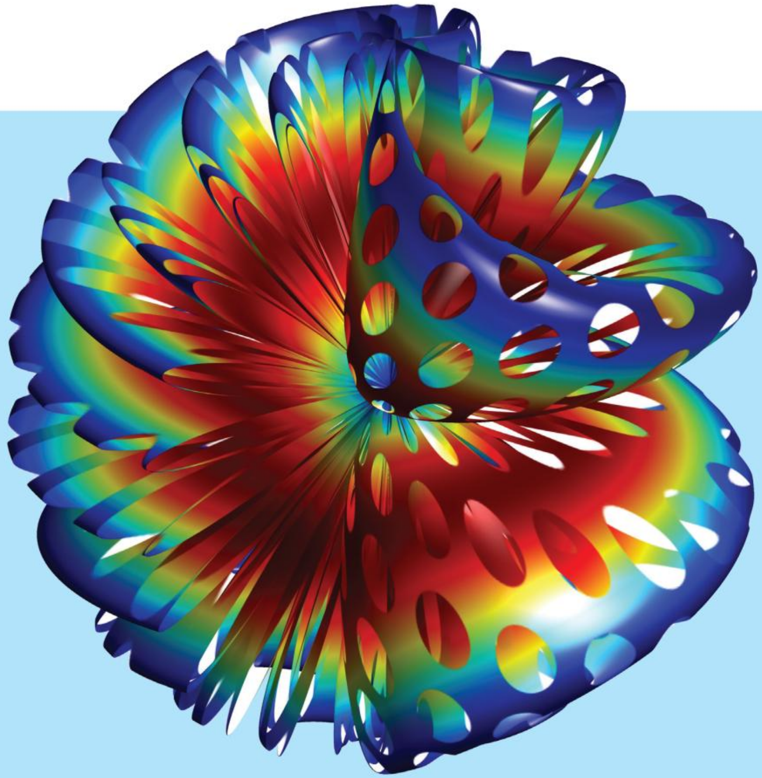
SCIENCE BY SIMULATION

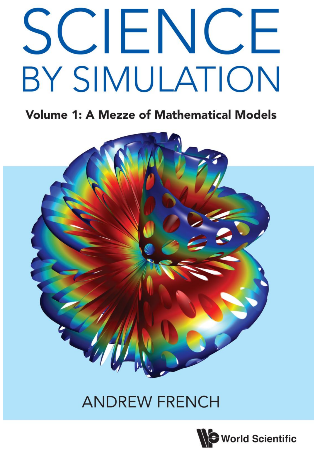
Volume 1: A Mezze of Mathematical Models



ANDREW FRENCH

World Scientific

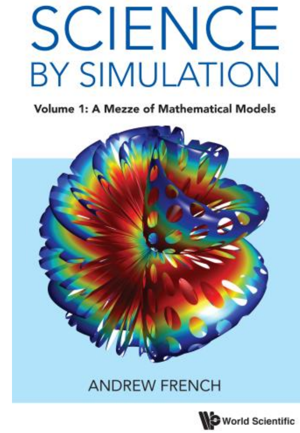
This is the first volume of **Science by Simulation**



As the title *A Mezze of Mathematical Models* suggests, it is a deliberate mixture of **contextualized** examples of **systems** that can be **modelled** using **mathematics**, and **simulated** using **computers**

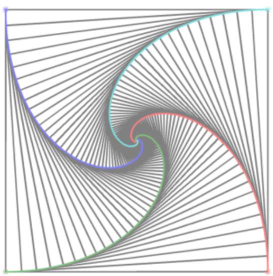
Who?

Dr Andy French. Physics teacher at Winchester College, UK.



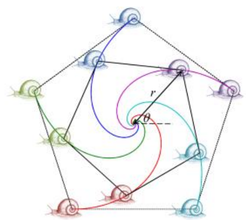
What?

