Homework #1 – Solutions

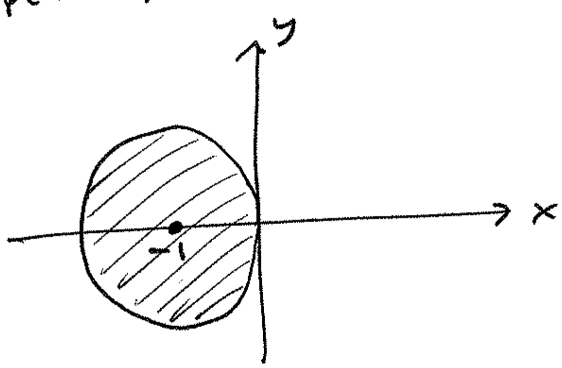
Problem 1 (a) For the explicit Euler scheme, the iteration for the model problem is

$$x^E_{n+1} = (1+\lambda\Delta t)\,x^E_n = (1+z)\,x^E_n$$

Hence, $x^E_n \to 0$ as $n \to \infty$ iff

$$|1+z| < 1$$

This corresponds to the disk of radius 1 around $z=-1$ in the complex plane:



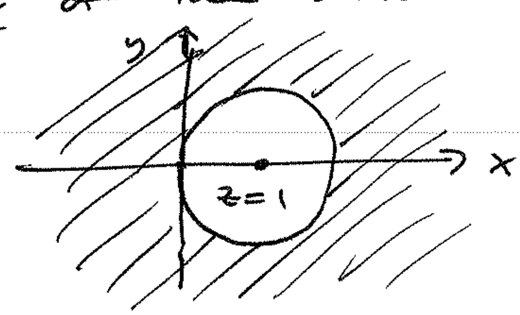
For the implicit Euler scheme,

$$x^I_{n+1}(1-\lambda\cdot\Delta t) = x^I_n \quad \text{or} \quad x^I_{n+1} = \frac{x^I_n}{(1-z)}.$$

Hence, $x^I_n \to 0$ as $n \to \infty$ iff

$$\left|\frac{1}{1-z}\right| < 1 \quad \text{or} \quad |1-z| > 1.$$

This is the <u>exterior</u> of the disk of radius 1 around $z=1$:



(b) It appears from the plots that the Euler approximation is acceptable for $N = 500$ and 600, but not $N=400$. This can be explained in terms of the absolute stability properties of the Euler scheme. From part (a) it is seen that the threshold of stability for the explicit Euler scheme is $z = -2$ along the real axis. In the present problem

