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# Advanced practical Programming for Scientists

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Zuse Institute Berlin

TU Berlin

SS2017

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**Overview:** Imperative, OOP, Functional, side effects, thread safe, Design by contract

**Design:** Information hiding, Dependencies, Coding style, Input checking, Error Handling

**Design:** Overall program design, Data structures, Memory allocation

**Tools:** git, gdb, undodb, doxygen

**Languages and correctness:** Design errors/problems C/C++, C89 / C99 / C11, Compiler switches, assert, flexelint, FP, How to write correct programs

**Testing:** black-box, white-box, unit tests, regression tests, error tests, speed tests

**Tools:** gcov, jenkins, cmake, doxygen, make, gprof, valgrind, cppcheck, clang

**Software metrics:** Why, Examples, Is it useful? Control flow complexity

**Parallel programming:** OpenMP, MPI, pthreads, OpenCL

**Program optimization:** Code optimization, linking libraries

**How to design large programs**

**Code-shootout and comparison:** Documentation, Release management

**All information is subject to change.**

Please register yourself via

<https://science-match.tagesspiegel.de/the-digital-future-may-2017>

Voucher/VIP Code: \*future17-1\*



All emails related to this lecture should start with **APPFS** in the subject.

Everybody participating in this lecture, please send an email to [<rehfeldt@zib.de>](mailto:rehfeldt@zib.de) with your Name and Matrikel-Nr.

We will setup a mailing list for announcements and discussion.

Everything is here [http://www.zib.de/koch/lectures/ss2017\\_appfs.php](http://www.zib.de/koch/lectures/ss2017_appfs.php)

If you need the certificate, regular attendance, completion of homework assignments, and in particular participation in our small programming project is expected. Grades will be based on the outcome and a few questions about it 😊 .

**No groups.**

## Exercises part I: Reading and writing Data

1. 21.04. Reading csv
2. 28.04. Reading xml
3. 05.05. Reading binary
4. 05.05. Checking input data

## Exercise part II: Time series prediction

5. 26.05. Making it work 1 (make)
6. 02.06. Making it work 2 (Documentation, fixing input data)
7. 09.06. Testing
8. 16.06. Measuring performance, serializing data structures
9. 23.06. Analyzing code quality
10. 30.06. Linking third party libraries (static vs. shared)
11. 07.07. Making it better

- **You can submit the exercises in any programming language.**
- It has to run on my Raspberry-pi running Linux
- Example solutions will be provided at least in one of the following languages: C99, C++14, python3, Ada2012.
- If you use anything else, you are on your own.
- I will judge your code nevertheless.

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[Register at github.com](https://github.com)

[Go to https://github.com/mattmilten/appfs](https://github.com/mattmilten/appfs)

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Create a new folder with your name and then make a pull request

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README.md

```
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```

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Address bar: <https://github.com/daniel-the-great/appfs/tree/master>

Repository: **daniel-the-great / appfs** (forked from [appfs/appfs](#))

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2 commits, 1 branch, 0 releases, 1 contributor

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**README.md**

