydata4[N];
double mydata4_avg[1];

// read or compute N 12-uples of doubles into mydata1[]
// read or compute N 7-uples of doubles into mydata2[]
// read or compute N 1-uples of doubles into mydata3[]
// read or compute N  doubles into mydata4[]

avg(N, 12, mydata1, mydata1_avg);
avg(N, 7, mydata2, mydata2_avg);
avg(N, 1, mydata3, mydata3_avg);
avg(N, 1, (double [N][1])mydata4, mydata4_avg);
```

Matrix Algebra, the C99 Way

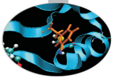
- Let's write a function to compute the trace of a matrix of `double`s
- And make it generic in the matrix size
- Again, variable length array parameters come to the rescue
- Again, you may get warnings on calls, and they could prove wrong

```
double tr(int n, const double a[n][n]) {
  int i;
  double sum = 0.0;

  for (i=0; i<n; ++i)
    sum += a[i][i];

  return sum;
}
```

Beware: compiler will not check the array dimensions match!

Matrix Algebra, the Old Way

- Before C99, there were no VLAs
- The solution was not that simple...
  - Only the ‘first dimension’ of an array parameter could be left unspecified at compile time
- To understand the solution, you have to learn more



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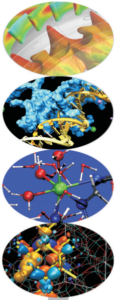

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Outline

You May Need More

- You may find yourself in need to return more than one result from a function
- And you may find yourself in need to pass a big `struct` to a function, without paying the price of copying its value
- And, believe it or not, in some part of your program you may find yourself in need to access a variable whose name is not known
- And to represent things as multiblock, unstructured grids, or building structures, or complex molecules, you may find yourself in need to access variables that don't even have a name

- In all these cases, you have to use memory addresses

Memory? Addresses?

- You can think of memory as a huge array of units of storage (usually 8 bits bytes)
  - The index in this array is termed *address*
- But how many bytes are needed to store a value?
  - It depends on value type and platform
- And it's even worse...
  - Not all locations are good for any value (at least performancewise)
  - Not all locations can be read/written
  - What are the starting and ending address?
  - The amount of memory seen by your program could vary during execution
  - You could have 'holes' in this ideal array
  - Or this ideal array could be made of separate, independent segments

Enter C Pointers

- Dealing directly with memory addresses is cumbersome
  - Easily makes the program non portable
  - Makes the program difficult to manage and confusing
  - Exhibits low level details you don't really want to care about
- How to avoid it?
- Named variables leave the whole issue to the compiler
  - You use the name and don't care about address
- C pointers let you manipulate addresses in a transparent and consistent way
  - They contain memory addresses
  - Allow you to manipulate addresses disregarding their actual values
  - Associate a C type to the memory location they point to
  - And give you a way to read or write this memory location, much like a named variable

Pointers Basics

- `int i, *p;`
  - declares an `int` variable `i`
  - and a 'pointer to `int`' variable `p`
  - in the latter, you can store the address of a memory location suitable to store an `int` type value
- `p = &i;`
  - `&i` evaluates to the address of variable `i`
  - `p` gets a valid address in
  - Got something familiar? Do you remember `scanf()`?
- `*p = 10;`
  - Expression `*p` is an *lvalue* of type `int`
  - You can performe assignment to it
  - You can use it in expressions to access the stored value
  - `*` has same precedence and associativity of unary `–`

Pointer vs. Pointee


```
int *p = NULL;
int a = 5;
```

p: 0
a: 5

```
p = &a;
```

p: address of a
a: 5

```
*p += 10;
```

p: address of a
a: 15

```
a += 1;
```

p: address of a
a: 16

Avoiding Costly Copies


```
struct vect3D {
  double x, y, z;
};

// REMINDER: I have to make vcross() more efficient! DONE!!
struct vect3d vcross(const struct vect3D *u, const struct vect3D *v) {
  struct vect3D c;

  c.x = u->y*v->z - u->z*v->y;
  c.y = u->z*v->x - u->x*v->z;
  c.z = u->x*v->y - u->y*v->x;

  return c;
}
```

- Copying 6 `doubles` for very little work
- Let's put pointers to good use
- `u->y` is a convenient shorthand for `(*u).y`
- But now we have the address of the arguments and could make a mistake and change their contents
- Let's make the pointees `const`

Did we say "valid"?

- A valid pointer value is an address that:
  - is in the process memory space
  - points to something which exists
  - and whose type matches
- Invalid pointers
  - uninitialized pointers (point to the wrong place, at best)
  - the address of a variable that does not exist anymore
  - the address of one type put in pointer to another type (unless you REALLY know what you are doing)
  - a null pointer, i.e. a 0 address
- Dereferencing (with `*`) a null pointer forces runtime error
- Good practice:
  - Always initialize pointers
  - If you don't know yet the right address, use `NULL` from `stddef.h`
  - `0` may also be used, but less readable

A Naive Mistake


```
struct vect3D {
  double x, y, z;
};

// REMINDER: I have to make vcross() more efficient! DONE!! Trying to do better...
struct vect3d *vcross(const struct vect3D *u, const struct vect3D *v) {
  struct vect3D c;

  c.x = u->y*v->z - u->z*v->y;
  c.y = u->z*v->x - u->x*v->z;
  c.z = u->x*v->y - u->y*v->x;

