PROGRAMMING FOR COMPUTATIONAL CHEMISTRY

Optimization & parallelization

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- Check the performances (profiling, see next slides)

Optimization options

- Use optimization options of the compiler: -Ok (k=0,1, 2, 3) (type man ifort and search "Specifies the code optimization for applications.")
- Automatic optimization improving code performance
- Example with profiling.f90
- Compile with -O0, -O1, -O2 and -O3 (n=100 and m=1000 as input)
- Run the executable by typing time ./profiling.x

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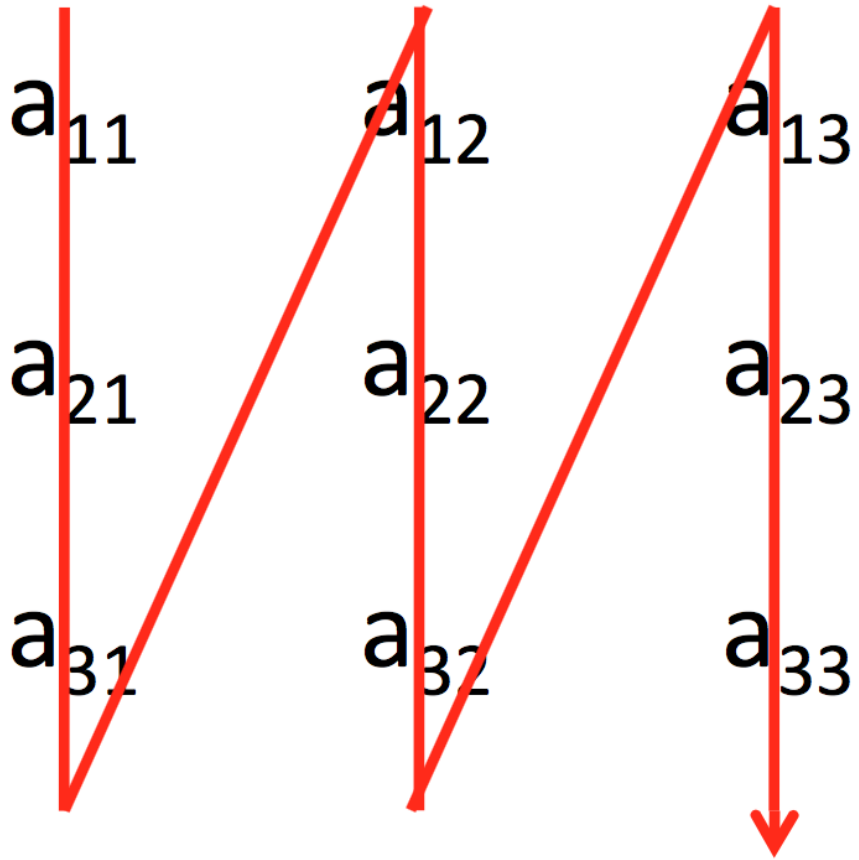

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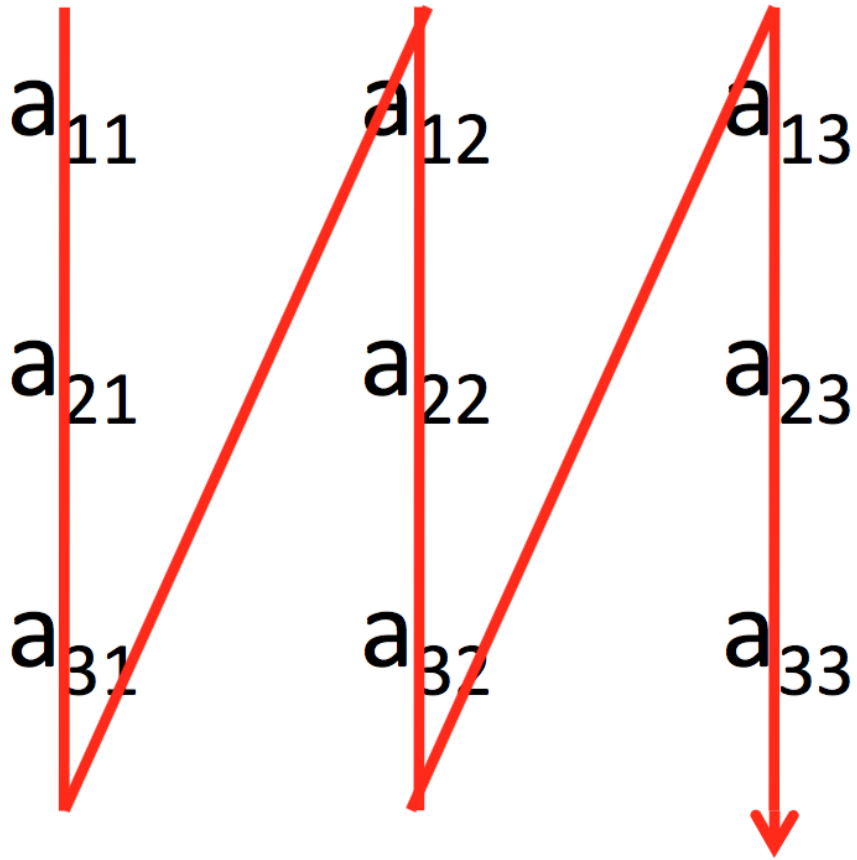

