PH353
Introduction to the Modeling of Physical Systems

Thursday 2-5pm, weeks 1-11

10 credits

Nominal hours :

33 hours in 11 supervised sessions

33 hours unsupervised work

34 hours report preparation

Assessment :

Project 1:	Weeks 1-4	Write-up	1/3
		(due in by the end of week 5)	
Project 2:	Weeks 5-11	Write-up	1/2
		(due in by the end of week 11)	
		Presentation	1/6
		(to be given on the 14/12)	

Modelling: Aims

1. Understanding of why/how a system works

2. Prediction of Future Experiments/Observations

Mathematical Models

Mathematical models need

1. Variables

2. Equations these satisfy

3. Constraints

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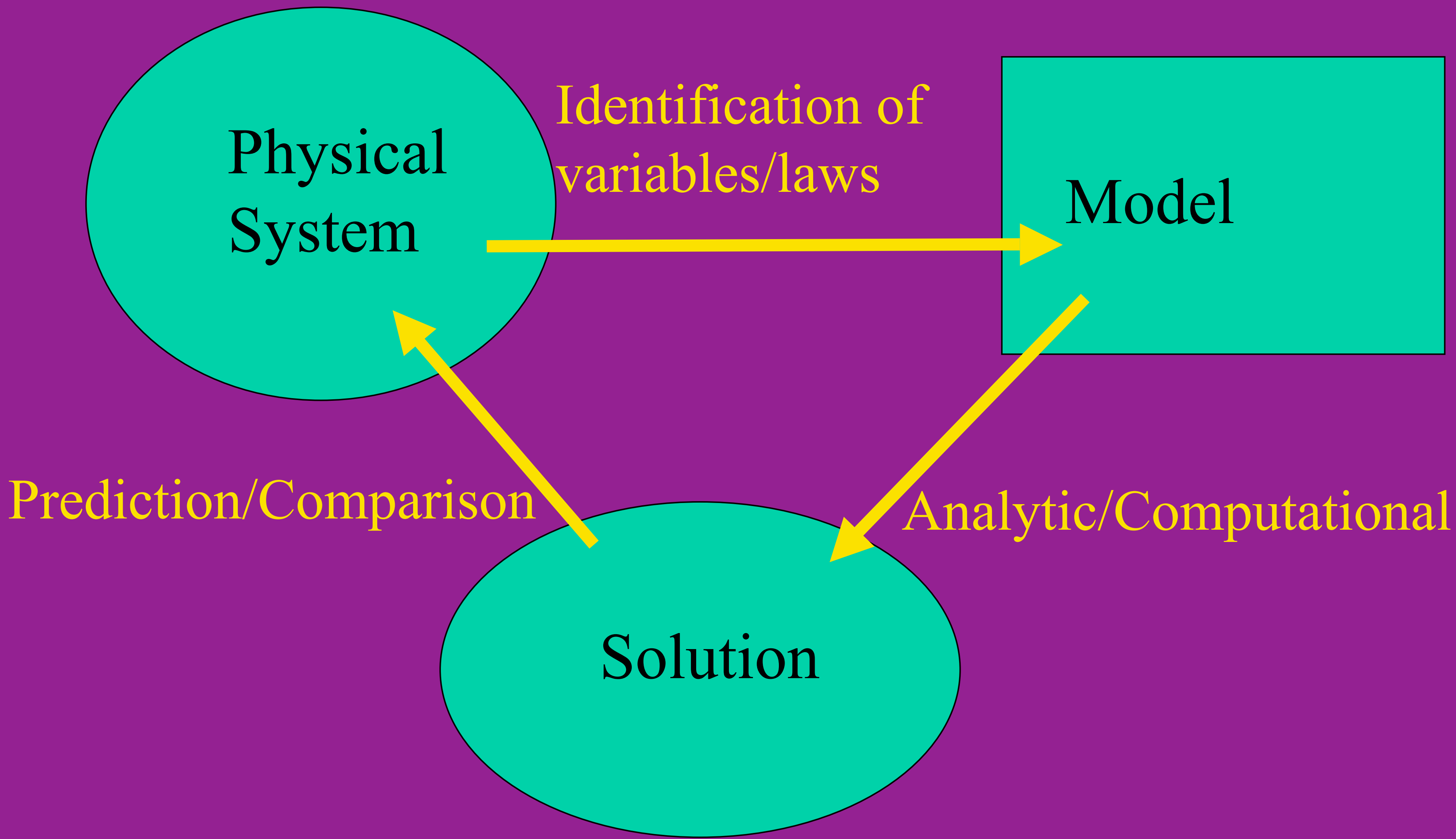

