

# BPhO Computational Challenge

# Thermodynamics

Dr Andrew French. March 2025.

















## These books are amazing!

## **Theodore Gray**

Bestselling author of *The Elements* and *How Things Work* Photographs by Nick Mann







$$\eta = \frac{W}{Q_{\text{in}}} \quad \text{Engine efficiency}$$
$$\therefore -\frac{T_C}{T_H} + 1 - \eta \ge 0 \quad \therefore \eta \le 1 - \frac{T_C}{T_H}$$



volume change

dV = -Adx

 $p = \frac{F}{A}$ 

The pressure acting upon the gas

dW = FdxWork done *on* the gas  $\therefore dW = pA \times -\frac{dV}{dW}$ 

 $\therefore dM$  $-\mathcal{D}$ 

If heat dQ is supplied to the gas then the **First Law of Thermodynamics** (that Energy in a closed system is conserved) means the internal energy change is



x, y, z translation)

The internal energy for *n* moles of an ideal gas is: **IDEAL GAS EQUATION** 

$$pV = nRT$$





Rudolf Clausius 1822-1888

## **ISENTROPIC (CONSTANT ENTROPY) PROCESS**

dS = dQ = 0 No heat exchanged

**ISOTHERMAL PROCESS**  dT = 0 pV = constant  $Q = W = nRT \ln\left(\frac{V}{V_0}\right)$ Heat input = work done by gas since no

change in U

 $\gamma = \frac{c_p}{c_V} = 1 + \frac{2}{\alpha}$ Ratio of constant constant capacitie  $W = \frac{p_0 V_0}{\gamma - 1} \left( 1 - \left(\frac{V_0}{V}\right)^{\gamma - 1} \right)$ 

Work done by gas on the surroundings

= constant

 $\gamma = \frac{c_P}{c_V} = 1 + \frac{2}{\alpha}$  Ratio of constant pressure to constant volume process heat capacities

 $c_{V} = \frac{R}{M} \frac{1}{\gamma - 1}$ 







Nicolas Léonard Sadi Carnot (1796-1832)

 $W = (T_H - T_C) nR \ln$ 

$$Q_{\rm in} = nRT_H \ln\left(\frac{V_2}{V_1}\right)$$
$$Q_{\rm out} = nRT_C \ln\left(\frac{V_3}{V_4}\right)$$

## Inputs

$$T_H, T_C, V_1, V_2, n$$

$$V_{4} = \left(\frac{T_{H}}{T_{C}}\right)^{\frac{1}{\gamma-1}} V_{1} \qquad V_{3} = \left(\frac{T_{H}}{T_{C}}\right)^{\frac{1}{\gamma-1}} V_{2}$$

## Next step: code up a Heat Cycle model! Start with a spreadsheet, then try MATLAB/Python etc ... The key idea is to VISUALIZE your solutions.

Carnot Cycle model

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	Nicolas Léonard Sadi Carnot (1796-1832)
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Input	paramete	ers
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Hot reservoir temperature /Celsius	19
Cold reservoir temperature /Celsius	
Mass of gas /g	1.0
Volume of gas at lowest volume and hightest pressure /litres	0.4
Volume of gas after isothermal expansion /litres	1.0
Degrees of freedom of molecular motion	
Molar mass of gas /gmol^-1	28.9
Outputs	

Heat input during isothermal expansion /kJ	
Heat output during isothermal compression /kJ	0.07
Total work done by gas on surroundings /kJ	0.03
Entropy change during isothermal stages /JK^-1	0.26
Efficiency (work done / heat input)	0.30

#### Theoretical efficiency



Note all temperatures incorporated into calculations will be converted to Kelvin first - i.e. add 273 to Celsius number.

#### Pressure, volume coordinates of heat cycle

p1	3.00	
V1	0.4	
p2	1.20	
V2	1.0	
р3	0.48	
V3	1.73	
p4	1.20	
V4	0.7	

Note all pressures are quoted in atmospheres. 1atm = 101,325 Pa. Volumes in litres. T in K.

