Tecniche di programmazione in chimica computazionale

Optimization & parallelization

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Optimization

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- Check the performances (profiling, see next slides)

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- Examples form1.f90 and form2.f90

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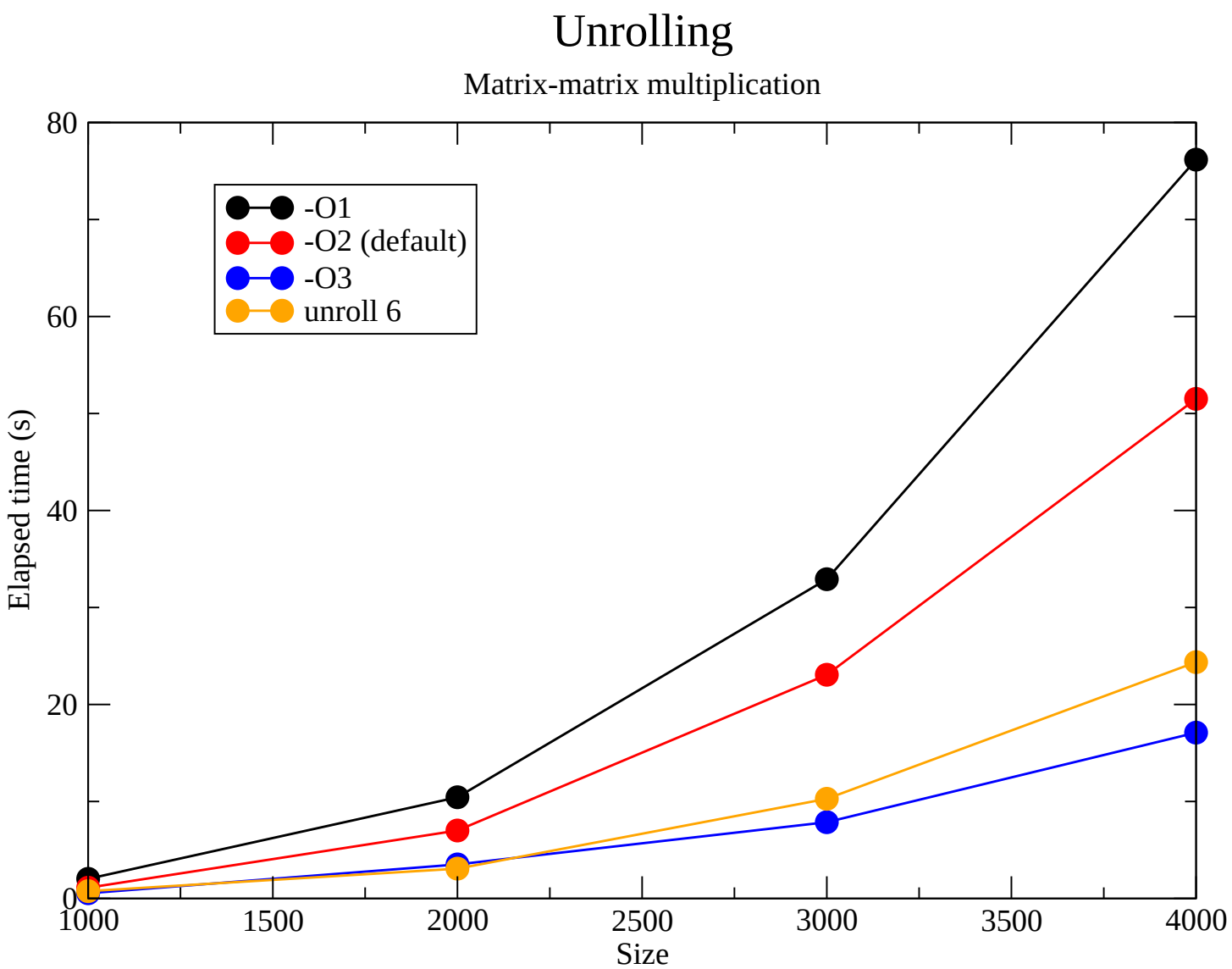
- Example unrolling.f90 (matrix-matrix multiplication)
- Use optimization options of the compiler: -On (n=0,1, 2, 3) (type *man ifort* and search "Specifies the code optimization for applications.")
- Automatic optimization improving code performance