A good model :

Encompasses the key physics of the situation

Is as simple as possible

Is tractable

Variables:

Variables are parameters (numbers) which describe the system,

Often these are obvious, such as the position of a particle however often they are collective e.g the centre of mass of a rigid body or the temperature and pressure of a gas

Constraints

Many mathematical systems contain a huge number of solutions.   Eg. Wave equation, heat equation etc.

Constraints allow us to choose the appropriate solution for our problem

Constraints may be initial conditions, boundary conditions, finiteness, single valued….

Computational methods

We should aim for flexibility!

You have used Mathematica before

We will focus on Visual Basic

(next semester – you decide!)

Project 1 : weeks 1-4

Project 2 : weeks 5-11

Each project will contain 2 or 3 intermediate steps/tasks. These should be approved before proceeding to the next step.

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Modelling Project 1: Gas Exchange in Humans

Applications:

1. Nitrogen Absorption/Release in sub-aqua diving and space travel

2. Uptake/Release of anaesthetics during operations/post operative care

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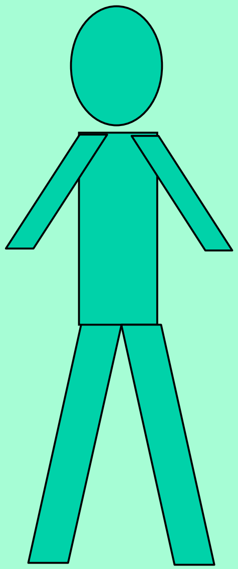
Environment:

Pressure: 1At (+/-0.05)

20.9% O_2

79% N_2

Trace CO_2



Changes to this enviroment?

HYPERBARIC: P>1

HYPOBARIC: P<1

NARCOTIC

FACT:

People exposed to HYPERBARIC conditions suffer illness when returning to normal conditions

EXPLAINATION:

This is due to absorption and release of gases (nitrogen) in the body tissues

BASIC GAS LAWS (variables P , V , T , n)

$$\frac{PV}{T} = nR$$

Gas of a single type

$$P = P_1 + P_2 + \ldots.$$

Mixture of gases

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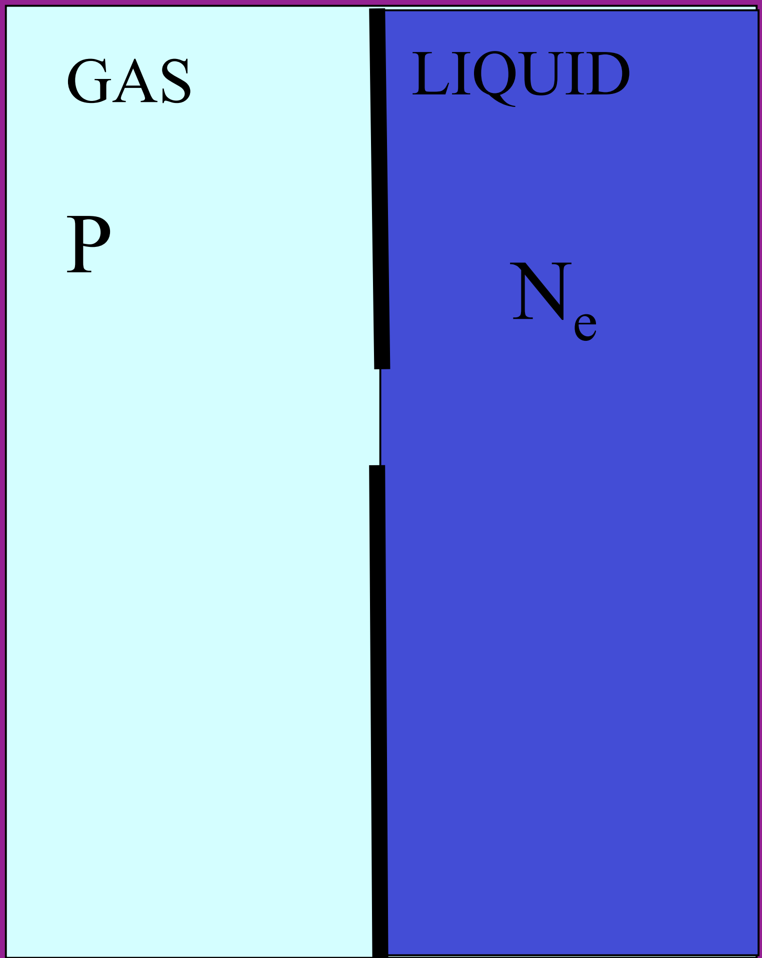