Reservoir	temperatures in K
T_H	423
T_C	293

Number of moles of gas in engine	
Ratio of specific heats gamma	1.667



	1 to 2		2 to 3		3 to 4		4 to 1	
	Isothermal		Adiabatic		Isothermal		Adiabatic	
	expansi	on	expan	sion	compr	ession	compre	ssion
V diff								
fraction	р	v	р	V	р	V	р	V
0	2.996	0.400	1.198	1.000	0.478	1.735	1.196	0.694
0.01	2.951	0.406	1.184	1.007	0.481	1.724	1.205	0.691
0.02	2.908	0.412	1.169	1.015	0.484	1.714	1.213	0.688
0.03	2.867	0.418	1.155	1.022	0.487	1.703	1.222	0.685
0.04	2.826	0.424	1.142	1.029	0.490	1.693	1.231	0.682
0.05	2.787	0.430	1.128	1.037	0.493	1.683	1.240	0.679
0.06	2.748	0.436	1.115	1.044	0.496	1.672	1.249	0.676
0.07	2.711	0.442	1.102	1.051	0.499	1.662	1.258	0.673
0.08	2.675	0.448	1.089	1.059	0.503	1.651	1.267	0.670
0.09	2.639	0.454	1.077	1.066	0.506	1.641	1.276	0.667
0.1	2.605	0.460	1.065	1.073	0.509	1.631	1.286	0.664
0.11	2.571	0.466	1.053	1.081	0.512	1.620	1.295	0.662
0.12	2.539	0.472	1.041	1.088	0.516	1.610	1.305	0.659
0.13	2.507	0.478	1.029	1.096	0.519	1.599	1.315	0.656
0.14	2.476	0.484	1.018	1.103	0.522	1.589	1.324	0.653
0.15	2.445	0.490	1.007	1.110	0.526	1.579	1.334	0.650
0.16	2.416	0.496	0.996	1.118	0.529	1.568	1.345	0.647
0.17	2.387	0.502	0.985	1.125	0.533	1.558	1.355	0.644
0.18	2.359	0.508	0.974	1.132	0.536	1.547	1.365	0.641
0.19	2.331	0.514	0.964	1.140	0.540	1.537	1.376	0.638
0.2	2.304	0.520	0.953	1.147	0.544	1.526	1.386	0.635
0.21	2.278	0.526	0.943	1.154	0.547	1.516	1.397	0.632
0.22	2.252	0.532	0.933	1.162	0.551	1.506	1.408	0.629
0.23	2.227	0.538	0.924	1.169	0.555	1.495	1.419	0.626
0.24	2.203	0.544	0.914	1.176	0.559	1.485	1.430	0.623
0.25	2.179	0.550	0.905	1.184	0.563	1.474	1.441	0.620
0.26	2.155	0.556	0.895	1.191	0.567	1.464	1.453	0.617
0.27	2.132	0.562	0.886	1.198	0.571	1.454	1.465	0.615
0.28	2.110	0.568	0.877	1.206	0.575	1.443	1.476	0.612
0.29	2.088	0.574	0.868	1.213	0.579	1.433	1.488	0.609
0.3	2.066	0.580	0.860	1.220	0.584	1.422	1.500	0.606
0.31	2.045	0.586	0.851	1.228	0.588	1.412	1.512	0.603
0.32	2.024	0.592	0.843	1.235	0.592	1.402	1.525	0.600
0.33	2.004	0.598	0.834	1.242	0.597	1.391	1.537	0.597
0.34	1.984	0.604	0.826	1.250	0.601	1.381	1.550	0.594
0.35	1.964	0.610	0.818	1.257	0.606	1.370	1.563	0.591
0.36	1.945	0.616	0.810	1.264	0.610	1.360	1.576	0.588
0.37	1.926	0.622	0.803	1.272	0.615	1.350	1.589	0.585
0.38	1.908	0.628	0.795	1.279	0.620	1.339	1.603	0.582
0.39	1.890	0.634	0.787	1.287	0.625	1.329	1.616	0.579
0.4	1.872	0.640	0.780	1.294	0.630	1.318	1.630	0.576