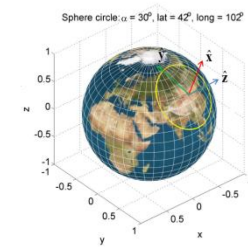
Book / website / educational concept / new BPhO course

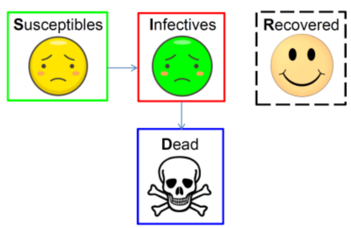


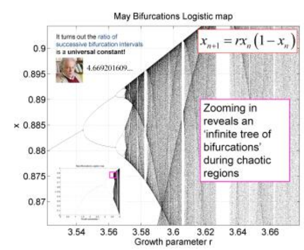
SCIENCE BY SIMULATION

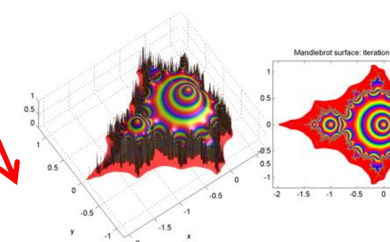
Dr Andrew French andy.french@physics.org www.eclecticon.info/scibysim.htm

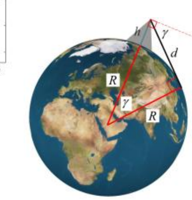






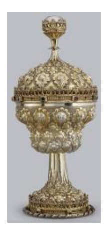


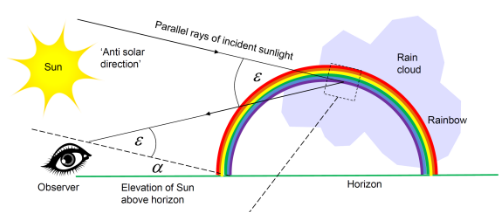




When?

Anticipated publication in 2022





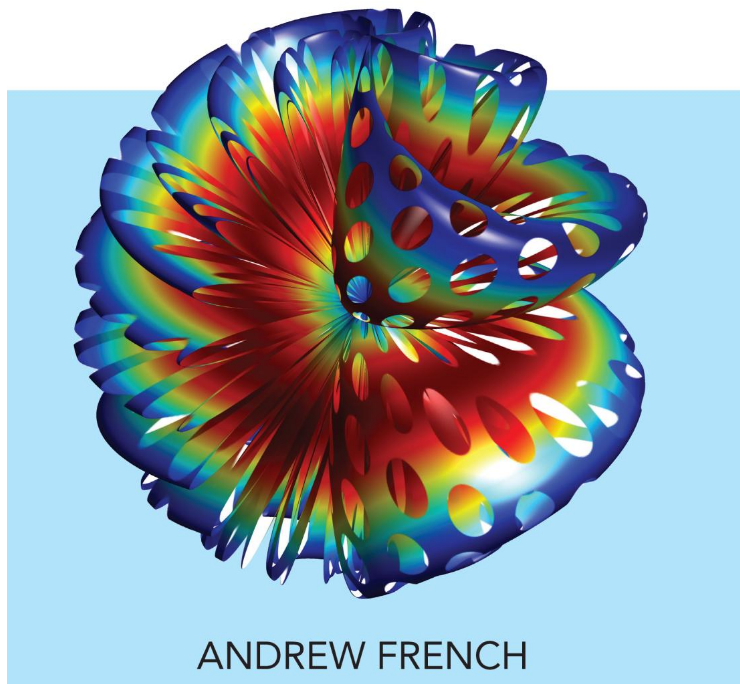
How?

