Software and Tools for Computational Engineering

RWTH AACHEN UNIVERSITY

The STCE Scripting Language

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- The STCE scripting language is a (very small) subset of C++ augmented with runtime support libraries (e.g. gnuplot[1] for visualization).
- The focus is on illustration of fundamental algorithmic aspects taught as part of STCE courses.
- The focus is not on efficiency nor on quality of software engineering.
- Learning the STCE scripting language will be straightforward if you are not new to (imperative) programming.
- The ability to use the STCE scripting language is a prerequisite for a number of exam formats for courses taught at STCE.

[1] www.gnuplot.info

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Requirements

- Shell, e.g.
  - RWTH High Performance Computing (Linux)
  - VirtualBox + STCE Linux image
  - Minimalist GNU for Windows
- Essential Linux

See tutorial.

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```
1  #include<iostream>
2  using namespace std;
3
4  int main() {
5    cout << "Leave me alone, "
6         << "world!" << endl;
7    return 0;
8  }
```

yields output

```
1  Leave me alone, world!
```

- Use a text editor to generate source, e.g. `:-) vi main.cpp`
- Include relevant chapters of the C++ standard library (line 1).
- Avoid specification of std:: namespace globally (line 2).
- The function **int** main() is required for executable program (line 3).
- An integer value is returned to the caller, e.g. Linux shell (line 7).

- A string is written to the standard output stream cout (screen) (line 5).
- A special end of line marker endl is used for formatting (line 6).
- An STCE script is a source file with extension .cpp containing at least the function main.

Building

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The sample code comes with a GNU makefile.[2]

Type `:-) make` to build; `:-) make clean` to clean up.

```
1  EXE=$(addsuffix .exe, $(basename $(wildcard *.cpp)))
2
3  COMPILER=g++
4  COMPILER_FLAGS=-Wall -Wextra -pedantic -O3
5
6  all : $(EXE)
7
8  %.exe : %.cpp
9    $(COMPILER) $(COMPILER_FLAGS) $< -o$@
10
11 clean:
12   rm -f $(EXE)
13
14 PHONY: all clean
```

[2] www.gnu.org/software/make/

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Types

- void
- int
- bool
- string
- float
- double

```
#include<iostream>
using namespace std;

int main() {
  int i=1;
  cout << i << endl;
  cin >> i;
  cout << i << endl;
  return 0;
}
```

yields output

```
1
0815 // user input
815
```

- Variables have types, e.g. **int** for integers.
- Variables should be initialized at the time of their declaration, e.g. with a constant (line 5).
- Users can supply values of variables via the standard input stream cin (keyboard) (line 7).
- Integer constants are sequences of digits.
- The range of integers is limited to $[-2147483648, 2147483647]$.
- See `types_int.cpp`.

```
1  #include<iostream>
2  using namespace std;
3
4  int main() {
5    bool b=true;
6    cout << b << endl;
7    cin >> b;
8    cout << b << endl;
9    return 0;
10 }
```

yields output

```
1  1
2  2 // user input
3  1
```

- Truth values (constants **true** and **false**) are stored as Boolean variables of type **bool** (line 5).
- In output they are represented as `1` (**true**) and `0` (**false**).
- Implicit conversion transforms `0` into **false** and any nonzero value into **true**.
- See `types_bool.cpp`.

Types: string

```
#include<string>
#include<iostream>
using namespace std;

int main() {
  string s1="Hi ",s2;
  cin >> s2;
  cout << s1 << s2 << "!" << endl;
  return 0;
}
```

```
folks // user input
Hi folks!
```

- Strings are stored as variables of type string defined in <string> (line 1).
- String constants are enclosed in quotes (lines 6,8).
- The C++ standard library offers a wide range of functionalities for strings.
- See www.cppreference.com for further details on <string>.
- See types_string.cpp.