## Four-stage engine (modelled by Diesel or Otto cycles)



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#### Otto Cycle model

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Input parameters	
Temperature T1 of air draw into piston /Celsius	20
Low pressure state p1 /atm	1.00
High pressure state p3 /atm	100
Volume V1 of uncompressed gas /litres	1
Volume V2 of compressed /litres	0.1
Degrees of freedom of molecular motion	3
Molar mass of gas /gmol^-1	28.966

Out	puts
-----	------

Heat input during isochoric heating /kJ	
Heat output during isochoric cooling /kJ	0.175
Total work done by gas on surroundings /kJ	
Efficiency (work done / heat input)	0.785

Theoretical efficiency



Note all temperatures incorporated into calculations will be converted to Kelvin first - i.e. add 273 to Celsius number.

#### Pressure, volume, temperature coordinates of heat cycle

p	1	1.00
V	1	1.000
T	1	293
p	2	46.42
V	2	0.100
T	2	1360
p	3	100.00
V	3	0.100
T	3	2930
p	4	2.15
V	4	1.000
T	4	631

Engine RPM	6500
Power output /kW	69.21979

Dower per culinder

0.785

Number of cylinders	1
Total power output /kW	69.22

Note all pressures are quoted in atmospheres. 1atm = 101,325 Pa. Volumes in litres. T in K.

Number of moles of gas in engine	0.042
Ratio of specific heats gamma	1.667
Constant volume specific heat capacity /Jkg^-1K^-1	431
Constant pressure specific heat capacity /Jkg^-1K^-1	718



Note real petrol engines have an efficiency of more like 20%, whereas diesels can be up to 40%. In other words, significant losses!



	1 to 2		2 to 3		3 to 4		4 to 1			
	I to 2           Adiabatic           compression           1.000         1.00           1.015         0.99           1.031         0.98           1.047         0.97           1.053         0.96           1.033         0.92           1.115         0.93           1.133         0.92           1.131         0.93           1.132         0.98           1.230         0.88           1.252         0.87           1.230         0.88           1.252         0.87           1.319         0.84           1.333         0.82           1.320         0.88           1.252         0.87           1.319         0.84           1.333         0.367           1.329         0.82           1.329         0.82           1.329         0.82           1.329         0.82           1.329         0.82           1.329         0.82           1.329         0.82           1.329         0.82           1.329         0.77           1.559         0.76 </td <td>Isochor</td> <td>ic</td> <td>Adiabati</td> <td>c</td> <td colspan="4">Isochoric</td>		Isochor	ic	Adiabati	c	Isochoric			
	compre	ssion	heating		expansio	on	cooling			
V or p										
diff										
fraction	р	v	р	v	р	v	р	v		
0	1.000	1.000	46.416	0.100	100.000	0.100	2.154	1.000		
0.01	1.015	0.991	46.952	0.100	86.621	0.109	2.143	1.000		
0.02	1.031	0.982	47.488	0.100	75.892	0.118	2.131	1.000		
0.03	1.047	0.973	48.023	0.100	67.142	0.127	2.120	1.000		
0.04	1.063	0.964	48.559	0.100	59.901	0.136	2.108	1.000		
0.05	1.080	0.955	49.095	0.100	53.834	0.145	2.097	1.000		
0.06	1.097	0.946	49.631	0.100	48.693	0.154	2.085	1.000		
0.07	1.115	0.937	50.167	0.100	44.295	0.163	2.074	1.000		
0.08	1.133	0.928	50.703	0.100	40.500	0.172	2.062	1.000		
0.09	1.151	0.919	51.238	0.100	37.199	0.181	2.051	1.000		
0.1	1.170	0.910	51.774	0.100	34.309	0.190	2.039	1.000		
0.11	1.190	0.901	52.310	0.100	31.762	0.199	2.027	1.000		
0.12	1.210	0.892	52.846	0.100	29.505	0.208	2.016	1.000		
0.13	1.230	0.883	53.382	0.100	27.494	0.217	2.004	1.000		
0.14	1.252	0.874	53.918	0.100	25.693	0.226	1.993	1.000		
0.15	1.273	0.865	54.454	0.100	24.074	0.235	1.981	1.000		
0.16	1.296	0.856	54.989	0.100	22.613	0.244	1.970	1.000		
0.17	1.319	0.847	55.525	0.100	21.288	0.253	1.958	1.000		
0.18	1.343	0.838	56.061	0.100	20.083	0.262	1.947	1.000		
0.19	1.367	0.829	56.597	0.100	18.984	0.271	1.935	1.000		
0.2	1.392	0.820	57.133	0.100	17.978	0.280	1.924	1.000		
0.21	1.418	0.811	57.669	0.100	17.054	0.289	1.912	1.000		
0.22	1.444	0.802	58.204	0.100	16.205	0.298	1.900	1.000		
0.23	1.472	0.793	58.740	0.100	15.421	0.307	1.889	1.000		
0.24	1.500	0.784	59.276	0.100	14.696	0.316	1.877	1.000		
0.25	1.529	0.775	59.812	0.100	14.024	0.325	1.866	1.000		
0.26	1.559	0.766	60.348	0.100	13.400	0.334	1.854	1.000		
0.27	1.590	0.757	60.884	0.100	12.819	0.343	1.843	1.000		
0.28	1 622	0 748	61 419	0 100	12 277	0 352	1 831	1 000		
0.2								00		
0.								00		
0.3								00		
0.3		11	1	-				00		
0.3	0							00		
0.3			-	>-				00		
0.3	P	-		J.	CONTRACT OF		-	00		
0.3					1			00		
0.3	Se -			MA	-	EX	66 YHP	00		
0.3	6					~		00		
0.3						-	-	00		
0.								00		
0.41	2.154	0.631	68.385	0.100	7.610	0.469	1.681	1.000		
0.42	2.206	0.622	68.921	0.100	7.373	0.478	1.670	1.000		
0.43	2.261	0.613	69.457	0.100	7.147	0.487	1.658	1.000		
0.44	2.317	0.604	69.993	0.100	6.932	0.496	1.646	1.000		
0.45	2.376	0.595	70.529	0.100	6.727	0.505	1.635	1.000		
0.46	2 437	0 586	71 065	0 100	6 5 3 2	0 514	1 623	1 000		



