Introduction to Scientific Computing Languages

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Languages for Scientific Computing

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- A set of **instructions and constructs** to communicate with a computing device
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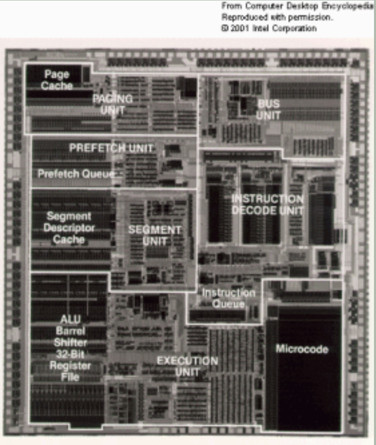
What is a “computing device”?

sequential processors, embedded processors, . . . , parallel computers, supercomputers.

Processor's Components



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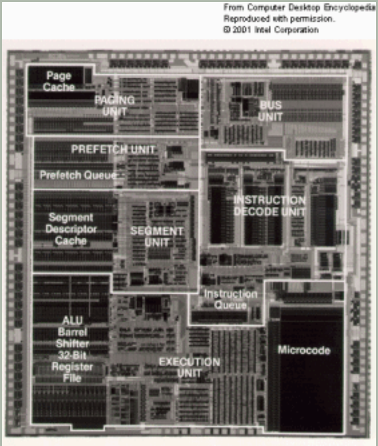

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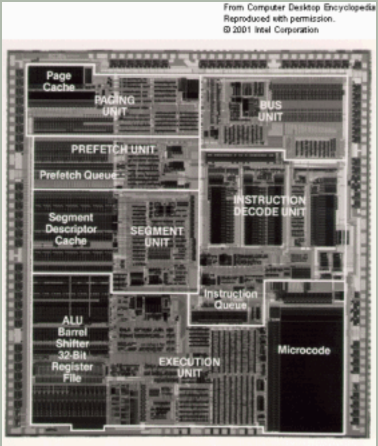

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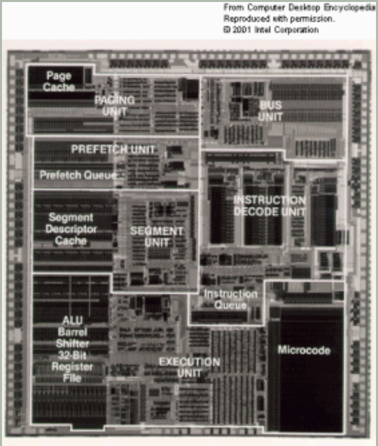

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- Languages let the users specify how to use these components
- Only **Assembly** operates on components: *"low-level"* language
- *"High-level"* languages only specify the computations to be performed
- A **compiler** and/or an **interpreter** translates high-level programs into a sequence of component actions

Assembly

Low-level language

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- Not the lowest level. Not directly executable.

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- **Assembler** translates assembly into machine code. Executable.
- Assembly consists of mnemonic codes.
  Machine code: only numbers.
- Translation Assembly $\leftrightarrow$ machine code is almost 1-1.
  This is not true for high-level languages.
- Assembler is hardware-specific. Control over chips' components.

Assembly

Example

```
        .text
        .globl poly
poly:
        li.s   $f0, 0.0           # y = 0, running & return result
        mtc1   $6  $f12           # x, move to float register
Loop:
        mul.s $f14, $f12, $f0     # compute (x * y)
        mul    $2, $5, 4          # $5 = i, compute address of a[i]
        addu   $3, $2, $4         # a + (i*4)
        l.s    $f16, 0($3)        # a[i], load coefficient
        add.s $f0, $f16, $f14     # y = a[i] + (x*y)
        addi   $5, $5, -1         # decrease i

        slt    $2, $5, $0         # $2 = 1 if i < 0
        beq    $2, $0, Loop       # goto Loop if i >= 0
Exit:
        j      $31
```

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# Evaluate the value of a polynomial using Horner's algorithm.
# f = a[0] + a[1] * x + a[2] * x^2 + ... + a[n] * x^n
```

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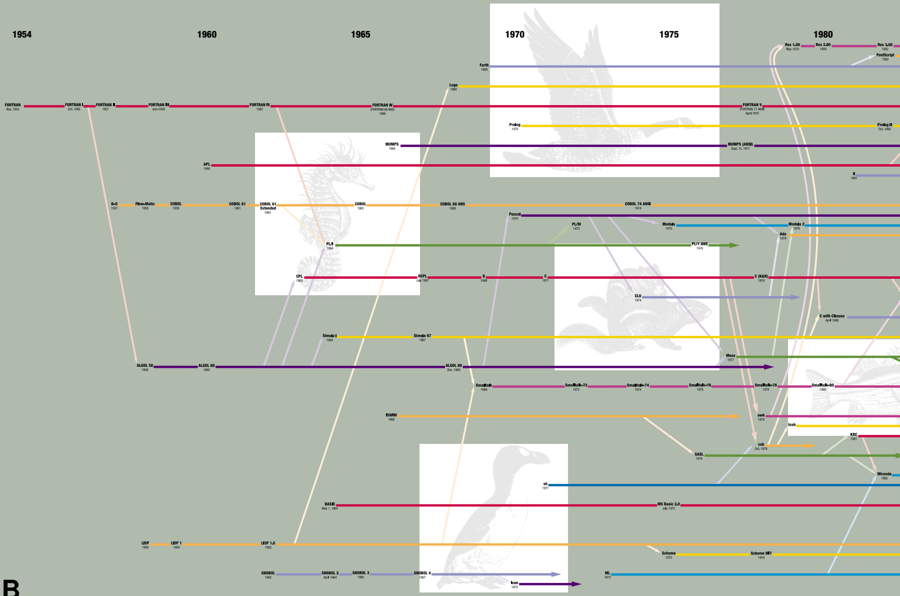
Plankalkül (1940s). For the Z1 computer, by Konrad Zuse.

History of Programming Languages



WEB

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- **Speed!**
- Examples: C, Fortran.

Computer Programs

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Program:

sequence of instructions expressing the operations to be performed on a target computing platform.

- Each program $\mathcal{P}$ has a meaning. It implements a function.
  $\{\text{Initial State}\} \quad \mathcal{P} \quad \{\text{Final State}\}$.

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  $[[\ ]]$ = Semantics operator. Operational, Denotational, Axiomatic.
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- Generally, we want $\mathcal{P}$ to compute $f(i)$, with $i \in I$.
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- Remember: when working with floating point numbers,
  the expression $x == y$ does not make sense!

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- BUT! One difference: side-effects.
  Many languages allow subroutines to have side-effects.
  The routine alters the state of the system even after its completion.

Side Effects

$\{\ (\texttt{res} = \ldots) \wedge \text{State}\ \}$

