Computer Programming

An Introduction for the Scientifically Inclined

Sander Stoks

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Chapter 1
Computers

Where a calculator on the ENIAC is equipped with 18,000 vacuum tubes and weighs 30 tons, computers in the future may have only 1,000 vacuum tubes and perhaps weigh $1\frac{1}{2}$ tons.

Popular Mechanics, March 1949

1.1 Do You Need To Know?

Many programming teachers deliberately refrain from going into details about computer hardware. Their reasoning is that intimate knowledge of the way computers work actually hinders the development of a proper programming style. In fact, many prefer working with pencil and paper instead of even *using* a computer. A quote by Edsger W. Dijkstra, a famous Dutch computer scientist, is that "Computer Science is no more about computers than astronomy is about telescopes." This is why the term 'computer science' is rather misleading. Some people have therefore adopted the slightly different term 'computing science'.

But this book is not about computer science. Instead, it treats computers in the same way an astronomer might treat telescopes. It certainly makes sense for an astronomer to know how telescopes work, and understand the basics of optics. Computers to us are *tools*, and any craftsman will explain to you that a thorough understanding of your tools can be vitally important.

Another famous quote is that it shouldn't matter whether your programs are performed by computers or by Tibetan monks. While this is certainly true, 'we scientists' are not necessarily in the business of creating the most elegant programs that would thrill Tibetan monks reading them. Our job is to get some kind of calculation finished—preferably before our computation time on the faculty's super computer reaches our quota. When our methods to achieve that goal resemble fastening a screw with a hammer, so be it.

On the other hand, it is worthwhile to keep the Tibetan monk quote in mind. Because surprisingly often, the program that a monk would be happiest to perform, is also the best solution.

1.2 Hardware Overview

1.2.1 Processor

The 'brain' of a computer is formed by the *Central Processing Unit,* or CPU, also simply called 'the processor'. The CPU can actually only do surprisingly simple things, but it can do it very fast. What a CPU does is execute a list of instructions which it fetches from memory. These instructions form the so-called 'machine language'. They are the smallest 'building blocks' of a program. The atoms, if you will[1].

Examples of the kind of instructions a CPU can perform are 'retrieve the contents of memory location p', 'compare this value to zero', 'add these two values', 'store this value in memory location p', 'continue running the program from memory location p', etc. Everything more 'high-level' that a computer does, is expressed in lists of instructions of this very simple kind. Things like 'print this file', 'store these data on disk', 'check whether the user has pressed a key', or 'plot these data in a graph on screen' are totally alien to the CPU and need to be expressed in machine language programs that can be hundreds or thousands of instructions long. Don't worry though, you won't need to write those. We can use higher-level *programming languages* and *libraries* that provide an abstraction layer above the machine language level.

[1]Since you are an (aspiring) scientist, you may be wondering whether the equivalents of nuclear particles also exist, and yes they do. Internally, most modern processors actually have instructions on an even lower level, and the machine language is implemented on top of this.

Machine language is usually referred to as *second generation programming language*, the first generation being the actual (binary) codes. The translation of more-or-less human-readable instructions to the actual machine codes is done using an *assembler*. The human-readable machine language instructions are called *mnemonics*, because they are easier to remember than the actual codes. So, the assembler might translate an instruction like `ADD A,(HL)` into 10000110[2].

A *third generation programming language*, which is the type we will be focusing on here, offers an even higher level of abstraction with named variables, English-like syntax, etc., which would let you write instructions like '`print y`' or '`result = (1 + epsilon)*sin(x)`'. Translation of your third-generation program into something the machine can handle is done by either a *compiler* or an *interpreter*—we'll get back to this later.

Research on *fourth generation programming languages* is in full swing; these would let you write 'meta-programs' like 'Write me a program to calculate the energy levels in a single quantum well with variable parameters.' Unfortunately, we're not quite there yet.

Typically, a CPU has in the order of a few dozen to about one hundred different instructions. The first processors did not even have instructions to, say, 'multiply these two values'; instead, this needed to be explicitly implemented in lower level instructions (using repeated addition, for example). Although modern processors can have quite elaborate instructions that multiply vectors or compare two values and exchange them, the real power of processors is that they are *fast*. Typically, they can process millions of these instructions per second, with billions being no exception.

The speed of processors is often measured in Hertz. The value you often see quoted for a certain computer system is their *clock frequency*. One 'clock tick' is the smallest time slice a system can operate with. This is actually not a very good measure to compare different types of processors. The problem is that different

[2]Although the following trivia is totally irrelevant for the present text, the instruction in fact means "Add the contents of the memory location at the address given by the register `HL` to the accumulator register `A`" in the machine code of the Zilog Z80 processor, as found in the Sinclair ZX80 and later computers (most notably the ZX Spectrum and the Tandy TRS80).

types of instructions can take a different number of clock ticks to perform, so the clock speed is not trivially related to the number of instructions per second the processor can perform. There is a measure of processor performance called MIPS (million instructions per second) which for this reason is also known as 'meaningless indication of processor speed'.

1.2.2 Memory

Computers store, retrieve, and operate on data. These data are stored in some form of *memory*. To write efficient programs, it is important to understand that a computer has a form of memory *hierarchy*. There are different kinds of memory in a system, each with different properties.

The fastest kind of memory available to a computer are its *registers*. These are located in the processor itself, and can often be accessed in a single clock tick. Usually, the processor has relatively few of them available, in the order of only four to 128 or even 256 in more advanced processor architectures. Usually it is in the order of 32. The 'size' of these registers (determining the range of numbers they can store) is dependent on the architecture of the processor. For example, when a processor is said to be *32 bit*, the main registers of that processor are 32 bits in size, and it can usually address 2^{32} bytes of memory (hence 4 gigabytes is the upper limit of the memory size of a 32-bit machine).

The 'normal', or 'working' memory of a computer is called RAM, for 'Random Access Memory'. One can view memory as a (large) array of *locations* that can each store a *value*. The locations are numbered, and this number is called the *address* of the memory location. The smallest 'addressable' memory unit is the *byte*. Each byte consists of eight *bits* (binary digits).[3] These bits can have only two values: 1 or 0 (or 'on' or 'off', if you wish). Since a byte has 8 bits, it can store any integer value between 0 (all bits are 0) through $2^8 - 1 = 255$ (all

[3]Actually, this number needn't be 8. There have been computer systems with a 'native' word size of 7 bits, or even 6. You can quite safely assume that a byte is 8 bits, however, and if some wise guy wants to make you look stupid for making that assumption, ask him to show you a machine with a different number. A *working* one.

bits are 1). See section 1.3 about binary arithmetic if this doesn't make sense to you.

To handle larger numbers, bytes can be grouped together to form a 16-bit *word* (storing up to $2^{16} - 1 = 65\,535$) or a 32 bit *long word* (storing up to $2^{32} - 1 = 4\,294\,967\,295$). On 64-bit systems, there also is a *long long word*, combining 8 bytes.

It is dangerous to mention typical memory sizes since that will make this book look hopelessly outdated in only a few years' time, but at the time of writing, memory capacities of a few gigabytes[4] were becoming commonplace for personal computers. Multi-user systems in use at computer centers at universities can have (much) more, and capacities in the many gigabyte range are not unusual. 64-bit systems have been available for quite a while in 'scientific machines', and at the time of writing this book they were being adopted in desktop systems (and even laptops) as well. These systems can address more than 4 gigabytes of memory.

It is important to realize that RAM is relatively slow. Although memory technology progresses and memory is getting faster, processors have accelerated far quicker. Typically, retrieving the contents of a memory location in RAM takes in the order of 10 ns. Compare this to a clock tick cycle of 1 ns in a 1 GHz system. The processor would spend most of its time waiting for data to become available from memory.

To remedy this problem, *cache memory* was introduced. This is memory that acts as an 'intermediate'. It is fast (in the order of, say, 3 ns) but also far more expensive than 'normal' memory, and therefore a typical system has far less of it. The way it works is that it stores data as a buffer between the CPU and main memory. If the CPU asks for the contents of a certain memory location, the memory subsystem first checks to see whether it happens to be in the cache memory, and only retrieves it from main memory if not (and stores it in the

[4]In line with the base-2 'nature' of computers, the SI prefixes are used in a (slightly) different meaning. A 'kilobyte' is not 1000 bytes but actually 1024 (2^{10}) bytes; similarly, a 'megabyte' is 1 048 576 (2^{20}) bytes, etc. The only exception is the size of your hard disk, which vendors usually express using the SI prefixes (because that yields larger numbers which look better on their spec sheet).

cache too, overwriting 'older' data there). Since many computer programs look at the same data more than once, next time that data is requested a lot of time can be saved because it is still in the cache memory. Most computer systems have several levels of cache memory, usually 'level 1 cache' directly on the CPU, running at the same speed as the CPU itself (or, say, half of that), or 'level 2 cache' which is slightly slower (and cheaper, and thus larger). Typical values are to the order of 32 kilobytes of level 1 cache and a megabyte for level 2 cache. There is actually even more cleverness involved in the way cache memories work (for example, RAM often is more efficient if it is asked for the contents of several adjacent memory locations in one 'burst', so the memory subsystem could gather *more* data than it is asked for at the time and store it in the cache, based on the prediction that the CPU might need that data in the near future anyway). For more information, you can take a look at more specialized literature like [5].

Whereas cache operation is completely transparent to the programmer (*i.e.* you don't need to know it's there), programs can run much faster (up to an order of magnitude) if the program and the data it operates on 'fit' in the cache.

It is also quite important to recognize that the types of memory mentioned so far are *volatile*. That is to say, this memory only 'remembers' its contents while the system is switched on. Often, you would like to store data for a longer period of time. There are different types of memory which are *persistent*, such as a Indexhard disk, CD-ROM, or flash storage.

Typically, capacities of the persistent storage available to a computer system are far larger than the RAM size. Consumer-level hard disks have capacities in the terabyte-order. It also needs to be noted that this kind of storage is several orders of magnitude slower still than RAM. When you are operating on data sets that are really large (so they won't fit in RAM), this is something to take into account. For several areas of science (such as astronomy or experimental high-energy physics), huge data sets are the rule.

Hard disks come in two major flavors, IDE and SCSI. The former stands for 'Integrated Drive Electronics' and is traditionally common on personal computers, while the latter stands for 'Small Computer Systems Interface' and is the system of choice for multi-user or high-performance computers. Traditionally, IDE drives have been cheaper but slower, and SCSI has offered some nice advantages like being able to chain more devices together, and offer 'redundant storage systems' (*i.e.* store the same data multiple times, so that when one drive breaks down, the data is not lost). IDE has caught up quite nicely, and although the fastest and meanest disk drives are still SCSI, IDE suffices for most applications; especially with the advent of high-speed 'Serial ATA' (ATA is the 'official name' for what everyone calls IDE). Again, this difference probably does not need to concern you unless you are deciding on a hardware system for your specific experiment or calculations. If your application involves huge amounts of measurement data that need to be stored in real time, you should consider equipping your system with SCSI. For completeness, it should also be mentioned that SCSI is not limited to hard disks only, as there are other peripherals (like scanners) which connect to the system via SCSI, although this is superseded with USB and FireWire (see below).