#### Diesel Cycle model

Dr A. French. September 2017



Input parameters	
Temperature T1 of air draw into piston /Celsius	2
Low pressure state p1 /atm	1.0
Volume V1 of uncompressed gas /litres	182
Volume V2 of compressed gas /litres	7
Volume V3 of compressed gas after isobaric heating /litres	17
Degrees of freedom of molecular motion	
Molar mass of gas /gmol^-1	28.96

#### Outputs

Heat input during isobaric heating /kJ	4267
Heat output during isochoric cooling /kJ	710
Total work done by gas on surroundings /kJ	3557
Efficiency (work done / heat input)	0.834

#### Theoretical efficiency



Note all temperatures incorporated into calculations will be converted to Kelvin first - i.e. add 273 to Celsius number.

#### Pressure, volume, temperature coordinates of heat cycle

p1	1.0
V1	1820
T1	298
p2	186.0
V2	79.1
T2	2410
p3	186.0
V3	169.7
Т3	5168
p4	3.6
V4	1820.0
Т4	1063

Single cylinder power outp	out
Engine RPM	84
Power output /kW	4,980
• •	

0.834

Number of cylinders	14
Total power output /kW	69,717

#### Note all pressures are quoted in atmospheres. 1atm = 101,325 Pa. Volumes in litres, T in K

Number of moles of gas in engine	74
Ratio of specific heats gamma	1.667
Constant volume specific heat capacity /Jkg^-1K^-1	431
Constant pressure specific heat capacity /Jkg^-1K^-1	718

### Note real petrol engines have an efficiency of more like 20%, whereas diesels can be up to 40%. In other words, significant losses!



