PROGRAMMING FOR COMPUTATIONAL CHEMISTRY

Introduction to Fortran

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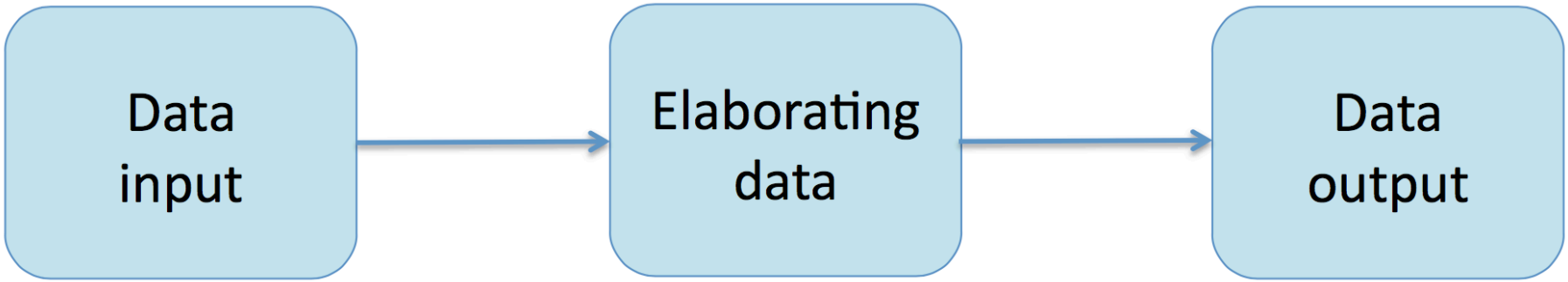
General flowchart

Goal for a computer: executing a set of instructions to solve a given numerical problem



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- Semantics: assign a meaning to the syntactic forms of the language

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- Start from the general instructions: input, do operations, output
- From the general problem to the identification of the main sections
- Simplify towards smallest pieces of code (stepwise refinement)

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  2. Coding the algorithm

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- Two main steps:
  1. Translating the source code into an object file, containing meta-instructions
  2. Converting the object (and possibly other ones in libraries) into an executable

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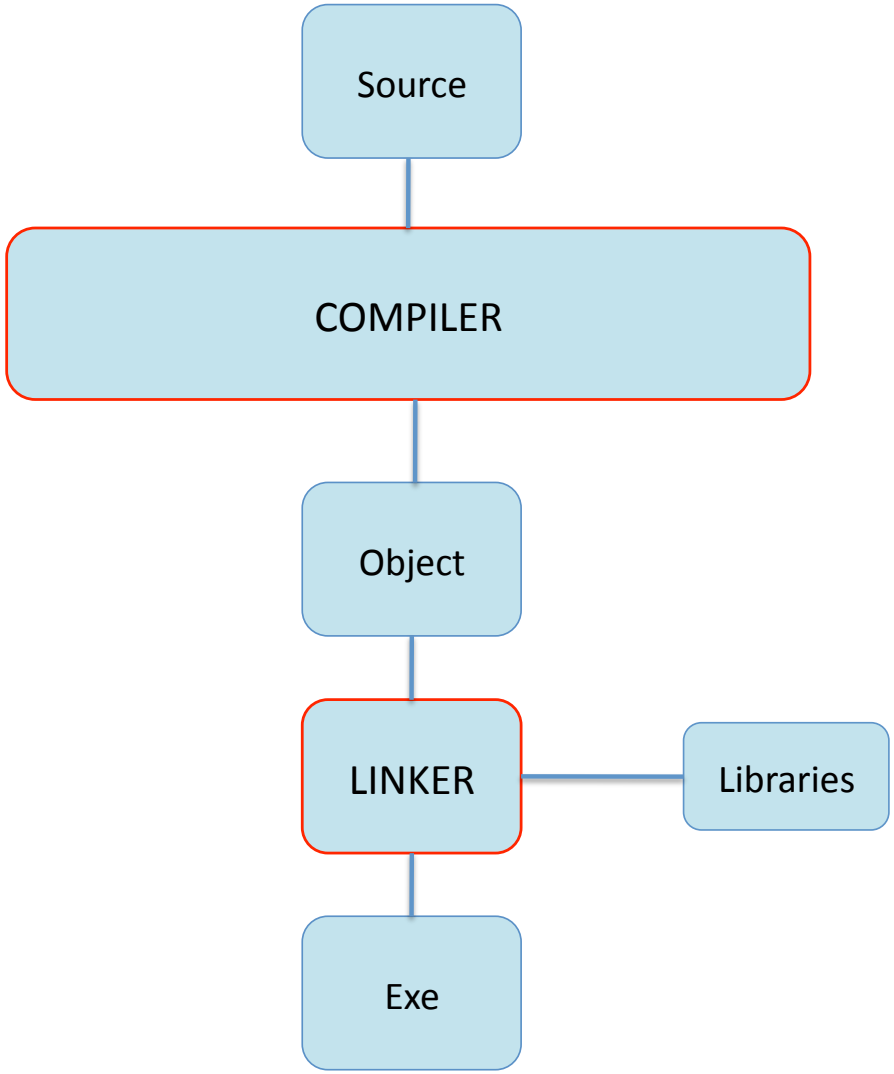

