MM2090: Introduction to Scientific Computing

Assignment 4

Team-3

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1 Abheshek(me20b005)

1.1 Arrhenius equation

This is the equation I have chosen.

$$k = Ae^{-E_a/RT} \tag{1}$$

It can also be written as

$$\ln k = -E_a/RT + \ln A \tag{2}$$

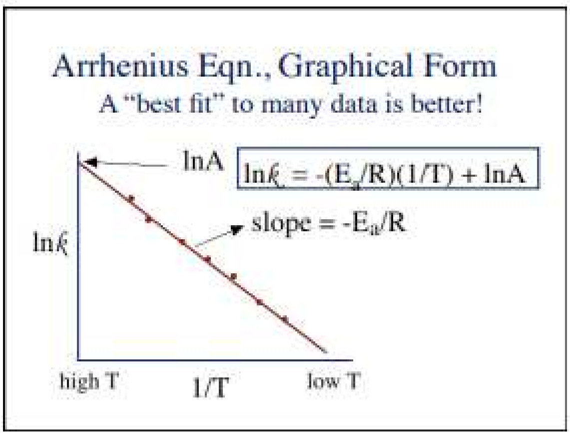

Figure 1: ME20B005

The Arrhenius equation 1 2 gives the dependence of the rate constant of a chemical reaction on the absolute temperature where

- k is the rate constant (frequency of collisions resulting in a reaction)
- T is the absolute temperature (in kelvins)
- A is the pre-exponential factor, a constant for each chemical reaction.The units of the pre-exponential factor A are identical to those of the rate constant and will vary depending on the order of the reaction. For a first-order reaction, it has units of s^{-1}. For that reason, it is often called frequency factor.According to collision theory, the frequency factor, A, depends on how often molecules collide when all concentrations are 1 mol/L and on whether the molecules are properly oriented when they collide.
- E_a is the activation energy for the reaction (in the same units as kBT).Activation energy can be thought of as the magnitude of the potential barrier (sometimes called the energy barrier) separating minima of the potential energy surface pertaining to the initial and final thermodynamic state. For a chemical reaction to proceed at a reasonable rate, the temperature of the system should be high enough such that there exists an appreciable number of molecules with translational energy equal to or greater than the activation energy.
- R is the universal gas constant

This equation has a vast and important application in determining rate of chemical reactions and for calculation of energy of activation [2]
In figure 1 we can see the relation of $\ln k$ and $1/T$ and also see the y intercept. From this graph, at a given temperature we can find the value of rate constant for a reaction [4].

2 Ankit kumar (me20b024)

2.1 Maxwell's Equations

The differential forms of Maxwell's equations as found by Heaviside, while completely valid, are now considered somewhat archaic, and have been replaced by the more useful (equivalent) integral forms. Each law is named according to the person(s) who originally discovered the connections represented by the equation. Here are the four equations:

$$\text{Gauss' law for electricity:} \quad \oint_{\substack{\text{closed}\\ \text{surface}}} \vec{E} \cdot d\vec{A} = \frac{Q_{enc}}{\epsilon_0} \tag{3}$$

$$\text{Gauss' law for magnetism:} \quad \oint_{\substack{\text{closed}\\ \text{surface}}} \vec{B} \cdot d\vec{A} = 0 \tag{4}$$

$$\text{Faraday's law:} \quad \oint \vec{E} \cdot d\vec{s} = -\frac{d\phi_B}{dt} \tag{5}$$

$$\text{Ampere-Maxwell law:} \quad \oint \vec{B} \cdot d\vec{s} = \mu_0 \epsilon_0 \frac{d\phi_E}{dt} + \mu_0 i_{enc} \tag{6}$$

Note: $\oint$ is used to specify a closed loop integral, also known as a line integral. It simply means that in the equation calculations, we must figure go all the way around the loop; we can't stop part way through or the equations won't be valid [11].