1.2.3 Peripherals and Interfaces

Of course, there need to be ways to get information into a computer and ways to view results. Typically, a computer has several *input devices* like a keyboard or a mouse, and *output devices* like a monitor or a printer.

In experimental science, computers are often also used for controlling an experimental set-up, or for data-acquisition. For this, there are a variety of ways to interface ('talk') to the computer. For relatively slow connections, with data rates in the order of up to 10 kilobytes/second, it is often easy to use the *serial port*. 'Serial' means that the data bits are transferred one after another, as opposed to 'parallel', when multiple bits (mostly 8, or some multiple of 8) are transferred simultaneously. Obviously, a parallel port requires more physical wires. Traditionally, printers have been connected to computers using a parallel interface.

Most computers have several serial ports available which operate following the RS-232 standard. This is quite a popular interface because it is both well documented and relatively easy to implement with cheap off-the-shelf electronics, and runs at speeds up to 115 kilobits/second (230 or even 460 on some systems). As an example, most external modems work via this interface.

Incidentally, 'legacy' parallel and serial interfaces are slowly being replaced by more modern interfaces such as USB (see below). This has the benefit of not having lots of different interfaces which can each take at most one or two devices, having special interfaces for your keyboard, mouse, modem, etc. The drawback is that the modern interfaces are more complex and need integrated circuitry to connect, whereas the 'old' interfaces can easily be used in an experimental setup using an old-fashioned soldering iron and a simple wiring diagram.

On the other end of the spectrum are high-data-rate interfaces such as GPIB which require installing separate extension cards in the computer, driven by special software, but enabling far higher throughput. This is needed to do real-time readouts of oscilloscopes, for example, with sampling rates up to the order of 100 MHz or more.

In between of these extremes, there are interfaces such as USB (Universal Serial Bus) and FireWire (officially called IEEE 1394), which several more recent peripherals and/or measurement systems are supporting. These interfaces support 'hot-plugging', *i.e.* the peripherals can be connected and disconnected while the system is switched on, and are detected and configured 'on the fly'. There is a trend towards using ethernet as an interface to peripherals (especially more 'elaborate' devices); they often include a small embedded computer which is configurable via a 'web interface'.

It is important to note that often, measurement equipment produces data in *analog* form, which needs to be converted to the *digital* form which a computer can work with. Many data acquisition cards have analog-digital converters that can convert hundreds of millions of samples per second.

In a pinch, it is worth noting that a *very* cheap and easy-to-use digital-to-analog and analog-to-digital converter is present in almost any consumer-level personal computer in the form of its sound card. Whereas this is probably not suited for serious lab work due to the limited amount of sample frequencies it can work with and its resolution, it has been used successfully in a wide range of high-school or first-year science lab type experiments.

1.2.4 Networks and Clustering

To get more computing power, you could get a bigger computer, but you could also try to somehow connect multiple computers together in a network, forming a *cluster*. This approach doesn't always work; only when the specific calculations you need to do lend themselves to be split up in multiple, independent parts, which can then be calculated on separate computers. This is of no use when each of your calculations depends on the outcome of a previous one, since the computers in your cluster would spend their precious time waiting for another computer to finish its calculation, then do their part of the job, and finally hand off the result to the next. Also, there is considerable 'overhead' associated with splitting up the calculations. Network connections are slower than intra-computer connections, so sending lots of data back and forth is going to take a relatively long time. Only for large and time-consuming calculations involving relatively little data, it is worthwhile to use multiple computers.

Excellent examples of this 'distributed computing' on a very large scale are the 'SETI at home' project and the RC5 project. Both harness the 'spare computer cycles' of computers all over the Internet, using computers which their owners have registered with the project maintainers. The former project **s**earches for **e**xtra-**t**errestrial **i**ntelligence by handing out packets of radio frequency readings to (home) computers, which then run a data analysis program on it when they would otherwise be sitting idle, and send the results back to the project maintainers (and then receive a new set, etc.). The latter project was more of a 'proof of concept', and was successfully used to crack a certain encryption scheme by brute force which would have taken tens of years in a conventional approach.

On a smaller scale, computer animation as used in films is often performed on clusters of computers called 'render farms', comprising hundreds of relatively low-cost computers and dramatically speeding up the rendering process.

Also, it is quite customary for computers to have more than one CPU, or have CPUs which internally have multiple complete processing units (so-called *multi-core* processors). This is an especially cost-effective way of increasing computer power, as prices increase exponentially with CPU speed (and CPU designers are running into physical limits regarding their clock speed) whereas performance increases only linearly. Performance does not scale exactly linearly with the number of CPUs though, since there is an overhead as well. Depending on the nature of the calculation and on how well the hardware and the operating system can cope with multiple CPUs, adding a second identical CPU will yield anywhere between 1.5 – 1.9 times the performance. Also, this extra performance does not come 'free': The programmer will have to make specific adjustments to the program to make it use the available CPUs.

1.3 Binary Arithmetic

Whereas most people use the decimal system, computers use a *binary* system. In this system, there are only two digits: 0 and 1. In our day-to-day decimal system, we are used to the fact that the *position* of a digit within a number determines its 'weight' when determining the value. The rightmost digit designates the 'ones', the one immediately to its left the 'tens', then the 'hundreds', etcetera. Formally, the value of a decimal number of n digits, numbered from right to left (!) as $d_n \cdots d_2 d_1 d_0$ is

$$\sum_{i=0}^{n} d_i 10^i.$$

So, the interpretation of the number 3207 in the decimal system is (going from right to left): 7 times 10^0 (7), plus 0 times 10^1 (0), plus 2 times 10^2 (200), plus 3 times 10^3 (3000), equals three thousand two hundred and seven. This is so trivial you don't usually stop to think about it.

Quite similarly, in the binary system, the rightmost digit designates the 'ones', the one immediately to its left the 'twos', then the 'fours', etc. So, for a binary number the formal interpretation would be

$$\sum_{i=0}^{n} d_i 2^i.$$

As an example, the interpretation of the binary number 1101 is (again, going from right to left): 1 time 2^0 (1), plus 0 times 2^1 (0), plus 1 time 2^2 (4), plus 1 time 2^3 (8), equals thirteen.

In the same way that powers of ten form 'natural orders of magnitude' for (most) humans, so are powers of *two* the 'natural orders of magnitude' for binary systems.

There is another system in regular use in computing, which is the *hexadecimal* system (often simply called 'hex'). This is a base-16 system, so it has a few *extra* digits besides our usual 0 – 9. In the hexadecimal system, these are designated using letters:

Hex	Decimal
A	10
B	11
C	12
D	13
E	14
F	15

Hence, the hexadecimal number 3E8B is interpreted as 'B' times 16^0 (*i.e.* 11 times 1), plus 8 times 16^1, plus 'E' times 16^2 (*i.e.* 14 times 256), plus 3 times 16^3, equals sixteen thousand and eleven (16011 in decimal). To differentiate hexadecimal from decimal numbers, they are often prefixed with '0x' (that's zero-x) or postfixed with 'H'. The above number would then be written as either 0x3E8B or 3E8BH. The hexadecimal system is not actually used by the computer itself, but rather in computer programming because the relation to binary values is clearer than when decimal numbers are used.

1.3.1 Negative Values

In our decimal system, we have a 'special digit' which can only occur at the leftmost position in a number, and which designates negative numbers. The previous sentence is, of course, just a convoluted description of the minus sign. In the binary system, there is no such special digit, and so far we have only seen how to represent positive integers (or zero) in binary. Clearly, there is a use for negative numbers, and there are several ways to represent them. The most often used system is called *two's complement*. It uses one bit (the leftmost) as a *sign bit*, using 0 for positive and 1 for negative. Also, to negate a number, each 1 in the binary representation is replaced with a 0 and vice versa, and finally 1 is added to the result. The main advantage of this 'agreement' is that you can subsequently perform arithmetic on these numbers without having to treat negative values in a 'special' way.

So, to negate the 8-bit binary value 0010 1101, we would first get 1101 0010, and then add 1 to the result, getting 1101 0011. Using this system, the largest negative value representable in 8 bits is -127 in decimal: 'minus' 0111 1111 becomes 1000 0001. The largest positive value is then 128 decimal; anything larger would have the 7th bit and another bit set, which would make it be interpreted as negative.

Therefore, it is important to realize that seeing only the digits of a certain binary number, say 1101 0011, doesn't tell you whether this number represents 211 or -45.

Incidentally, there is another system called *one's complement* in which a negative value is simply formed by inverting all the bits (*i.e.*, without adding one). This system has the drawback that there are two ways of representing 'zero', namely 'all bits cleared' but also 'all bits set'. The latter would correspond to 'minus zero'. This ambiguity has led to the adoption of two's complement instead in the majority of systems.

1.3.2 Floating Point Numbers

Apart from integer numbers of various sizes, computers can also work with *floating point numbers*, often simply called *floats*, or, in some computer languages, *reals*. It is quite important for scientific programming to realize that computer reals are not 'real' reals, in that they have a *finite* precision. More on that, and why it is important, in the next subsection.

The way a computer stores floating point values is rather clever because it allows a wide range of values to be stored in the same number of bits. Of course, to us scientists it is actually nothing new, as we often use a similar trick when dealing with either very large or very small numbers: We note a certain factor (with a certain precision) and add 'times ten to the power of n'. For floating point values, the computer simply divides the available space in two parts, and stores the factor (called the *mantissa*) in one part, and the exponent in the other. Both are signed with a single bit. Most systems offer two or even three varieties of floating point number types, with increasing numbers of bits available for increased accuracy, in a tradeoff for memory requirements and/or execution speed.

1.3.3 Range and Accuracy

For the integer types (bytes, words, and long words) it is quite obvious that there is a limit to the actual value they can store. Trying to store 70 000 in a 16-bit word simply won't fit. Nor will 40 000 in a 16-bit signed word. Trying to do so anyway will result in the computer signaling an error condition called *overflow*. What specific type of variable you will need to use in your programs to prevent this phenomenon looks to be simple enough at first sight. However, you must realize that this limit also has an effect on *intermediate results*.

As an example, consider you are writing a program to calculate the average distance to the sun for all the planets of our solar system. You decide to use integer variables (just for the sake of the argument), and since a quick glance at the distances table learns that the average probably comes out at about 2×10^9 km, you decide that it is safe to use 32-bit, unsigned integers (since these can hold over 4×10^9).

Now, depending on how you write your computer program, you might still run into trouble. If you would do it the 'naive' way, by simply adding up the various distances from the sun for each of the planets, and finally dividing by nine to get the average value, an overflow will occur during the calculation. This is because the *sum* of all these distances is close to 1.6×10^{10} km, and that intermediate result *doesn't fit*, no matter whether you are going to be dividing it into something more manageable later on.

Of course, the correct thing to do in this rather contrived example would be to use floating point values. They are called 'floating point' for a reason: when the value grows 'too big', the exponent changes to keep the mantissa within range. You can view it as if a float value 'resizes to fit'. For most systems, even the smallest type of floats can vary between 10^{-37} and 10^{+38}, and the mantissa has 24 digits of precision. If that is not enough, there is usually a 'double precision float' (or simply 'double') available, that often goes from 10^{-308} to 10^{+308} with 53 digits of precision.