- Example matrix_swap.f90 (compile using -O0)

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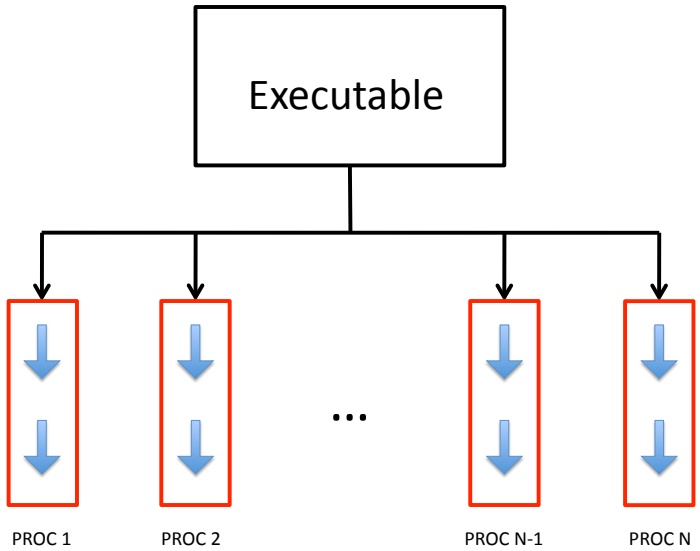

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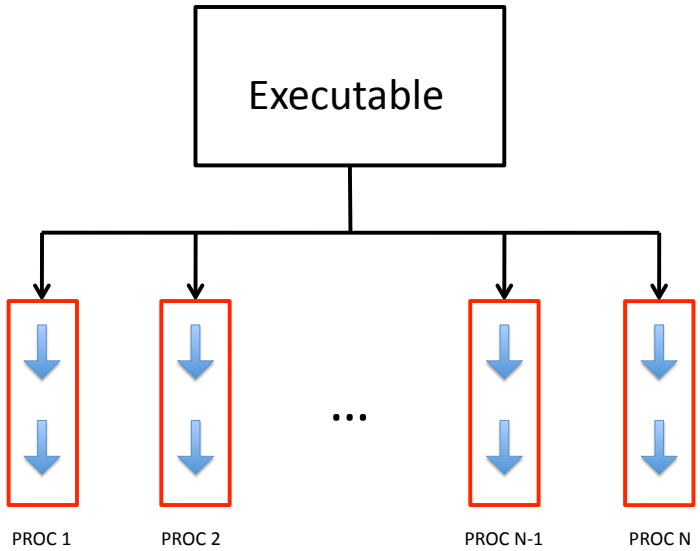

- Each process has a unique identifier (rank)

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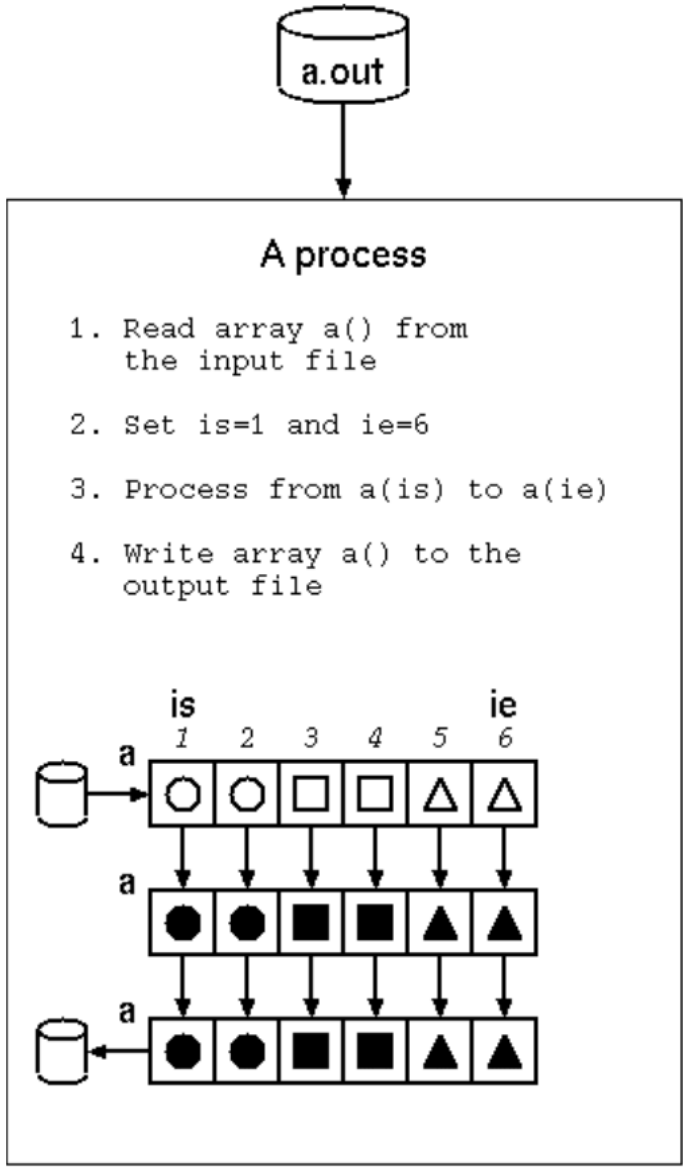

