

Tecniche di programmazione in chimica computazionale

Esame 5/9/24

- 1) Read from the same file an integer number n , and a square matrix $A(n \times n)$ with complex elements in double precision;
- 2) Compute the sum: of the real part of the elements of the antidiagonal ($s1$); of the imaginary part of the elements of the upper triangular part ($s2$); of the imaginary part of the elements of the first and last column ($s3$);
- 3) if ($s1-s2$) is larger than ($s2-s3$) compute the transpose conjugate of A without using the `implicit transpose()` Fortran function; otherwise, define a one-dimensional array $b(n)$ obtained with the integer part of the real parts of the elements of the diagonal of A , and sort it in increasing order;
- 4) print on a file the results from point 3).