Gas dissolves in a liquid

Equilibrium amount is proportional to pressure (partial) of the gas

$$N_e = \lambda P$$

New variable :

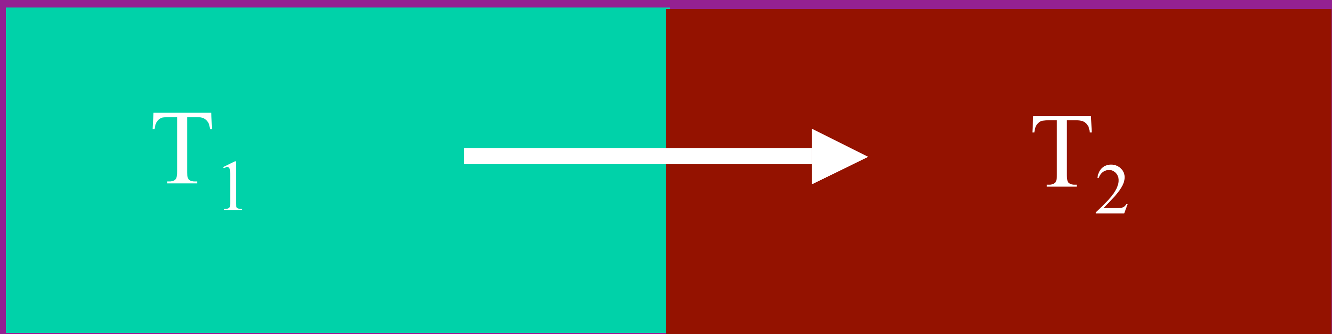
TENSION instead of N

``The tension is the equivalent pressure corresponding to that density of gas'' (units of At)