```
appfs
```

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<https://github.com/daniel-the-great/appfs/pull/new/master>

*Algorithm engineering refers to the process required to transform a pencil-and-paper algorithm into a **robust, efficient, well tested**, and easily usable **implementation**.*

— Bader, Moret, Sanders

*Real Programmers don't comment their code. If it was hard to write, it should be hard to understand and harder to modify.*

— Fortune (6)

*Beware of bugs in the above program. I have only proved it correct, not tried it.*

— D.E.Knuth

*The single most important rule of testing is to **do** it.*

— Kernighan, Pike

- **Laws** describe the feasible region of a solution
- **Objectives** (are directions) describing which solution to prefer
- **Rules** try to exclude (rule out) bad solutions

*“Look, that's why there's rules, understand?  
So that you think before you break 'em.”*  
— Terry Pratchett, Thief of Time

In general I recommend to follow rules, until you are sure you understand what the rules wanted to achieve and you believe your objectives are served better by not obeying the rule.

**But think first!**

If the union of all rules defines an empty space, resist the temptation to change the objective to look for a solution that violates the least number of rules. Slack solutions usually have a horrible objective value.

The speed of light  $c$  in vacuum is a universal physical constant. Its exact value is 299792458 m/s. According to special relativity,  $c$  is the maximum speed at which all conventional matter and hence all known forms of information in the universe can travel. (Wikipedia)

**“Everything should be made as simple as possible, but no simpler.”**

— Albert Einstein

Don't use goto!

See <https://softwareengineering.stackexchange.com/questions/125715/do-we-still-have-a-case-against-the-goto-statement>

A designer knows he has achieved perfection not when there is nothing left to add, but when there is nothing left to take away.

— Antoine de Saint-Exupery

In computer science terminology, **imperative programming** is a programming paradigm that describes computation in terms of **statements** that change a **program state**. In much the same way that imperative mood in natural languages expresses commands to take action, **imperative programs define sequences of commands for the computer to perform.**

Imperative programming, [http://en.wikipedia.org/w/index.php?title=Imperative\\_programming&oldid=624302389](http://en.wikipedia.org/w/index.php?title=Imperative_programming&oldid=624302389) (last visited Sept. 21, 2014)

Imperative Programmierung ist ein Programmierparadigma. Danach werden Programme so entwickelt, dass „ein Programm aus einer Folge von Anweisungen besteht, die vorgeben, in welcher Reihenfolge was vom Computer getan werden soll“.

Die imperative Programmierung ist das am längsten bekannte Programmierparadigma. Diese Vorgehensweise war, bedingt durch den Sprachumfang früherer Programmiersprachen, ehemals die klassische Art des Programmierens. Sie liegt dem Entwurf von vielen Programmiersprachen, zum Beispiel ALGOL, Fortran, Pascal, Ada, PL/I, Cobol, C und allen Assemblersprachen zugrunde.

Seite „Imperative Programmierung“. In: Wikipedia, Die freie Enzyklopädie. Bearbeitungsstand: 20. September 2014, 14:27 UTC. URL: [http://de.wikipedia.org/w/index.php?title=Imperative\\_Programmierung&oldid=134202110](http://de.wikipedia.org/w/index.php?title=Imperative_Programmierung&oldid=134202110) (Abgerufen: 21. September 2014, 20:41 UTC)

*I am in command!*

input->putput->output

Data separated from instructions (more or less 😊 as instructions are data)

Von-Neumann Architecture/Stored-Program-Computer

Access Memory, do computations incl. conditional, PC program counter

-> allows: goto (jump), if (conditional), while (loop)

1. Do it!
2. Anyway!

Structured programming vs. goto

Blocks, subroutines, scopes.

*Building your own world of objects*

**Object-oriented programming** attempts to provide a model for programming based on objects. OO programming integrates code and data using the concept of an “object”. An object is an abstract data type with the addition of **polymorphism** and **inheritance**.

**An object has both state (data) and behavior (code).**

- > Information hiding
- > polymorphism comes naturally
- > single vs. multiple inheritance.
- > templates and generics

*The way mathematicians think.*

Functional programming is a style of building the structure and elements of computer programs, that treats computation as the evaluation of mathematical functions and avoids changing state and mutable data.

In functional code, the output value of a function depends only on the arguments that are input to the function, so calling a function  $f$  twice with the same value for an argument  $x$  will produce the same result  $f(x)$  both times.

Eliminating side effects, i.e. changes in state that do not depend on the function inputs, can make it much easier to understand and predict the behavior of a program, which is one of the key motivations for the development of functional programming.

-> side effects / mutable state -> `rand()`, `getchar()`, `putchar()`

-> call by value, call by reference

-> thread safeness -> `errno`

- **Imperative programming** – defines computation as statements that change a program state (Assembler)
- Procedural programming, structured programming – specifies the steps the program must take to reach the desired state (C, Pascal, Fortran 77)
- **Functional programming** – treats computation as the evaluation of mathematical functions and avoids state and mutable data (Lisp, ML, Haskell, Erlang, Ocaml)
- **Object-oriented programming (OOP)** – organizes programs as objects: data structures consisting of datafields and methods together with their interactions (Smalltalk, C++, Java, Eiffel)
- **Declarative programming** – defines computation logic without defining its control flow (Prolog)
- **Event-driven programming** – the flow of the program is determined by events, such as sensor outputs or user actions (mouse clicks, key presses) or messages from other programs or threads (JavaScript)

- wasted a lot of time coding the wrong algorithm?
- used a data structure that was much too complicated?
- tested a program but missed an obvious problem?
- spent a day looking for a bug you should have found in five minutes?
- needed to make a program run three times faster and use less memory?
- struggled to move a program from one architecture to another?
- tried to make a modest change in someone else's program?
- rewritten a program because you couldn't understand it?

## Was it fun?

From: Kernighan, Pike „The practise of programming“

These include

- **simplicity**, which keeps programs short and manageable;
- **clarity**, which makes sure they are easy to understand, for people as well as machines;
- **generality**, which means they work well in a broad range of situations and adapt well as new situations arise; and
- **automation**, which lets the machine do the work for us, freeing us from mundane tasks.

From: Kernighan, Pike „The practise of programming“