However, it is important to realize that floats have a *finite* precision. For a human, the question 'how much is $10^{100} + 1$?' is just as easy to answer as 'how much is $10^{10} + 1$?' or 'how much is $10^{200} + 1$?'. For the computer, though, these pathological numbers pose a problem. Because they are big, the exponent shifts to make room (or 'the point floats', if you will), but adding that 1 will then be problematic because there is not enough precision left. This results in the somewhat disturbing conclusion that to a computer, $N + 1 = N$ for sufficiently large N.

It is quite important to keep these anomalies in mind when designing scientific computer programs.

1.3.4 Rational and Complex Numbers

Although some computer languages also have a special type of variable for storing complex numbers, many do not. This was added to the C standard relatively late (and not all compilers support it yet). This is one of the reasons scientists usually scoffed at computer scientists trying to sell them C over FORTRAN (which has had complex numbers for ages, as well as high-precision floats). We will see that it doesn't *really* matter as you can add your own types to most serious programming languages (including, in a limited and somewhat concocted way, C).

A more fundamental issue is that computers tend not to know about rational numbers. To a computer, $\frac{1}{2} = 0.5$, no matter how much the difference has been beaten into our heads at school (saying that $\frac{1}{2}$ is 'infinitely precise' and that 0.5 represents anything between $0.4500\cdots$ and $0.5499\cdots$). The computer cannot accurately represent $\frac{1}{3}$, for example. That means that there are fundamental rounding errors that could possibly cause trouble. This phenomenon is investigated later in this book.

Now, it needs to be said that with clever programming, one *can* make computers work with rational numbers (in fact, they can do algebra just fine). This has even appeared in the realm of handheld calculators. But at the lowest (hardware) level, the most advanced type of numbers a computer 'knows' about are floats (or possibly vectors of them, in more modern machines).

1.4 Operating Systems

The operating system your scientific program runs on is usually even less of an issue than the particular computer hardware. There is one notable exception which is in experiment control, which is why we will briefly dwell on the subject.

The first (big) programmable computers were quite literally 're-wired' for each new program. The operator would plug in cables, like an old-style telephone operator. Later, computers were re-programmable more easily by reading the programs from punch cards. These computers were operated in *batch mode*. That is to say, the programmer would write a program (usually in a low-level language at that time), get it punched in a stack of punch cards, and hand this to the computer operator. When it was this program's turn to run, the operator would load the program into the computer, run it, and when it was done, collect the output and run the next one.

This method of running computers turned out not to be the most efficient one, since when a program was loading a large data set off a (relatively slow) storage medium, the CPU would just sit there, twiddling its expensive thumbs waiting for that operation to finish.

With the advent of faster and larger memory, computers could hold several programs in memory at once, and 'switch' between them. *I.e.,* when one program would issue a ‘slow’ operation, the computer would pay attention to another program while, for example, the disk was loading the requested information into memory for the first program. Once that was done, the computer would switch back to the first one. This ensured that the CPU was always running at full throttle.

Running several programs ‘at once’ (note that it wasn’t *really* ‘at once’, but rather ‘small parts of them in rapid succession’) introduced all kinds of other problems—for example, when one of the programs would have an error in it, say, overwriting the contents of random memory locations, other programs running along with it could be influenced by that, producing erroneous results, even though they were themselves fully correct.

Another problem is that of *limited resources*; suppose two programs request a chunk of memory for intermediate results 3/4 the size of the total memory. Were each of these running on the machine alone, this would not be a problem. But when running on the same machine simultaneously, the second program trying to get the requested chunk of memory would somehow have to be either told this failed, or suspended until the first program finished with it. The same goes for multiple processes requesting access to, say, a plotter or printer connected to the computer.

So, gradually the *operating system* expanded from a simple scheduler for various jobs, into a complex system taking care of memory management, resource allocation, etc. It also provides a variety of services to programs, such as ‘abstracting’ various types of computer hardware (so that your program does not need to know exactly what kind of sound card the computer system has, or what video card, etc.), and provides support for showing your program’s output in a window on screen, which the user can move, resize, etc. It also takes care of file management on the computer’s hard disks, provides network connections (to other machines on your local network or to the Internet), and much more. It is safe to say that for the vast majority of computers nowadays, the operating system itself is probably the most complex piece of software running on it.

Usually, an operating system tries to be as *transparent* as possible, *i.e.* programs would spend most of their time running as if they were the only program on the system, apart from some ‘agreements’ that a program never accesses hardware directly, but always ‘asks’ the operating system for it (to prevent the *limited resources* problem mentioned above), etc.

However, there are some situations in which it is important to realize that running on a system together with other programs imposes subtle differences with having the system all to yourself. Suppose the computer is being used to drive some kind of experimental set-up in which some apparatus is controlled, and some measurement data needs to be collected a certain amount of time after an event occurs. There are plenty of examples for such a set-up, such as firing a laser into a cell containing a gas mixture, and reading an image from a CCD camera exactly x milliseconds later.

Now, your computer program might in broad lines be structured like this:

1. Fire laser
2. Wait x milliseconds
3. Read data from camera

which looks easy enough. However, if the operating system decides to interrupt your program after it has just fired the laser, then turn its attention to several other jobs running on the same computer (for example, because you have moved the mouse, or because some network activity was detected and the computer needs to store incoming data somewhere, or whatever else might be going on on your computer), and only returns to your experiment-driving program a couple of milliseconds later, the data read in from the camera would be ‘stale’.

Because of this problem, there exists a special class of operating systems called *real time operating systems*, which make certain *guarantees* about how long certain operations will take at most. In such an operating system, you could ask to wait *exactly* x milliseconds, and while the system would be free to do other stuff in that time span, it *guarantees* it will return to your program within that limit.

While this all may seem rather trivial, it is surprising how many experiments are driven using a computer running an operating system that is thoroughly unsuited for that task.

For an excellent text on operating systems, see [6].

1.5 Specialized Machines

It is worth mentioning that there are specialized computers that can do a certain type of operations very efficiently. For example, some computers have special arithmetic units that can perform calculations on whole vectors at a time. In many areas of science, vector (and matrix) calculations form an important part of daily life, and thus a machine which can speed up these calculations can save a lot of time. Another example is *parallelism*, *i.e.* having multiple CPUs running simultaneously.

Some of these ‘extras’ are handled transparently to the programmer by the operating system (for example, by scheduling different concurrent processes to various processors) or by the specific programming language used or the compiler used to translate it to machine code (for example, the compiler might recognize that you are doing vector arithmetic and could insert built-in machine code instructions for these). However, sometimes the programmer needs to specifically use these advanced features.

Although it is outside the scope of this book to dwell on these specialized subjects too long, it is worth noting that several of these features, which used to be strictly the domain of high-end computers, are finding their way to the user desktop as well. Machines with two or more processors in them are available off-the-shelf (although it is not unusual for high-end computers to have 64 processors or even more), and many processors have used ideas from vector-processing systems in their instruction set, usually under the name of ‘multimedia extensions’ or some-such.

1.6 Synopsis

Whereas designing your programs as machine-independent as possible will generally result in more elegant programs, blatantly ignoring the features and limitations of computers could result in inefficient programs, or even incorrect and unexpected results.

This chapter gave a brief overview of computer hardware and operating systems, and pointed out some pitfalls to avoid when designing scientific programs.

Also, computer arithmetic and native data types were explained, along with some caveats as to precision and range of them.

1.7 Questions and Exercises

1.1 Write your birth year in binary and hexadecimal notations.

1.2 Most processors have specialized circuitry for performing multiplications, and the specific values of the operands of a multiplication do not make much difference in the speed at which the operation is performed. However, 'older' computers could multiply by a factor of 2^n significantly faster than by a factor of, say, 3^n or 7^n. Can you explain why? Hint: can you multiply by a factor of 10^n faster than by a factor of 3^n or 7^n?

1.3 To get a feeling for data acquisition and the data rates involved, calculate how many bytes per second are transferred when capturing audio at CD quality (which is sampled at 44.1 kHz, 16 bits per sample, stereo). Could this be transferred over a serial connection as mentioned in §1.2.3, without any compression techniques?

Chapter 2

Programs

The process of preparing programs for a digital computer is especially attractive, not only because it can be economically and scientifically rewarding, but also because it can be an esthetic experience much like composing poetry or music.

Donald E. Knuth

2.1 Computer Recipes

To explain what a computer program is, invariably the metaphor of a recipe comes up. This metaphor is quite bearded, but since it also makes good sense, we'll add a few hairs to the beard.

At a low level, when a computer 'runs a program', it basically just executes a list of instructions, just like a cook might follow the instructions on a recipe. This metaphor describes only a certain kind of programs, since there are other, more modern 'paradigms' of programming. However, programs written using these other styles are ultimately converted to lists of instructions for the computer to execute, and a large part of scientific programming challenges can be adequately tackled using this paradigm.

So, let us take a look at a typical student recipe.

Noodles

Ingredients

- 1 plastic cup of dried noodles
- optional: 1 sachet of sauce (probably inside the plastic cup)
- water

Preparation

- Open plastic cup of dried noodles
- Remove sachet of sauce from the cup, if it's there
- Boil a sufficient amount of water
- Pour boiling water into the cup up to the designated fill line
- Close the plastic cup
- Wait 3 minutes
- Add the sauce
- Stir
- Wait another 2 minutes
- Stir again
- Add some more hot water if desired
- Enjoy! (Wine suggestion: Chateau Lafitte)

Now, although this recipe might appear very simple, there are quite a few things that can be remarked about this example. First and foremost, note that this recipe is a procedure to produce a desired output (a delicious and wholesome meal) from a specific set of ingredients, neatly listed at the top, via a well-defined set of steps.

Secondly, the recipe involves making *decisions* based on *tests*—even if they are not spelled out. One test, for example, would have been 'Prod in the noodles after the designated amount of time, and see whether they have the desired structure. If they don't feel right, add some more water' instead of just 'Add some more hot water if desired'.

Thirdly, and perhaps most importantly at this stage, notice how the recipe does not explain *everything*. For example, it just says 'Boil a sufficient amount of water', and not 'Place a sufficient amount of water in a kettle, put the kettle on the stove, take a matchbox, strike the match against the box until it lights, turn the gas knob, light the gas under the kettle, wait until the temperature of the water reaches 100°C.' It is assumed here that the chef knows how to boil water. This might seem a trivial observation, but it is a most important concept. A recipe explaining *everything* (imagine having to explain how to operate the tap to put water in the kettle—all the way down to describing the motor muscle control in the chef's hand when turning the knob on the tap) would quickly be far too long to be usable. This would be equivalent to the 'machine language' mentioned in the previous chapter.

Similarly, a recipe not explaining enough is of little use either. For example, while an experienced chef might find an instruction like 'serve with hollandaise sauce' totally adequate, a student cooking all by himself (or herself) for the very first time might be at a loss when the recipe says 'fry an egg'. If the student runs into something like 'serve with hollandaise sauce', there had better been a separate recipe for hollandaise sauce somewhere in the cookbook.