A selection of example models and contexts

Learn to build mathematical models

SCIENCE BY SIMULATION

Volume 1: A Mezze of Mathematical Models



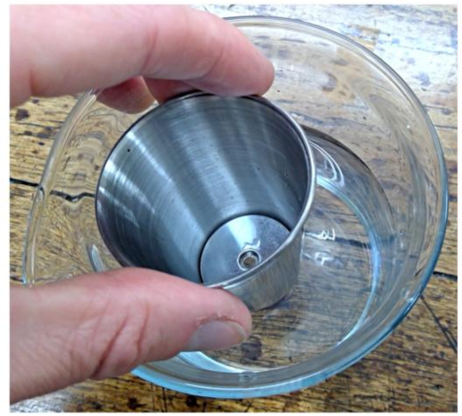
World Scientific

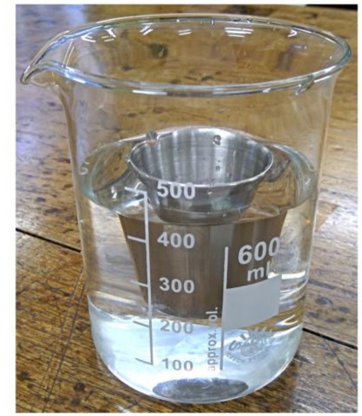
The power of context

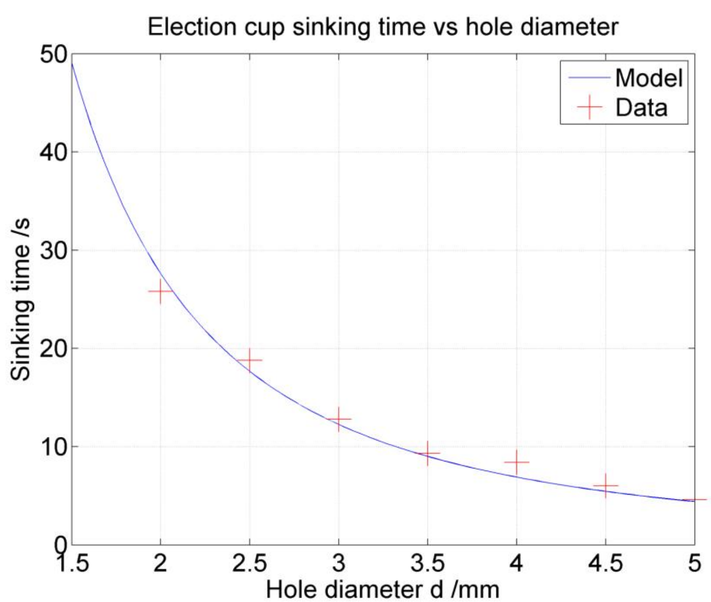
Science by storytelling!

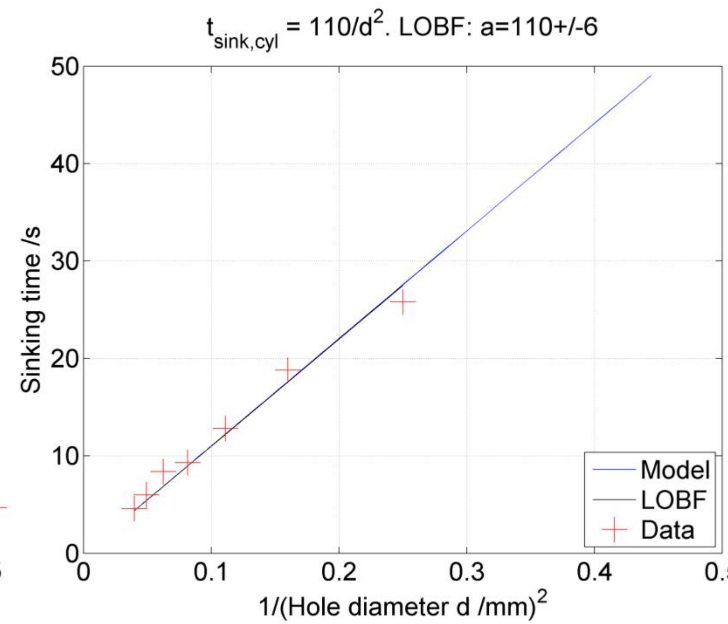
Learn to code dynamic computer simulations

