Tecniche di programmazione in chimica computazionale

Expressions, operations and variables

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Constants

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- Define a constant using parameter (param.f90)

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- Example assign.f90

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- Better to always start a Fortran code with implicit none

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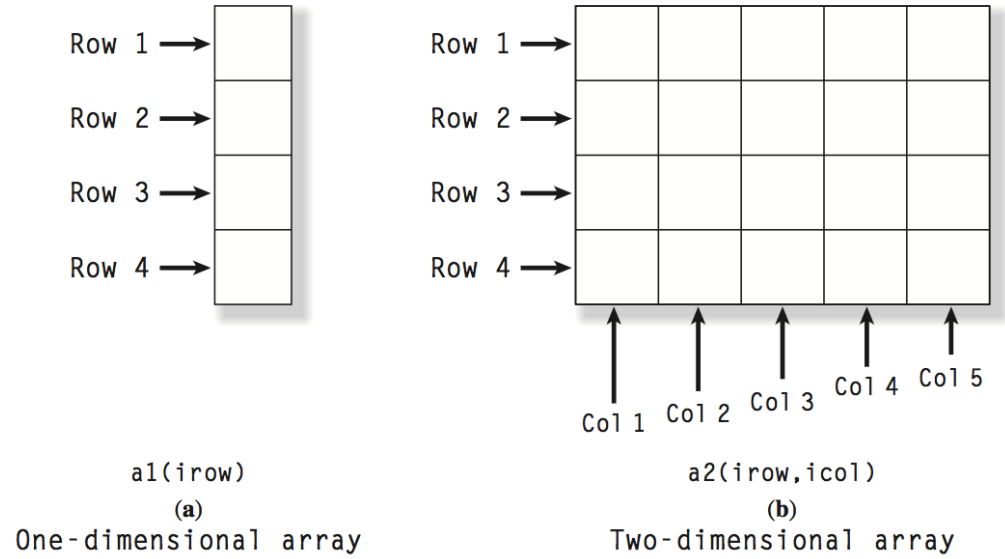
- add d (e.g., dcos(x)) for real*8

Arrays

- Structured data type: vectors, matrices, more complicated structures



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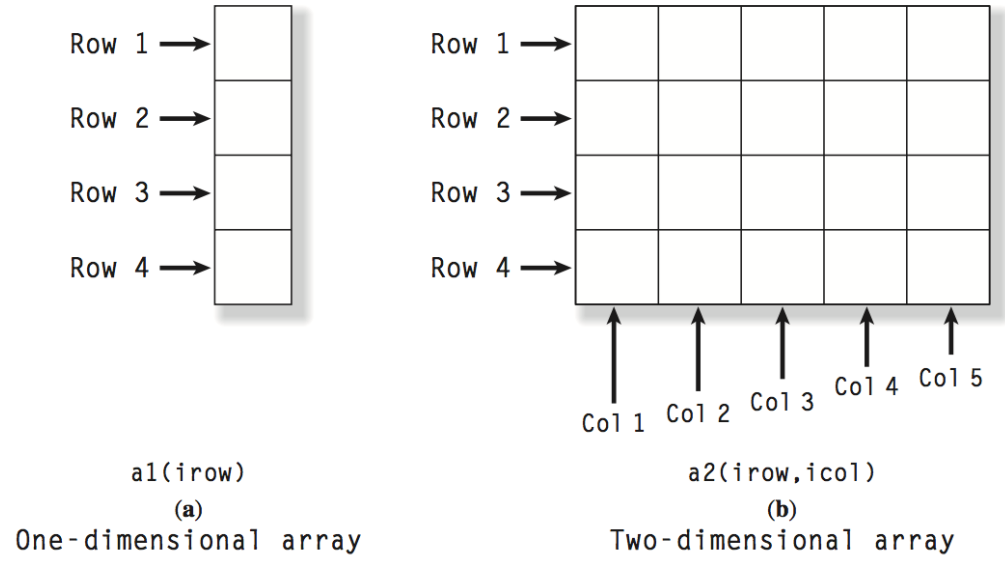

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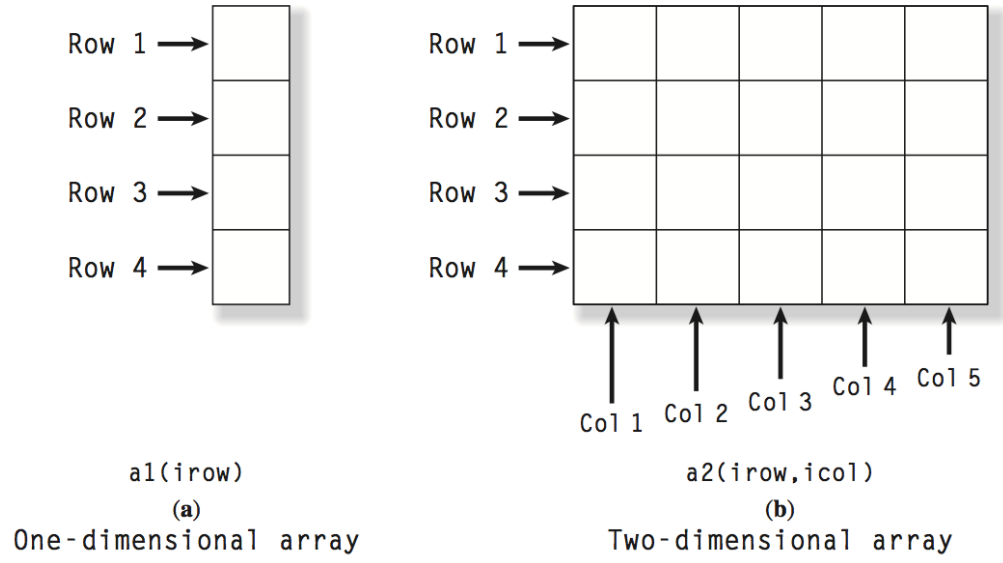

- Array of any type (integer, single and double precision etc.)
- Intrinsic Fortran functions:
  - maxval(x)
  - minval(x)
  - sum(x)
  - dot_product(a,x)
  - matmul(A,B)

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- Dynamical arrays: example alloc.f90

Arithmetic expressions

$$n1 + n2$$

- Composed of terms (n1 and n2) and operators (+)
- Computational form to run operations into the computer
- Evaluation: executing the operations specified in a given expression

Arithmetic operators

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- Power > multiplication/division > addition/subtraction

Other operators

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  - .ne. (/=)
  - .lt. (<)
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- String: // to concatenate two strings

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- Priority: arithmetic > relational > logical

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- Explicit conversion: int(), real(), dble()
- Example conv.f90