```
res := routine_name( args );
```

$\{\ (\texttt{res} = \ldots) \wedge \text{State}'\ \}$

- If (State = State′) $\rightarrow$ no side-effects.
- Most languages allow constructs with side-effects.
- Print statements; iterative constructs; ...

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- Structure:

```
routine_name( args )
    //
    body
    //
return( value )
```

depending on the language,
`args`, `body` and `value` are optional

Questions about Subroutines

```
routine_name_1(args_1)        routine_name_2(args_2)
    //                            //
    body_1                        body_2
    //                            //
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  Recursion ≡ iteration!

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BLAS	LAPACK	PETSc	MPI	...
FFTW	LINPACK		OpenMP	
	EISPACK		Pthreads	
- Libraries can be written in one or more languages.
  Can they be accessed from a program written in a different language?

Imperative vs. Functional Languages

Imperative Languages

- Concept of **Variables** and **State**.
- Program is an ordered sequence of commands and **assignments**.
- Commands modify state. Side-effects.
- C, C++, Fortran, Java, Python, Matlab, . . .

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Functional Languages

- No variables or assignments.
- Program consists of **Functions** and **Recursion**.
- No side-effects!
- Subset of Declarative Languages.
- Lisp, APL, ADA, Haskell, Mathematica, Clojure, F# . . .

Scope

```
Program A;
Var I:Integer;
    K:Char;
    R:Real;

    Procedure B;
    Var K:Real;
        L:Integer;

        Procedure C;
        Var M:Real;
        Begin
        // Body #1
        End;
    Begin
    // Body #2
    End;
Begin
// Body #3
End;
```

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- Where is `K` used as `Real`?

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- Can `L` be referenced in `Body #2`? `Body #3`?

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    Begin
    // Body #2
    End;
Begin
// Body #3
End;
```

- Which variables (of which type) are defined in `Body #1`?

  `I:Integer`, `R:Real`, `K:Real`, `L:Integer`, `M:Real`

- Where is `K` used as `Real`?

  `Body #1` and `Body #2`

- Can `L` be referenced in `Body #2`? `Body #3`?

  `Body #2`: yes; `Body #3`: no

Scope (2)

```
program main
var y: Real;
    procedure compute()
    var x : Integer;
        procedure initialize()
        var y: Integer;
        var z: Real;
        begin {initialize}
        // Body #1
        end {initialize}

        procedure transform()
        var x: Real;
        begin {transform}
        // Body #2
        end {transform}
    begin {compute}
    // Body #3
    end {compute}
begin {main}
// Main body
end {main}
```

Scope (2)

```
program main
var y: Real;
    procedure compute()
    var x : Integer;
        procedure initialize()
        var y: Integer;
        var z: Real;
        begin {initialize}
        // Body #1
        end {initialize}

        procedure transform()
        var x: Real;
        begin {transform}
        // Body #2
        end {transform}
    begin {compute}
    // Body #3
    end {compute}
begin {main}
// Main body
end {main}
```

- What is the scope of the variable `x` declared in the procedure `compute`?

Scope (2)

```
program main
var y: Real;
    procedure compute()
    var x : Integer;
        procedure initialize()
        var y: Integer;
        var z: Real;
        begin {initialize}
        // Body #1
        end {initialize}

        procedure transform()
        var x: Real;
        begin {transform}
        // Body #2
        end {transform}
    begin {compute}
    // Body #3
    end {compute}
begin {main}
// Main body
end {main}
```

- What is the scope of the variable `x` declared in the procedure `compute`?

  `Body #1` and `Body #3`

Scope (2)

```
program main
var y: Real;
    procedure compute()
    var x : Integer;
        procedure initialize()
        var y: Integer;
        var z: Real;
        begin {initialize}
        // Body #1
        end {initialize}

        procedure transform()
        var x: Real;
        begin {transform}
        // Body #2
        end {transform}
    begin {compute}
    // Body #3
    end {compute}
begin {main}
// Main body
end {main}
```

- What is the scope of the variable `x` declared in the procedure `compute`?

  `Body #1` and `Body #3`

- What is the environment for the procedure `transform`?

Scope (2)

```
program main
var y: Real;
    procedure compute()
    var x : Integer;
        procedure initialize()
        var y: Integer;
        var z: Real;
        begin {initialize}
        // Body #1
        end {initialize}

        procedure transform()
        var x: Real;
        begin {transform}
        // Body #2
        end {transform}
    begin {compute}
    // Body #3
    end {compute}
begin {main}
// Main body
end {main}
```

- What is the scope of the variable `x` declared in the procedure `compute`?

  `Body #1` and `Body #3`

- What is the environment for the procedure `transform`?

  `y:Real` and `x:Real`