  return &c; // MADNESS!!
}
```

- Sparing another copy it's tempting...
- But it's very naive!
- `c` is an automatic variable, and it's gone when the pointer is used
- And probably the memory locations have been already reused and overwritten!

Pointers and Arrays

- **`double *p[10]`**
  - it's an array of 10 pointers to **`double`**
- and **`double *p[10][3]`**
  - it's an array of 10 arrays, each of 3 pointers to **`double`**
- while **`double (*p)[10]`**
  - it's a pointer to array of 10 **`doubles`**
- and **`double (*p)[10][3]`**
  - it's a pointer to an array of 10 arrays, each of 3 **`doubles`**
- Confusing? It's logical: operator **`[]`** has higher precedence than **`*`**
- But easily becomes nasty!
  - What's **`double (*p[10])[3]`**?
  - And **`double (*(*p[10])[3][5])[8][2]`**?
- Best practice: use **`cdecl`** tool to familiarize and decrypt

Pointers Arithmetic

- Useful to poke around in arrays
- `p + 7`
  - will give you an address
  - that is `7*sizeof(*p)` after the one in `p`
- You can also use `-`, `+=`, `-=`, `++`, and `--`
- `p1 - p2`
  - if of the same pointer type, will give you an integer value
  - more precisely, of `ptrdiff_t` type (from `stddef.h`)
  - the displacement from `p2` to `p1` in units of `sizeof(*p1)`
- Pointer comparison
  - `==` (equal), `!=`, `>`, `<`, `>=`, `<=` can be used on pointers of the same type
- Pointer casting
  - Pointer values can be cast to pointers of different type
  - Do it VERY carefully, it's easy to do the wrong thing
  - Pointers may also be cast to some integer type, but it's highly non portable, don't do it

Pointers and Array Equivalence

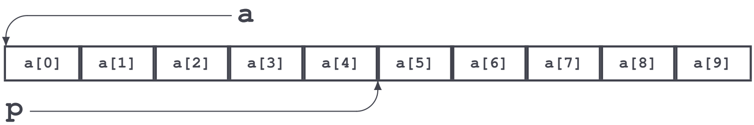
- `*(p+7)` can be shortened to `p[7]`
- Aha!
- Can a pointer be used as an array?
  - `true`
- I see... so is the array name a pointer?
  - `true`, but it's constant, you can't change it
- But if I have `int a[N]`, and `int *p`, may I assign `p=a`?
  - `true`, you can
- Then, what's the difference between an array variable and a pointer variable declarations?
  - An array declaration allocates memory for data
  - A pointer declaration allocates memory for a data address only
- And between array and pointer function parameters?
  - Irrelevant, an array argument passes a pointer
  - You are now ready to understand good old C tricks

Skeptical? Try to Believe

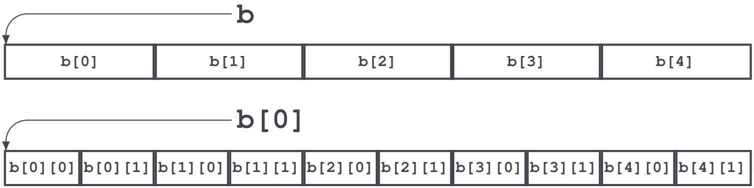

```c
#include <stdio.h>

double a[] = {1.0, 2.0, 3.0, 4.0, 5.0};

int main() {

  double *p;

  p = a; // variable p now stores the address of array a

  printf("%lf\n", a[2]); // will print 3.0
  printf("%lf\n", *(p+2)); // will print 3.0

  p[2] = 7.0; // reassigns a[2]

  printf("%lf\n", p[2]); // will print 7.0
  printf("%lf\n", a[2]); // ditto, it's the same location

  return 0;
}
```

Array Names and Pointers


```
int a[10];
int *p = a + 5;
```




```
int b[5][2];
```



Averaging, with Pointers

- This one should be quite obvious
- Perfectly equivalent to using `const double a[]`
- You'll often encounter something like this, particularly in libraries

```
double avg(int n, const double *a) { /* which one is const? */
  int i;
  double sum = 0.0;

  for (i=0; i<n; ++i)
    sum += a[i];

  return sum/n;
}
```

`const int *p` is a pointer to `const`, `int *(const p)` is a `const` pointer

Averaging Arrays, with Pointers

- Let's generalize to sets of *m* numbers
- And make it generic, as usual
- Now you are ready for the traditional solution
- And for an application of pointer casting

```
void avg(int n, int m, const double (*a)[], double *b) {
  int i, j;
  const double *p = (const double *)a;

  for (j=0; j<m; ++j)
    b[j] = 0;

  for (i=0; i<n; ++i)
    for (j=0; j<m; ++j)
      b[j] += p[i*m + j];     /* mapping two indexes */
                              /* to one 'by hand' */
  for (j=0; j<m; ++j)
    b[j] /= n;
}
```

Calling Generic **avg()**

- New or old style, arrays or pointers, simply pass array dimension and name
- Using casts for arrays of doubles
- If `avg()` is written using VLAs, pedantic compilers may give a warning on function call, even if it's correct: they are wrong, check with Standard document or good book

```
double mydata1[N][12];
double mydata1_avg[12];
double mydata2[N][7];
double mydata2_avg[7];
double mydata3[N][1];
double mydata3_avg[1];
double mydata4[N];
double mydata4_avg;

// read or compute N 12-uples of doubles into mydata1[]
// read or compute N 7-uples of doubles into mydata2[]
// read or compute N 1-uples of doubles into mydata3[]
// read or compute N  doubles into mydata4[]

avg(N, 12, mydata1, mydata1_avg);
avg(N, 7, mydata2, mydata2_avg);
avg(N, 1, mydata3, mydata3_avg);
avg(N, 1, (double [N][1])mydata4, &mydata4_avg);
```

Averaging Arrays, Another Classic Flavor

- Again averages sets of *m* numbers
- For arbitrary *m*
- This idiom arose when compilers were not good at optimization

```
void avg(int n, int m, const double (*a)[], double *b) {
  int i, j;
  const double *p = (const double *)a;

  for (j=0; j<m; ++j)
    b[j] = 0;

  for (i=0; i<n; ++i)
    for (j=0; j<m; ++j) {
      b[j] += *p;    /* array elements `walked by' */
      ++p;           /* in the same sequence */
    }

  for (j=0; j<m; ++j)
    b[j] /= n;
}
```

Matrix Algebra, the Old Way

- Let's write a function to compute the trace of a matrix of `double`s
- And make it generic in the matrix size
- And use a traditional way
- Again, you'll often encounter something like this, particularly in libraries

```
double tr(int n, const double (*a)[]) {
  int i;
  double sum = 0.0;
  const double *p = *a;  /* works like casting here, why? */

  for (i=0; i<n; ++i)
    sum += p[i*n + i];

  return sum;
}
```

Matrix Algebra, Another Old Way

- Let's write a function to compute the trace of a matrix of `double`s
- And make it generic in the matrix size
- And use another traditional way, from times when compilers didn't optimize well

```
double tr(int n, const double (*a)[]) {
  int i;
  double sum = 0.0;
  const double *p = *a;

  for (i=0; i<n; ++i) {
    sum += *p;
    p += n + 1;   /* next element on diagonal */
  }

  return sum;
}
```

Matrix Algebra, yet Another Classic Flavor

- Bottom line, we are working on `doubles`
- Call it like `tr(8, (double *)mp)`
- Or call it like `tr(8, mp[0])`
- Widely used in numerical libraries, but write new code using VLAs