$$J = \frac{\partial f}{\partial x} = -\frac{1}{\epsilon}$$

and

$$\Delta t = \frac{1}{N}$$

so that stability requires

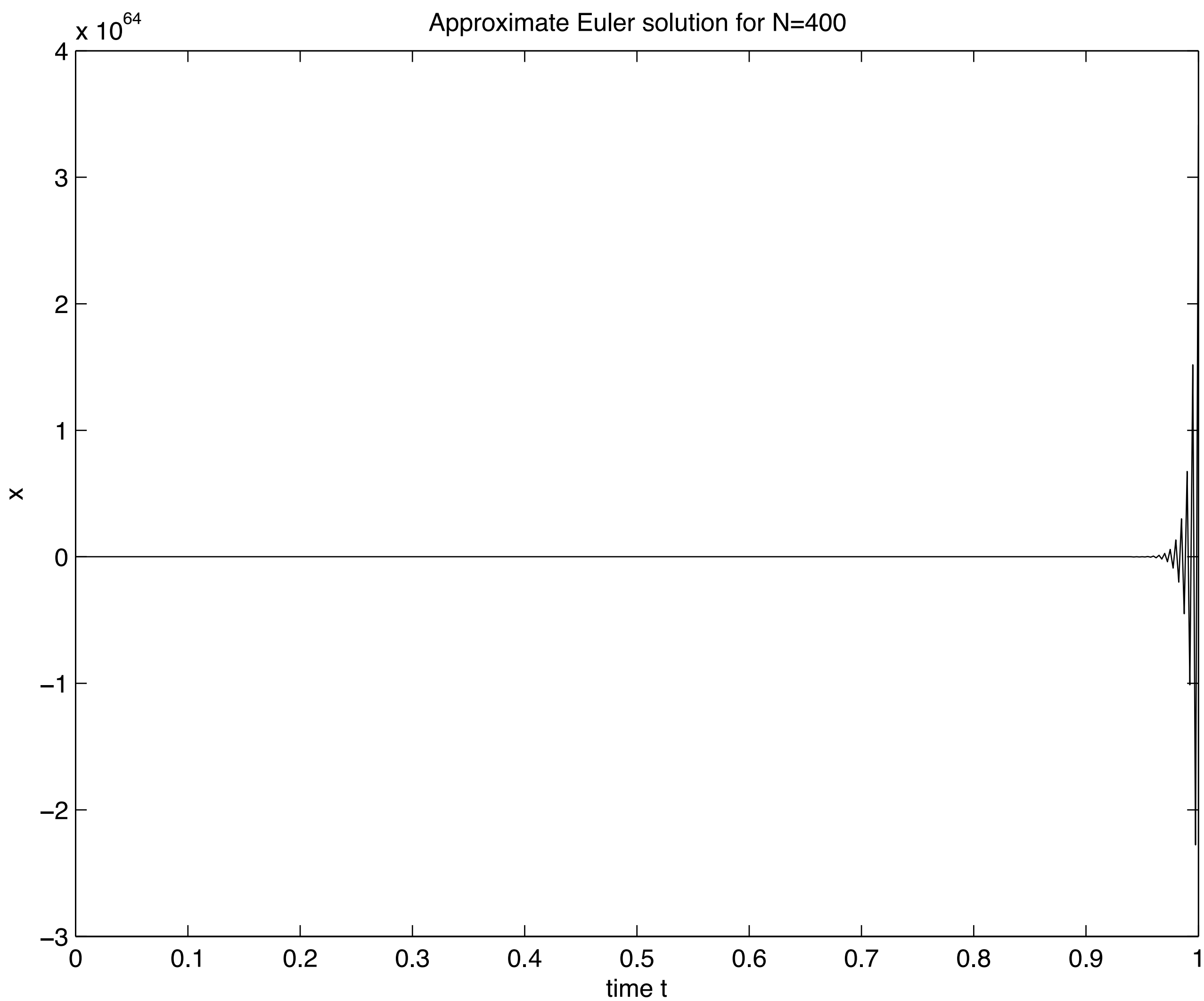
$$2 > |J \cdot \Delta t| = \frac{1}{\epsilon N}$$