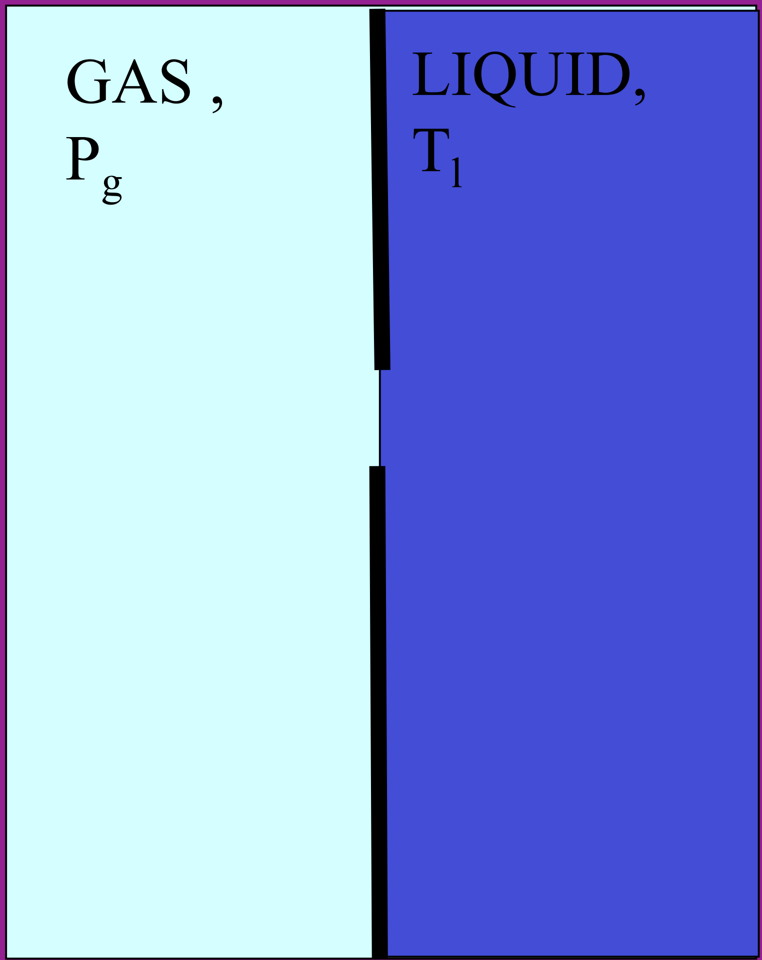
Why?

1. Easy interchange between pressure and tension

2. Gas flows from areas of high tension to low tension



Out of Equilibrium Flow



If T_l is not equal to P_g:

$$\frac{dT_l}{dt} = -\lambda \left(T_l - P_g \right)$$

Step 1:

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Solve

$$\frac{dT}{dt} = -\lambda(T - T_e)$$

For T_e = constant , $T(0) = 1$

Parameters : T_e , λ , t_{max} t_{step}

Analtic solution is easy – find it

Numerical solution

Use Visual Basic and Runge-Kutta (PH206)

Discrete time step: Δt , order of Runge-Kutta N

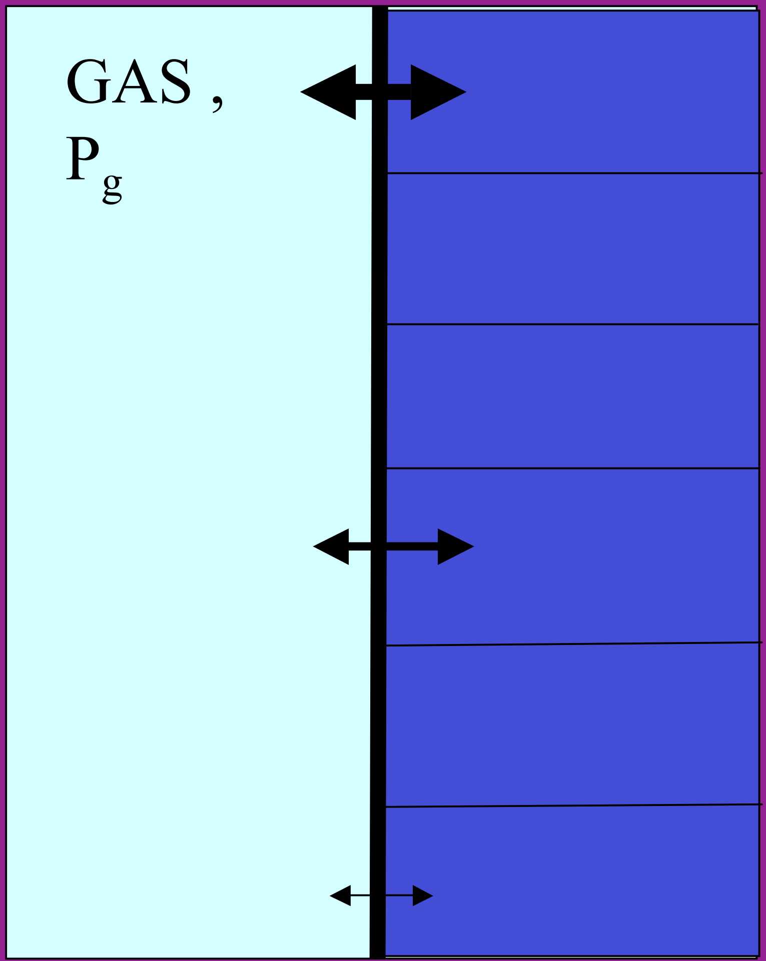
Investigate ``errors'' as function of Δt and N

Completion of step one-

A working programme, easily changeable to produce $T(t)$, given $T(0)$, T_e and λ and to plot $T(t)$.