```
double tr(int n, const double *a) {
  int i;
  double sum = 0.0;

  for (i=0; i<n; ++i) {
    sum += *a;
    a += n + 1; /* next element on diagonal */
  }

  return sum;
}
```

Matrix Algebra, a Bad Way

- A way of getting rid of all complexity
- It's the "third" use of type **`void`**
- Sometimes you'll find sloppy code like this
- But not a good idea in this case, it's dangerous

```
double tr(int n, const void *a) {
  int i;
  double sum = 0.0;
  double *p = a;

  for (i=0; i<n; ++i) {
    sum += *p;
    p += n + 1; /* next element on diagonal */
  }

  return sum;
}
```

`void` and Pointers

- `void *p;` declares a *generic pointer*
- I.e. a pointer pointing to unknown type
- If type is unknown, size is unknown
- So no arithmetic is possible, only assignment and comparisons
- The value of any pointer can be converted to a generic one
- A generic pointer can be converted to any pointer type

- So, what's the danger with `tr()`?
  - `tr()` assumes something pointing to `doubles`
  - With `void *`, pointers at any type will do
  - A pedantic compiler would warn you at any use of `tr()`
  - And you'd get annoyed and switch off warnings
- But generic pointers are essential to other purposes

qsort()

- Declaration (from `stdlib.h`):

```
void qsort(
  void *base,
  size_t count,
  size_t size,
  int (*compare)(const void *el1, const void *el2) );
```

- Sorts an array of `count` elements of unknown type, starting at `base`
- Each element has size `size`
- What's `compare`?
  - `qsort()` doesn't know elements type
  - And has no clue at how to compare them
  - `compare` is a pointer to a function that knows more
- Yes, a function has an address and function name evaluates to it

Sorting with `qsort()`

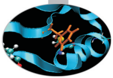
- Define a comparison function like:

```
int comparedoubles(const double *a, const double *b) {
  if (*a == *b)
    return 0;

  if (*a > *b)
    return 1;

  return -1;
}
```

- Can you see how it matches the **`compare`** parameter?
- Then, if **`g`** is an array of 10000 **`double`**s, you can sort it in ascending order like this:

```
qsort(g, 10000, sizeof(double), comparedoubles);
```

- Want it sorted in descending order?
  - Substitute < to >
- Have an array sorted in ascending order?
  - You can use **`bsearch()`** to find an element

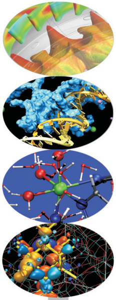


Scientific and Technical Computing in C

Day 2

Stefano Tagliaventi   Isabella Baccarelli

CINECA Roma - SCAI Department



Roma, 6-7 November 2014

Outline

Characters

- In C, characters have type `char`
- I.e. an integer type holding the numeric character code
- But it's implementation defined if `char` is signed or not
- Encoding may depend on implementation and OS
- In most implementations, characters numbered 0 to 127 match the standard ASCII character set
- Literal character constants are specified like this: `'C'`
  - `'\n'` is new line
  - `'\t'` is tab
  - `'\r'` is carriage return
  - `'\\'` is backslash \
  - `'\''` is '
  - `'\"'` is "
  - and `'\0'` is ASCII NUL, with code 0, quite important despite of its value

#include <ctype.h>

Function	Returns
`int isalpha(int c)`	true if alphabetic character
`int isdigit(int c)`	true if a digit character
`int isalnum(int c)`	`isalpha(c) || isdigit(c)`
`int isprint(int c)`	true if printable character (including `' '`)
`int iscntrl(int c)`	`!isprint(c)`
`int islower(int c)`	true if lowercase alphabetic character
`int isupper(int c)`	true if uppercase alphabetic character
`int isspace(int c)`	true if `' '`, `'\t'`, `'\n'`, ...
`int tolower(int c)`	converts uppercase ones to lowercase others unchanged
`int toupper(int c)`	converts lowercase ones to uppercase others unchanged

- Do you remember? `char` types are converted to `int` in all arithmetic expressions
- Do not play with character codes, use these functions, they make the code portable

Strings

- Strings are not first-class citizens in C
- Simply arrays of `chars`
- The string must be terminated by a `'\0'` character
- Commonly referred to as *null terminated* strings
- This has annoying consequences
  - String lengths must be computed by scanning
  - No way for bounds checking
  - And a source of program weaknesses

- String constants are specified like this:
  `"A null terminated string"`
- A terminating `'\0'` is automatically appended
- You already met them using `printf()`
- Use a \ at end of lines to write multiline string constants

The Biggest Mistake


```
char decdigits[10];
//...
strcpy(decdigits, "0123456789");
```

- The string is 10 characters long
- But it has a terminating `'\0'`
- So its internal representation is **11** characters long

Fixing the Biggest Mistake