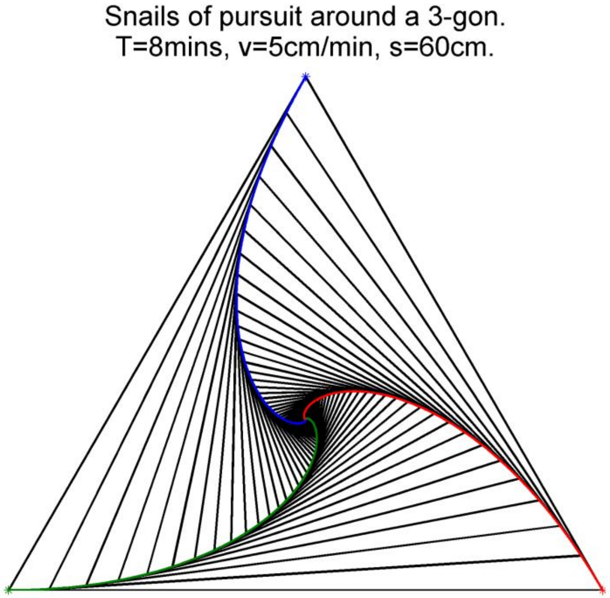

Unknown



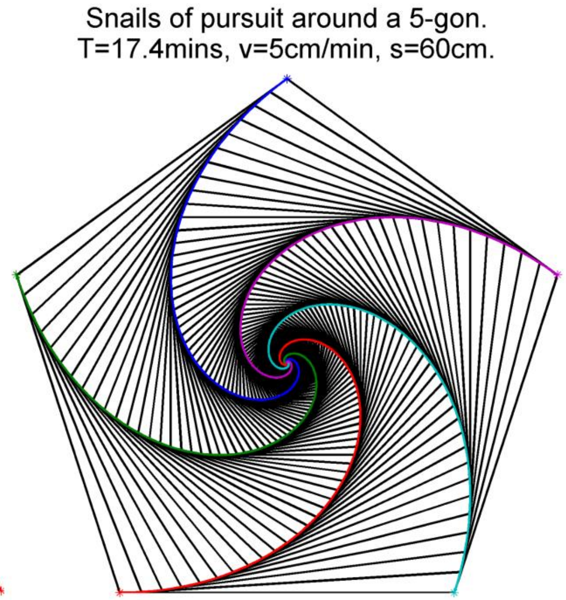

500
400
300
200
100
600
ml


Election cup sinking time vs hole diameter
Model
Data
Sinking time /s
Hole diameter d /mm
0
10
20
30
40
50
1.5
2
2.5
3
3.5
4
4.5
5

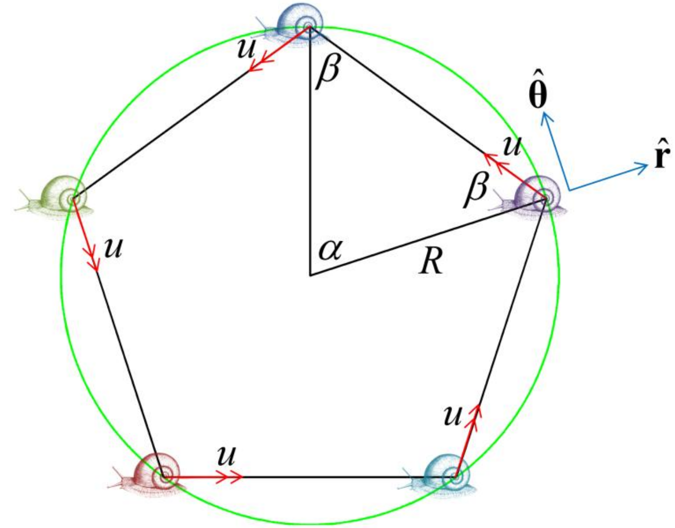

$t_{sink,cyl}$ = 110/d^2. LOBF: a=110+/-6
Model
LOBF
Data
Sinking time /s
1/(Hole diameter d /mm)^2
0
10
20
30
40
50
0
0.1
0.2
0.3
0.4
0.5