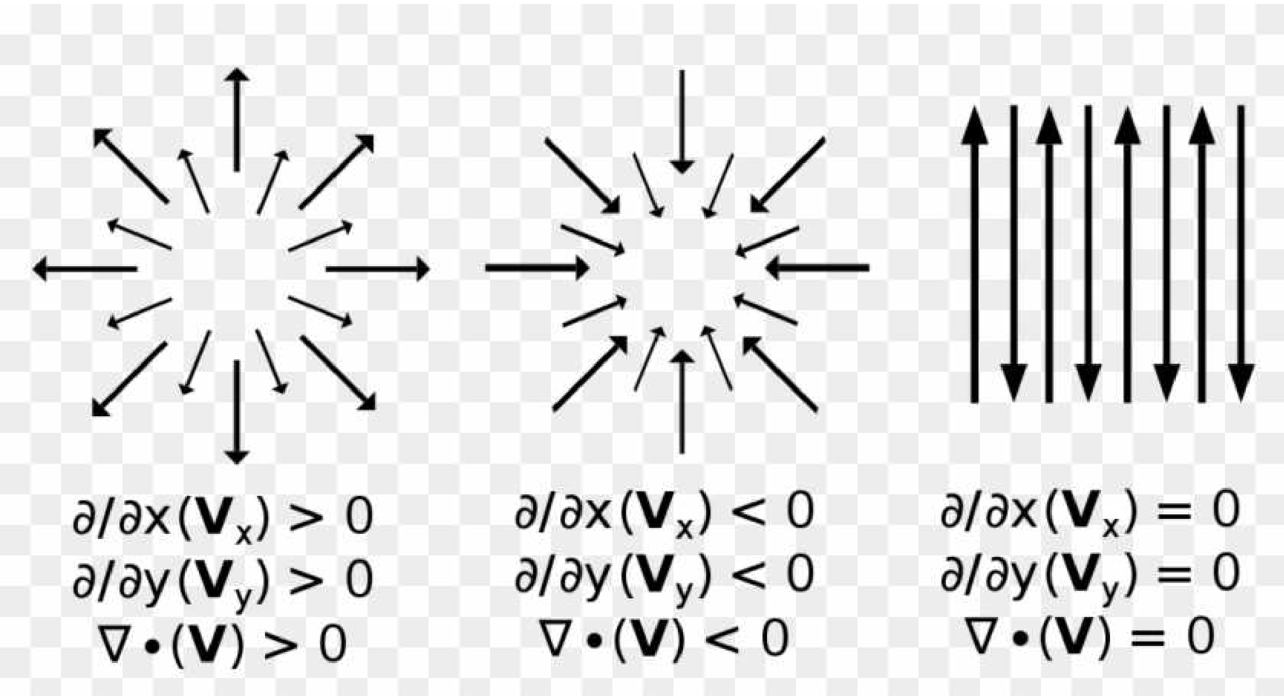

Figure 2: Applications of Maxwell's equation

2.2 Importance of Maxwell's Equations

Equation 3, also known as Gauss' Law, is stating that the divergence of the electric field is equal to the charge density inside of a closed surface of interest, multiplied by a constant. The divergence is how much the electric field “spreads out” from a given point. If there is more charge inside, the divergence is greater. If it’s zero, the divergence is zero [1].

What this equation 4 is saying is that the curl of the electric field is equal to the negative of the change in the magnetic field in time. In other words, if the magnetic field isn’t changing, electric field lines are straight. If it is changing, the electric field “swirls” appropriately, depending on if the field is increasing or decreasing. A changing magnetic field can induce an electric field! (i.e. Faraday induction). The negative sign is called Lenz’s law.

There are no magnetic monopoles (equation 5). The divergence of B is always zero. As such, there is no “sink” or “source” for B - the field lines have no beginning and no end. There is no source for them like there is for an electric field (i.e. an electric monopole). All magnetic “charge” is found in a dipole, with a North and a South.