So, an important lesson here is that a recipe (and a computer program) is written with a certain 'assumed knowledge'. You don't explain everything every time; you explain it once, and then refer to it. Given recipes for noodles and for hollandaise sauce, you could easily combine these into a recipe for noodles with hollandaise sauce—preferably not by *copying* the respective recipes, but by saying something like

Noodles with Hollandaise Sauce

- Prepare noodles
- Prepare hollandaise sauce

- Put noodles in a bowl
- Add hollandaise sauce
- Mix thoroughly
- Enjoy!

The ‘Prepare noodles’ and ‘Prepare hollandaise sauce’ are instructions of a higher level than the others, because they refer to other recipes. A similar thing is very common in computer programs. Even if specific ‘sub-tasks’ are only used in one place in a program, it can be quite useful to ‘break them out’ into separate parts of the program, because this makes the core of your program much more readable and gives a nice overview of what the program is supposed to do.

2.2 A Real Program

Enough with the metaphors; without further ado, let’s proceed with a ‘real’ program. The following program lets you type two numbers and prints out the sum. It is written in BASIC, which stands for Beginners’ All-purpose Symbolic Instruction Code. BASIC is one of the earlier programming languages, and is not considered suitable for any ‘real work’. However, its syntax is closer to ‘plain English’ than that of C, and we’ll compare the equivalent program in C in a while.

```
PRINT "Please enter two numbers"
INPUT a
INPUT b
LET c = a + b
PRINT "Their sum is "; c
END
```

It is almost possible to read this as a recipe written in plain English. Even if this is the very first time you’ve seen a program, you can probably guess what it does. We'll walk through the program explaining what everything does in detail below.

What you see here is a list of 'statements' (or 'commands'), one per line. In older BASIC dialects, every line had a line number. In more modern ones, this is not necessary. The line number also functioned as a 'label' and you could change the 'flow' of your program by using a `GOTO` *line number* command, after which the program execution would continue at the specified line. The use of `GOTO` is religiously frowned upon by computer scientists, because it facilitates a programming style which is affectionately known as 'spaghetti code'.

The `PRINT` command simply prints what comes after it to the screen. In this case, the text after it is surrounded by double quotes to denote that it is a *text string*, *i.e.* a piece of text that should be printed verbatim to the screen without further interpretation by the computer.

Next come two lines with `INPUT`. As you have probably guessed, these ask you to enter something into the computer. The little `a` and `b` are *variables* – just what you'd expect them to be. So, the numbers you type to the computer (closed with Enter or Return, or whatever your computer keyboard calls it), are stored in the variables named `a` and `b`. Variables are of the floating point type by default in BASIC. How the computer denotes that you are expected to enter something is implementation-specific; on some systems and dialects of BASIC, it might print out a question mark; on others, it might just flash a blinking cursor at you.

Next comes a line containing the `LET` command. What it does is assign the value of the expression `a + b` to the new variable named `c`. In most dialects of BASIC, you can actually leave out the `LET` command, so the line would just read `c = a + b`.

Then, the value of `c` is printed to the screen. You see that the text string '`Their sum is`' is followed by a semicolon, which in most BASIC dialects means 'more data follows, and you should print the rest on the screen immediately following what you just printed'. Had it been a comma, there would have been a 'tab' spacing on screen. Forget about these details though. What's important is that, since `c` is not surrounded by quotes, it is interpreted to be a variable, not a text string, and its value is printed to the screen.

Finally, the last line says that the program ends here. This particular statement is also not always needed – most BASIC dialects understand that the end of the program is denoted by the end of the text.

To actually execute this program, you'd have to find a computer with a BASIC interpreter, key it in, and type `RUN`. Yesteryear's computers of the 'home computer' crop, like the Sinclair ZX Spectrum or the Commodore 64, had a BASIC interpreter built in, so immediately after switching on the system, you would be able to key in our little program (each line prefixed with a line number, though), and run it.

2.3 The Same Program in C

At first glance our little program, now written in the computer language C (which we will use for the remainder of our book), will perhaps look rather intimidating compared to the friendly BASIC. Don't worry; although we won't do a similar walk-through as we did in the previous section, you will shortly be able to understand the details. For now, if you can vaguely recognize the main characteristics, you'll be fine.

```
#include <stdio.h>

int main(void)
{
    float a, b, c;
    printf("Please enter two numbers: ");
    scanf("%f %f", &a, &b);
    c = a + b;
    printf("Their sum is %f\n", c);
    return 0;
}
```

The first thing you have probably noticed is that the C program looks more 'complicated' than the equivalent BASIC one. There are more strange characters (percent signs, number signs, curly braces, and ampersands), and every statement ends in a semicolon (this means you are free to put multiple statements on the same line, each terminated with a semicolon, but that is considered bad programming style because it makes your programs harder to read).

This 'syntactical complexity' is one of the main complaints many people have against C as a first language, but 'power comes at a price' and once you have a firm grasp of the language, you can write compact and powerful code. Also, many languages developed after C have 'borrowed' this syntax style, including the curly braces to delimit 'scopes' (more on that later), the semicolon, the function call syntax with a comma-separated list of arguments between brackets, etc. Knowing C, you can read programs in a variety of other programming languages as well.

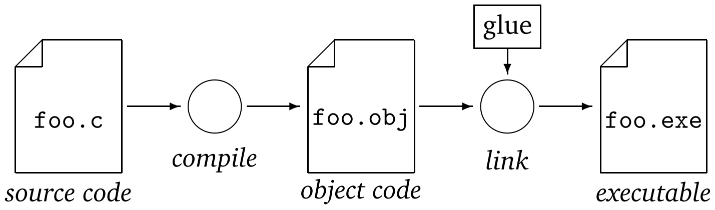
2.4 Running Your Programs

By now, you are probably interested in actually running a program on a computer. Unfortunately, the precise steps required to do this vary quite a bit from one system to another. You will need a computer system with a C compiler installed (if you don't know what a compiler is, don't worry: you will two paragraphs from now). It falls outside of the scope of this book to expand on various compiler flavors, and we will limit our treatment of C as much as possible to ANSI C, which should run on any system.

Since you are probably interested in what goes on exactly when you make your computer run one of your programs, we will briefly go over the various steps here. This is necessary to get your first experimental C program running on your system, and some of the details will become more important later. Once these steps are defined, we will finally type up our first little C program, compile it, and run it. That's a promise.

Since the term *program* is used to mean both the code you typed and the final, runnable program, we will introduce some precise terminology here to eliminate confusion. By *source code*, we mean the program 'text' as you type it. This doesn't mean much to the computer. It's just a text file, and it cannot be executed. Instead, you use a special program called a *compiler*, which translates your source code to *object code*. Finally, a second program called a *linker* massages your object code, along with some 'glue', into an *executable* which can run on your computer system. The final product is also called a *binary*. The entire process is sometimes called *building* a program. It is worth noting that your source code is (strictly speaking) machine-independent, whereas your object code is tied to the specific machine you compiled it for.

In general, the process to build a program can be visualized with the following figure:



The file extensions in this figure have been chosen from the Windows system. On UNIX systems, the default extension for object files is `.o`, and executables usually have no extension at all.

Basically, getting a running program requires the following steps:

1. Type in your source code
2. Compile it to object code
3. Repeat the above steps until the compiler can't find any more errors
4. Link the object code to form an executable program
5. Execute the program.

For now, you can view the compile and link steps as one. For programs consisting of a single file (the majority of our programs, and in fact quite a large number of programs as used for scientific calculations), the compile and link steps are actually done with a single command.

Let us now finally type in our first program. The precise steps needed to compile and run it will be specified below for both a Microsoft Windows system and a generic UNIX system. So, open up your favorite text editor, and type the code below. Be wary of typos, because most will cause your compiler to 'emit scary warnings'. Also, note that I said 'text editor' and not 'word processor'. It is important to understand that a C program is just a regular text file, and there's nothing 'magical' about it. On the other hand, if you use a word processor (such as Microsoft Word), usually there are 'hidden' control codes embedded in your document (for instance, to specify the layout of the text, whether a certain phrase is in italics, etc.) and these would confuse the compiler. On Windows, you could use Notepad, for instance (crude though it is); if you're using a UNIX system you probably have a favorite plain-text editor already. There are many programming-oriented editors on either platform, and many good ones are even free. A quick Google for 'programming editor' or something like that should give quite a few hits.

```
#include <stdio.h>

int main(void)
{
    printf("Hello, world!\n");
    return 0;
}
```

After you've made sure you typed in your program exactly as shown above, including the weird `#` character and the semicolons, save this file under the name `hello.c`. It is a general convention to designate C programs by appending a `.c` extension to the file name, and there are operating systems which get hopelessly confused if you do not comply, so it is best to stick to it.

Don't worry if you don't understand all the details of the program. The occurrence of a `\n` character at the end of your greeting, and the curly braces, and the `int`, `void`, and `return` stuff – it is all explained in the next chapter. This is only to get something happening on your computer, and to get the pesky details about building programs on your particular systems out of the way.

Now, you have entered your program into your computer, but you cannot run it.

You can email it to some Tibetan monks to admire, or compile it for execution on your own computer. We will assume you will want to do the latter. Depending on whether you are working on a UNIX system or on a personal computer with Windows, you can find below how to compile (and link) this program.

2.4.1 Building on Windows

If you have a computer with Microsoft Windows and have Developer Studio (MS Visual C++) installed, there is a compiler available under the name `cl` ('cee ell', not 'cee one'). This is a C++ compiler, but it also compiles 'plain' C. To be able to run this compiler from the command line (*i.e.* from a DOS prompt), you need to set some paths correctly. This is easily done by running the `VCVARS32.BAT` batch file, which comes with MSVC. It can probably be found at a location like `\Program Files\Microsoft Visual Studio 8\VC\bin\VCVARS32.BAT`, but the actual location may vary. If you have installed MSVC yourself, you are probably more than smart enough to find it. If you are working on a system that is remotely administered, there are probably some people in your organization who get paid to help you find it. Depending on how Developer Studio was installed, there may even be a handy shortcut in the Start menu to launch a command prompt window with the paths already set up correctly.

Once you've run this batch file in a command prompt window, you can then run `cl hello.c` (assuming you are in the directory containing your `hello.c` source code), which will invoke the compiler on your little program. It will perform compiling and linking in one go, and generate `hello.exe` in the same directory, which is the executable program. In the process, the compiler will generate a `hello.obj` file, which is the object file. You can safely throw this away; it is re-built every time you compile your program again.

If you are using MSVC, you can switch on the maximum warning level using the `/W4` switch:

```
cl /W4 hello.c
```

This is a good habit, and you should always compile at the maximum warning level. In §2.6 we will talk about these warnings.

By the way, if you indeed have Developer Studio installed, there are easier ways to edit, build, and run your program. Developer Studio is actually what is called an 'Integrated Development Environment' (IDE), and you can invoke the compiler with a keyboard shortcut. The editor does 'syntax highlighting' (it will give keywords it recognizes a certain color, which is a nice aid to catch typing errors while editing, since if a keyword in your program is spelled wrong, it will not get the color you expect). Also, it helps you find errors by jumping directly to the line in which the error occurred.

If you're using Developer Studio, you can use the 'project wizard' to set up a new project. For all the examples in this book, you should pick 'empty console project', which will set up a new project without filling in any code. You can also select 'Hello World project', but that would be cheating. If you select 'Run' from the appropriate menu, it will automatically re-build the executable if you have edited the code since the last time it was built. We'll get back to features like this in chapter 10.