Unrolling loops



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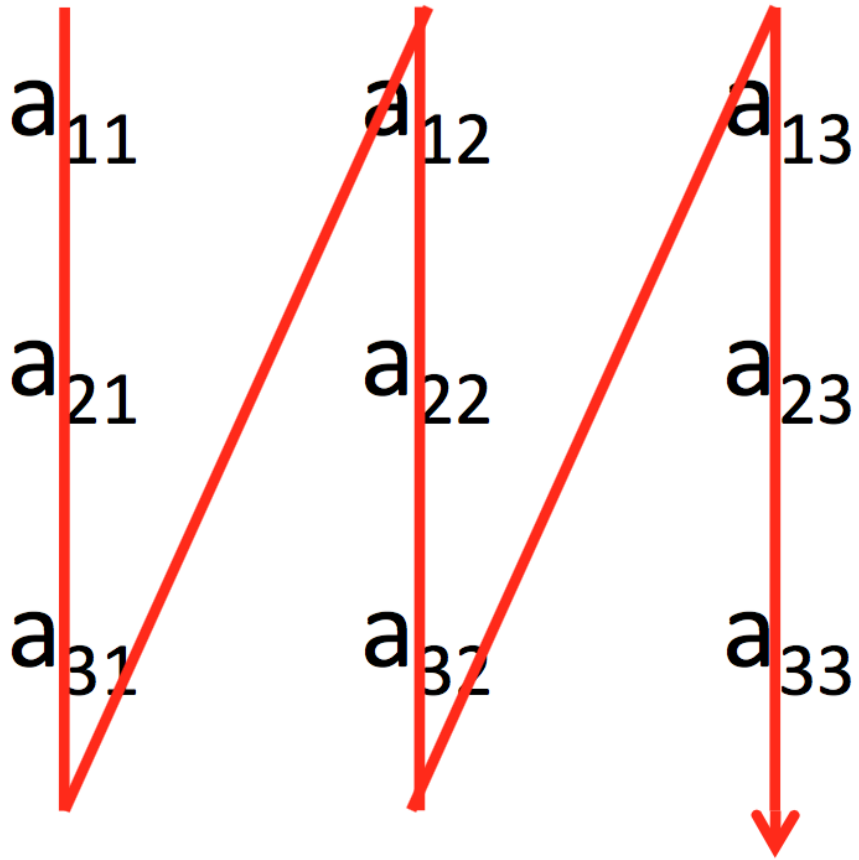