```
char decdigits[] = "0123456789";
```

- An 11 characters array will be automatically allocated
- (Yes, you could do this for any array)
- But this only fixes the problem on initialization
- Not when you build string dynamically or do simple minded I/O
- Ever heard of '*buffer overflows*'?

#include <string.h>

Function	Does
`size_t strlen(const char *s)`	returns actual string length
`char *strncpy(char *d, const char *s, size_t n)`	copies **n** characters from **s** to **d**, returns **d**
`char *strncat(char *d, const char *s, size_t n)`	appends **n** characters from **s** to **d**, returns **d**
`int strcmp(const char *s1, const char *s2)`	lexicographic comparison of **s1** and **s2**
`int strncmp(const char *s1, const char *s2, size_t n)`	lexicographic comparison of **s1** and **s2**, up to **n** characters
`char *strchr(const char *s, int c)`	returns pointer to first occurrence in **s** of character **c**, **NULL** if not found
`char *strrchr(const char *s,) int c)`	returns pointer to last occurrence in **s** of character **c**, **NULL** if not found
`char *strcspn(const char *s, const char *set)`	returns pointer to first occurrence in **s** of any character in **set**, **NULL** if not found
`char *strspn(const char *s, const char *set)`	returns pointer to first occurrence in **s** of any character not in **set**, **NULL** if not found
`char *strstr(const char *s, const char *sub)`	returns pointer to first occurrence in **s** of string **sub**, **NULL** if not found
`char *strtok(const char *s, const char *set)`	allow to separate string **s** into tokens, read documentation

- Do you remember? `char` types are converted to `int` in many cases
- You'll also find in use `strcpy()` and `strcat()`: dangerous! avoid them
- Way too common mistake: forgetting about and writing code doing the same
- Don't reinvent the wheel, use library functions!

More Friends from `stdlib.h`

Function	Returns conversion of initial portion of `s` to
`strtof(const char *s, char **p)`[3]	`float`[1]
`strtod(const char *s, char **p)`	`double`[1]
`atof(const char *s)`	`double`
`strtold(const char *s, char **p)`[3]	`long double`[1]
`atoi(const char *s)`	`int`
`strtol(const char *s, char **p, int base`[2]`)`	`long`[1]
`atol(const char *s)`	`long`
`strtoul(const char *s, char **p, int base`[2]`)`	`unsigned long`[1]
`strtoll(const char *s, char **p, int base`[2]`)`[3]	`long long`[1]
`atoll(const char *s)`[3]	`long long`
`strtoull(const char *s, char **p, int base`[2]`)`[3]	`unsigned long long`[1]

1. If `p` is not null, sets it to point to first character after converted portion of `s`
2. The `base` used in string representation ranges from 2 to 36 (!).
3. C99

- More practical than `scanf()` family in many cases
- `strto...()` form preferred
- Use `sprintf()` to convert the other way around
- Where `char **p` appears, pass the address of a `char *` pointer variable...

Yes, Pointers can be Pointees!

Aggregate
Structures
Defining Types
Arrays
Storage & C.
More Arrays
Pointers
Basics
And Arrays
void
Strings
Chars
Strings
Manipulations
Command Line
I/O
Files
Text
Binary
Memory
Allocation
Data Structures
Finale

```
int **p = NULL;
int *q = NULL;
int a = 5;
```

p:	0
q:	0
a:	5

```
p = &q;
```

p:	address of q
q:	0
a:	5

```
*p = &a;
```

p:	address of q
q:	address of a
a:	5

```
**p += 10;
```

p:	address of q
q:	address of a
a:	15

`argc` and `argv`

- Up to now, we disregarded `main()` parameters
  - Which is legal
  - And writing `int main(void)` is legal too
- In its full glory, `main(int argc, char *argv[])` receives two arguments
  - An integer count, `argc`
  - And an array of `argc` pointers to string, `argv`
  - Names are not mandatory, just a solid tradition
- On most systems
  - `argv[0]` contains the name of program executable
  - `argv[1]` through `argv[argc-1]` contain the command line parameters specified at program invocation
- Form `int main(int argc, char **argv)` is fully equivalent

Use of argc and argv


```
void print_help_and_exit(){
        printf("Usage: ./shapp [-l|-t|-h]\n");
        exit(EXIT_FAILURE);
}
int main(int argc,char *argv[]){

        if(argc < 2 || argv[1][0]!='-')
                print_help_and_exit();
        switch(argv[1][1])
        {
                case 't':
                        timestamp_ordering();
                        break;
                case 'r':
                        reverse_order();
                        break;
                case 'h':
                        print_help_and_exit();
                default:
                        print_help_and_exit();
        }

}
```

More Alternatives with `switch ()`

- **switch** (*integer-expression*) **{**
  case *constant-expression*:
  statements
  [**case** *constant-expression*:
  statements]
  [**default:**
  statements]
  }
  1. Evaluates *integer-expression*
  2. If value equals one *constant-expression*, execution jumps to the statement following it
  3. Otherwise, if **default:** exists, execution jumps to statement following it
  4. Otherwise execution leaves **switch()** and proceeds to the following code

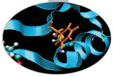
A `switch ()` 'Feature'

- Beware: once 2 or 3 above happened, encounter of another `case` or of `default` does not imply exit from `switch`!
- A `break;` statement is needed to this purpose

- This is way too easily forgotten
- Best practices:
  - Always add a `break;` statement at end of each '`case`'
  - Even if it's unreachable, you'll appreciate on code changes
  - Unless you really intend to execute two or more '`cases`' at once

More **`break`**, and **`continue`**

- A **`break;`** statement forces execution to bail out from innermost enclosing statement among:
  - **`switch ()`**
  - **`while ()`**
  - **`do...while ()`**
  - **`for (;;)`**
- A **`continue;`** statement terminates execution of current iteration of innermost enclosing statement among:
  - **`while ()`**
  - **`do...while ()`**
  - **`for (;;)`**
- Execution continues with next iteration



Scientific and Technical Computing in C

Day 2

Stefano Tagliaventi Isabella Baccarelli

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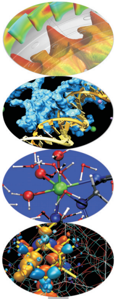


Outline

Files

- C thinks of files as *streams* of data you can read/write from/to
- C has no notion of file content or structure: user knows about
  - You read what you know is there
  - You write what you want to put there
- Files are managed by internal data structures of `FILE` type
  - Whose details may be implementation defined
- All functions are declared in `stdio.h`
- Most functions return or accept pointers to `FILE` structures
- You simply declare variables of `FILE *` type and use these functions
  - And usually may disregard details

Three Files for Free

- When `main()` is called, three files have already been opened for you
- Accessible by three expressions of `FILE *` type
  - `stdin` for standard input
  - `stdout` for standard output
  - `stderr` for error messages output
- Usually map to user's terminal, unless they were redirected at command launch

Using More Files is not Free

- If `myfile` is a `FILE *` variable, open a file using:
  `myfile = fopen("mydata.dat", "r");`
- Second string is a mode:
  - `"r"` to read existing text file
  - `"w"` to create a new text file or truncate existing one to zero length
  - `"a"` to create a new text file or append to existing one
  - Use `"rb"`, `"wb"`, or `"ab"` for binary files
  - `"r+"` and `"r+b"` to both read and write to existing file
- Biggest mistake: assuming `fopen()` succeeded
  - `fopen()` returns NULL on failure
  - Always check and use `errno` to know more
- `fclose(FILE *f)` orderly closes an open file, do it when you are done with it
- A string `FILENAME_MAX` long is big enough for any file name

Simple String I/O

- `char *fgets(char *s, int n, FILE *stream)`
  - Reads in at most one less than `n` characters from stream and stores them into the buffer pointed to by s. Reading stops after an EOF or a newline.
  - Returns `s` on success, `NULL` on failure
  - A robust I/O function. Use it in your code.
- Use `int feof(FILE *stream)` to check if `NULL` was returned because end of file was reached
- `char *fputs(const char *s, FILE *stream)`
  - Writes `s` string to file
  - Returns `EOF` on error
- `char *puts(const char *s)`
  - Like `fputs()` on `stdout`, but adds a `'\n'`
- You'll encounter `gets()` in codes: offers no control on maximum input size, don't use it

Talking to Humans

- `fprintf()` converts internal formats of basic data types to human readable formats
- `fprintf(`*`file`*`, "`*`control string`*`", `*`arguments`*`)`
    - Characters in *`control string`* are emitted verbatim
    - But conversion specifications beginning with `%` cause the conversions and output of arguments
    - Arguments (i.e. expressions) must match conversion specifications in number, types, and positions
    - Conversion specification `%%` emits a `%` character and consumes no arguments
- `printf()` outputs to `stdout`
- `snprintf()` and `sprintf()`
    - Write to string instead of file
    - `snprintf()` is preferable as maximum string length can be specified

Common Mistakes

- Beware: if you want to remove item `c` from output in

