

Fortran Programming for Scientific Computing

September 25–27, 2019

CSC – IT Center for Science Ltd, Espoo

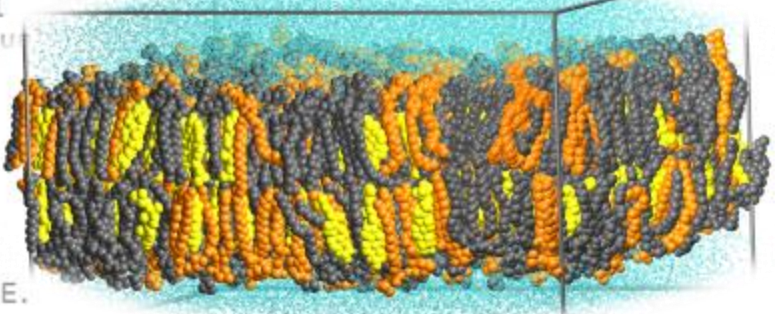
Sami Ilvonen

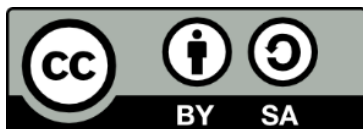
Jussi Enkovaara

```

DO imolecule_kind_a=1,nmolecule_kind
  molecule_kind_a => molecule_kind_set(imolecule_kind_a)
  CALL get_molecule_kind(molecule_kind=molecule_kind_a, molecule_list=molecule_list_a,&
    natom=natom_mol_a)
DO imolecule_a=1,SIZE(molecule_list_a)
  imol_a = imol_a + 1
  DO iatom_mol_a=1,natom_mol_a
    iatom_a = molecule_set(molecule_list_a(imolecule_a))%first_atom + &
      iatom_mol_a - 1
    imol_b = 0
    DO imolecule_kind_b=1,nmolecule_kind
      molecule_kind_b => molecule_kind_set(imolecule_kind_b)
      CALL get_molecule_kind(molecule_kind=molecule_kind_b,&
        molecule_list=molecule_list_b, natom=natom_mol_b)
      DO imolecule_b=1,SIZE(molecule_list_b)
        imol_b = imol_b + 1
        DO iatom_mol_b=1,natom_mol_b
          iatom_b = molecule_set(molecule_list_b(imolecule_b))%first_atom +&
            iatom_mol_b - 1
          ! is this block active
          IF (symmetric) THEN
            IF (iatom_a > iatom_b)
              include_ab = .FALSE.
            ELSE
              include_ab = .TRUE.
            END IF
          ELSE
            include_ab = .TRUE.
          END IF
        END DO
      END DO
    END DO
  END DO
END DO

```





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Agenda

Wednesday

Morning	Getting started with Fortran
Noon	Lunch break
Afternoon	Procedures and modules

Thursday

Morning	Fortran arrays
Noon	Lunch break
Afternoon	Input/output

Friday

Morning	Derived types Generic procedures and procedure pointers
Noon	Lunch break
Afternoon	Language interoperability Further features

**Coffee breaks at
10:00 and 14:30**

**Lectures are intertwined with hands-on
exercises**

Web resources

- CSC's Fortran95/2003 Guide (in Finnish) for free
<https://goo.gl/xE9847>
- Fortran wiki: a resource hub for all aspects of Fortran programming
<http://fortranwiki.org>
- GNU Fortran online documents
<http://gcc.gnu.org/onlinedocs/>