Prof. A. Massini Exam – July 20, 2016 Part A - Student's Name - Matricola number Exercise 1 (5 points) Question 1 (6 points) Question 2 (5 points) Exercise 2 (5 points) Exercise 2 (5 points) Question 3 (5 points)

Exercise 3 (6 points)

Total (32 points)

Intensive computation

Exercise 1 (5 points) - Sparse matrices

Consider the sparse matrix 10x10 here below

0,608806	0	0	0	-0,3044	0	0	0	0	0
0	15080,45	0	0	0	-7540,22	94,2528	0	0	0
0	0	3,14176	0	0	-94,2528	0,78544	0	0	0
0	0	0	12566400	0	0	0	-6283200	0	0
-0,3044	0	0	0	0,608806	0	0	0	-0,3044	0
0	-7540,22	-94,2528	0	0	15080,45	0	0	0	-7540,22
0	94,2528	0,78544	0	0	0	3,14176	0	0	-94,2528
0	0	0	-6283200	0	0	0	12566400	0	0
0	0	0	0	-0,3044	0	0	0	0,608806	0
0	0	0	0	0	-7540,22	-94,2528	0	0	15080,45

a)	Show its Skyline representation (using symbolic names m_{ij} for nonzero elements) .
b)	Show the Skyline representation after cancellation of element $m_{8,4}$ and its symmetric
c)	Show the Skyline representation after the insertion of element m _{9,3} and its symmetric

Question 1 (6 points) - Sparse matrices & Matlab

Question 2 (5 points) GPU & CUDA

Explain wl	hat a CUDA kernel is and how it is executed.

Exercise 2 (5 points) - Linear systems

Apply the Cholesky factorization method to the matrix $\begin{pmatrix} 1 & 2 & 4 \\ 2 & 13 & 23 \\ 4 & 23 & 77 \end{pmatrix}$.

Question 3 (5 points) - Linear systems Briefly describe the Gauss elimination method and the possible strategies of pivoting.

Exercise 3 (6 points) - Linear systems

Solve the system

$$\begin{cases} 9x_1 + x_2 + x_3 = 1 \\ 2x_1 + 10x_2 + 3x_3 = 2 \\ 3x_1 + 4x_2 + 11x_3 = -1 \end{cases}$$

with Jacobi's Method using $\mathbf{x}^{(0)} = (0, 0, 0)$ as starting solution.

Complete the table below, doing three iterations.

k	X ₁ ^(k)	X ₂ ^(k)	X ₃ ^(k)
0	0	0	0
1			
2			
3			

Exam – July 20, 2016	
Part B	
	- Student's Name
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	Exercise 1 (4 points)
	Exercise 2 (4 points)
	Exercise 3 (4 points)
	Exercise 4 (5 points)
	Question 1 (5points)
	Question 2 (5 points)
	Question 3 (5 points)

Total (32 points)

Intensive computation

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Exercise 1 (4 points) - Errors

a) Given $y'=2,2$ as the approximation of $\sqrt{5}$, compute the absolute and relative forward error and absolute and relative backward error.
absolute forward error
<i>relative</i> forward error
absolute backward error
<i>relative</i> backward error
b) Compute the value of the condition number.
Exercise 2 (4 points) - Errors
Show the contribution of <i>computational error</i> and <i>propagated data error</i> when computing $\sin(7\pi/8)$.

Exercise 3 (4 points) - Eigenvalues and eigenvectors

Apply four iterations of the Power Method to the matrix: $\begin{pmatrix} 1 & 1 & -1 \\ 1 & 2 & 1 \\ 2 & -1 & 1 \end{pmatrix}$				

Exercise 4 (5 points) - Methods for Differential equations

Consider the initial value problem $y' = \frac{y \ln y}{x}$ $y(2) = e$
Use Euler's Method for four iterations (e.g. compute the approximation y_4) with a step size of $h=0.1$ to find approximate values of the solution. The exact solution is: $y=e^{x/2}$
Compare the approximate solution obtained for $h = 0.1$ after four iterations with the exact value of the solution giving the percentage error.

Question 1 (5 points) - Molecular Dynamics Describe the three principal models used in Molecular dynamics (Hooke's law, Lennard-Jones, hard sphere).

Question 2 (5 points) - Global optimization

Describe what the global optimization aim is, in particular with respect to local optimization, and briefly describe some techniques.				

Question 3 (5 points) - Simulation Describe what is meant by model verification and model validation and some possible techniques.