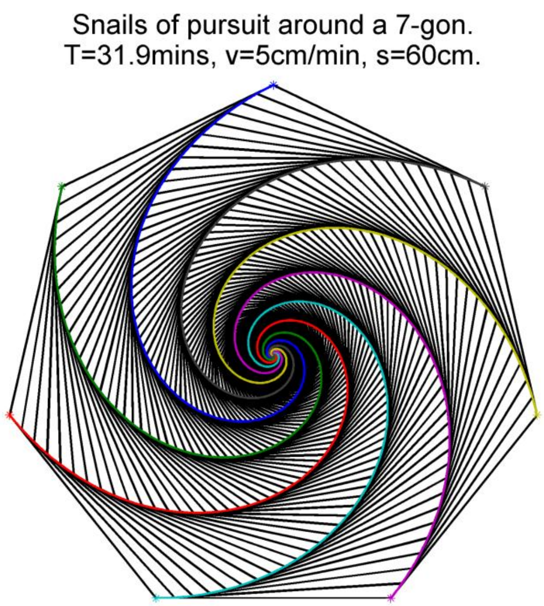

Snails of pursuit around a 3-gon.
T=8mins, v=5cm/min, s=60cm.

(a)

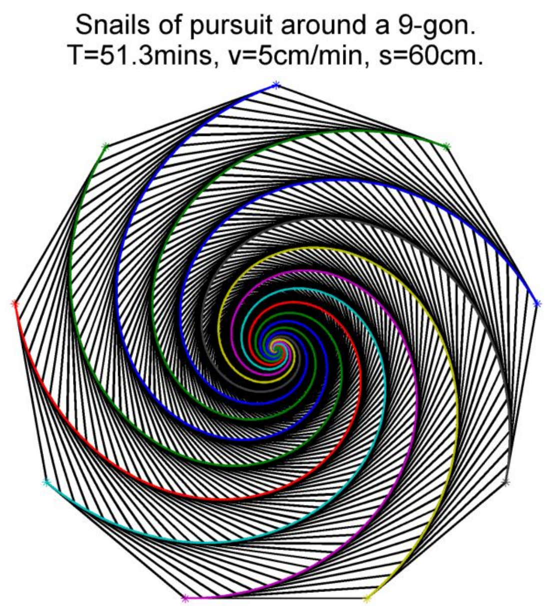

Snails of pursuit around a 5-gon.
T=17.4mins, v=5cm/min, s=60cm.

(b)

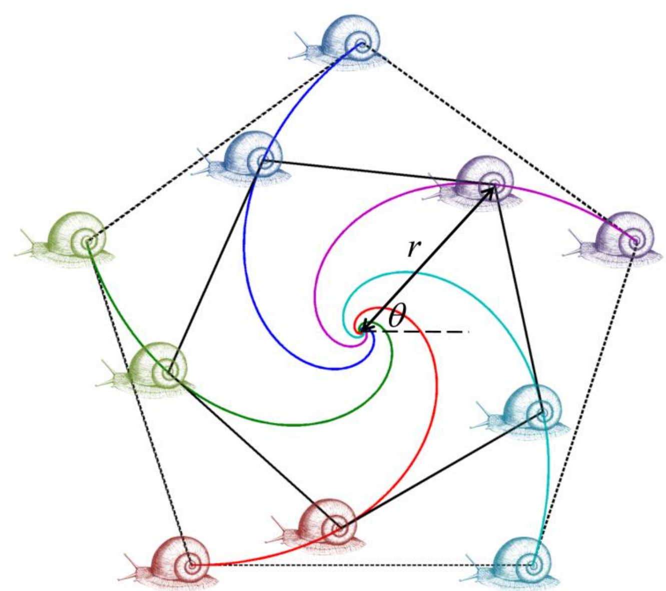

u
β
$\hat{\theta}$
$\hat{r}$
u
β
u
α
R
u
u


Snails of pursuit around a 7-gon.
T=31.9mins, v=5cm/min, s=60cm.