For $\lambda = 0.2\ \mathrm{min}^{-1}$, $T(0)=1$, $P_e=5$, $t=10$mins, study of the ``error'' versus Δt and N (You need the analytic solution to compare to.)

Model of the Body



Model body by a series of compartments with a variety of values of λ , λ_i

Variables: T_i the tensions in the different tissues

The compartments are representative of tissue types – differentially linked by blood flow to atmosphere

Step 2:

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Solve

$$\frac{dT_i}{dt} = -\lambda_i(T_i - T_e)$$

For T_e = constant , $T_i(0) = 1$

Variables : T_e , λ_i , t_{max} t_{step}

Technical points:

1. Use of Arrays obviously!!!!!

Variables become array-value. New variable – the size of array (number of compartments.)

2. Important that Step 1 was written carefully (rewrite!)

Completion of step two-

A working programme, easily changeable to produce $T_i(t)$, given $T_i(0)$, T_e and λ_i and to plot $T_i(t)$.

For λ_i =(0.2, 0.1, 0.05, 0.01, 0.002) min^{-1} evaluate and plot $T_i(t)$ for $T_i(0)=1$, and

T_e =5, for t between 0 and 20 minutes

T_e =1, for t between 20 and 60 minutes

Step 3

Solve for $T(t)$ with a complicated $T_e(t)$

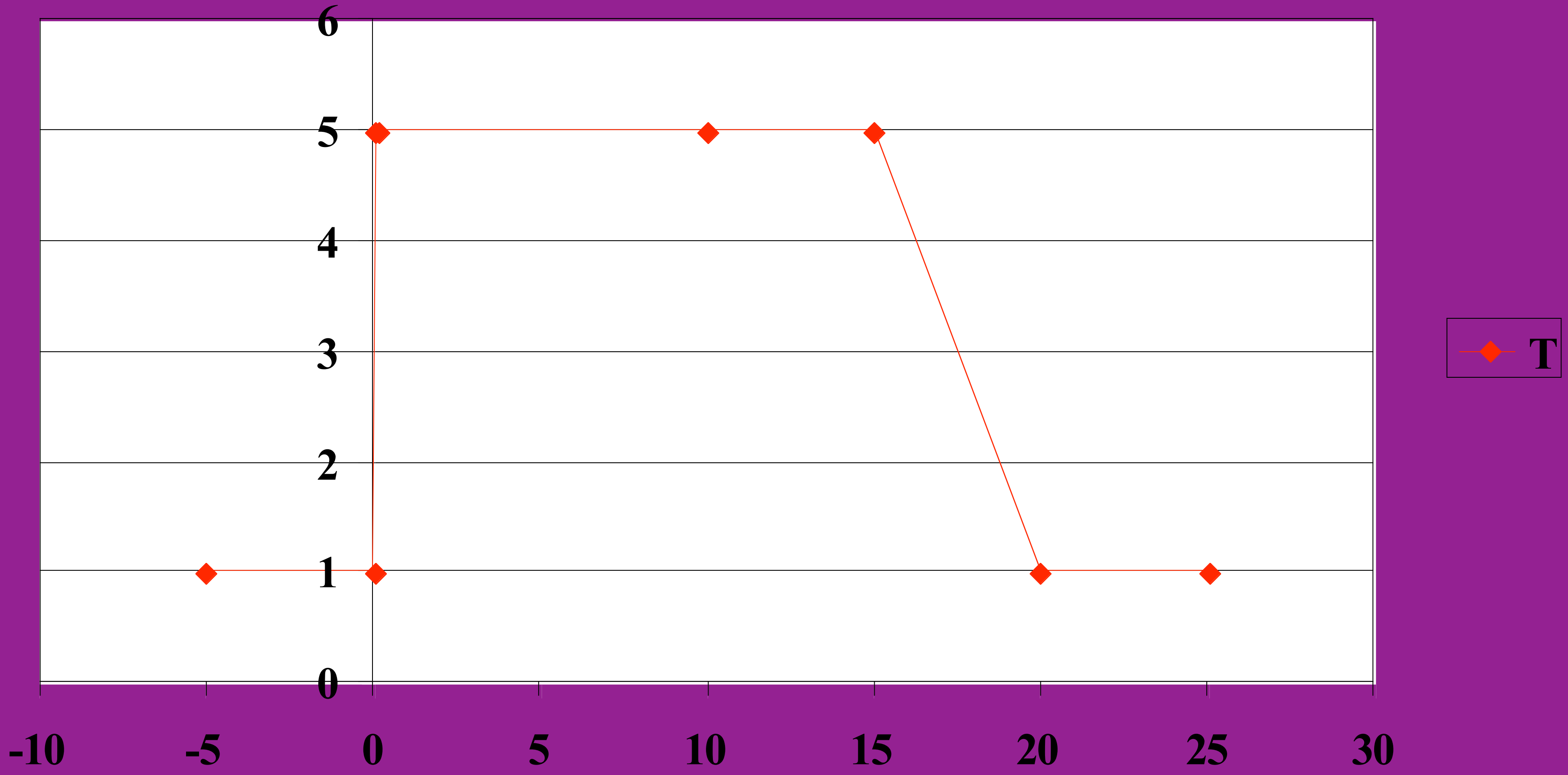
Eg. $T_e(t) = T_2$, $0<t<A$, $T(0)=T_0$

$T_e(t) = T_2 + r(T_0 - T_2)(t-A)$, $A<t<A+1/r$

$T_e(t) = T_0$, $t > A+1/r$

still analytic!

Tension is time-dependant as



Completion of step three-

A working programme, easily changeable to produce $T(t)$, given $T(0)$, T_e , λ, r and to plot $T(t)$.

For $T(0)=1$, $T_e=5$, $\lambda=0.05\ \text{min}^{-1}$, determine the value of $T(A+1/r)$ for various values of r. Compare to the analytic solution

Step 4 : Decision Making

