

Intensive computation

Prof. A. Massini

Midterm Exam – April 16, 2021

- Student's Name -

- Matricola number -

Question 1 (5 points)	
Exercise 1 (8 points)	
Exercise 2 (6 points)	
Question 2 (4 points)	
Exercise 3 (4 points)	
Question 3 (4 points)	
Total (31 points)	

Question 1 (5 points) - Molecular Dynamics

Briefly describe: **a)** the Hooke Law Model, **b)** how to solve it using the modeling based on differential equations **c)** how to obtain the exact solution. *Consider the 1-dimensional case with at most 4 particles.*

Exercise 1 (5+3 points) - Methods for Differential equations and errors

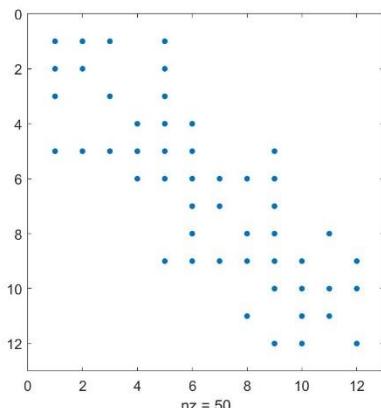
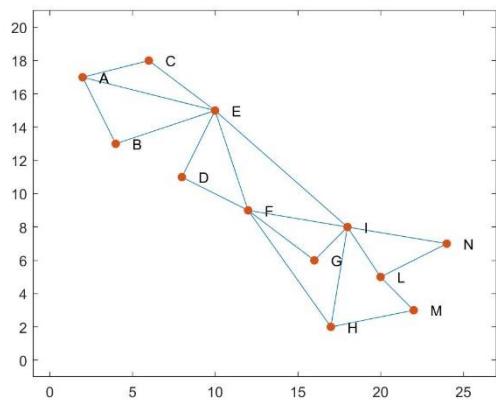
- a) Consider the initial value problem $y' = \frac{4x^3}{y}$ $y(1) = 2$

Use Euler's Method with a step size of $h_1 = 0.2$ and a step size of $h_2 = 0.3$ to find the approximate value of the solution for $x=1,6$.

Use two fractional digits (decimal places).

- b) Compute the relative forward error and the relative backward error, giving percentage values, using the approximate solution obtained for $x=1,6$ in both cases h_1 and h_2 , using the exact solution: $y = \sqrt{2x^4 + 4}$

Exercise 2 (6 points) Consider the graph G and the corresponding adjacency matrix M shown here below. Consider the (symmetric) matrix D containing distances among nodes (double precision values).



- a) Specify which arrays you need for the following compressed representations and how many bytes they occupy in memory.

Ellpack-Itpack

CSR

BSR – choose the most convenient block size > 2

b) Explain how arrays change after in the graph a new edge is added between nodes I and N and what is the new memory occupation for the compressed representations of matrix D.

Ellpack-Itpack

CSR

BSR – choose the most convenient block size > 2

Question 2 (4 points) Explain how the Power method and the Deflation method work to compute eigenvalues and eigenvectors.

Exercise 3 (4 points) a) Explain how to find the most connected node in a graph. **b)** If the vector of eigenvalues and the matrix of eigenvectors for the graph in Exercise 1 are the following, specify what the most connected node in the graph is and explain why.

-1.5390	-0.7380	-0.6023	-0.3677	-0.0691	0.6277	1.0000	1.3152	1.7651	2.4249	3.3915	4.7917
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	1	2	3	4	5	6	7	8	9	10	11	12
1	0,0588	-0,0836	0,1940	-0,5891	-0,4654	-0,0468	0,0000	0,2270	-0,0627	0,2939	-0,4472	0,2104
2	0,1678	0,2355	-0,2938	0,3427	0,0346	-0,0180	-0,7071	0,1289	-0,0400	0,2081	-0,3454	0,1740
3	0,1678	0,2355	-0,2938	0,3427	0,0346	-0,0180	0,7071	0,1289	-0,0400	0,2081	-0,3454	0,1740
4	0,1081	0,4575	0,1735	-0,0019	-0,2782	-0,1558	0,0000	-0,6937	-0,0273	-0,3065	-0,1270	0,2347
5	-0,4848	-0,3257	0,2769	0,1204	0,4284	0,0535	0,0000	-0,1863	0,0321	0,0026	-0,3788	0,4496
6	0,2103	-0,4695	-0,5549	-0,1178	-0,1310	0,0045	0,0000	-0,0324	-0,0530	-0,4394	0,0750	0,4403
7	-0,2869	0,1604	0,1394	0,1894	-0,2024	-0,5874	0,0000	0,4763	0,2543	-0,2806	0,1501	0,2404
8	-0,3885	0,3331	-0,0321	-0,0055	-0,1552	0,4739	0,0000	0,2109	-0,5471	-0,0812	0,2511	0,2736
9	0,5182	0,1907	0,3315	-0,1412	0,3473	0,2142	0,0000	0,1826	0,2475	0,0396	0,2840	0,4712
10	-0,2667	0,1885	-0,4084	-0,3591	0,2091	-0,3268	0,0000	-0,2373	0,0779	0,4861	0,3265	0,2045
11	0,2581	-0,3001	0,2749	0,2666	-0,0505	-0,3951	0,0000	-0,0837	-0,6132	0,2841	0,2415	0,1261
12	-0,0990	-0,2181	0,0480	0,3658	-0,5205	0,3026	0,0000	-0,1737	0,4253	0,3689	0,2552	0,1782

Question 3 (4 points) Describe the Jacobi method and the Gauss-Seidel method.