```
1  #include<iostream>
2  using namespace std;
3
4  int main() {
5    float f=1e-1;
6    cout << f << endl;
7    cin >> f;
8    cout << f << endl;
9    return 0;
10 }
```

yields output

```
1  0.1
2  3.14159265358979 // user input
3  3.14159
```

- Non-integer numerical values are stored in floating-point format.
- Real values are rounded to the grid of floating-point numbers yielding various unpleasant numerical effects.
- The range of **float** is limited to $\pm[1.17549 \cdot 10^{-38}, 3.40282 \cdot 10^{38}]$.
- **float** constants can be written in fixed-point (e.g. `3.1415`) or floating-point (e.g. `314.15e-2`$=314.15 \cdot 10^{-2}$) notation (line 5)
- The precision of **float** yields 6 significant digits in fixed-point notation.
- Implicit conversion of float-point values to **int** or **bool** uses rounding.
- See `types_float.cpp`.

```
1  #include<iostream>
2  using namespace std;
3
4  int main() {
5    double d=31.415e−1;
6    cout.precision(15);
7    cout << d << endl;
8    cin >> d;
9    cout << d << endl;
10   return 0;
11 }
```

yields output

```
1  3.141
2  3.14159265358979 // user input
3  3.14159265358979
```

- The range of **double** is limited to $\pm[2.22507 \cdot 10^{-308}, 1.79769 \cdot 10^{308}]$.
- **double** constants can be written in fixed-point or floating-point notation (line 5).
- The precision of **double** yields 15 significant digits in fixed-point notation.
- The precision of the cout needs to be changed from its default (6 digits) to inspect full precision of **double** (line 6).
- See `types_double.cpp`.

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```
#include<iostream>
#include<cmath>
using namespace std;

int main() {
  float x=1e-0,y=1e1;
  y=exp(x+sin(x)/y);
  cout << y << endl;
  return 0;
}
```

yields output

```
2.95692
```

- Following resolution of flow of control imperative programs amount to sequences of assignments of results of numerical expressions to variables (line 7).
- Arithmetic operators include +,−,∗,/,%.
- Arithmetic functions include sin,cos,exp,log,fabs,fmax.
- See `www.cppreference.com` for further details on arithmetic operators and <cmath>.
- See `cmath.cpp`.

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Flow of Control

- **if**
- **if—else [if—else ...]**
- **while**
- **do—while**
- **for**

```
#include<cmath>
#include<iostream>
using namespace std;

int main() {
  float x,y;
  cin >> x;
  if (x<0) {
    y=x+sin(x);
  }
  y=x-cos(x);
  cout << y << endl;
  return 0;
}
```

yields output

```
-1.5403
```

for input x=-1

- The code in curly brackets (e.g. y=x+sin(x)) is executed if the condition (e.g. x<0) evaluates to **true** (lines 8-10).
- Potentially very complex conditions can be formulated using relational (<,>,==,!=,<=,>=) and logical (!,&&,|| corresponding to negation, AND, inclusive OR) operators.
- The curly brackets can be omitted if they enclose a single statement (as it is the case here).
- See `if_1.cpp`.

```
#include<cmath>
#include<iostream>
using namespace std;

int main() {
  float x,y;
  cin >> x;
  if (x<0) {
    y=x+sin(x);
  } else {
    y=x-cos(x);
  }
  cout << y << endl;
  return 0;
}
```

See `if_2.cpp` and `if_3.cpp`.

```
#include<cmath>
#include<iostream>
using namespace std;

template<typename T>
void f(const T& x, T& y) {
}

int main() {
  float x,y;
  cin >> x;
  if (x<0) {
    y=x+sin(x);
  } else if (x>0) {
    y=x-cos(x);
  } else {
    y=exp(x);
  }
  cout << y << endl;
  return 0;
}
```

```
1  #include<cmath>
2  #include<iostream>
3  using namespace std;
4
5  int main() {
6    float x=1,y;
7    y=x-cos(x);
8    while (y<1) {
9      y=y+sin(x);
10   }
11   cout << y << endl;
12   return 0;
13 }
```