World's largest container ship in 2014 MV CSCL Globe



MAN B&W 12S90ME-C Mark 9.2 diesel engine. 69,720kW at 84RPM

Assume about 1820 litre cylinder volume V1

Max compression ratio: V1/V2 = 23

V3 guessed at: V1/10.726

	1 to 2		2 to 3		3 to 4		4 to 1				
	Adiabat	tic			Adiabati	с					
	compre	ssion	Isobaric	heating	expansio	on	Isochoric cooling				
V or p											
diff											
fraction	р	v	р	v	р	v	р	v			
0	1.000	1820.000	186.014	79.130	186.014	169.681	3.566	1820.000			
0.01	1.016	1802.591	186.014	80.036	159.354	186.184	3.540	1820.000			
0.02	1.033	1785.183	186.014	80.941	138.322	202.688	3.514	1820.000			
0.03	1.050	1767.774	186.014	81.847	121.404	219.191	3.489	1820.000			
0.04	1.067	1750.365	186.014	82.752	107.569	235.694	3.463	1820.000			
0.05	1.085	1732.957	186.014	83.658	96.095	252.197	3.437	1820.000			
0.06	1.104	1715.548	186.014	84.563	86.461	268.700	3.412	1820.000			
0.07	1.122	1698.139	186.014	85.469	78.285	285.203	3.386	1820.000			
0.08	1.142	1680.730	186.014	86.374	71.279	301.707	3.360	1820.000			
0.09	1.162	1663.322	186.014	87.280	65.225	318.210	3.335	1820.000			
0.1	1.182	1645.913	186.014	88.186	59.954	334.713	3.309	1820.000			
0.11	1.204	1628.504	186.014	89.091	55.332	351.216	3.284	1820.000			
0.12	1.225	1611.096	186.014	89.997	51.256	367.719	3.258	1820.000			
0.13	1.248	1593.687	186.014	90.902	47.639	384.223	3.232	1820.000			
0.14	1.271	1576.278	186.014	91.808	44.414	400.726	3.207	1820.000			
0.15	1.295	1558.870	186.014	92.713	41.525	417.229	3.181	1820.000			
0.16	1.319	1541.461	186.014	93.619	38.925	433.732	3.155	1820.000			
0.17	1.344	1524.052	186.014	94.524	36.577	450.235	3.130	1820.000			
0.18	1.370	1506.643	186.014	95.430	34.447	466.739	3.104	1820.000			
0.19	1.397	1489.235	186.014	96.335	32.508	483.242	3.078	1820.000			
0.2	1.425	1471.826	186.014	97.241	30.739	499.745	3.053	1820.000			
0.21	1.453	1454.417	186.014	98.146	29.119	516.248	3.027	1820.000			
0.22	1.483	1437.009	186.014	99.052	27.631	532.751	3.001	1820.000			
0.23	1 5 1 2	1410 000	100 014	00.057	20 201	F 40 2F 4	2 070	1020.000			
0.24	:			A	E	Mainht 17.2 m		20.000			
0.25			L -	-	Cal			20.000			
0.26								20.000			
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0.28	<u> </u>	-		641				20.000			
0.29	C 🗆		1					20.000			
0.3		1				from monthly	-	20.000			
0.31			-				100	20.000			
0.32	<b>[</b> :						-	20.000			
0.33		10	4				-	20.000			
0.34		1	-	7	A STATE		10	20.000			
0.35				1 1	1			20.000			
0.36	Г	m	1	115				20.000			
0.37		ment .	and the	4		19 "		20.000			
0.38	_ I	-		T	-	4		20.000			
0.39			A		an -			20.000			
0.4				5 6	1			20.000			
0.41	1		1	CAL UNIT	10			20.000			
0.42			1			P		20.000			
0.43			-		-	3		20.000			
0.44				1 -	1 :	5		20.000			
0.45					TA C	- 1 -		20.000			
0.46						14		20.000			
0.47	-		-					20.000			
0.48				-		1	Height 1,85	20.000			
0.49			100.01*		111.11.34						