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- Semantic errors: use debugging options to find and fix them, structured programming to avoid them

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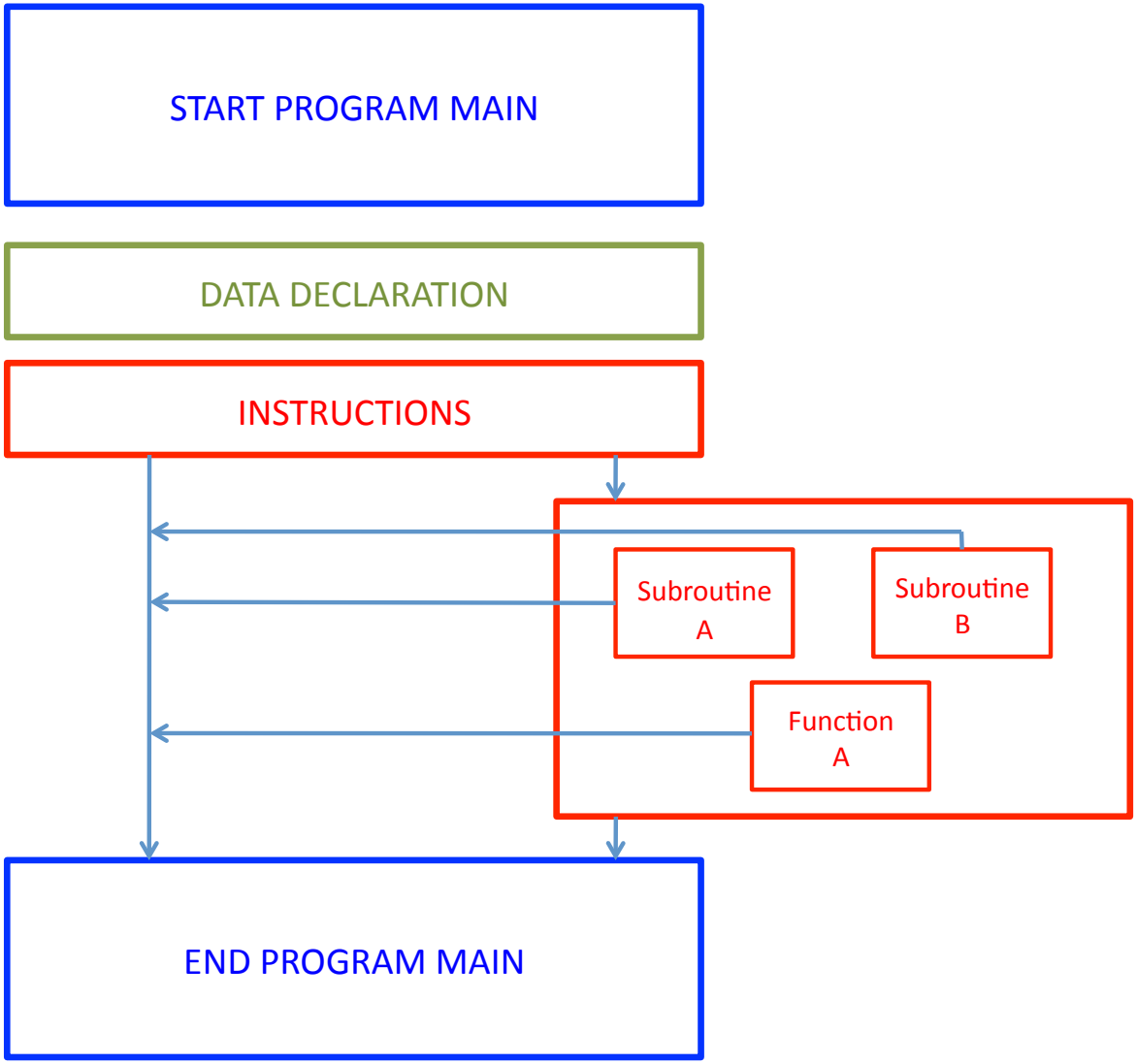
- Standard releases:
  - FORTRAN4
  - FORTRAN66
  - FORTRAN77
  - Fortran90
  - Fortran95
  - Fortran03
  - Fortran08
  - ...

Generic (Fortran) code



Our first code

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- Let us do it together (hello_world.f90)

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  5. ...

Source and binaries

- Two types of files: binary or text
  - Binaries can be programs or data files written by programs or the operating system
  - Text files are those that can be read by us human beings
- Two categories of files: programs or data
- Either a file contains a set of instructions to be executed by the CPU (a program) or it contains information (data)