If we move from and environment P_1 to P_2 then gas will flow in and out of tissues. If the outflow is too large then bubbles may form in our tissues with disastrous consequences. (Ranging from inconvenience to death.) The potential problems arise in subaqua diving and space travel. We need some criteria to enable us to make decisions to avoid problems.

For humans breathing air, after being exposed to a hyperbaric environment decompression illness can occur on return to normal. (This was first observed in tunnel workers but is also a problem for divers and astronauts.)

Decompression illness is caused by bubbles of Nitrogen which occur is the pressure is lowered too quickly.

Criteria exist to avoid this

Haldane Criteria

Tissue at tension T → Environment with gas at pressure P

Safe provided, T < 2.0 P

(This refers to Nitrogen and decompression Illness)

Application : Space Walking

When undertaking spacewalks astronauts face decompression illness because the environment in their space suits is different from that in the space craft.

Spacecraft: Normal conditions i.e. Air at 1At

Spacesuit: Atmosphere is pure O_2 at 1/3 At

Step 4: planning a spacewalk

Investigate the possible ways of preparing an astronaut for a space walk. Use the Haldane criteria to avoid decompression illness.

We can avoid decompression by a) spending time at an intermediate pressure or b) changing pressure continuously (possibly at a constant rate.) Investigate both. For (a), you should determine the times that must be spent at intermediate pressures and measure how these times depend upon the choice of intermediate pressures. For (b) you should determine the maximum rate at which the pressure can safely change.

Repeat if the Haldane Criteria is altered with 2.0 to 1.6

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Modelling Project 2:

Finding Quantum Bound States

Applications:

1. Finding the spectrum of Quarkonium

2. Chemistry