CS 230, Quiz 4

Name: _____ ID: _____

You will have 15 minutes to complete this quiz. This quiz contains 2 problems of equal value; **only the highest-scoring question will contribute to your grade**. Choose carefully.

Problem 1 (4 points)

The Lennard-Jones potential is simple model describing the interaction between two molecules. With this model, two molecules have potential energy ϕ given by

$$\phi(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right),$$

where ϵ and σ are constants and $r = \|\mathbf{x}_1 - \mathbf{x}_2\|$ is the distance between two molecules at locations $\mathbf{x}_1$ and $\mathbf{x}_2$. Find the force $\mathbf{f}_1$ felt by the molecule at $\mathbf{x}_1$ as a result of this interaction.

Problem 2 (4 points)

In class, we saw a few schemes for solving the differential equation $x' = f(x)$, where the function $f(x)$ is given. One of these was the midpoint rule, which is *implicit*. We analyzed the stability by considering the differential equation $x' = -\lambda x$ with $\lambda > 0$, where we found $x^{n+1} = Ax^n$ for some number A that depended on λ and Δt. We then concluded that the method would be stable if $|A| < 1$. There is also an *explicit* midpoint rule, which is given by the rule

$$x^{n+1} = x^n + \Delta t f\left(x^n + \frac{\Delta t}{2} f(x^n)\right).$$

(a) If we apply this scheme to $x' = -\lambda x$, show that $x^{n+1} = Ax^n$ for some number A; find A (it should depend on λ and Δt). (b) What restrictions are required of Δt so that $|A| < 1$?