The curl of B, or the “swirliness of B” is equal to the Current Density (the amount of current per unit volume) plus any change in the electric field (equation 6). This second part is often called the “displacement current, since it helps with dealing with capacitors [11].

Figure 2 is showing different situation of Maxwell equation.

3 Chinmayee - ME20B053

3.1 Newton's Second Law

[8]

$$F = ma(= changeinmomentum) \tag{7}$$

F = Force acting on the body
m = Mass of the body
a = Acceleration of the body

Newton's second law states that the acceleration of an object is directly related to the net force and inversely related to its mass. Acceleration of an object depends on two things, force and mass. It allows you to calculate the acceleration (and therefore velocity and position) of an object with known forces. The force acting on a body is equal to the change in momentum of the body per unit time, which in turn gives us "F=ma".

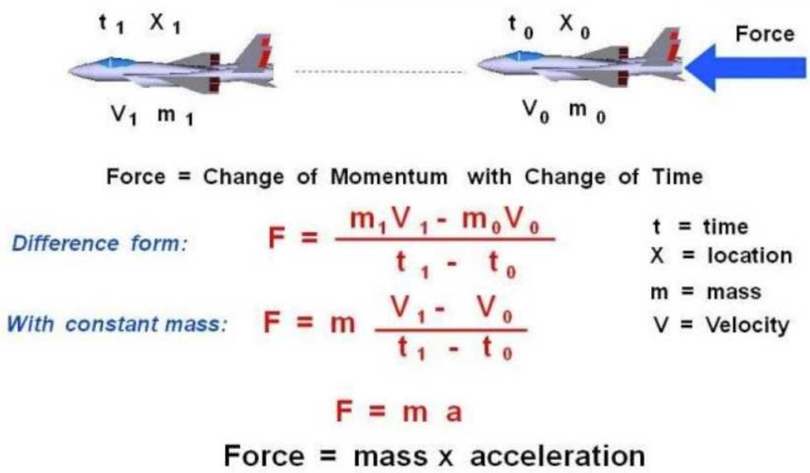

Figure 3: ME20B053

[9]

4 Siddhesh - MM20B019

For the assignment 4, I have chosen the following equation.

$$j^{\star} = \sigma T^4 \tag{8}$$

The following equation can be derived from the above equation.

$$P = Aj^{\star} = A\varepsilon\sigma T^4 \tag{9}$$

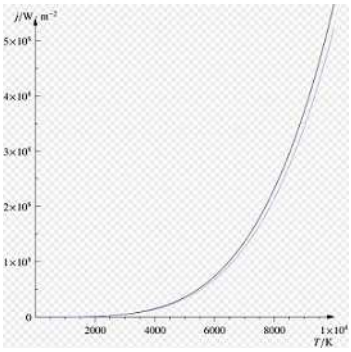

Figure 4: MM20B019

The Stefan–Boltzmann law describes the power radiated from a black body in terms of its temperature where

- $j^{\star}$ is the black-body radiant emittance (radiant flux emitted by a surface per unit area).
- T is the thermodynamic temperature (in kelvins).
- P is the total power radiated from an object.
- A is the surface area of the object.
- ε is the emissivity of the grey body.

4.1 Description

- The equation 8 is Stefan-Boltzmann's law and the equation 9 can be derived for a general grey body.
- The Stefan–Boltzmann law states that the total energy radiated per unit surface area of a black body across all wavelengths per unit time $j^{\star}$ is directly proportional to the fourth power of the black body's thermodynamic temperature T.
- Graph 4 of a function of total emitted energy of a black body $j^{\star}$ proportional to its thermodynamic temperature T. In blue is total energy according to the Wien approximation.