  ```
  printf("Parameters: %lf, %lf, %lf\n", a, b, c);
  ```

  the following is not enough:

  ```
  printf("Parameters: %lf, %lf, %lf\n", a, b);
  ```

  you need to update the format string too:

  ```
  printf("Parameters: %lf, %lf\n", a, b);
  ```

- And on adding an item you have to add a proper conversion specifier
- Ditto for type mismatches: no argument checking is required
- In some cases, dire consequences could follow
- A clever compiler may be able to warn you, if you ask

`printf()`: Integer Types

- In `%d` and `%u`, `d` and `u` are conversions
  - Internal to base 10 text representation
- `l`, `ll`, `h`, and `hh`, are size modifiers
  - Look back at integer types table if you need a refresh
- Variations on a theme
  - `%10d`: at least 10 characters, right justified, space padded
  - `%.4d`: at least 4 digits, right justified
  - `%010d`: at least 10 characters, right justified, leading `0`s
  - `%-10d`: at least 10 characters, left justified, space padded
  - `%+d`: sign is always printed (not relevant for `u`)
  - `% d`: same, but a space if positive (not relevant for `u`)
- `printf("%-5d%+6.4d", 12, 12);`
  Prints?

`printf()`: Floating Types

- Conversions
  - `%f`: `float` to base 10 decimal text
  - `%E`: `float` to base 10 exponential text
  - `%G`: most suitable of the above ones
- `l` and `L` are size modifiers
  - Look back at floating types table if you need a refresh
- Variations on a theme
  - `%10f`: at least 10 characters, right justified, space padded
  - `%.4f`: 4 digits after decimal point (`f` and `E` only)
  - `%.7G`: 7 significant digits
  - `%010f`: at least 10 characters, right justified, leading `0`s
  - `%-10f`: at least 10 characters, left justified, space padded
  - `%+f`: sign is always printed
  - `% f`: same, but a space if positive
- `printf("%+8.2lf %.4lE", 12.0, 12.0);`
  Prints?

`printf()`: Characters and Strings

- `%c`: emits character with specified code
- No variations

- `%s`: emits a string
- Variations on a theme
  - `%10s`: at least 10 characters, right justified, space padded
  - `%.7s`: exactly(!) 7 characters from string
  - `%-10s`: at least 10 characters, left justified, space padded
- `printf("%-7s%4.3s", "Vigna", "Vigna");`
  Prints?

- And more conversions are defined, but we'll not cover them

Listening to Humans

Aggregate
Structures
Defining Types
Arrays
Storage & C.
More Arrays
Pointers
Basics
And Arrays
void
Strings
Chars
Strings
Manipulations
Command Line
I/O
Files
Text
Binary
Memory
Allocation
Data Structures
Finale

- `fscanf()` converts human writable formats of basic data types to internal ones
- `fscanf(`*`file`*`, "`*`control string`*`", `*`arguments`*`)`
  - Arguments must be pointers!
  - Arguments must match conversion specifications in number, types, and positions
  - White-space in *`control string`* matches an arbitrary sequence of zero or more spaces
  - All other characters must match verbatim with characters in input
- `scanf()` reads from `stdin`
- `sscanf()` reads from string instead of file

`scanf()` Conversions

- Conversions discussed for `printf()` work, the other way around
- They skip white-space characters before reading and converting, except for `%c`
- Number too big for the type? Result is implementation defined
- Fewer variations on the theme (for most conversions)
  - `%10d`: no more than 10 characters considered (not for `%c`)
  - `%*d`: looks for text matching an `int`, but ignores it
- `scanf("%4d%*6d%3d", &i1, &i2);`
  Input: `12   34567890` (notice: 3 space characters)
  Reads?

Common Mistakes

- Any mismatch in input to a **`scanf()`** will stop input and conversions
- **`scanf()`** always returns the number of conversions performed, do not discard it:

  ```
  itemsread = scanf("%lf ,%lf", &a, &b);
  ```

  check the result, and take correcting actions (or fail gracefully)
- Giving fewer arguments than conversion specifiers, as in:

  ```
  itemsread = scanf("%lf ,%lf ,%lf", &a, &b);
  ```

  is a very good recipe for disaster, and one difficult to debug
- So is giving the wrong pointer or a pointer to the wrong type

User Input


```
//...
    printf("Enter t max: ");
    scanf("%lf", &tmax);
```

- User mistypes `U.0` for `7.0`
- Program behaves in unintended ways
- Could check `scanf()` return value and fail gracefully, but let's give user a chance

Wrong Solution


```
  int itemsread;
//...
  do {

    printf("Enter t max: ");

    itemsread = scanf("%lf", &tmax);

  } while (itemsread == 0);
```

- Again, user mistypes `U.0` for `7.0`
- Program stops responding, burning CPU cycles
- `scanf()` is very finicky about input
  - As soon as a character doesn't match the format string, puts it back in input buffer
  - To find it again at each iteration

Better Solution


```
  int itemsread;
//...
  do {
    char s[257];

    printf("Enter t max: ");
    if (fgets(s, sizeof(s), stdin) == NULL)
      exit(EXIT_FAILURE);

    itemsread = sscanf(s, "%lf", &tmax);