Note that there are several other C compilers available for Windows, which vary wildly in price, performance, and quality. Some have different licensing options for non-commercial use, or offer special academic discounts. Examples are the Digital Mars compiler, the Intel compiler, and the Borland compiler. A quick Google for 'free Windows C compiler' may turn up some interesting results.

2.4.2 Building on UNIX Systems

Most vendors of UNIX systems ship a compiler with their system. Usually, you can invoke it with the `cc` command. On some systems, typing `cc hello.c` will actually only compile, but on most, it will also link the executable for you as a convenience. If not, you will have to link it yourself. In this case, you will find that the compiler generated a `hello.o` file, which is the object code for your program. To link this into an executable, you will need to invoke the linker. On some systems, this is also done with the `cc` command; often you can specify the name of the resulting executable with a `-o` switch, so you would type `cc -o hello hello.o`. On other systems, the linker has to be invoked with `ld`. You will need to do some experimenting to find out what the exact incantation for your particular system is. Sometimes, the name of the resulting executable will be `a.out` (for historical reasons) if you do not specify a name yourself.

Incidentally, there are actually some freely available UNIX-like operating systems out there such as Linux or FreeBSD. These often come with GCC, for 'Gnu Compiler Collection'. This includes an excellent C compiler. GCC is also available for many other operating systems, such as BeOS, and can even be installed on a Windows machine (with some extra effort – Google for 'MinGW').

With Mac OS X, you have access to a free-of-cost development environment as well (called Xcode), which is based on GCC.

If you are using GCC, it is a good habit to specify the `-Wall` flag, which turns on all warnings (we'll get to these warnings in §2.6). So the example above would be

```
  cc -Wall -o hello hello.c
```

In chapter 10, we will take a look at some more advanced software building tools, in case your computer programs span several files. For the most part of this book, programs will usually be small enough to fit in one single `.c` file.

2.4.3 Running Your Hello World

To execute your first masterpiece of programming, simply type its name at your command prompt (you may have to prefix it with `./` if you're on a UNIX system). Your computer will run your program, and the text 'Hello, world!' should appear in all its glory.

While you are still all proud and warm and fuzzy, let us take a short detour and look at programming languages in a bit more detail. After that, we will take a look at what would have happened if you were unfortunate enough to make a typing error in your program. This would most likely have caused the compiler to complain with an error, which we will examine in the section after the next.

2.5 Programming Languages

We have now seen a similar program in two programming languages, BASIC and C. There are *lots* of programming languages, each with their own pros and cons. In general, you can divide programming languages in two broad categories; languages which are *compiled* and languages which are *interpreted*.

During the above paragraphs on how to build and run your program, you may have observed that there are quite a number of steps to take before you can actually run your program. Especially when you are making small changes to your code to see what effect they have on the program, it is a nuisance to continually have this cycle of 'edit, save, compile, link, run', and it would be nice to have a more 'interactive' way. When working like this, interpreted languages are nice. They don't need to be compiled and linked; instead, there is a 'runtime' which reads the program source and executes it line-by-line as it goes along. Examples of programming languages that work this way are BASIC and most scripting languages (most notably javascript). The latter is often used in small web-based applications since it can be embedded in a web page. In this case, the 'runtime' is part of your Internet browser.

There are two major drawbacks to interpreted languages. One is speed; you always have the overhead of the interpreter itself. For this reason alone, nobody uses interpreted languages for any significant scientific work. The other is that a compiler actually provides a first 'sanity check' on your code. If you make a typing error, for example typing `prinft` where you mean `printf`, the compiler will catch that (see next section). In an interpreted language, it will only be found at run time. In a program with considerable complexity, the typo may be in a line which gets executed rarely – meaning your program can be running fine for days, and suddenly stop. Also, for the same reason, it is hard for interpreted languages to implement *type-safety* (more on that later).

The most common languages compiled to machine code are Pascal, C, C++, and FORTRAN. Traditionally, the former is used in programming courses because it is clean, strict, and verbose, leading to structured and well-behaved programs. FORTRAN is the language of choice for many scientific programmers because it handles complex numbers natively and treats matrices and vectors as 'first class citizens', has millions of lines of code available in scientific libraries for many applications, and because the raw performance of its compiled code has always been the mark to beat for other languages. Unfortunately, it is also diagonally opposed to Pascal in imposing 'arbitrary' constraints on the way you write your code (actually, *because* of some of these constraints it can optimize so aggressively), leading to code which is hard to understand and maintain. With newer FORTRAN 'dialects' like FORTRAN90, many of these drawbacks are no longer there. Unfortunately, FORTRAN compilers are not nearly as ubiquitous as, say, C compilers.

There are also languages which are a bit of both. Most notably Java (which, despite the name, has nothing in common with javascript) and C# (pronounced 'C-sharp') are compiled, yet not to native machine language but to an 'intermediate' code which runs on a 'virtual machine'. Apart from only having to compile your programs once and being able to run this 'pseudo' machine code on multiple platforms (as long as there is a virtual machine available for that particular platform), it has the added advantage of only allowing a subset of what one would allow a 'real' program. For instance, one can deny such virtual machines any write-access to your hard disk. These kind of programs are often used as 'applets' you can download via the web.

C was traditionally intended for 'systems programming'; for writing, say, an operating system. It originally lacked scientific niceties such as the built-in complex type of FORTRAN, and it allows far more 'direct to the metal' programming than Pascal. This sounds like C is 'worst of both worlds'. The nice thing about C though is that you can write programs which are (nearly) as performant as FORTRAN programs, you can see 'what's going on' in terms of how the computer will actually do things (which would be considered a drawback to most 'purists' but without which a typical science student would be left with nagging questions), and that C compilers are everywhere. *Every* serious computing platform has a C compiler available, and C has become the 'lingua franca' of computers. Some would say this places it in the same category as Latin or Ancient Greek: Interesting for historical reasons, but not used anymore 'in the real world'. On the other hand, mastering these languages can be a great help when learning modern languages. The same goes for C: many more recently designed computer languages borrow heavily from C. Also, C continues to be used for many current projects, among which are some of the most high-profile computer programs in the world (such as the Linux kernel and many applications running on it).

Lastly, C++ is an 'extended version' of C which allows for *object oriented programming* and *generic programming*, both of which are outside the scope of this book. For most scientific type of programs, neither way of programming adds many benefits. A nice thing to note is that any valid C program is also a valid C++ program.

At certain points in this book, we will compare how other languages handle the concepts just introduced. If you are not interested in other programming languages or you are afraid you will become confused, you can skip these sections without missing anything important.

2.5.1 Variations in C

C is not the youngest of languages, and since its inception has undergone a few changes. The first major version of C was marked by the publishing of a book (in 1978) by its inventors, Brian Kernighan and Dennis Ritchie. After their names, this version of C is called 'K&R C'. There was no formal standardization of the language, and various implementations interpreted the book in slightly different ways. When the popularity of C grew (borrowing back features from C++ in the process), it became clear that a proper standard was needed, and the resulting version is usually referred to as 'ANSI C' or 'C89'. Kernighan and Ritchie updated their book to reflect this new standard ([2]). This book is highly recommended and can usually be obtained rather cheap, since book stores figure that a computer book this old can't be worth much anymore.

In the late 1990s, the C standard was revised again by an ISO committee, and the resulting standard is usually called 'C99' (the official document is ISO/IEC 9899:1999) because the standard was ratified by ISO in 1999.

Most compilers support C99, but not all compilers support it entirely. Therefore, the examples in this book will be based on C89 as much as possible, with a note explaining if anything changed in C99.

2.6 Errors and Warnings

Computer programs need to conform to a rather strict syntax for the compiler to understand them. It is important to note that the compiler can not catch any *semantic* errors. There are even compilers who will say 'None of the errors found' when successfully compiling a program. To understand the difference more closely, take a look at the following programs.

```
#include <stdio.h>

int main(void)
{
    float a, b, c;
    a = 10;
    b = 3.1415;
    c = a + b;
    printf("The sum of a and b is %f\n", b);
    return 0;
}
```

Even if you can't follow all the details (which is understandable, especially for the `printf` statement), you should see that it prints out '`The sum of a and b is` followed by the value of `b`, instead of `c`. This program, however, is perfectly legal C and no compiler will complain. The compiler cannot know that this program prints out something silly. Semantic errors like this are also sometimes called *bugs*: the program is 'correct' according to the compiler, but doesn't produce the intended result.

Now, if you have made a *syntax* error, the compiler will be able to produce an error message, usually telling you what it was expecting, and where in your source code the error occurred. The format of these error messages is not standardized, and they vary wildly between compilers.

For example, take the following program:

```
int main(void)
{
    float a, b, c
    a = 10;
    b = 20;
    c = a + b;
    return 0;
}
```

Apart from the fact that this program doesn't really do anything useful (since it doesn't print out the result of the calculation), note that there is no semicolon at the end of the first line. In C, all statements must end with one, so this is a syntactical error. Let's try to compile it anyway (forgetting semicolons is one of the things beginning C programmers do all the time, so it's better to get used to it).

Trying to compile it might give an error message like the following:

```
error.c: In function ‘main’:
error.c:4: parse error before ‘a’
```

Note that it mentions the file it was working on (in this case, we assumed that the source code was in a file named `error.c`), what function it was working on (we'll get to this in the next chapter), and even what line it was on (line 4) when it encountered a 'parse error'. Your actual compiler output may vary, but it is typical that it didn't say something like 'missing semicolon on line 3'. In C, statements may span multiple lines, so for all the compiler knew, everything was fine and dandy at line 3, and only when it suddenly found that 'a' at the beginning of line 4, it suspected something was wrong. So a first tip when getting rid of syntax errors is to check out the preceding line(s) of your program.

Also, it is worth noting that a single mistyped line can mess up the compiler's understanding of all the code below it, in a sort of 'domino effect'. So, don't get scared if you get an enormous list of errors the first time you compile your program. It may well be that they all disappear once you fix the first one.

Apart from errors, the compiler can also emit warnings. In case of a warning, the compiler can continue compiling your program, but found some code which it found 'suspicious'. Most compilers let you specify a warning level (where a higher level means that it will be more verbose in venting its opinion about your code). *Always* compile at the highest warning level, and never ignore the compiler's warnings. After all, it knows quite a bit more about C than you do, and if it detects something fishy, you'd better take a second look.

Different compilers generate different warnings. Some people even use several different compilers on their code, each at maximum warning level, and only rest once none of these compilers finds anything to warn about.

Now that we have basic knowledge about building and running programs, let us cover the fundamentals of the C programming language in more detail. This will be the subject of the following chapter.

2.7 Synopsis

This chapter gave an introduction to computer programs, and how to compile and build them into executable binaries on different computer systems. You have met the 'hello world' program, saw an overview of various programming languages, and had a brief introduction to compiler errors and the difference between syntactic and semantic errors.

As many other languages, C is what is called a *compiled language*. A program written in C cannot be directly executed by the computer. It must be *compiled* (translated from *source code* into *object code*) and *linked* (combined with some 'glue' and made into a proper executable for this particular computer system) before it can be run.

2.8 Questions and Exercises

2.1 Insert some deliberate syntax errors in a program and try to compile it. Examine the error messages your C compiler gives you. Can you easily find the location of the error in your source file?