4.2 Further Reading

- Laboratory experiments to demonstrate the Stefan–Boltzmann radiation law using the tungsten filament of a traditional incandescent lamp have been described several times. [3]
- The Bureau International des Poidset Mesures (International Bureau of Weights and Measures) recognized that the Planck's law is not accurate at temperatures below the silver point (infrared radiation) and recommended using the Sakuma-Hattori equations instead of the Planck's equation. These changes should lead naturally to modifications of the integral law of thermal radiation, the Stefan-Boltzmannn law, but apparently no such empirical correction was suggested, even though the deviations are significant or even larger than the Stefan-Boltzmann radiation. [5]

1 arxiv.org
2 researchgate.net
3 wikipedia.org

5 Shriya Shukla (ME20B163)

5.1 Bernoulli's Equation

[6]

$$P_1 + \frac{1}{2}\rho v_1^2 + \rho g h_1 = P_2 + \frac{1}{2}\rho v_2^2 + \rho g h_2 = constant \tag{10}$$

ρ = fluid density
P_1=pressure at elevation 1
g= acceleration due to gravity
v_1 =velocity at elevation 1
h_1 =height of elevation 1
P_2 =pressure at elevation 2
v_2 =velocity at elevation 2
h_2 =height at elevation 2

In fluid dynamics, Bernoulli's principle states that an increase in speed of the fluid occurs simultaneously with decrease in static pressure or decrease in the fluid's potential energy. The above Bernoulli's equation 10 was derived by Leonhard Euler. A better visual explanation of the equation is given in figure 5

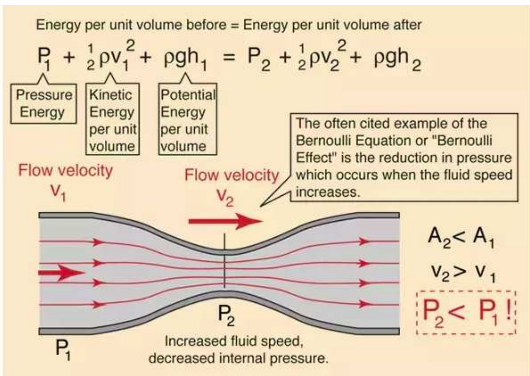

Figure 5: ME20B163
[7]

6 Sumanth Hegde - MM20B059

6.1 The Gamma Function Equation

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt$$

6.2 Variables

$\Gamma(x)$=The value of Gamma Function
x=value at which Gamma Function is to be evaluated

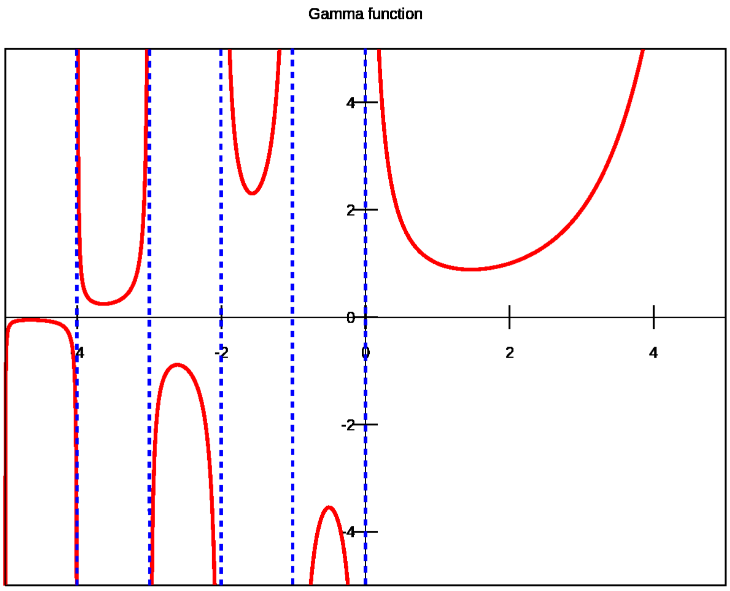

Figure 6: Gamma Function Plot

6.3 Description

In mathematics, the gamma function (represented by Γ) is one commonly used extension of the factorial function to continuous and complex numbers. The gamma function is defined for all complex numbers except the non-positive integers as an improper integral as given in the equation above. For positive integers, $\Gamma(x) = (x-1)!$ [10]

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