  } while (itemsread == 0);
```

- This form causes wrong input to be consumed and removed
- Use `fscanf()` for rigidly formatted files
- With imprecise formats (as user input is), use `fgets()`, then `sscanf()`

Dealing with Many Data

- Text I/O is human readable
- Text I/O is platform independent
- But text I/O is huge
  - Because of issues in base 2 vs. base 10 representation
- To recover exact binary form of a floating type, you need:
  - at least 9 decimal digits in text I/O for a **`float`**
  - at least 19 decimal digits in text I/O for a **`double`**
- And text I/O is slow
  - Because of size
  - And because conversions take time
- Best practice:
  - Use text I/O to talk to humans or as a last resort for some programs
  - Use binary I/O otherwise

Binary Reads and Writes


```
size_t fread(void *data, size_t elsz,
                  size_t count, FILE *f);
size_t fwrite(const void *data, size_t elsz,
                  size_t count, FILE *f);
```

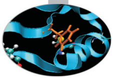
- Read/write ***count*** elements of size ***elsz*** from/to file ***f*** to/from address ***data***
- Both return the number of elements actually read/written
  - Can be less than requested if error occurred, or (**fread()** only) end of file was encountered
  - Use **feof()** or **ferror()** to determine cause
- Best practice:
  - do binary I/O in chunks as large as possible
  - performance will sky-rocket

Walking Around in a File

- Each I/O operation takes place from the position in the file where the last one ended
- But position can be changed
- Not special to binary files, but mostly used with them
- `fseek(f, 4096L, `*`wherefrom`*`)` moves forward by 4096 bytes relative to:
  - file beginning, if *`wherefrom`* is `SEEK_SET`
  - current position, if *`wherefrom`* is `SEEK_CUR`
  - file end, if *`wherefrom`* is `SEEK_END`
  - and returns zero if successful, non zero otherwise
- `ftell(f)` returns the current position (`long`)
  - on failure, returns -1L and sets `errno`
- This is a 64 bits world: files can be huge!
  - In case, use `fsetpos()` and `fgetpos()`
  - They use an `fpos_t` type large enough

Dealing with Fortran Binary Files

- You may need to read Fortran binary files
- And Fortran adds two extra 32 or 64 bits integers, one at beginning and one at end of each record (i.e. of each **`WRITE`** for unformatted files)
- Option 1: skip them with **`fseek()`**
- Option 2: read them and forget the values
- Option 3: write the file from Fortran opening it in **`STREAM`** mode
  - Designed to match the C file concept
  - Introduced in Fortran 2003
  - But already available in most implementations

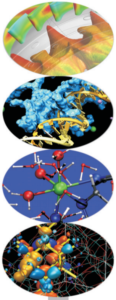


Scientific and Technical Computing in C

Day 2

Stefano Tagliaventi Isabella Baccarelli

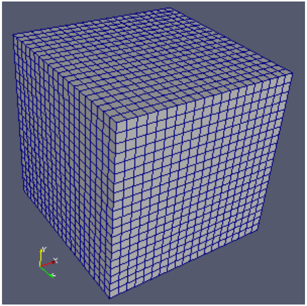
CINECA Roma - SCAI Department



Roma, 6-7 November 2014

Outline

A PDE Problem



- Let's imagine we have to solve a PDE
- On a dense, Cartesian, uniform grid
  - Mesh axes are parallel to coordinate ones
  - Steps along each direction have the same size
  - And we have some discretization schemes in time and space to solve for variables at each point

A Rigid Solution


```
#define NX 200
#define NY 450
#define NZ 320

double deltax; // Grid steps
double deltay;
double deltaz;
//...
double u[NX][NY][NZ]; // x velocity component
double v[NX][NY][NZ]; // y velocity component
double w[NX][NY][NZ]; // z velocity component
double p[NX][NY][NZ]; // pressure
```

- We could write something like that at file scope
- But it has annoying consequences
  - Recompile each time grid resolution changes
  - A slow process, for big programs
  - And error prone, as we may forget about
- Couldn't we size data structures according to user input?

Looking for Flexibility


```
int main(int argc, char *argv[]) {
  double deltax, deltay, deltaz; // Grid steps
  int nx, ny, nz
//...
  double u[nx][ny][nz];
  double v[nx][ny][nz];
  double w[nx][ny][nz];
  double p[nx][ny][nz];
```

- We could think of declaring variable length arrays inside `main()` or other functions
- This is unwise
  - Automatic arrays are usually allocated on the process stack
  - Which is a precious resource
  - And limited in most system configurations

A Better Approach


```
#define MAX_NX 400
#define MAX_NY 400
#define MAX_NZ 400

double u[MAX_NX*MAX_NY*MAX_NZ];
double v[MAX_NX*MAX_NY*MAX_NZ];
double w[MAX_NX*MAX_NY*MAX_NZ];
double p[MAX_NX*MAX_NY*MAX_NZ];

void my_pde_solver(int nx, int ny, int nz,
                   double u[nx][ny][nz],
                   double v[nx][ny][nz],
                   double w[nx][ny][nz],
                   double p[nx][ny][nz]);
```

- We could use VLA parameters
- But we should cast on calls, to avoid compiler warnings
  - How would you cast `u[MAX_NX*MAX_NY*MAX_NZ]` into `double u[nx][ny][nz]`?
- Maximum problem size is program limited: `nx*ny*nz` must be less than `MAX_NX*MAX_NY*MAX_NZ + 1`

Slightly More Comfortable, the Old Way


```
void my_pde_solver(int nx, int ny, int nz,
                   double u[],
                   double v[],
                   double w[],
                   double p[]) {
  // variable declarations and solver code...

  u[(i*ny + j)*nz + k] = ...;
  v[(i*ny + j)*nz + k] = ...;
  w[(i*ny + j)*nz + k] = ...;
  p[(i*ny + j)*nz + k] = ...;

  // more solver code...
```

- We could write code as the above, no need for casting on `my_pde_solver()` calls
- And you'll encounter code like this, that was a C89 way
- But so old fashioned!! Don't do that for new codes
- And remember, maximum problem size is limited

More Comfortable, Thanks to C99


```
void my_pde_solver(int nx, int ny, int nz,
                   double um[],
                   double vm[],
                   double wm[],
                   double pm[]) {

  double (*u)[ny][nz] = (double (*)[ny][nz])um;
  double (*v)[ny][nz] = (double (*)[ny][nz])vm;
  double (*w)[ny][nz] = (double (*)[ny][nz])wm;
  double (*p)[ny][nz] = (double (*)[ny][nz])pm;