or

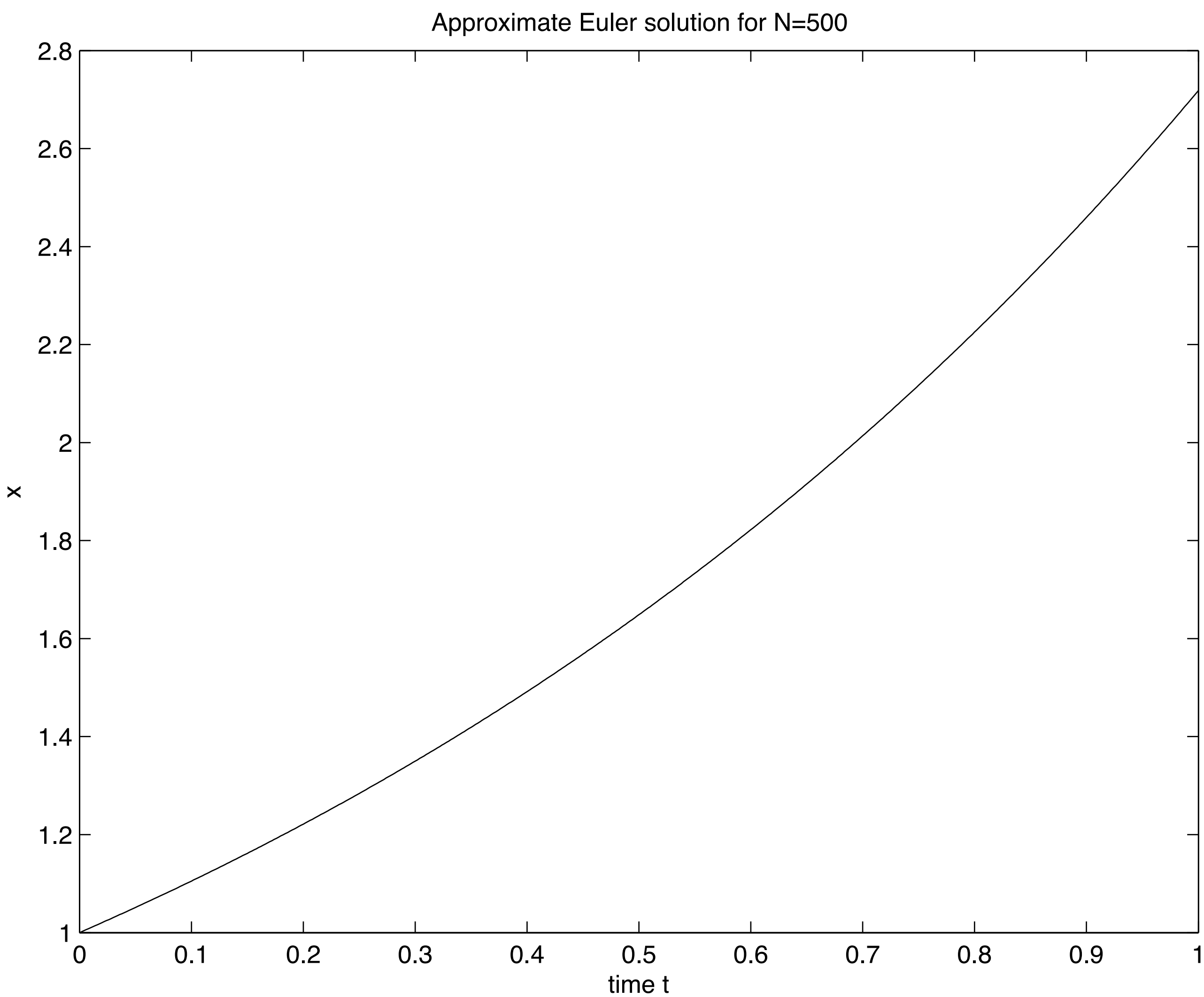
$$N > \frac{1}{2\epsilon} = 500.$$

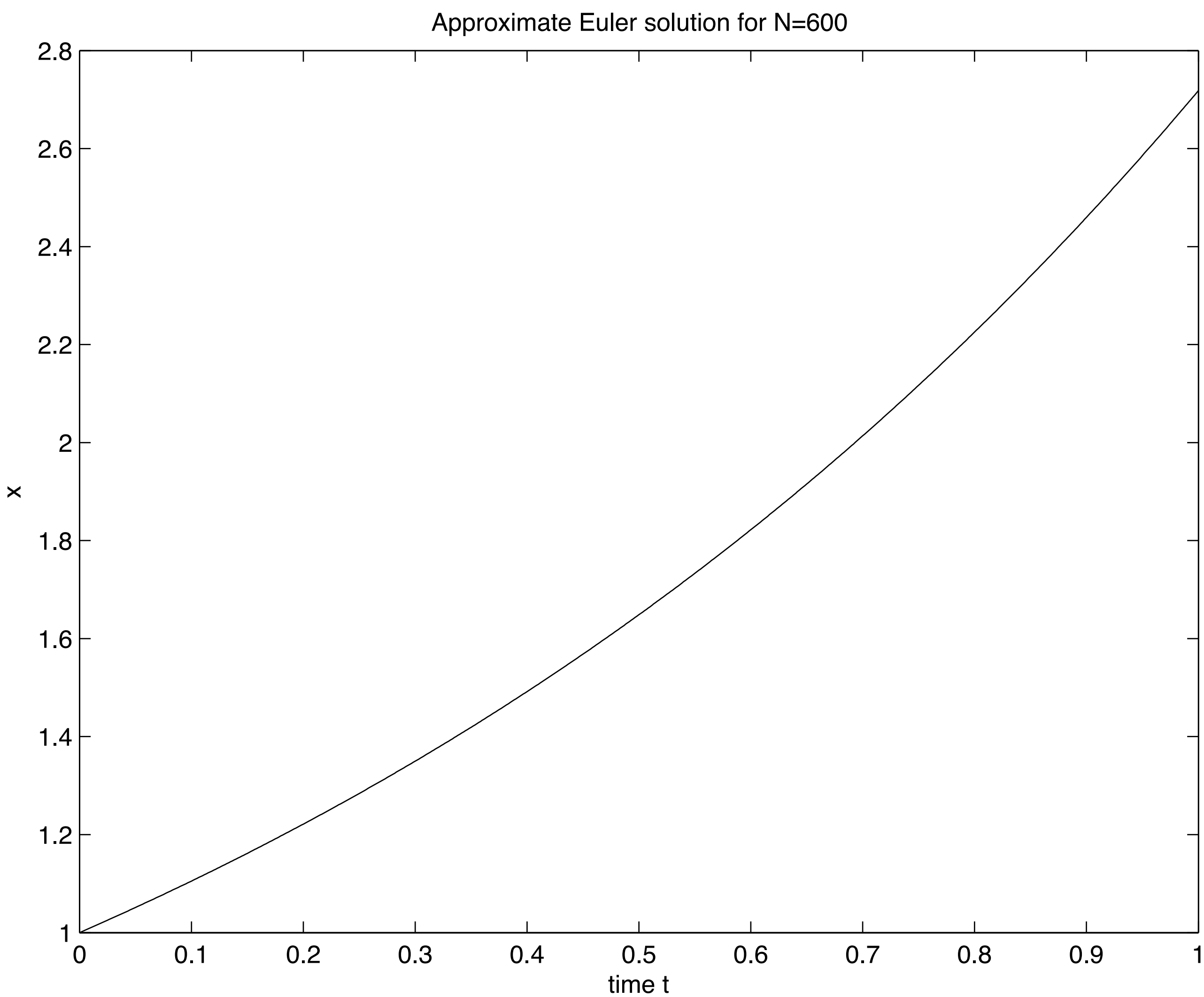
The case $N = 500$ is marginal for stability.