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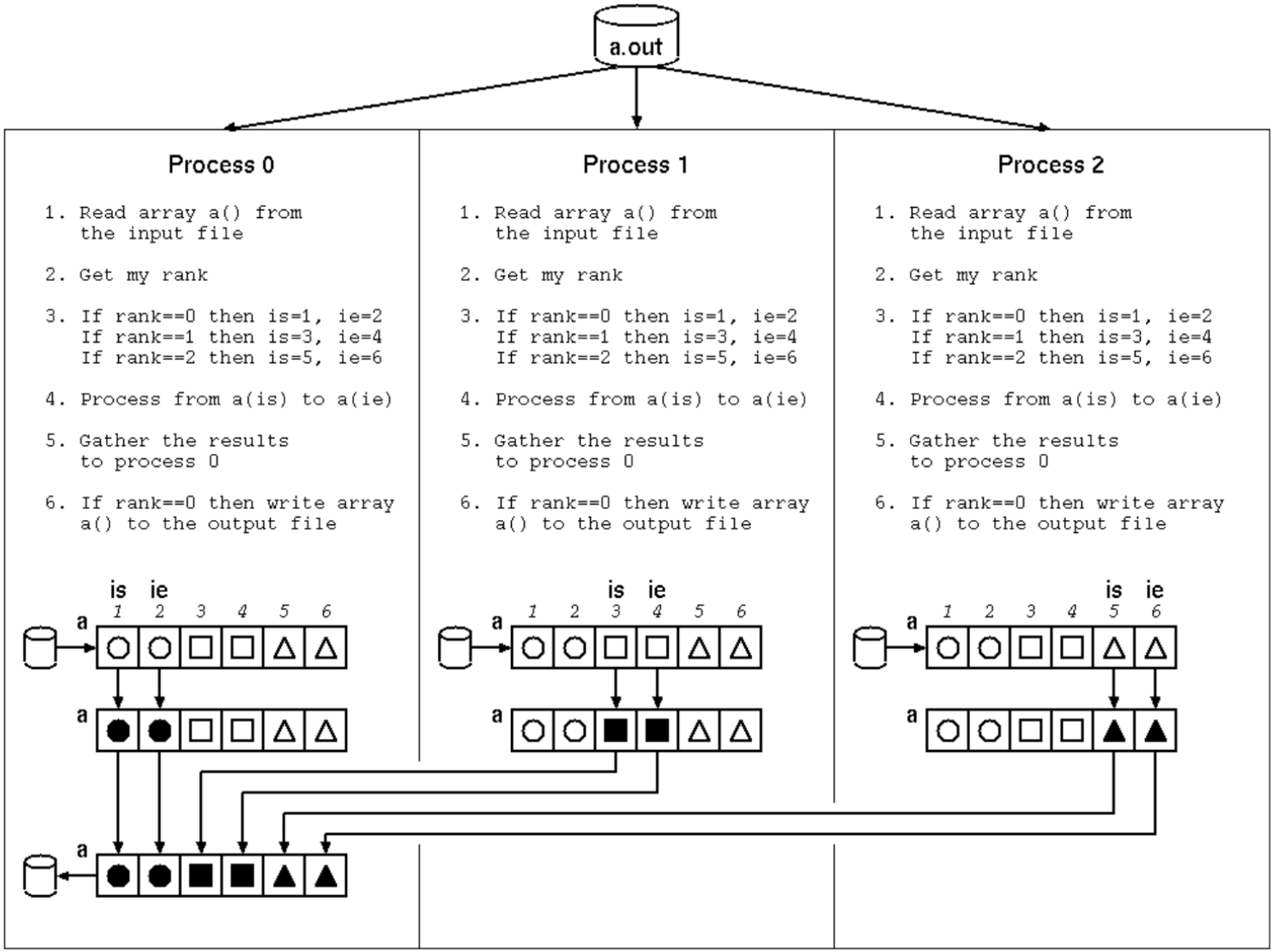

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- Example hello_world.f90

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- Examples: bcast.f90, simd.f90