  // solver code using u, v, w, and p as humans do
```

- Let's rewrite `my_pde_solver()` like this (and update function declaration as well!)
- Definitely easier to use
  - No casting on `my_pde_solver()` calls
  - And writing `my_pde_solver()` is easier too
- Maximum problem size still program limited, however

Removing Limitations

Aggregate
Structures
Defining Types
Arrays
Storage & C.
More Arrays
Pointers
Basics
And Arrays
void
Strings
Chars
Strings
Manipulations
Command Line
I/O
Files
Text
Binary
Memory
Allocation
Data Structures
Finale

- Being program limited is annoying
- It's much better to accommodate to any user specified problem size
  - Right, as long as there is enough memory
  - But if memory is not enough, not our fault
  - It's computer or user's fault
- And there are many complex kinds of computations
  - Those in which memory need cannot be foreseen in advance
  - Those in which arrays do not fit
  - Those in which very complex data structures are needed

Enter Dynamic Allocation (from `stdlib.h`)


```
void *malloc(size_t size)
void *calloc(size_t el_count, size_t el_size)
```

- **`malloc()`** allocates a memory area suitable to host a variable whose size is **`size`**
  - Allocated memory is uninitialized.
  - Use it like this:

```
a_ion_ptr = (ion *)malloc(sizeof(ion));
```

- **`calloc()`** allocates a memory area suitable to host an array of **`count`** elements, each of size **`size`**
  - Allocated memory is initialized to zero: can be slow, but useful
  - Use it like this:

```
a_flt_ptr = (float *)calloc(nx*ny*nz, sizeof(float));
```

- Best practice: always cast return values, gives less compiler warnings and helps readability

The Biggest Mistake

- Assuming `malloc()` or `calloc()` succeeded!
- Where all these 'dynamic allocated memory' comes from?
  - From an internal area, often termed "*memory heap*"
  - When that is exhausted, OS is asked to give the process more memory
  - And if OS is short of memory, or some configuration limit is exhausted...
- On failure, `malloc()` and `calloc()` return null pointers
  - Dereferencing it forces program termination (usually a "segmentation fault")
  - We could say you deserve it
  - But all time spent in previous computations would be lost
- Best practice: ALWAYS, ALWAYS, always check

```
if ((p = malloc(some_size)) == NULL) {
   // save your precious data, if any
   // and fail gracefully
 }
```

Resizing


```
void *realloc(void *ptr, size_t new_size)
```

- `realloc()` takes a previously allocated memory area, and gives you a new area whose size is `size`
  - Original area contents are copied in the new area, up to min(*oldsize*, `size`)
  - Use it like this:

```
new_ptr = (float *)realloc(a_flt_ptr,
                           nx*ny*2*nz*sizeof(float));
```

- Particularly handy to shrink or lengthen arrays
- On failure, returns null pointer and leaves old area unchanged
- Biggest mistakes
  - Assuming `realloc()` succeeded: always check
  - Assuming only size changes and address remains the same: it can happen, but only in particular cases

Getting Rid of Memory Areas


```
void free(void *ptr)
```

- An allocated memory area persists until it is “freed”
- Of course, heap allocated memory is claimed back at process termination
- But better give back a memory area to the dynamic memory “pool” for reuse, as soon as you are over with it
  - Just imagine you are processing one item at a time...
  - Allocating new memory areas at each item without freeing previously allocated ones...
  - Your process size will grow until...
  - In jargon, this is a *memory leak*
- Remember: programmers causing memory leaks have particularly bad reputation

The First Big Mistake with `free()`


```
  char s[BIG_STRING + 1];
  char *p;
//....
  if ((p = malloc(BIG_STRING + 1)) == NULL) {
    // save your precious data, if any
    // and fail gracefully
  }
  strncpy(p, s, BIG_STRING);

  while (++p) {
    // process characters
  }
  free(p);  // p has been incremented!
  free(s);  // MADNESS: s not ‘malloced’!
```

- `free()` MUST be passed a pointer returned by `malloc()` and friends
- Otherwise behavior is implementation defined
- In most practical cases, program execution is aborted

The Second Big Mistake with `free()`


```
int *p, i;
long long *q;

if ((p = malloc(sizeof(int)*n)) == NULL) { /*take action*/ }
// process some data
free(p);

if (!(q = malloc(sizeof(long long)*m))) { /*take action*/ }
for(i=0; i<m; ++i)
  p[i] = i - m;   // a typo!
//...
```

- Memory still there, but could have been reused!
- Or could have not been reused as well...
- Could appear to work, very difficult to catch
- Good advice: always zero a pointer after freeing it
  - Can be done “automagically” if you

    `#define free(ptr_var) (free(ptr_var), ptr_var = NULL)`

The Third Big Mistake with `free()`


```
typedef struct mydata {
  int n;
  double *somedata;
  int *moredata;
} mydata;

mydata *p = calloc(1, sizeof(mydata));
if (!p) { /* take action */ }

p->n = datasize;
p->somedata = calloc(datasize, sizeof(double));
p->moredata = calloc(datasize, sizeof(int));
if (!p->somedata || !p->moredata) { /* take action */ }

//input and process data

free(p);  // forgot something?
```

- Freeing `p`, `p->somedata` and `p->moredata` are gone, so we can't free their pointees, memory leak!
- Free `p->somedata` and `p->moredata` first, then `p`

Memory Friends from `string.h`

Function	Does
`void *memmove(void *d, const void *s, size_t len)`	copies a `len` bytes sized memory area from `s` to `d`, returns `d`
`void *memset(void *p, int val, size_t len)`	writes `len` copies of `(unsigned char)val` starting from address `p`, returns `p`

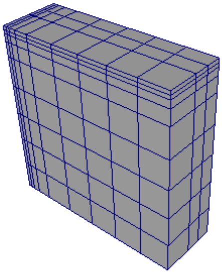
- You'll happen to encounter `memcpy()` too
  - Copies almost as `memmove()` does
  - If memory areas happen to overlap, `memmove()` is safe and does the right thing
  - While `memcpy()` could be faster, but is unsafe
  - Be prudent, and prefer `memmove()`
  - Surprisingly, `memmove()` is also faster in quite a few implementations!
- Way too common mistake: forgetting about and writing code doing the same
- Don't reinvent the wheel, use library functions!

Comfortable, and User Friendly