```
v,i,j,k,l,s,a[99];
main()
{
for(scanf("%d",&s);*a-s;v=a[j*=v]-a[i],k=i<s,
j+=(v=j<s&&!k&&!printf(2+"\n\n%c"-(!l<<!j),
"#Q"[l^v?(l^j)&1:2])&&++l||a[i]<s&&v&&v-i+j&&
v+i-j))&&!(l%=s),
v||(i==j?a[i+=k]=0:++a[i])>=s*k&&++a[--i]);
}
```

What might it possibly do?

- Be able to **follow control flow** (-imperative, +structured, -OO, +functional)
- Structuring programs into units (-imperative, +structured, +OO)
- Minimize dependencies (between components)
  - Minimize scope
  - Minimize side effects (+functional)
  - Data hiding (+OO)
  - How about things happening automatic?  
(member functions in C++, Garbage collection)
  - Being clever?: `while(*s++ = *t++);`
  - DbC

```
int data[10000]; // all 0..255
long long fun = 0;
unsigned i;
[...]
int t = (data[i] - 128) >> 31;
fun += ~t & data[i];
```

```
/* The Computer Language Benchmarks Game http://benchmarksgame.alioth.debian.org/  
Contributed by Dmitry Vyukov  
*/  
#define _GNU_SOURCE  
#include <stdlib.h>  
[...]  
#define CL_SIZE 64  
  
void* cache_aligned_malloc(size_t sz)  
{  
    char*          mem;  
    char*          res;  
    void**         pos;  
  
    mem = (char*)malloc(sz + 2 * CL_SIZE);  
    if (mem == 0)  
        exit(1);  
    res = (char*)((uintptr_t)(mem + CL_SIZE) & ~(CL_SIZE - 1));  
    pos = (void**)(res - sizeof(void*));  
    pos[0] = mem;  
    return res;  
}
```

(DbC), is an approach for designing software.

It prescribes that software designers should define formal, precise and verifiable interface specifications for software components, which extend the ordinary definition of abstract data types with preconditions, post-conditions and invariants.

These specifications are referred to as “contracts”, in accordance with a conceptual metaphor with the conditions and obligations of business contracts.

Pre-conditions

Post-conditions

Invariants

Please check out the data for this exercise located here:

<https://github.com/mattmilten/appfs>

You will find a program named **ex1\_gen** used to generate the input data.

Run this program as follows:

```
./ex1_gen 100000000 >ex1.dat
```

The file **ex1.dat** should then contain roughly 100 million lines.

You can check by

```
wc -l ex1.dat
```

Size should be around 2GB.

The first number is 123456789.

Each line should consists of

- a sequence-number,
- a location (1 or 2), and
- a floating point value  $> 0$ .

Empty lines are allowed. Comment lines start with a "#".

Everything after a "#" on a line should be ignored.

Read in the data and compute the geometric mean for each location.

Be aware that there might be some errors in the data.

Write a program named **ex1** in C or your favorite language, which

1. Reads in the data from **ex1.dat**
2. Compute the **Geometric Mean** for both locations  
Output should look like:

File: ex1.dat with 100001235 lines

Valid values Loc1: 50004598 with GeoMean: 36.7817

Valid values Loc2: 49994703 with GeoMean: 36.7825

1. Check in the source code into github as explained
2. use `time ex1 ex1.dat`  
to get the runtimes of your program
3. Copy the output of your program

Send the output of `time`, and your `ex1` with  
subject of **APPFS ex1 vorname nachname**  
per email to `<koch@zib.de>`

**Deadline: 27.04. 16 Uhr** (earlier would be better)