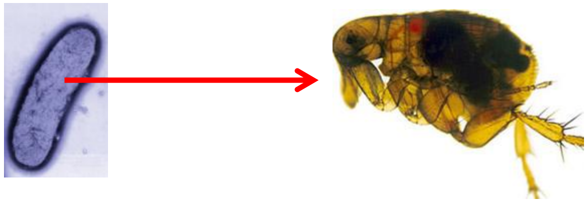
(c)


Snails of pursuit around a 9-gon.
T=51.3mins, v=5cm/min, s=60cm.

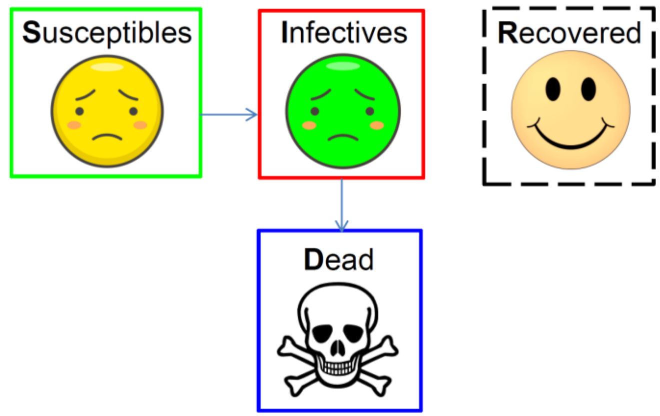
(d)

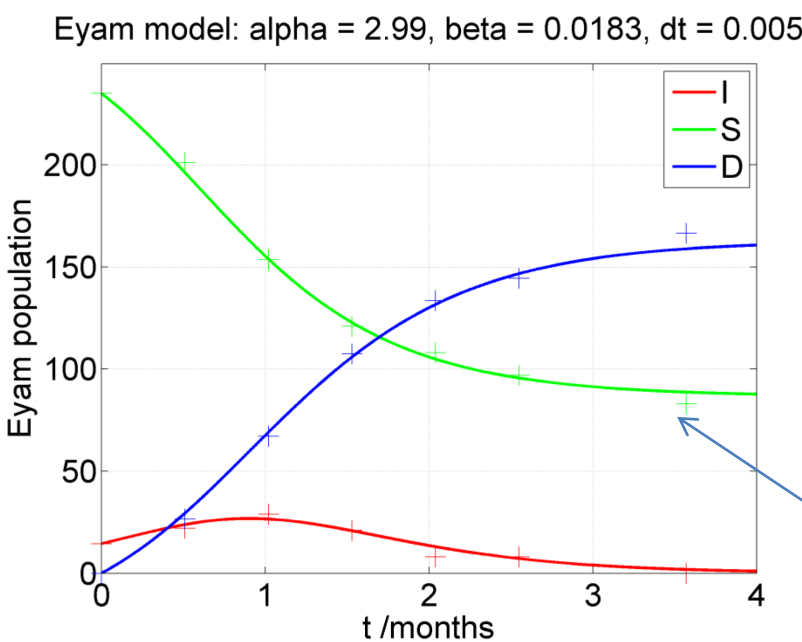

r
θ

1665. A bale of damp cloth is delivered to the Derbyshire village of **Eyam**... George Viccars, the tailor's assistant, dries the cloth and releases fleas infected with *Yersinia Pestis* bacteria – **Plague**



Rector **William Mompesson** *quarantines* Eyam and records **Infected**, **Susceptible** and **Dead** populations *as time progresses*





Can we develop a mathematical model to predict I,S,D vs time? What does this tell us about *Epidemiology* in general? → e.g Flu, Ebola

