

Tecniche di programmazione in chimica computazionale

Optimisation

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- Check the performances (**profiling**)

Optimization options

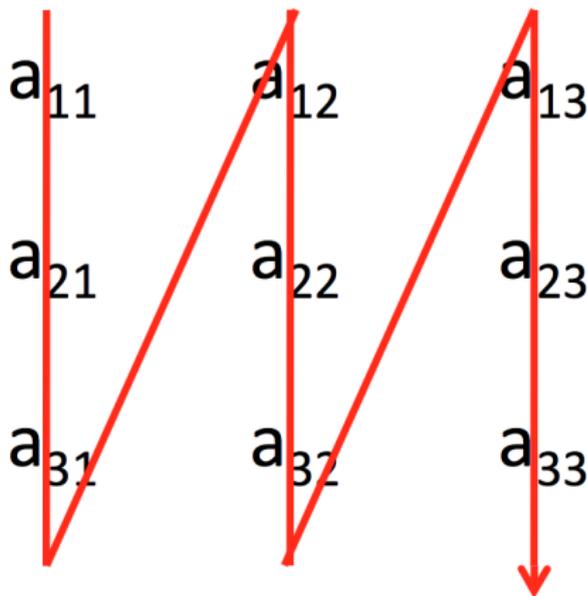
- Use **optimization options** of the **compiler**: `-Ok` ($k=0,1,2,3$) (type `man ifort` and search “Specifies the code optimization for applications.”)
- **Automatic** optimization improving code performance
- Example with **profiling.f90**
- Compile with `-O0`, `-O1`, `-O2` and `-O3` ($n=100$ and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

Swap indexes in matrices

- Methods to linearly store multidimensional arrays in RAM
- Fortran memory management: **column-major order**

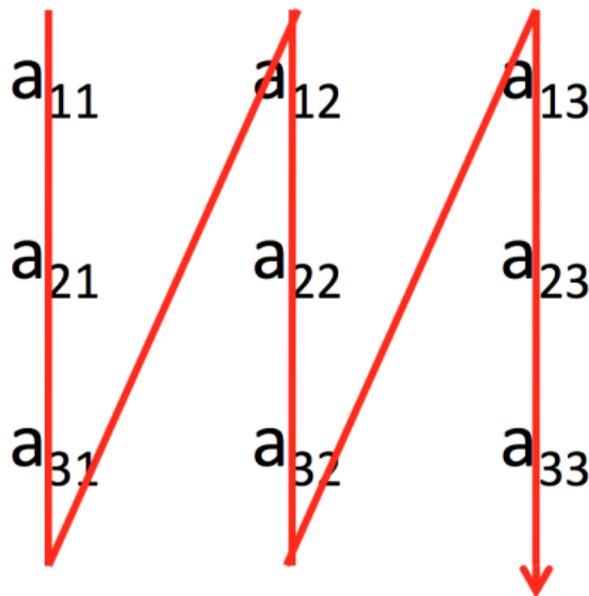
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- Example `matrix_swap.f90` (compile using `-O0`)

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- Example **profiling.f90**