
Homework - Introduction to Frontiers of Computational Science

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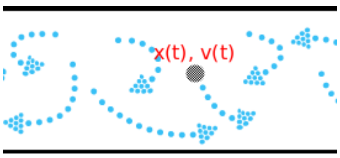
Problem 1.
In a fluid we can define a fluid parcel, a very small amount of fluid which is moving with the fluid flow.



Fluid parcel moving around with a flow velocity $\mathbf{v}(\mathbf{x}, t)$ at position $\mathbf{X}(t)$.

Flow velocity at $\mathbf{X}(x(t), y(t), z(t))$ at time t is described by a function:

$$\mathbf{v}(\mathbf{X}(t), t) = \frac{\partial \mathbf{X}(t)}{\partial t}$$

and the temperature of fluid at position $\mathbf{X}$ is described by a function $\theta = \Theta(\mathbf{X}, t)$
Prove:

$$\frac{D\theta}{Dt} = \frac{\partial \Theta}{\partial t} + \mathbf{v} \cdot \nabla \Theta$$

Using chain rule:

$$\begin{aligned} \frac{D\theta}{Dt} &= \frac{D\Theta(\mathbf{X}, t)}{Dt} \\ &= \frac{\partial \Theta}{\partial t} + \frac{\partial \Theta}{\partial x}\frac{dx}{dt} + \frac{\partial \Theta}{\partial y}\frac{dy}{dt} + \frac{\partial \Theta}{\partial z}\frac{dz}{dt} \\ &= \frac{\partial \Theta}{\partial t} + (\mathbf{v} \cdot \nabla)\Theta \end{aligned}$$

with $\mathbf{v} = (\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt})$ and $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$.

Problem 2.
Solve this equation using Euler method:

$$\frac{dx}{dt} = -\lambda x$$

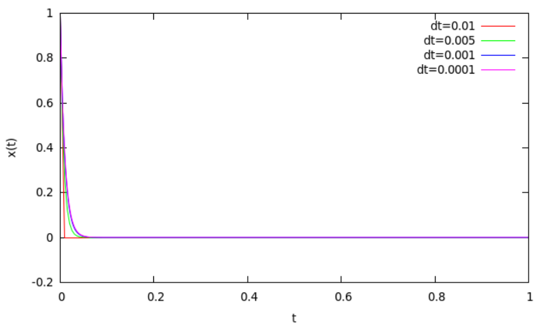
with initial condition $x(0) = 1$ and $\lambda = 100$, find $x(1)$! Try different Δt (0.03, 0.01, and 0.001).
Using Euler method means that we can solve this by:

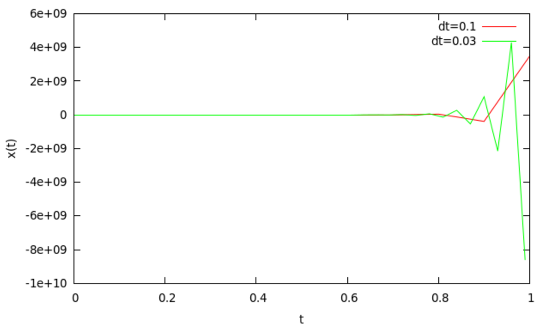
$$\begin{aligned} x(t+\Delta t) &= x(t) - \lambda x(t)\Delta t \\ &= (1-\lambda\Delta t)x(t) \end{aligned}$$

and the exact solution for this differential equation is $x(t) = e^{-\lambda t}$, so $x(1)$ should be 3.720076×10^{-44}.
Result:

Δt	$x(1)$
0.1	3.48678e+09
0.03	-8.58993e+09
0.01	0
0.005	6.22302e-61
0.001	1.74787e-46
0.0001	2.24877e-44

Euler method is numerically unstable (conditionally stable) especially for stiff equations. Stable condition if $|z+1| \leq 1$, with $z = -\lambda dt$ for above equation.





Program

```
#include <iostream>
#include <stdlib.h>
#include <math.h>
#include <fstream>
using namespace std;

void plot();
int main(int argc, char * argv[]){
    double lambda = 100., x0 = 1.;
    double ti = 0., tf = 1.;
    double dt = 0.001, x = x0, t = ti;

    if (argc <= 1){
        printf("Usage: %s dt\n", argv[0]);
    }
    if (argc > 1){
        dt = atof(argv[1]);
    }

    double N = (tf - ti)/dt;
    ofstream out("output.txt");
    out << t << " " << x << endl;
    for (int i=1;i<=N;i++){
        x = (1. - lambda*dt)*x;
        t = t+dt;
        out << t << " " << x << endl;
    }
    out.close();
    cout << "Exact value x(1) = 3.720076e-44\n";
    cout << "x(" << tf << ") = " << x << endl;

    plot();
    return 0;
}

void plot(){
    ofstream ploter("inp.plt");
    ploter << "#gnuplot input file\n";
    ploter << "set term png size 600,400\n";
    ploter << "set output \"euler.png\"\n";
    ploter << "set xlabel \"t\"\n";
    ploter << "set ylabel \"x(t)\"\n";
    ploter << "plot \"output.txt\" u 1:2 w l t \"x(t)\"\n";
    ploter.close();

    system("gnuplot inp.plt");
    system("rm inp.plt");
}
```