2.805 500.574 180.014 125.500 10.054 578.557 2.505 1820.000





If the specific heat capacity of the fluid is c, and the vessel contains m kg of fluid

$$dQ = -mcdT$$

If we assume the heat capacity is independent of temperature

$$\frac{dT}{dt} = -\frac{kA}{mc\Delta x} (T - T_a)$$
$$\int_{T_0}^T \frac{dT}{T - T_a} = -\frac{kA}{mc\Delta x} \int_0^t dt$$
$$\left[ \ln |T - T_a| \right]_{T_0}^T = -\frac{kAt}{mc\Delta x}$$

Q is the heat transferred from the vessel to the surroundings k is the thermal conductivity of the vessel  $\Delta x$  is the thickness of the vessel A is the surface area of the vessel

$$\frac{dQ}{dt} = kA\frac{\left(T - T_a\right)}{\Delta x}$$



"Heat flow via conduction is proportional to temperature gradient"

T

Joseph Fourier (1768-1830)

$$\ln\left(\frac{T-T_a}{T_0-T_a}\right) = -\frac{kAt}{mc\Delta x}$$
$$\frac{T-T_a}{T_0-T_a} = e^{-\frac{kAt}{mc\Delta x}}$$
$$T = T_a + \left(T_0 - T_a\right)e^{-\frac{kAt}{mc\Delta x}}$$



Isaac Newton (1643-1727)

### Brownian motion – a random walk

Brownian motion, initially observed as the random jittering of pollen grains in a microscope slide, is due to the random jostling of molecular motion. In the base of the pollen grains, it is the smaller (invisible) air molecules which are colliding at random. How far will a given particle move in a specified time, given its motion is random?

Consider motion in one direction in *N* steps of fixed length *l*. The caveat is that each step is either forward or backwards, and the direction is 'chosen' randomly.

The total displacement is

$$x = l \sum_{i=1}^{N} a_i$$
 where  $a_i = -1$  or 1

A sensible measure of the distance travelled is the root-mean-square (RMS) displacement:

$$\sqrt{\langle x^2 \rangle} = l \sqrt{\left\langle \left(\sum_{i=1}^N a_i\right)^2 \right\rangle} = l \sqrt{\left\langle \sum_{i=1}^N a_i^2 + \sum_{i=1, i \neq j}^N \sum_{j=1}^N a_i a_j \right\rangle}$$
Robert Brow (1773-1858)  

$$\left\langle \sum_{i=1}^N a_i^2 \right\rangle = N \quad \text{and} \quad \left\langle \sum_{i=1, i \neq j}^N \sum_{j=1}^N a_i a_j \right\rangle = 0 \quad \longleftarrow \quad \text{Since } a \text{ is a random choice between -1 and 1}$$

$$\therefore \sqrt{\langle x^2 \rangle} = l \sqrt{N}$$



Brownian motion simulation



Brown 1858)

Hence the RMS random walk displacement in *t* seconds is predicted to be:

$$\sqrt{\left\langle x^2 \right\rangle} = l\sqrt{N} = \sqrt{l\left\langle v \right\rangle t}$$

The step size l can be associated with the **mean free path** between molecular collisions. We can define the mean free path to be the average distance travelled by a molecule in time t divided by the number of molecules it will likely collide with in that time.





The interaction volume is root 2 larger because all molecules are in *relative* motion. Hence the length of the 'interaction tube' is proportional to the average *relative* speed

Mean free path

 $\pi\sqrt{2}d^2n$ 

Mean free path

Average

distance

between

collisions

Colliding particles, assumed to be circular with diameter d

We can determine the **mean free path** for an ideal gas by using the **Ideal Gas Equation** 



Hence 
$$l = \frac{k_B T}{\pi \sqrt{2} d^2 p}$$

If we divide this by the particle diameter *d* we arrive at **Knudsen's number (Kn)**. This dimensionless constant determines whether our statistical mechanics argument is valid, or whether a 'continuum' concept is needed.

The latter model is what is used to describe much of **fluid mechanics** i.e. where we consider the fluid as a continuously varying entity rather than a series of discrete, and randomly moving, molecules colliding.