This is verified by plotting the errors in the Euler solution for $N = 499, 500$ and 501. In addition to a gradual growth in the magnitude of the errors with time, there are also oscillations in the error. These have growing amplitude for $N=499$, constant amplitude for $N=500$ and decaying amplitude for $N=501$. This change in the amplitude of oscillations for N increasing beyond 500 illustrates the change in the stability properties of the Euler scheme.

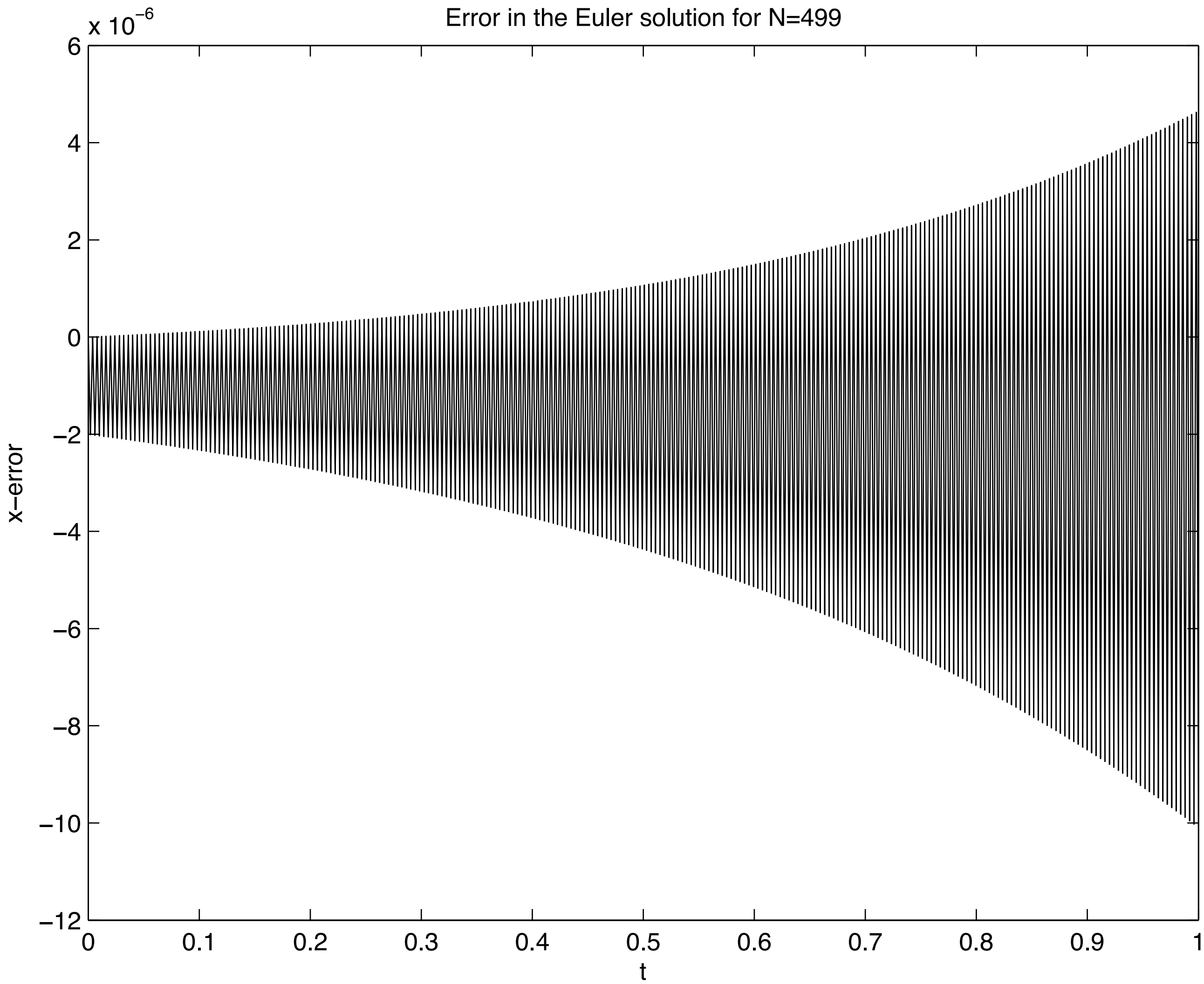


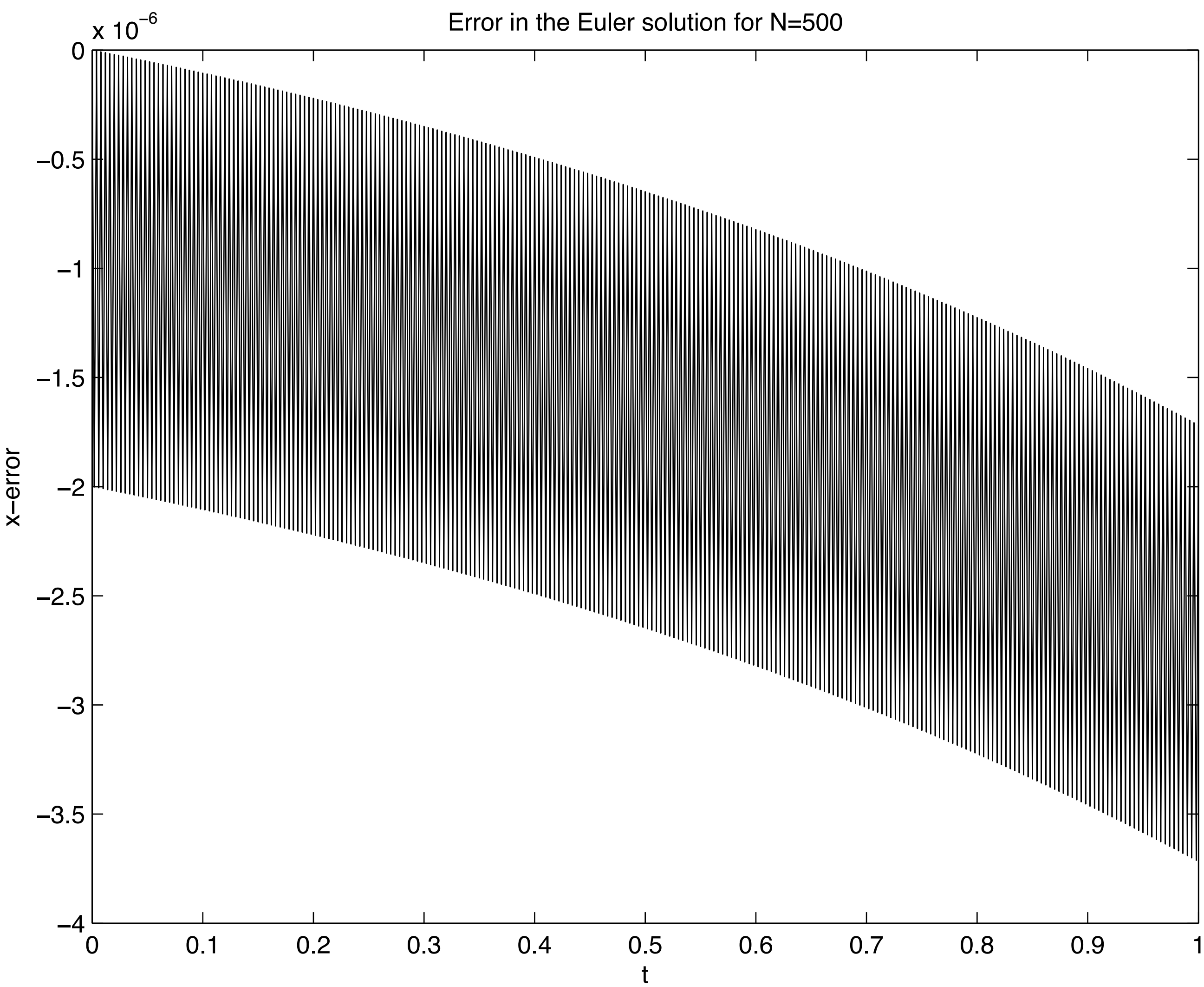
Approximate Euler solution for N=400
x 10^64
4
3
2
1
0
−1
−2
−3
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
time t