2.2 Would it be feasible to try and build a compiler which could detect semantical errors?

Chapter 9
Simulations

What happens if a big asteroid hits earth? Judging from realistic simulations involving a sledge hammer and a common laboratory frog, we can assume it will be pretty bad.

Dave Barry

9.1 Virtual Experiments

In science, theory and experiment are two equally important facets in trying to understand the world around us. On the one hand, experiments are devised to test certain hypotheses. On the other hand, sometimes experiments yield results which call for a new theory.

In many cases, experiments can be performed 'in real life'. Ideally, one can perform a series of trials varying only a single parameter, and establish a correlation between this parameter and the observed behavior. An example would be dropping a series of balls from a certain height, all with the same dimensions but having a different mass, to see whether its mass has any influence on the time it takes for a ball to hit the ground. Another example would be determining the solubility of some solid in a liquid as a function of the temperature, or letting a series of seedlings grow in varying lighting conditions to observe the effect of light on plant growth.

In many other cases, experiments are not so easy to do. Imagine an astrophysicist wanting to test a theory on the behavior of colliding galaxies. One can't simply 'set up' such an experiment, and if there doesn't happen to be any astronomical data available for such an event, the scientist is more or less ‘out of luck’.

When this astrophysicist is willing to make some assumptions though, such as ‘galaxies are so enormous and so sparse that their individual stars can be thought of as having their mass concentrated in a single point’, and ‘stars adhere to Newtonian gravitation mechanics’, he could sit down with a stack of paper and *calculate* what would happen. For ‘simple’ systems of interacting particles, this is quite feasible. However, even when there are only a few particles involved, this rapidly becomes undoable. Let alone when we are dealing with hundreds of thousands of particles, each interacting with all the others.

Here, computer simulations can help. In this chapter, we’ll look at a few ‘computer-simulated experiments’. First, a word of caution. When performing experiments ‘in the real world’, if you forget a certain important aspect in your hypothesis, your experiments will most likely prove it wrong (unless you forget *two* important aspects which happen to cancel each other out). In a computer simulation however, if your program is wrong, your results will be wrong. Sometimes this can be on purpose: ‘Suppose we eliminate the effects of friction, what would happen?’ But sometimes this is simply an error, rendering the entire experiment meaningless. It is therefore often advisable to start out with a setup for which the outcome is known, so you can at least check whether your simulation is in accordance with reality for that particular case before heading off in unexplored territory.

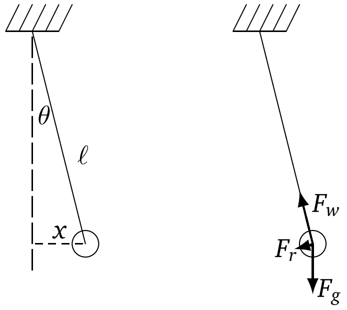
There won’t be many new language features treated in this chapter, but with the material covered so far you can already write quite a few useful scientific programs.

9.2 A Pendulum

In this section, we will examine a *pendulum:* a mass suspended on a wire, swinging back and forth. This is a nice first example, because it is straightforward to derive an analytical solution to this problem in the case of ‘relatively small’ amplitudes. This makes it possible to compare the simulation results with the 'known' solution before extending the simulation to areas where the analytical solution is considerably more difficult.

9.2.1 Analytical Derivation

Consider a mass m suspended on an (inelastic, mass-less) wire of length ℓ. The earth pulls on this mass m with a gravitational force $F_g = mg$, and when it is in 'resting position', this force is exactly cancelled by the pulling force in the wire F_w. When the mass is moved out of its center position by a distance x, the gravitational force and the pulling force in the wire no longer cancel, and there is a remaining force F_r pulling the mass back to the center position. This is shown in the figures below.



Simple trigonometry shows that $F_r = -F_g \sin\theta = -F_g x/\ell$. The mass will be accelerated by $a = F_r/m$, and since $F_g = mg$, the end result is that $a = -gx/\ell$.

Now, for small θ (*i.e.*, when the pendulum is moved only a little bit from its resting position before it is let go), we can ignore the fact that a and x are not entirely parallel, and simply state that

$$a = \frac{\mathrm{d}^2}{\mathrm{d}t^2}x(t) = -\frac{g}{\ell}x(t),$$

which is a familiar differential equation: Some function $x(t)$, twice differentiated, yields the same function again but with a minus sign and some factor. We know the solution to such a differential equation: the sine (or cosine) function. It is more natural in this case to take the cosine, since at $t = 0$ we are releasing the pendulum from a nonzero starting position x_0:

$$x(t) = x_0 \cos\left(\sqrt{\frac{g}{\ell}}\, t\right).$$

It is usually surprising to physics students when they first find out that the mass of the pendulum has no influence on its frequency (which is $\frac{1}{2\pi}\sqrt{g/\ell}$), nor does its initial position x_0.

9.2.2 Numerical Simulation

We will characterize the pendulum by its position x and its velocity v (still pretending that the problem is essential one-dimensional). To visualize the position of the pendulum, we will use some crude graphics:

```
void print_pos(double x)
{
    int i;

    if (x > 39 || x < -39)
        return; /* position doesn't fit on screen */
    for (i = 0; i < 40 + x; ++i)
        printf(" ");
    printf("*");
}
```

Assuming a screen width of 80 columns, this routine prints an asterisk at the position of the pendulum (so we are limited to positions ranging from −39 to 39, putting the ‘resting position’ in the middle of a line). Note that the function does not print a ‘newline’ character (`\n`) after the asterisk, which you might have expected – we’ll see why below.

The ‘body’ of the simulation consists of an endless loop which uses the function above to print out the current position of the pendulum and then updates its position and velocity:

```
int main(void)
{
    double length = 200;
    double g = 9.8;
    double x = 38;   /* initial position */
    double v = 0;
    while (1)    /* endless loop */
    {
        double Fr = -g*x/length;
        print_pos(x);
        v += Fr;
        x += v;
        getchar();
    }
    return 0;
}
```

When you run this program, a new value is calculated (and displayed) each time you press the enter key. You'll have to exit the program by pressing Control-C or Control-Break (depending on whether you are on a UNIX system or a Windows system). Since pressing the enter key normally also causes a newline to be displayed on screen, we didn't have to do this ourselves in in the `print_pos()` function.

The output on screen after a few runs should look somewhat like this:

```
                                                             *
                                                            *
                                                         *
                                                     *
                                               *
                                          *
                                   *
                            *
                      *
               *
          *
      *
  *
 *
*
  *
    *
        *
              *
                   *
                          *
                                 *
                                       *
                                              *
                                                   *
                                                       *
```

This looks quite nicely like the expected cosine wave.

9.2.3 Extending the Simulation

In the current model, the pendulum will keep swinging forever. In reality, this is not so, and that is mainly due to friction of the mass as it passes through the air surrounding it.[1] Therefore, let's extend our model of the pendulum to include friction.

The mass at the end of the pendulum experiences a frictional force which is proportional to its velocity squared:

$$F_f = \frac{1}{2} C_f A \rho v^2$$

where C_f is a constant depending on the shape of the object (the factor car designers try to get as low as possible), A is its area perpendicular to its direction of movement, and ρ the density of the medium the element is passing through. For our purposes, we can simplify this by combining all the constants:

$$F_f = C v^2$$

where C becomes another parameter of our model.

Now, we modify the expression calculating the acceleration by subtracting the frictional force from the force exerted by the neighboring elements, and using this new resulting force instead:

```
    double Fr = -g*x/length;
    double Ff = C*fabs(v)*v;
    double Ft = Fr - Ff;
    v += Ft;
```

The function `fabs()` returns the absolute value of its `double` argument. It is part of the standard C library and can be used by including `math.h`. We've seen how such a function could be implemented in §4.1.

[1]This is not the *only* reason; a pendulum in vacuum still doesn't keep swinging *forever* as it loses energy due to internal friction as well. We will ignore this effect because it is much smaller than the air friction.

We use this function because otherwise the resulting friction force would always be positive, in which case negative velocities (*i.e.*, the pendulum moving 'to the left' in our case) would experience an *extra* acceleration due to friction, instead of a deceleration.

Setting C to about 0.02 gives a nice 'dampening' effect.

Before moving on to the next section, it is probably a good idea to take a look at the first few exercises at the end of this chapter. Especially question 9.4 is important, since it deals with an important limitation of numerical simulations.

9.3 Random Values

In §3.6, an example was given of a function with a return value but without any parameters. The example there was a `random()` function, and such a function exists indeed. The function `rand()` returns a (pseudo) random integer value between 0 and `RAND_MAX` (the definition of `RAND_MAX` is in `stdlib.h`). Of course, it is impossible to 'calculate' a random value, so this is *pseudo* random: making clever use of the characteristics of the way numbers are handled in computers, including their overflow behavior, the result of successive calls to `rand()` are a series of numbers which are *in principle* deterministic, but which *appear* to be random. For *real* random values, there should be a hardware device connected to the computer which delivers the values. You can even order CD-ROMs containing millions of random values, which were taken from physical random generators. For many purposes, however, pseudo-random values suffice.

Often, it is easier to deal with floating-point random values in the interval $[0, 1)$; for this, you can use the macro[2]

```
  #define frand() (rand()/((double)RAND_MAX + 1))
```

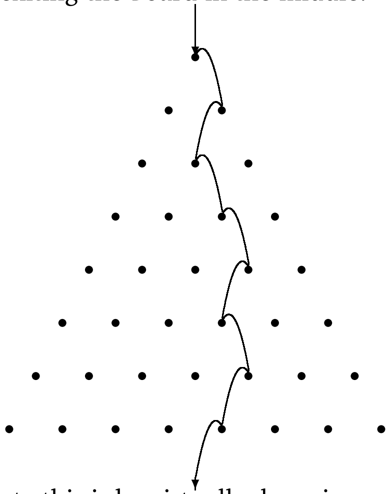
We will use this function to simulate a 'marble board': Take a wooden board and hammer in nails in the shape of a triangle, with one nail at the top, two on

[2] In the original K&R book, this macro is defined slightly different, but the version presented here works also on systems where `RAND_MAX` is equal to `INT_MAX`.

the second row, three on the third, etc. (see the figure on the next page). Then, drop a series of marbles from above onto the topmost nail. Each marble will bounce on the topmost nail, either fall to the left or the right of it, then bounce on one of the nails on the second row, bounce to its left or its right again, etc. When it finally reaches the bottom of the board, each marble has made left or right bounces as many times as there are rows in the board.

Given enough marbles and a big enough board, the resulting positions at which the marbles drop off the board at the bottom form a *Gaussian distribution:* If the nails are placed at the exact right positions, the chances of bouncing either left or right are equal, and the chances of ending up near the middle of the board, after an approximately equal number of 'left bounces' and 'right bounces', are much greater than the chances of making only left bounces and ending up at the far left of the board, or only right bounces and ending up at the far right. This is used in several games of chance, of which the 'pachinko' variety is very popular in Japan.

The figure below page shows a 'marble board' with 36 nails, and one possible trajectory of a marble exiting the board in the middle.