- The code in curly brackets (loop body; e.g. y=x+sin(x)) is executed while the condition (e.g. x<0) evaluates to **true** (lines 8-10).
- Zero or more loop iterations are performed; termination may not be guaranteed.
- The curly brackets can be omitted if they enclose a single statement (as it is the case here).
- See `while.cpp`.

```
 1  #include<cmath>
 2  #include<iostream>
 3  using namespace std;
 4
 5  int main() {
 6    float x=1,y;
 7    y=x-cos(x);
 8    do {
 9      y=y+sin(x);
10    } while (y<1);
11    cout << y << endl;
12    return 0;
13  }
```

- The loop body (e.g. y=x+sin(x)) is re-executed while the condition (e.g. x<0) evaluates to **true** (lines 8-10)
- one or more loop iterations are possible; termination may not be guaranteed
- the curly brackets can be omitted if they enclose a single statement (as it is the case here)
- See `do_while.cpp`.

```
1  #include<cmath>
2  #include<iostream>
3  using namespace std;
4
5  int main() {
6    float x=1,y;
7    y=x-cos(x);
8    int j=10;
9    for (int i=0; i<j; i=i+1) {
10     y=y+sin(x);
11   }
12   cout << y << endl;
13   return 0;
14 }
```

- The loop body (e.g. `y=x+sin(x)`) is executed while the condition (e.g. `i<j`) evaluates to **true** (lines 9-11).
- Variables local to the loop statement can be declared and initialized (e.g. `int i=0`) (line 9).
- Values of variables can be updated after each loop iteration (e.g. `i=i+1`) (line 9).
- Zero or more loop iterations are performed; termination may not be guaranteed.

- The curly brackets can be omitted if they enclose a single statement (as it is the case here).
- Typical use cases include the iteration through vectors or matrices.
- See `for.cpp`.

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- definition
- type generics
- arguments passed by value
- arguments passed by reference

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```
 1  #include<cmath>
 2  #include<iostream>
 3  using namespace std;
 4
 5  float g(float x, int i) {
 6    x=x+i;
 7    float y=x+sin(x);
 8    return y;
 9  }
10
11  int main() {
12    float f=sin(1e1);
13    cout << g(f,1) << endl;
14    return 0;
15  }
```

yields output

```
1  0.89632
```

- Subprograms have a name (e.g. g), a (return) type (e.g. **float**; **void** for missing return value), and a list of arguments (e.g. **float** x, **int** i; here passed by value; see below) (line 5).
- They can declare local variables (e.g. **float** y) (line 7).
- The return value (e.g. y) is passed back to the caller (e.g. main) (line 8).
- See `subprograms_1.cpp`.

```
1  #include<cmath>
2  #include<iostream>
3  using namespace std;
4
5  template<typename T1, typename T2>
6  T1 g(T1 x, T2 i) {
7    x=x+i;
8    T1 y=x+sin(x);
9    return y;
10 }
11
12 int main() {
13   float f=sin(1e1);
14   int i=1;
15   cout << g(f,i) << endl;
16   return 0;
17 }
```

yields output

```
1  0.89632
```

- Types of arguments and results can be made variable (e.g. `T1` and `T2`) (line 5).
- Type-generic subprograms become templates for the compiler to instantiate automatically for the given scenario; e.g. the compiler realizes that in line 15 `g` is called with arguments of types `T1`=**float** and `T2`=**int**; the corresponding instance of `g` is generated automatically by the compiler (lines 13-15).
- Replace **float** → **int** and **int** → **double** to see a different result (1).
- See `subprograms_2.cpp`.

Arguments Passed by Value


```
1  #include<cmath>
2  #include<iostream>
3  using namespace std;
4
5  template<typename T>
6  T g(T x) { // pass by value
7    x=x+1;
8    T y=x+sin(x);
9    return y;
10 }
11
12 int main() {
13   float f=sin(1);
14   cout.precision(15);
15   cout << g(f) << " " << f << endl;
16   double d=sin(1);
17   cout << g(d) << " " << d << endl;
18   return 0;
19 }
```

- By default all arguments are passed by value (line 6).
- Arguments passed by value result in a local copy used inside of the function.
- Potential modifications of this copy have no effect on the value of the original argument passed by the caller; hence, the code on the left yields the output

```
1 2.80506181716919 0.841470956802368
2 2.80506170934973 0.841470984807897
```

- See `subprograms_3.cpp`.

Arguments Passed by Reference