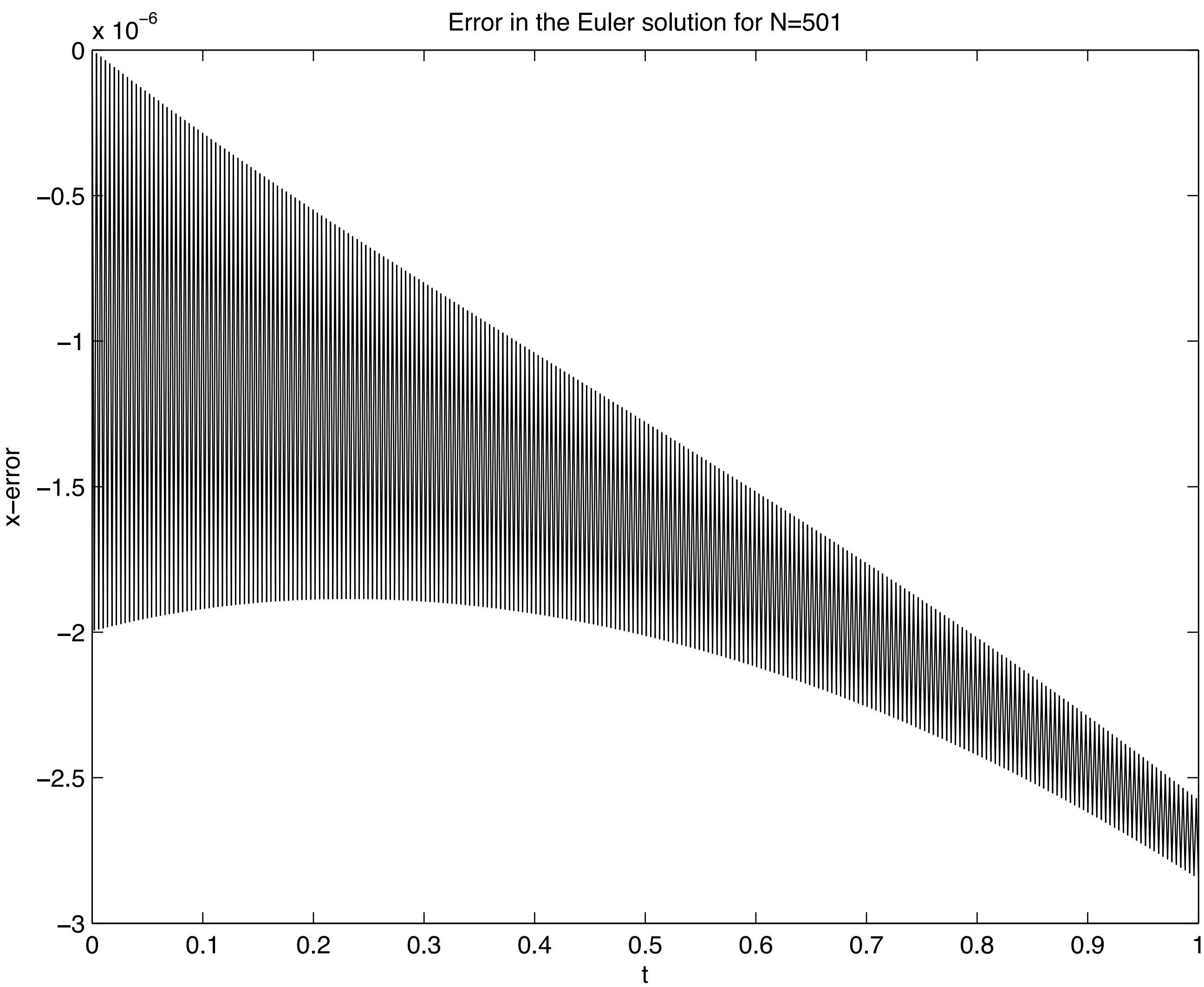

Approximate Euler solution for N=500
x
time t
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1



Approximate Euler solution for N=600
x
time t
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8


Error in the Euler solution for N=499
x 10^−6
x−error
t
6
4
2
0
−2
−4
−6
−8
−10
−12
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


Error in the Euler solution for N=500
x 10^-6
0
−0.5
−1
−1.5
−2
−2.5
−3
−3.5
−4
x−error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
t



Error in the Euler solution for N=501
x 10^−6
0
−0.5
−1
−1.5
−2
−2.5
−3
x−error
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
t

