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Python in High-Performance Computing

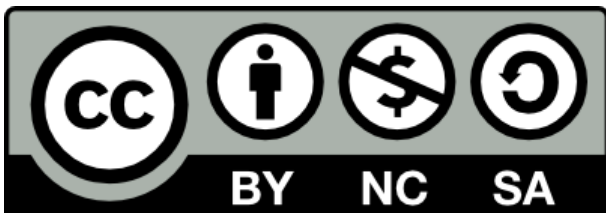
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```
import sys, os
try:
    from Bio.PDB import PDBParser
    __biopython_installed__ = True
except ImportError:
    __biopython_installed__ = False

__default_bfactor__ = 0.0      # default B-factor
__default_occupancy__ = 1.0    # default occupancy level
__default_segid__ = ''        # empty segment ID

class EOF(Exception):
    def __init__(self): pass

class FileCrawler:
    """
    Crawl through a file reading back and forth without loading
    anything to memory.
    """
    def __init__(self, filename):
        try:
            self.__fp__ = open(filename)
        except IOError:
            raise ValueError, "Couldn't open file '%s' for reading." % filename
        self.tell = self.__fp__.tell
        self.seek = self.__fp__.seek
    def prevline(self):
        try:
            self.prev()
```



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Agenda

Thursday

9:00-9:15	Python and HPC
9:15-10:00	NumPy – fast array interface to Python
10:00-10:30	Exercises
10:30-11:00	Coffee Break
11:00-11:30	Vectorized operations & broadcasting
11:30-12:00	Exercises
12:00-13:00	Lunch break
13:00-13:30	Advanced indexing, I/O, and misc utilities
13:30-14:30	Exercises
14:30-15:00	Coffee Break
15:00-16:00	Visualisation with Python
16:00-17:00	Exercises

Friday

9.00-9.45	MPI introduction
9:45-10:30	MPI and Python – mpi4py
10.30-11.00	Coffee break
11:00-12:00	Exercises
12.15-13.00	Lunch break
13.00-13:30	Multiprocessing, i.e. process-based "threading"
13:30-14:30	Exercises
14.30-15.00	Coffee break
15.00-15.30	C extensions – integrating efficient C routines in Python
15:30-16:30	Exercises
16:30-17:00	Summary of Python HPC strategies