```
void my_pde_solver(int nx, int ny, int nz,
                   // physical parameters
                    ) {
//...
  double (*u)[ny][nz] = (double (*)[ny][nz])calloc(nx*ny*nz, sizeof(double));
  double (*v)[ny][nz] = (double (*)[ny][nz])calloc(nx*ny*nz, sizeof(double));
  double (*w)[ny][nz] = (double (*)[ny][nz])calloc(nx*ny*nz, sizeof(double));
  double (*p)[ny][nz] = (double (*)[ny][nz])calloc(nx*ny*nz, sizeof(double));

  if (u == NULL || v == NULL || w == NULL || p == NULL) {
    fprintf(stderr, "Not enough memory!\n");
    exit(exit_failure);
  }

  // solver code using u, v, w, and p in as humans do
```

- Now available memory is the limit
- And still easy to use

Nonuniform Grids



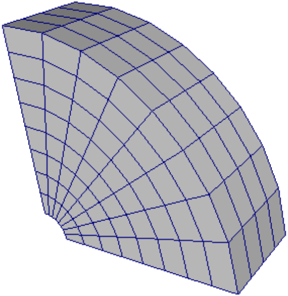
- Let's imagine we have to solve a PDE
- On a dense, Cartesian, non uniform grid
    - Mesh axes are parallel to coordinate ones
    - Steps along each direction differ in size from point to point

Keeping Information Together


```
typedef struct nonuniform_grid {
  int nx, ny, nz;

  double *deltax; // Grid steps
  double *deltay;
  double *deltaz;
} nonuniform_grid;
//...
nonuniform_grid my_grid;

//...

mygrid.deltax = calloc(nx - 1, sizeof(double));
mygrid.deltay = calloc(ny - 1, sizeof(double));
mygrid.deltaz = calloc(nz - 1, sizeof(double));
// Check immediately for NULL pointers!
```

- Related information is best kept together
- Grid size and grid steps are related information

Structured Grids in General Form



- Let's imagine we have to solve a PDE
- On a dense structured mesh
  - Could be continuously morphed to a Cartesian grid
  - Need to know coordinates of each mesh point

Sketching a Mesh Description


```
typedef vect3D meshpoint;
typedef vect3D normal;

typedef struct mesh {
  int nx, ny, nz;

  meshpoint *coords;

  normal *xnormals;
  normal *ynormals;
  normal *znormals;

  double *volumes;
} mesh;
//...
nonuniform_grid my_grid;

mygrid.coords = calloc(nx*ny*nz, sizeof(meshpoint));
mygrid.xnormals = calloc(nx*ny*nz, sizeof(normal));
mygrid.ynormals = calloc(nx*ny*nz, sizeof(normal));
mygrid.znormals = calloc(nx*ny*nz, sizeof(normal));
mygrid.volumes = calloc((nx-1)*(ny-1)*(nz-1), sizeof(double));
// Check immediately for NULL pointers!
```

- No VLAs allowed in structures
- Cast to VLA array pointer in functions using it

Multiblock Meshes and More

- A multiblock mesh is an assembly of connected structured meshes
  - You could dynamically allocate a `mesh` array
  - Or build a `block` type including a `mesh` and connectivity information
- Adaptive Mesh Refinement
  - You want your blocks resolution to adapt to dynamical behavior of PDE solution
  - Which means splitting blocks to substitute part of them with more resolved meshes
- Eventually, you'll need more advanced data structures
  - Like lists (and recursion comes handy)
  - Like binary trees, oct-trees, n-ary trees (and recursion becomes essential)

If You Read Code Like This...


```
struct block_item;

typedef struct block_item {
  block *this_block;

  struct block_item *next;
} block_item;

//...
   while (p) {
     advance_block_in_time(p->this_block);
     p = p->next;
   }
```

- It is processing a singly-linked list of mesh blocks
- You need to learn more on abstract data structures
- Don't be afraid, it's not that difficult

And If You Read Code Like This...


```
struct block_tree_node;

typedef struct block_tree_node {
  block *this_block;

  int children_no;
  struct block_tree_node **childrens;
} block_tree_node;

//...
void tree_advance_in_time(block_tree_node *p) {
   int i;

   for(i=0; i<p->children_no; ++i)
     tree_advance_in_time(p->childrens[i]);

   advance_block_in_time(p->this_block);
}
```

- It is processing a tree of mesh blocks (AMR, probably)
- You need to learn more on abstract data structures
- Don’t be afraid, it’s not that difficult

SuperComputing Applications and Innovation

Outline

What We Left Out (1 of 2)

- More preprocessor magic, like:
  - lots of predefined macros to automatically adapt your code to platforms and compilers
  - macros to write function with variable number of arguments
- More types, like:
  - extended integer types
  - wide and Unicode characters and related facilities
  - unions and bit fields, mostly used for OS programming
- More facilities to:
  - control the floating point environment
  - interact with the process environment
  - localize your program
- More facilities for robustness:
  - static and dynamic assertions
  - bounds checking functions for I/O and string management (C11 Annex K)
  - precise control of process termination

What We Left Out (2 of 2)

- More facilities for performance:
  - `inline` functions
  - control of data alignment in memory
- C11 threads support
- More functions
- More C practice
  - That's your job
- More about programming
  - Code development management tools
  - Debugging tools
  - Look among Cineca HPC courses

Looking for More

- ANSI WG14
  C Standard and Technical Corrigenda
  `http://www.open-std.org/jtc1/sc22/wg14/www/standards`
  `http://www.open-std.org/jtc1/sc22/wg14/www/docs/n1570.pdf`
- S. Summit
  comp.lang.c Frequently Asked Questions
  `http://www.c-faq.com/`
- D. Dyer
  The Top 10 Ways to get screwed by the "C" programming language
  `http://www.andromeda.com/people/ddyer/topten.html`
- S. Harbison, G. Steele
  C A Reference Manual
  Prentice Hall, 5th ed., 2002
- A. Kelley, I. Pohl
  C by Dissection: The Essentials of C Programming
  Addison Wesley, 4th ed., 2000
- A. Koenig
  C Traps and Pitfalls
  Addison Wesley, 1989

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Slides and examples were authored by:

- Michela Botti
- Federico Massaioli
- Luca Ferraro
- Stefano Tagliaventi