The way we will simulate this is by virtually dropping marbles, making a series of 'left-right' decisions using the `frand()` macro we have just seen, and noting the current position as we go. We will use a similar trick to draw the resulting distribution on the screen as we used in the pendulum simulation of the previous section. We will place a virtual row of 'bins' below the virtual marble board in which each dropped marble ends up, by increasing the value in in an `int` array corresponding to the 'bin' the marble ends up in, and we will use a (large enough) number of experiments to build up the probability distribution.

First, let's set up the distribution to be all-zero using a fixed number of 'bins'. This number is a measure of the size of the marble board, and it is a parameter of our simulation. Since we will use a similar trick to display the resulting distribution as we did in the pendulum example in the previous section, we'll pick a number which nicely fills one screen-full.

```
#include <stdio.h>
#include <stdlib.h>

#define BINS 24
#define N_EXPERIMENTS 400

#define frand() (rand()/((double)RAND_MAX + 1))

void draw_distribution(int distribution[], int size)
{
    int i, j;
    for (i = 0; i < size; i++)
    {
        for (j = 0; j < distribution[i]; j++)
            printf("*");
        printf("\n");
    }
}

int main(void)
{
    int distribution[BINS];
    int i;
    /* clear the initial distribution */
    for (i = 0; i < BINS; i++)
        distribution[i] = 0;

    /* perform the simulation a number of times */
    for (i = 0; i < N_EXPERIMENTS; i++)
    {
        int j = BINS;    /* j tracks the current position */
        int k;

        /* "walk" the marble board */
        for (k = 0; k < BINS; k++)
        {
            if (frand() < 0.5)    /* flip a virtual coin */
                j++;    /* take a right */
            else
                j--;    /* take a left */
        }

        /* note where the marble exited */
        distribution[j/2]++;
    }

    draw_distribution(distribution, BINS);

    return 0;
}
```

The chances of `frand()` returning less than 0.5 are 50%, so we are giving equal probabilities to either a left-bounce or a right-bounce. Note that we start out with `j = BINS` and we increase the distribution at `j/2` at the end of each simulation, instead of starting out at `BINS/2`, the 'real' center position, and increasing the distribution at bin `j`. This is because `j` is either increased or decreased at each bounce and never stays unchanged, meaning that depending on the number of bins we use, either only the even bins or only the odd bins get filled, resulting in a distribution with 'holes' in it.

If you run this program, something like the following distribution should appear on your screen:

```
*
***
*******
******************
******************************
************************************************
************************************************************
********************************************************
********************************************************
************************************************
****************************************
*****************
************
****
```

This approaches the familiar bell-shaped Gaussian distribution (tipped on its side). However, if you run the program again and again, you may notice something interesting: You get the same curve each time! How is this possible, given that the decisions are supposed to be random?

The reason is that the `rand()` function returns *pseudo*-random numbers, as was mentioned at the start of this section. The algorithm behind `rand()` works by 'remembering' the previous value returned, and in each successive call performing a calculation using this number which causes an overflow, so that the resulting new number appears to be unrelated to the previous one. However, the calculations are the same each time, so if a series starts out with a certain value, called the *seed* of the random generator, the resulting series of pseudo-random numbers will be identical. At each program start, the seed is reset to the same value, hence you'll get the same random series each time you run the program.

Sometimes this is desirable, because this way you can 'replay' an experiment; but in this case, we'd rather have new results each time we try the simulation. We can arrange this by setting the seed ourselves (using the `srand()` function). The problem is that we need to figure out a different seed each time we run the program, so we are facing a 'chicken-and-egg' problem! There is no use calculating a random value for this seed, because that random value will be the same every time we run the program...

One thing which *does* change from run to run is the current *time*. Most computer systems have an internal clock, and C offers functions to read out its value, often in the form of a single integer number representing the number of seconds passed since the 'beginning of time', for example January 1st, 1970 – an arbitrary choice, and not even the same one on every system, but that doesn't matter as long as it is a different value each time we run the program. If we `#include <time.h>`, we have the function

```
time_t time(time_t *tp);
```

It returns the current time[3]. If `tp` is non-`NULL`, the current time is also assigned to `*tp`. By using this value as the seed of our random generator, we can get a different series each time we run the program. Simply adding

```
srand(time(NULL));
```

to the beginning of our simulation makes sure we see different distributions at each program run, unless we run the program quicker than the granularity of `time_t`. On most systems this is one second.

Incidentally, the `time.h` header file also makes available a whole range of other time-related functions, including functionality to convert a `time_t` value to a human-readable 'calendar' string, and for dealing with time zones and daylight saving. More information will be given in §12.3.4.

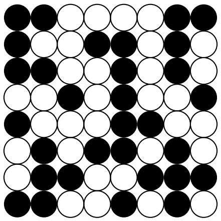
Finally, it is worth noting that many systems offer a random generator with significantly better statistical properties than the simple `frand()` macro we were using here. For some situations, this can be important. For example, for the simulation of this section it wouldn't be too much of a problem if the random generator had the property that every, say, tenth 'coin flip' would always be the opposite result of the one immediately preceding it, as long as the chances for 'heads' or 'tails' would be approximately equal for the rest of the coin flips.

[3]Officially, it may return -1 if there is no system clock available on this particular system, but unless you are on a really exotic or ancient system, this is not an issue.

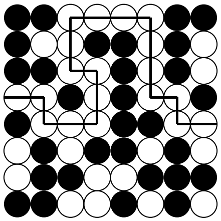
However, you wouldn't use such a random generator to run an online casino, because such a 'pattern' would soon be found out and taken advantage of.

9.4 Percolation

In this section, we will use simulations to examine a class of phenomena known as *percolation*. In the most elementary sense, the problem consists of finding a set of connected locations (*i.e.*, a pathway) through a medium. Let us start with a 2D example in which we have an equal-spaced grid. On each grid location, there can be a 'pass-through' or a 'block'. The distribution of these is determined by a single parameter: the chance of there being a 'pass-through' at any given location. In the figure below, a small 8×8 grid is shown, where open circles denote the 'pass-through' locations, and closed ones denote the 'blocks':



This particular grid has 31 blocks and 33 pass-throughs, so apparently the pass-throughs were distributed with approximately 50% probability. Below is the same grid, but with a pathway shown which connects the left side of the grid to the right side:



The goal of our simulation is to find pathways like these automatically, and figure out what the chances are of such pathways existing as a function of the distribution of 'pass-throughs' in the grid. We know by common sense that a pass-through distribution probability of 0 yields a zero chance of finding any pathways, and a probability of 1 gives a 'completely open field'. What the curve in between looks like is interesting, and this is the subject of this section.

This may seem like frivolous 'maze-solving', but there are interesting real-world applications in which similar situations apply. For example, if the 'pass-throughs' represent conducting particles and the 'blocks' represent insulating particles, then simulations like these help figure out what the chances are that a certain mixture of conducting and non-conducting particles is electrically conducting as a whole. Another example is to estimate the probability of a certain thickness of a porous, foam-like material with a certain density being airtight.

To do the maze-solving part, we will use the recursion concept treated in §4.9 along with a new 'trick' called *backtracking*.

First, we will set up the grid. We like to print out the resulting solution to the screen, so we take a grid size which nicely matches the screen. We fill a two-dimensional `int` array (see §5.4). At each grid position, a zero means a block (or a non-conducting cell, or a piece of solid material in a foam), and a 1 represents a 'pass-through' (or a conducting particle, or an air bubble). We will first look at a program generating and displaying a single grid:

```
#include <stdio.h>
#include <stdlib.h>
#include <time.h>

#define WIDTH 79
#define HEIGHT 24

#define frand() (rand()/((double)RAND_MAX + 1))

void draw_grid(int grid[][WIDTH])
{
    int i, j;
    for (i = 0; i < HEIGHT; i++)
    {
        for (j = 0; j < WIDTH; j++)
        {
            if (grid[i][j] == 0)
                printf(" ");
            else
                printf(".");
        }
        printf("\n");
    }
}

int main(int argc, char *argv[])
{
    int grid[HEIGHT][WIDTH];
    int i, j;
    double chance = 0.5;
    if (argc == 2)
        chance = atof(argv[1]);
    srand(time(NULL));
    for (i = 0; i < HEIGHT; i++)
    {
        for (j = 0; j < WIDTH; j++)
        {
            if (frand() < chance)
                grid[i][j] = 1;
            else
                grid[i][j] = 0;
        }
    }
    draw_grid(grid);
    return 0;
}
```

If you run this program a few times with different probability values, you will get a feeling for the 'density' of such grids.

Incidentally, the loop filling the grid could have been written a lot more compact (and cryptic) as

```
      for (i = 0; i < HEIGHT; i++)
          for (j = 0; j < WIDTH; j++)
              grid[i][j] = (frand() < chance);
```

See §4.3 about boolean expressions if this doesn't make sense straight away.

Now for the 'meat' of our simulation: automatically finding out whether there is any pathway from the left side of the grid to the right side.

Looking at this problem with recursion in mind, the notion of a 'pathway to the right side' can be formulated a little differently: *A certain grid point is part of a pathway to the right side if at least one of its neighboring grid points is part of a pathway.* In other words: *You can reach the other side of the grid from a certain point if you can reach the other side of the grid from one of its neighbors.*

Therefore, we will simply walk along all points on the left side of the grid, and determine whether any of these fulfills the descriptions above. If so, we can stop: we needn't find *all* pathways nor the shortest.

Let us construct the recursive function to do this 'pathway check'. First, let's define its return value: It should be zero if it's not part of a pathway, and one if it is:

```
  int percolate(int grid[][WIDTH], int i, int j)
  {
      if (i < 0 || j < 0 || i >= HEIGHT)
          return 0;    /* invalid position: fell off the grid */
      if (i >= WIDTH)
          return 1;    /* we have reached the right side! */

      if (grid[i][j] == 0)
          return 0;    /* we ran into a block */

      /* check whether our neighbors are part of a pathway    */
      if (percolate(grid, i, j + 1)    /* right neighbor?     */
       || percolate(grid, i, j - 1)    /* or the left one?    */
       || percolate(grid, i + 1, j)    /* or below us?        */
       || percolate(grid, i - 1, j))   /* or above?           */
          return 1;  /* If so, we're part of the pathway too  */
      /* otherwise, this is a dead end */
      return 0;
  }
```

It may be strange to see four recursive calls of the same function, but you are free to make as many as you like. It can be mind-boggling if you try to perform this ‘in your head’, but the compiler does a good job of it so you don’t have to.

The bottom part of the function performs the test we described above: If we aren’t on a block, and one of our neighboring grid points is part of a pathway, then we are part of a pathway too. The top part of the function makes sure we don’t run off the grid, and takes care of stopping the recursion when we reach the other side of the grid. Be sure to let this function ‘sink in’ for a while, perhaps using the example grid presented earlier in this section, and see whether you can develop a good feeling for how this algorithm works.

It may be helpful to keep the following analogy in mind. Suppose you are dropped at the entrance of a maze, and your task is to say whether this maze has an exit. Further suppose that you have the capability of splitting off identical clones of yourself. One way to solve your task is to split off a clone of yourself and send him into the maze, with simple instructions:

1. At each junction in the maze, pick one corridor for yourself and send clones of yourself into the others, giving each of these clones this exact list of instructions
2. report back at the previous junction when you either run into a dead end or find the exit
3. when you arrive back at the previous junction, wait for all your clones to arrive there too and ‘re-join’ with them into a single entity again, remembering whether you or any of your clones has found the exit, and finally
4. report back at the previous junction.