Problem 2. (a) With

$$\hat{O}(t) \equiv e^{it\hat{H}/\hbar}\,\hat{O}\,e^{-it\hat{H}/\hbar},$$

we verify by differentiation that

$$\frac{d}{dt}\hat{O}(t) = \frac{i\hat{H}}{\hbar}\,e^{it\hat{H}/\hbar}\,\hat{O}\,e^{-it\hat{H}/\hbar} + e^{it\hat{H}/\hbar}\,\hat{O}\,e^{-it\hat{H}/\hbar}\left(-\frac{i\hat{H}}{\hbar}\right)$$

$$= \frac{i}{\hbar}\left(\hat{H}\,\hat{O}(t) - \hat{O}(t)\,\hat{H}\right)$$

$$= \frac{i}{\hbar}[\hat{H}, \hat{O}(t)].$$

It follows that

$$\langle \Psi, \hat{O}(t)\Psi \rangle = \langle \Psi, e^{it\hat{H}/\hbar}\,\hat{O}\,e^{-it\hat{H}/\hbar}\Psi \rangle.$$

We now use the property, easily verified by direct calculation that

$$\langle \Psi, \hat{H}\Psi \rangle = \langle \hat{H}\Psi, \Psi \rangle,$$

which implies that $H^* = H$ or H is hermitian. Thus,

$$\left(e^{it\hat{H}/\hbar}\right)^* = e^{-it\hat{H}/\hbar}$$

and

$$\langle \Psi, \hat{O}(t)\Psi \rangle = \langle e^{-it\hat{H}/\hbar}\Psi, \hat{O}\cdot e^{-it\hat{H}/\hbar}\Psi \rangle$$

$$= \langle \Psi(t), \hat{O}\,\Psi(t) \rangle$$

with

$$\Psi(t) \equiv e^{-it\hat{H}/\hbar}\,\Psi .$$

Then,

$$\frac{d}{dt}\Psi(t) = -\frac{i\hat{H}}{\hbar}\, e^{-it\hat{H}/\hbar}\Psi = -\frac{i}{\hbar}\hat{H}\Psi(t)$$

or

$$i\hbar \frac{d}{dt}\Psi(t) = \hat{H}\Psi(t).$$

(6) The Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

are satisfied iff the smooth function $f = u + iv$ is complex-analytic. This is easily seen to coincide with the condition that

$$\begin{aligned} 0 &= \frac{\partial}{\partial \bar{z}} f(z,\bar{z}) \\ &= \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)(u+iv) \\ &= \frac{1}{2}\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) + \frac{i}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right). \end{aligned}$$

The definitions

$$\frac{\partial}{\partial z} = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right), \quad \frac{\partial}{\partial \bar{z}} = \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)$$

are immediately seen to satisfy the product rule of calculus, since they are linear combinations of $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$.

To verify the chain rule is trickier. By definition

$$\frac{\partial h}{\partial z} \stackrel{?}{=} \frac{\partial g}{\partial w}\frac{\partial w}{\partial z} + \frac{\partial g}{\partial \bar{w}}\frac{\partial \bar{w}}{\partial z}$$

$$= \frac{1}{4}\left(\frac{\partial g}{\partial u} - i\frac{\partial g}{\partial v}\right)\left(\frac{\partial f}{\partial x} - i\frac{\partial f}{\partial y}\right) + \frac{1}{4}\left(\frac{\partial g}{\partial u} + i\frac{\partial g}{\partial v}\right)\left(\frac{\partial \bar{f}}{\partial x} - i\frac{\partial \bar{f}}{\partial y}\right).$$

Substituting

$$\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)f = \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + i\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)$$

$$\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\bar{f} = \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) - i\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)$$

gives

$$\begin{aligned}
\frac{\partial h}{\partial z} \stackrel{?}{=}\ & \frac{1}{4}\left[\frac{\partial g}{\partial u}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + \frac{\partial g}{\partial v}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\right] \\
& + \frac{i}{4}\left[\frac{\partial g}{\partial u}\left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) - \frac{\partial g}{\partial v}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right)\right] \\
& + \frac{1}{4}\left[\frac{\partial g}{\partial u}\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) + \frac{\partial g}{\partial v}\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right)\right] \\
& + \frac{i}{4}\left[-\frac{\partial g}{\partial u}\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) + \frac{\partial g}{\partial v}\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)\right] \\
= \ & \frac{1}{2}\left(\frac{\partial g}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial g}{\partial v}\frac{\partial v}{\partial x}\right) - \frac{i}{2}\left(\frac{\partial g}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial g}{\partial v}\frac{\partial v}{\partial y}\right) \\
= \ & \frac{1}{2}\left(\frac{\partial h}{\partial x} - i\frac{\partial h}{\partial y}\right) \quad \text{by the usual chain rule.}
\end{aligned}$$

The verification of $\frac{\partial h}{\partial \bar{z}} = \frac{1}{2}\left(\frac{\partial h}{\partial x} + i\frac{\partial h}{\partial y}\right)$ is similar.