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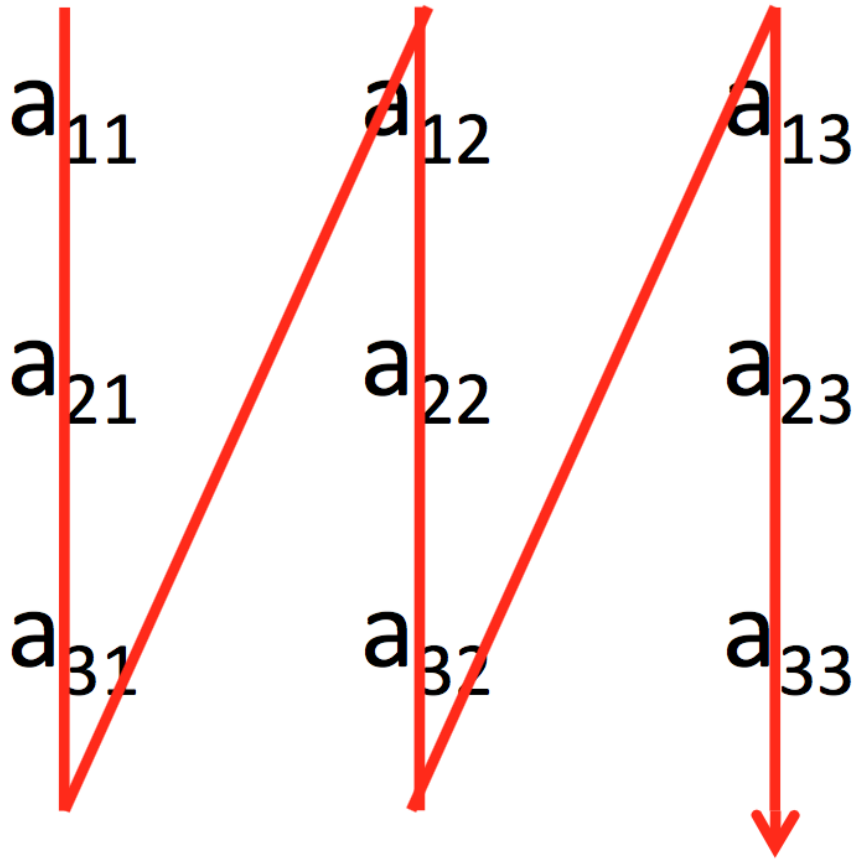

- Example matrix_swap.f90 (compile using -O0)

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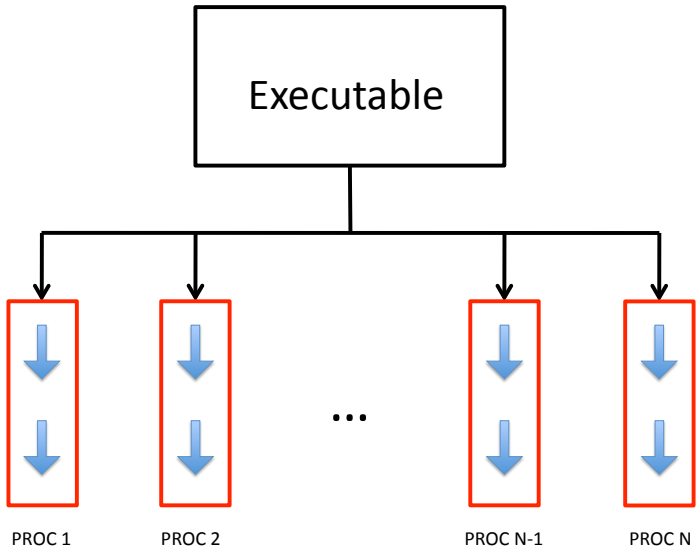

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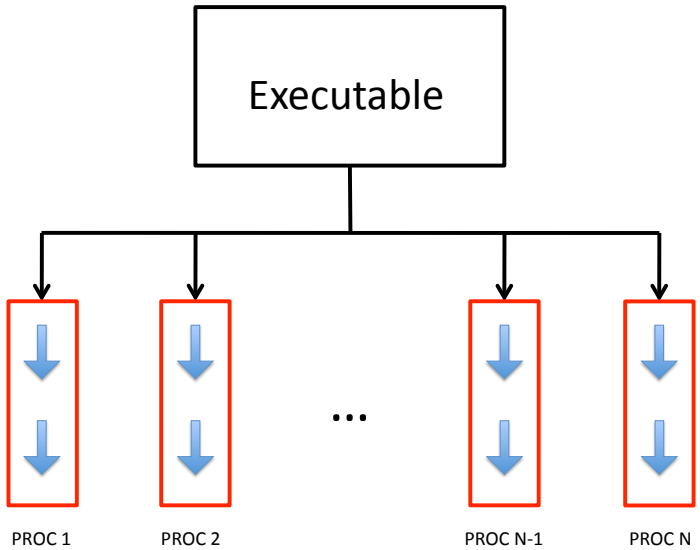