```
#include<cmath>
#include<iostream>
using namespace std;

template<typename T>
T g(T &x) { // pass by reference
  x=x+1;
  T y=x+sin(x);
  return y;
}

int main() {
  float f=sin(1);
  cout.precision(15);
  cout << g(f) << " " << f << endl;
  double d=sin(1);
  cout << g(d) << " " << d << endl;
  return 0;
}
```

- Arguments to be passed by reference need to be preceded by & (line 6).
- Arguments passed by reference are used directly inside of the function.
- Potential modifications inside of the function also apply to the value of the argument passed by the caller; hence, the code on the left yields the output

```
2.80506181716919 1.84147095680237
2.80506170934973 1.8414709848079
```

- See `subprograms_4.cpp`.

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```
#include<cmath>
#include<cassert>
#include<iostream>
using namespace std;

template<typename T>
T f(T x) {
  assert(x>=0);
  return sqrt(x);
}

int main() {
  float x;
  cin >> x;
  cout << f(x) << endl;
  return 0;
}
```

- Assertions are conditions to be fulfilled while executing the script; they are defined in <cassert> (line 2).
- E.g. the argument of the square root function must be non-negative (line 8).
- Assertions should be inserted into the script whenever such a condition can be formulated sensibly; understanding / debugging is simplified significantly.
- See `assert.cpp`.

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```
1  #include<fstream>
2  using namespace std;
3
4  template<typename T>
5  void in(T& x, string filename) {
6    ifstream ifs(filename);
7    ifs >> x;
8    ifs.close();
9  }
10
11 template<typename T>
12 void out(T x, string filename) {
13   ofstream ofs(filename);
14   ofs << x;
15   ofs.close();
16 }
17
18 int main() {
19   float x; in(x,"x.in"); out(x,"x.out");
20   return 0;
21 }
```

- Data can be read from / written to text files via file streams defined in <fstream> (line 1).
- Declaration of an input file stream of type ifstream requires specification of the name (of type string) of the file to be read from (line 6).
- Output file streams of type ofstream are declared analogously (line 13)
- Usage is then similar to cin and cout (lines 7,14).
- See `fstream.cpp`.

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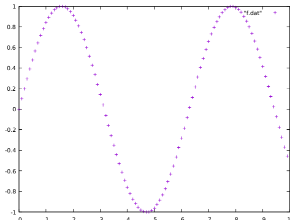
```
1  #include<cmath>
2  #include<fstream>
3  using namespace std;
4
5  template<typename T>
6  T f(T x) { return sin(x); }
7
8  int main() {
9    float xmin=0, xmax=10;
10   int nsamples=100;
11   ofstream ofs("f.dat");
12   for (float x=xmin;
13     x<xmax;
14     x=x+(xmax−xmin)/nsamples) {
15     ofs << x << " "
16         << f(x) << endl;
17   }
18   ofs.close();
19   return 0;
20 }
```

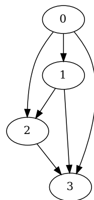
- Input files for gnuplot can be generated, e.g. by sampling a given function (lines 12-17)
- Run :-) `gnuplot` to open the gnuplot shell.
- Type `plot "f.dat"` to get



- See `www.gnuplot.info` for detailed information on gnuplot.
- See `vizualisation_1.cpp`.

```
1  #include<fstream>
2  using namespace std;
3
4  int main() {
5    ofstream ofs("g.dot");
6    ofs << "digraph {" << endl;
7    int n=4;
8    for (int i=0;i<n;i=i+1)
9      for (int j=i+1;j<n;j=j+1)
10       ofs << i << " -> "
11           << j << endl;
12   ofs << "}" << endl;
13   ofs.close();
14   return 0;
15 }
```

- Input files for graphviz can be generated, e.g. a directed acyclic complete graph with four vertices (line 6-12).
- :-) `dot -Tpdf g.dot -o g.pdf` generates the following `g.pdf`



- See `www.graphviz.org` for detailed information on graphviz and dot.
- See `vizualisation_2.cpp`.

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