<u>Problem 3</u>. We begin by writing the Hamiltonian as

$$\hat{H} = \hat{T}_N + \hat{V}_{NN} + \hat{H}_e$$

with $\hat{H}_e = \hat{T}_e + \hat{V}_{ee} + \hat{V}_{Ne}$. Then, with $\Psi_{BO}(\mathbf{R}, \mathbf{r}, t) = \psi(\mathbf{R}, t)\,\Phi(\mathbf{r}, \mathbf{R})$ we get

$$\hat{H}\,\Psi_{BO}(t) = \hat{T}_N\,\Psi_{BO}(t) + \hat{V}_{NN}\psi(t)\cdot\Phi + \psi\cdot\hat{H}_e\Phi$$

Using $\hat{H}_e\Phi = \varepsilon(\mathbf{R})\Phi$, this becomes

$$\hat{H}\,\Psi_{BO}(t) = \hat{T}_N\,\Psi_{BO}(t) + (\hat{V}_{NN} + \varepsilon(\hat{\mathbf{R}}))\psi\cdot\Phi$$

Hence,

$$\langle \Psi_{BO}(t), \hat{H}\,\Psi_{BO}(t)\rangle = \langle \Psi_{BO}(t), \hat{T}_N\Psi_{BO}(t)\rangle + \langle \psi(t), (\hat{V}_{NN} + \varepsilon(\hat{\mathbf{R}}))\psi(t)\rangle\cdot\cancelto{1}{\langle\Phi,\Phi\rangle}$$

Likewise,

$$\langle \Psi_{BO}(t), \partial_t\Psi_{BO}(t)\rangle = \langle \psi(t), \partial_t\psi(t)\rangle\cdot\cancelto{1}{\langle\Phi,\Phi\rangle}$$

since Φ is time-independent and

$$\langle\Phi,\Phi\rangle = \int d\mathbf{r}\;\Phi^2(\mathbf{r},\mathbf{R}) = 1 \quad \text{for all } \mathbf{R}.$$

We conclude by observing that

$$\langle \Psi_{BO}(t), \hat{T}_N \Psi_{BO}(t) \rangle$$

$$= \sum_{k=1}^{N} \int d\mathbf{R} \int d\mathbf{r} \; \frac{1}{2M_k} \nabla_{\mathbf{R}_k} \big(\psi^*(\mathbf{R},t) \Phi(\mathbf{r},\mathbf{R}) \big) \cdot \nabla_{\mathbf{R}_k} \big(\psi(\mathbf{R},t) \Phi(\mathbf{r},\mathbf{R}) \big)$$

$$= \sum_{k=1}^{N} \int d\mathbf{R} \; \frac{1}{2M_k} \left| \nabla_{\mathbf{R}_k} \psi(\mathbf{R},t) \right|^2 + \int d\mathbf{R} \; |\psi(\mathbf{R},t)|^2 \left(\sum_{k=1}^{N} \frac{1}{2M_k} \int d\mathbf{r} \; \left| \nabla_{\mathbf{R}_k} \Phi(\mathbf{r},\mathbf{R}) \right|^2 \right).$$

The cross-terms all vanish, i.e.

$$\int d\mathbf{R} \int d\mathbf{r} \; \big(\nabla_{\mathbf{R}_k} \psi^*(\mathbf{R},t) \cdot \nabla_{\mathbf{R}_k} \Phi(\mathbf{r},\mathbf{R}) \big) \psi(\mathbf{R},t) \Phi(\mathbf{r},\mathbf{R}) + \int d\mathbf{R} \int d\mathbf{r} \; \big(\nabla_{\mathbf{R}_k} \psi(\mathbf{R},t) \cdot \nabla_{\mathbf{R}_k} \Phi(\mathbf{r},\mathbf{R}) \big) \psi^*(\mathbf{R},t) \Phi(\mathbf{r},\mathbf{R}) = 0,$$

since the normalization condition $\int d\mathbf{r} \; \Phi^2(\mathbf{r},\mathbf{R}) = 1$ implies

$$\int d\mathbf{r} \; \nabla_{\mathbf{R}_k} \Phi(\mathbf{r},\mathbf{R}) \cdot \Phi(\mathbf{r},\mathbf{R}) = \frac{1}{2} \nabla_{\mathbf{R}_k} \left[\int d\mathbf{r} \; \Phi^2(\mathbf{r},\mathbf{R}) \right] = 0.$$