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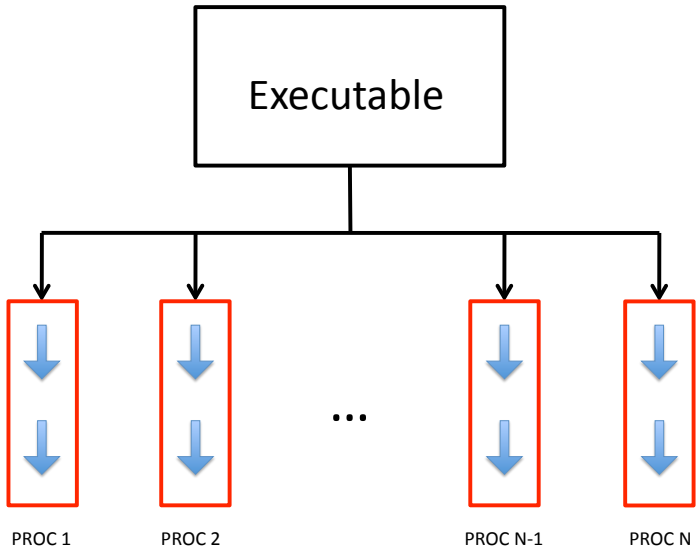

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- Where: RS/6000: Practical MPI Programming

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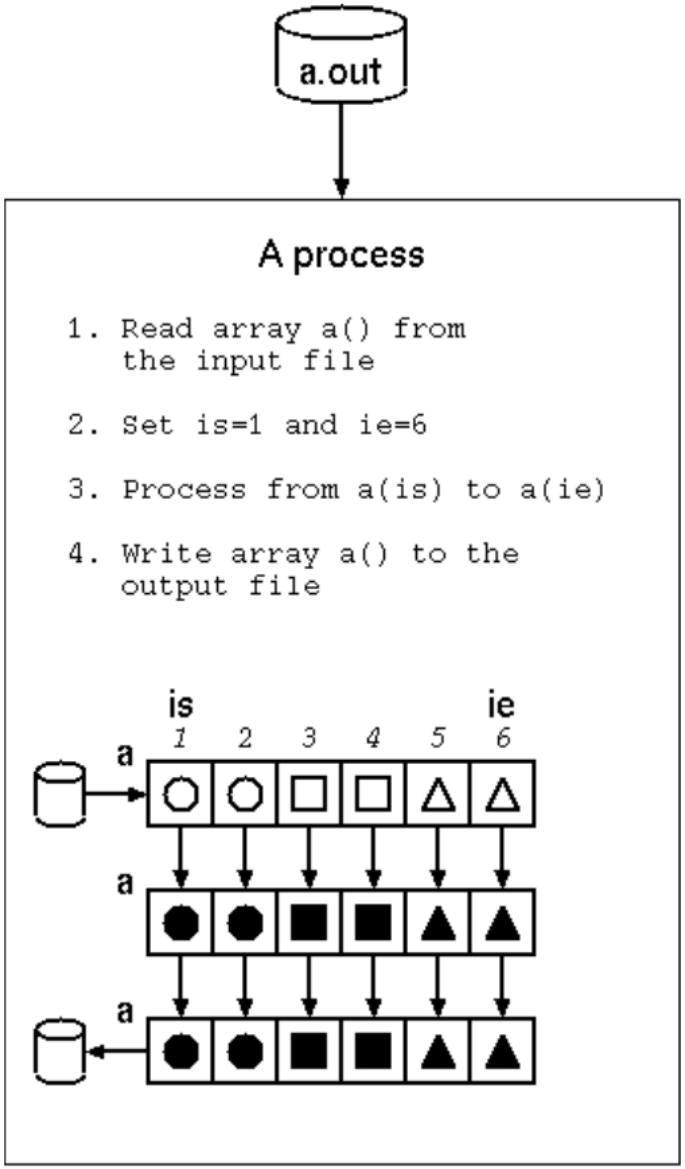