Kn≪1 Continuum

Kn > 1 Statistical mechanics

For a typical air molecule on Earth

$$d = 0.3$$
nm,  $p = 10^{5}$  Pa,  $T = 293K$   
 $\therefore l = 1.0 \times 10^{-7}$  m

$$\therefore \mathrm{Kn} = \frac{l}{d} = 333$$

So a statistical argument is justified





PhET States of Matter

1D F	RANDOM	WALK	SIM		A. I	Frenc	h Nov	2019																			
STEF	P SIZE = 1																										
			1 2	2 3	3	4	5	6	7	8 9	) 10	) 1	1 12	2	1	2	3	4	4 5	6	5 7	8	3 9	) 10	11	. 12	
n	sqrt(n)	x	x	x	x	x	x	x	x	x	x	x	x	x^	2 x^2	x	^2 )	x^2	x^2	x^7	x^2	x^2	x^2	x^2	x^2	x^2	rms x
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	) (	)	0	0	0	0	0	0	0	0	0
1	1	1	-1	1	1	1	-1	1	1	-1	-1	1	-1	1	1	1	. 1	1	1	1	1	1	1	1	1	1	1
2	1.4142	2	-2	2	2	2	0	0	2	-2	0	0	0	4	4	4	L 1	4	4	0	0	4	4	0	0	0	1.528
3	1.7321	3	-3	1	3						1	rm	s distanc	e x of rand	om walk				1	1	1		1	1	1	1	1.915
4	2	4	-4	2	4	160							saistante										4	0	0	0	2.38
5	2.2361	5	-5	1	5														4				1	1	1	1	2.887
6	2.4495	4	-4	0	4	140													J.M.			5	0	4	0	0	2.708
7	2.6458	3	-5	-1	5											- May	I. I. M	N. J					1	9	1	1	2.887
8	2.8284	4	-4	-2	6	120								A. A.			VW	WW.					0	4	4	4	3
9	3	3	-5	-3	5								MY	JAY "	Ŵ								1	9	1	1	3.109
10	3.1623	2	-6	-2	4	100						<b>م</b> عال			Y								4	4	4	4	2.944
11	3.3166	1	-7	-1	5					M		1											1	9	9	9	3.512
12	3.4641	0	-8	0	6	× 80			n vy		Ŵ												0	16	16	4	4
13	3.6056	-1	-7	-1	7	E		1													rms	x	1	25	25	1	4.359
14	3.7417	0	-6	-2	8	60																(n)	4	16	36	4	4.546
15	3.873	-1	-5	-1	9			V					Γ	1					/	_			9	25	25	9	4.865
16	4	-2	-4	0	8	40		1						/ 2	2		1		ר א				16	36	16	4	4.655
17	4.1231	-3	-3	-1	7	40								( X -			:/	<b>1</b>	/V				9	25	25	1	4.655
18	4.2426	-4	-2	-2	8	20	1						$\mathbf{N}$	1.00			v	V	•••				16	36	16	0	5.196
19	4.3589	-3	-3	-1	7	20	/						N	l.	/								25	25	25	1	5.066
20	4.4721	-2	-2	-2	8																		36	36	36	0	5.715
21	4.5826	-1	-3	-3	7	0,			500	0		10000	)	1	5000		2	0000		25000			25	49	25	1	5.627
22	4.6904	-2	-4	-4	8								step r	number n									16	64	16	0	5.538
23	4.7958	-1	-5	-3	9	9	-3	11	-3	3	-9	5	-1	1	25	9	) {	31	81	9	121	9	9	81	25	1	6.137
24	4.899	-2	-4	-2	8	8	-4	10	-2	4	-10	4	0	4	16	4	. (	54	64	16	100	4	1			17	
25	5	-3	-5	-1	7	9	-3	11	-3	3	-9	5	-1	9	25	1		49	81	9	121	9	9			N	
26	5.099	-2	-4	-2	8	8	-4	10	-4	4	-8	6	-2	4	16	4	. (	54	64	16	100	16	1		1		
27	5.1962	-3	-5	-1	7	7	-3	11	-3	5	-9	7	-1	9	25	1	. 4	49	49	9	121	9	2	r =	_ /		$\alpha$
28	5.2915	-2	-6	0	6	6	-2	12	-4	4	-8	6	-2	4	36	0	) 3	36	36	4	144	16		v —	- ı		$\mathcal{M}_{i}$
29	5.3852	-1	-5	1	7	5	-1	11	-5	3	-9	5	-3	1	25	1	. 4	49	25	1	121	25	9				L L
30	5.4772	-2	-4	0	8	4	0	10	-6	2	-10	4	-2	4	16	0	) (	54	16	0	100	36	4			i=1	
31	5.5678	-3	-5	1	9	3	1	11	-5	3	-9	5	-1	9	25	1	. 8	81	9	1	121	25	9				
-		1	1	1	-				-	1	1	1	1	+ +	1				1	1	1	1				1	1
																							C	1 :		— I	orl
																								i		-	
•	1 N i	ra	nr		m	v	va		ci	m		at	in	n ir	Ē	'vr	20										
	ושו	a				V	v Cl		3		<b>MI</b>	ul						•					1		1		
																								_			
																							v		-		