When a clone returns to his spawning point, he can either report that "one of the paths I just came from reaches an exit" or "none of the paths I just came from reaches an exit". Finally, the first clone you split off comes walking out of the maze and reports to you whether *any* of his clones has found an exit.

With the help of the analogy, perhaps you can also find the fatal flaw in this algorithm before reading the next paragraph.

This algorithm will quickly end up in infinite recursion. Why? Because a clone cannot determine whether a certain maze junction has been visited before. One of the clones is bound to reach a junction already visited, split off new clones, and send them off following 'older clones'. In fact, one of them will run into the very corridor his 'parent' just came from! Clearly, recursion alone isn't enough to solve this task.

Enter *backtracking*. This is the computational equivalent of the fairy tale of Little Thumbkin, leaving a trail of bread crumbs on his way through the forest. What we have to do is *mark* the grid points we've already visited. Below is a modified version of the `percolate()` function which does just that.

```
int percolate(int grid[][WIDTH], int i, int j)
{
    if (i < 0 || j < 0 || i >= HEIGHT)
        return 0;
    if (j >= WIDTH)
        return 1;

    if (grid[i][j] == 0)
        return 0;

    /* have we visited this point before? */
    if (grid[i][j] > 1)
        return 0;  /* in that case, don't bother continuing */

    /* Mark this grid as visited */
    grid[i][j] = 2;

    if (percolate(grid, i, j + 1)
     || percolate(grid, i, j - 1)
     || percolate(grid, i + 1, j)
     || percolate(grid, i - 1, j))
    {
        /* mark as visited AND part of a pathway */
        grid[i][j] = 3;
        return 1;
    }

    return 0;
}
```

We need to modify the `draw_grid()` function a bit to deal with these 'marked' grid points:

```
  void draw_grid(int grid[][WIDTH])
  {
      int i, j;
      for (i = 0; i < HEIGHT; i++)
      {
          for (j = 0; j < WIDTH; j++)
          {
              if (grid[i][j] == 1 || grid[i][j] == 2)
                  printf(".");
              else if (grid[i][j] == 3)
                  printf("*");
              else
                  printf(" ");
          }
          printf("\n");
      }
  }
```

Below is a typical output of the program with a pass-through density of 0.7:

```
 . .... ......... .... .... ... . ... ...... . .... ...... .. .  ..... . .....
.... ... .. .......   .   ... ......... .... . ..... .. .  ....  ..     ... ....
......  . .... ....   . .  ..... .. ............. .. ...........  . ... . ... ..
   . . . ......... ... .... ..  . .......... ....... ..... .  .....  . . .. ....
    .  ..    . . ... ..  .. . ... .. .  .  . .. .   . . . ..   ...  .......... .
********* . ...   ..... .  .. ... .... ............ . .. .. .. ... ..   ...  ...
. ... ..**. . .  ...... ......   .... ...........  .. . . .. ..... . .  ... ..
........ *   ..... .  ..  . ....     ..  ...... . ******* ...  .......... .....
   ......** .   . . . .. .. ......  ... ... ..  ..*** . ****   ......... .. .  ..
  .. .  ..******  ... ... .............  ...   ..***.   .. ************* . ....
.. ...  .. . ..**  ..  ... .  ... . .... ... ....****    .. ..  ... .  ** .*****
.....  .**** ****. .... ..  ....... ......... ...  ***   .... ***********   *   .
. . ..  ** *** .. .  ..... . ............. .... . .** . ..   .**   ........*.. .
..  .... *.   .. .  .... .. ....... ... .  . . ...*** . .. . .** .. .  ..***  .
........ * .   .. . .. . . .. . ...... .........***  ......   *. .. .. . *** . .
 . . ....****** .. ....... ..    . .... ******  .. . ...  ** .... *******.. .
... ........  *  ..  . . ....********** . **  ... .. .. . .  .****.   * .. .. ..
... ...... ...***. .... .. . **** ...*****  ... . .........   ** . **.   . ..
 ....... .. ... *  ... .....*****   ......  ...  . .. ... . ****. ..*    .    ..
 ......... . ...** .......** ****  ............  ... . ... .*** ..  ***.. .....
 ..... ...... ...** ...... **** **. ..   ... . ..  ... ..  ...**  ... ** .. .. .
. .. ....  ....  .***********  **  .......... ...... . . .  ..*********. . . .
............. ........   ...****  .... . ... .  ....  ........ ... . ..  ......
 .... .  ....... .. ....  ..... . ...... .. .......  .. ....  .   ... .  .......
 ......   .. ... .. ... .........  .... . . ...  ... . . . .. .. .. ..... ..
```

Note that the code above simply finds the *first* pathway, not necessarily the shortest. For our current experiments, we aren't particularly interested in the length of the pathway; just in whether there *is* one.

There are several questions and exercises at the end of this chapter, starting with exercise 9.7, in which the simulation of this section is used to examine some interesting properties of these grids.

As a final note: we are using an `int` array for the grid, and this is a bit 'overkill' since we only use four different values for each grid position (out of the four *billion* values available for an `int`). For the grid size we've been considering, this is not an issue. However, on many systems the amount of memory available on the stack is limited to a much smaller size than heap memory (memory available through `malloc()`, see page 147). If you are running the simulation with larger grids, or extend it to examine three-dimensional grids, you may get a compiler error that the `grid` array is getting too big for the stack. In that case, you could modify it to use `char`s instead of `int`s, which will buy you a factor of four. Ultimately, you will need to modify the program to work with dynamically allocated memory (see §5.7).

9.5 Synopsis

This chapter presented several 'real-world' examples of simulations and computer experiments. In all cases, it is important to find a mapping of a real-world situation to a model which is suitable for computer simulations, *i.e.*, a *discrete* model. It is important to realize that this discretization step has some implications to the reliability of the simulation, and there is often a trade-off between speed and accuracy. For an accurate simulation, you'd rather take very small discretization steps, requiring many iterations of the algorithm, and which may get 'stuck' due to 'underflow': The differences in each step are so small that they get lost in the limited precision of the computer. For fast results you would use large discretization steps, with the risk of 'overshoot' where the simulation may 'explode'.

In many simulations, *random behavior* is required. Since 'generating random numbers on a computer' is a contradiction in terms, you normally have to settle for *pseudo-random* behavior. The computer can generate a series of numbers which *appear* to be random; the quality of the random generator is measured by how easy it is to spot certain 'patterns' in the sequence of numbers.

A certain class of problems can be tackled by using 'maze-solving' algorithms. Here, an important extension to *recursion* is *backtracking*, in which the recursive search for solutions is augmented by marking which solutions have already been examined, and 'reversing the steps' once it turns out that a certain path doesn't lead to a solution.

A simulation using only 'first principles', is called an *ab initio* experiment. It can be dangerous to interpret the results of such simulations because you must be sure you haven't left out any important effects. In a 'real' experiment, you usually assume that the measurements are right – if they don't stroke with your hypothesis, it is quite likely that the hypothesis is incomplete. In a computer simulation, there may be other effects to deal with, like limited precision, overflow or underflow, or even simple miscalculations.

9.6 Other Languages

C was not designed with scientific simulations in mind, but the language does lend itself quite nicely to such experiments. For some experiments, an object-oriented language (see §6.5) might be more suitable, because you can directly map concepts of the real-world situation to classes of objects in the language.

Most languages offer sufficient mathematics support for most experiments, and most support recursion (and thus backtracking).

Traditionally, most ‘scientific’ programs are written in FORTRAN (which is older than C). In fact, its name comes from FORmula TRANslator, and it was specifically designed so that scientists could write programs which looked more ‘mathematical’ instead of using the machine language of a particular machine (see §1).

Because FORTRAN has been the ‘language of choice’ for scientists for several decades, there exists an enormous amount of ‘mature’ (*i.e.*, highly optimized and reliable) code in so-called *libraries* (see chapters 10 and 12), but it is often possible to call functions from these libraries from your C programs.

9.7 Questions and Exercises

9.1 In the pendulum simulation of §9.2, determine the period of the pendulum, either by simply counting the number of times you need to press the enter key before the pendulum reaches its original position again, or by modifying the program to keep track of the maximum position. How does it compare to the theoretical value? Also modify the length of the wire and see whether the resulting frequencies correspond to the theory.

9.2 Determine the effect of the ‘friction term’ on the frequency of the pendulum.

9.3 Varying the friction constant C in the pendulum simulation determines how quickly the pendulum is at rest again. When C is very low, the pendulum will not experience much friction and keep swinging for a long time; When C is above a certain value, the pendulum will not even swing at all (*i.e.*, it slowly approaches its resting position and never swings to the other side). This would correspond to a pendulum placed in a container full of syrup or some other viscous liquid. When C has the smallest value for which the pendulum *just* doesn't swing anymore, the system is said to be *critically dampened*. Determine this value of C.

9.4 The constant g used in the pendulum simulation is only valid here on Earth. On different planets, there would be a different g. Change the value of g to be ten times as big and see what influence that has on the frequency of the pendulum. Then, change it to be a hundred times as big (to simulate, say, a pendulum near a heavy star). What happens? Can you explain? How could you modify the code to handle extreme gravity like this?

9.5 $\star$ Making the length of the pendulum comparable to the initial position x_0 will render the derivation invalid, but the code of the simulation does not take this into account. Modify the simulation so that it takes vertical acceleration into account as well (*i.e.*, distinguish between v_x and v_y) and keep track of the vertical position of the mass. You will need to take centripetal acceleration into account ($a_c = v^2/r$), or the pendulum will keep 'falling down'. You may notice that it is very hard to get good results with your simulation, because the errors made in each step keep adding up, rendering the simulation useless.

9.6 In the marble board simulation of §9.3, modify the left-right decision criterion to give different chances for left and right (*i.e.*, use a 'loaded die') and observe how this changes the resulting distribution.

9.7 The first thing to examine with the 'percolation grids' of §9.4 is the probability to find a pathway as a function of the probability used to distribute 'pass-throughs' and 'blocks'. Examine all such distribution probabilities from 0 to 1 in increments of 0.05, perform several simulations at each probability, and plot the probability of finding a pathway. You will quickly find out that there is a 'critical density' around which the pathway probability rises steeply. What is this 'critical density' for the grid size used in the examples?

9.8 Obviously, the grid size is an important factor too. Examine the effect of grid dimensions on the 'critical density'.

9.9 In the clone analogy, one could argue that it would be much easier to simply leave one clone at each junction, who 'remembers' where he came from, and only send off his clones in the *other* directions. Modify the program to be more like this. Can you get it simpler this way?

9.10 ⋆ Modify the pathway-finding algorithm to find the *shortest* pathway through a given grid. Given this modified algorithm, plot the *average* pathway length against the pass-through probability, not counting simulations which couldn't find a pathway at all. Hint: the `percolate()` function as it is now only returns *whether* there was a pathway in this direction. Can you modify it to return the number of steps needed to reach it? At each grid point, compare the return values of `percolate()` and let the shortest non-zero value win. One is added (for the current grid point) and the result returned again.