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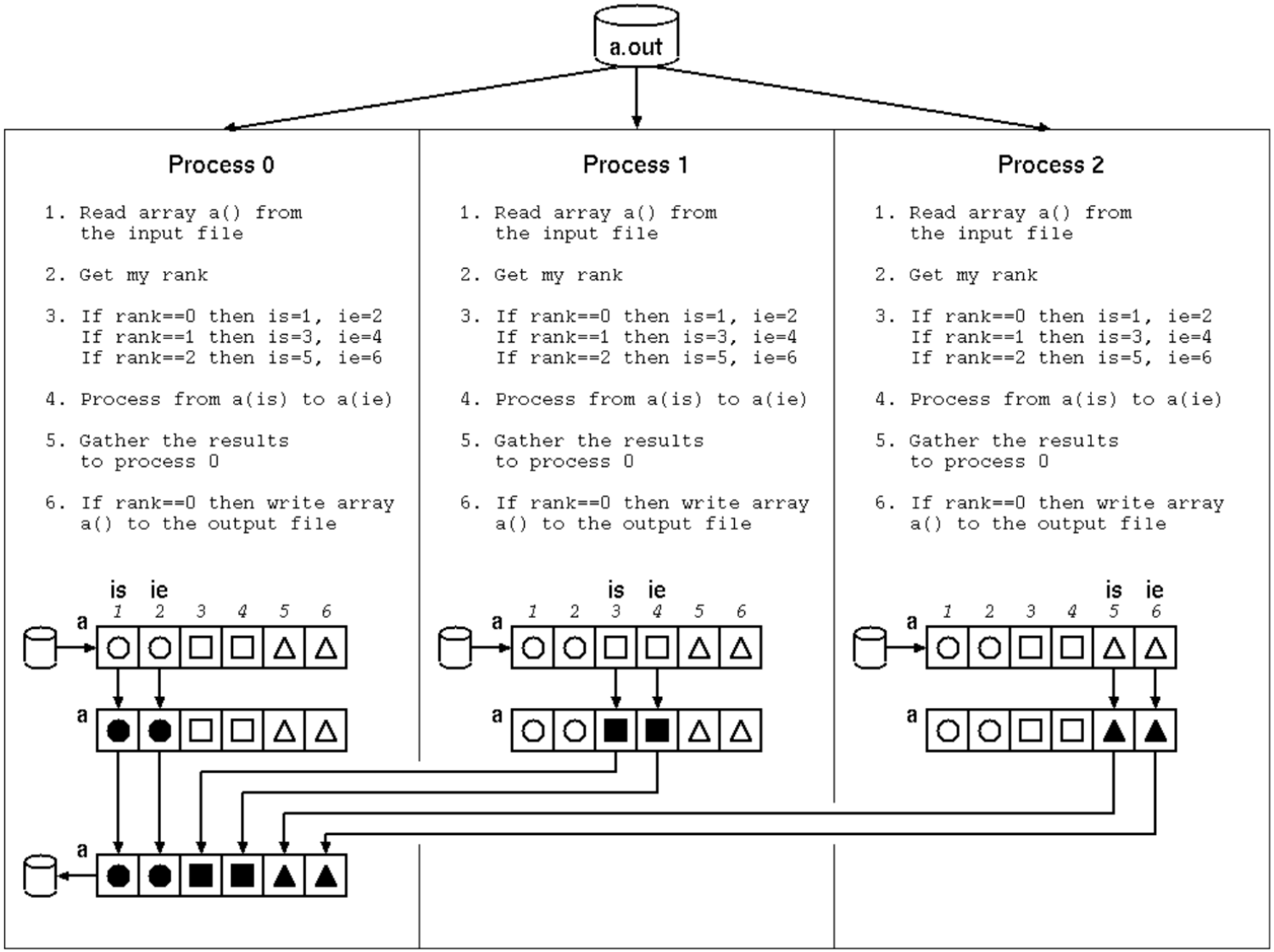

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- Example: hello_world.f90

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