Random walk. Max step size = 1, N = 10000



```
Random walk. Step size = 1
       & A visual representation of a random walk.
 1
                                                                 200
 2
       % Step sizes are fixed, but directions are random.
                                                                 150
 3
                                                                 100
       %Number of steps
 4
                                                                  50
                                         2D random walk
                                                                >
 5 -
       N = 1e6;
                                         MATLAB
 6
                                                                 -50
                                         simulation
 7
       %Fixed step size
                                                                 -100
8 -
       s = 1;
                                                                 -150
-200
 9
                                                                      -100
                                                                                100
                                                                                     200
                                                                                         300
10
       SInitilize x, y position vectors, starting from the origin.
11 -
       x = zeros(1,N); y = zeros(1,N);
12
13
       %Determine random walk
14 -
     \Box for n=2:N
           theta = 2*pi*rand;
15 -
16 -
           x(n) = x(n-1) + s*cos(theta); y(n) = y(n-1) + s*sin(theta);
17 -
       end
18
19
       &Plot random walk
20 -
       plot(x,y,'b-'); hold on;
21 -
       plot( x(1),y(1),'q*' ); plot( x(end),y(end),'r*' );
22 -
       xlabel('x'); ylabel('y'); title( ['Random walk. Step size = ',num2str(s)]);
23 -
       grid on;
24
25
       %Print a PNG file of the random walk
26 -
       print( gcf, 'random walk.png','-dpng','-r300' );
27
28
       %End of code
```





```
7
     [] function random walks
8
      P = 42; %Numbers of random walks
                                                          MATLAB implementation
9 -
LO —
      N = 5000; %Number of steps
                                                          of multiple random
L1 —
      s = 1; %Fixed step size
                                                          walks (in a loop)
L2 —
      fsize = 18; %Graph fontsize
L3
L4
       %Initialize axes and then plot random walks
L5 —
       axes('nextplot','add','fontsize',fsize);
L6 —
     \exists for n=1:P
L7 —
           [x, y] = randomwalk(N, s);
L8 —
           RGB = rand(1,3); plot(x,y,'-','color',RGB);
L9 —
       end
20 -
       xlabel('x'); ylabel('y'); title( ['Random walk. Step size = ',num2str(s)] );
21 -
      grid on; axis equal; box on;
22
23
       %Print a PNG file of the random walk
24 -
      filename = ['random walks ', strrep(datestr(now), ':', '-'), '.png'];
25 -
      print( gcf, filename, '-dpng', '-r300' );
26 -
      close(gcf);
27
28
       ક્રક્ર
29
30
       %Random walk generator
31
     [ function [x,y] = randomwalk(N,s)
32 -
      x = zeros(1,N); y = zeros(1,N);
     = for n=2:N
33 -
34 -
          theta = 2*pi*rand;
35 -
           x(n) = x(n-1) + s*cos(theta); y(n) = y(n-1) + s*sin(theta);
36 -
       end
```

7





We can compute a 3D **diffusion** model *efficiently* by using a random walk.

The random walk gets around the need to keep track of thousands of particles and their collisions.







i.e. absolute temperature is proportional to mean KE of molecules

Ludwig Boltzmann 1844-1906