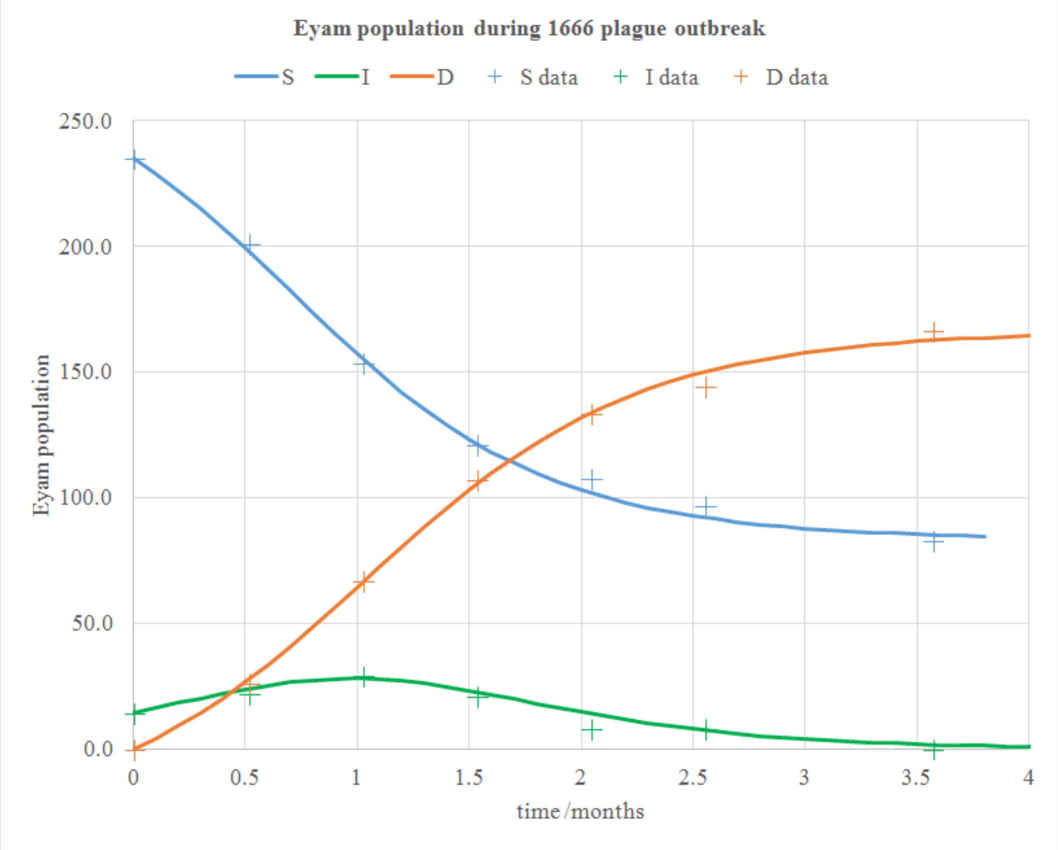
Calculus methods, differential equations numerical methods, line of best fit, iteration, loops ...

We performed the Eyam analysis in **Python**, then in **MATLAB**.
You can also construct an Euler model via a spreadsheet (**Excel**).

Black Death Epidemiological model using the Eyam data
Andy French & John Cullerne. 24th February 2018.

Initial population N0	249.5
Initial number of succeptables S0	235
Initial number of infectives I0	14.5
Transmission rate constant beta	0.017759
Death rate constant alpha	2.9
timestep dt /months	0.1

t /months	S	I	D	N	N+D = N0
0	235.0	14.5	0.0	249.5	249.5
0.1	228.9	16.3	4.2	245.3	249.5
0.2	222.3	18.3	8.9	240.6	249.5
0.3	215.1	20.2	14.2	235.3	249.5
0.4	207.4	22.0	20.1	229.4	249.5
0.5	199.3	23.7	26.5	223.0	249.5
0.6	190.9	25.3	33.4	216.1	249.5
0.7	182.3	26.5	40.7	208.8	249.5
0.8	173.7	27.4	48.4	201.1	249.5
0.9	165.3	27.9	56.3	193.2	249.5
1	157.1	28.0	64.4	185.1	249.5
1.1	149.3	27.7	72.5	177.0	249.5
1.2	141.9	27.0	80.6	168.9	249.5
1.3	135.1	26.0	88.4	161.1	249.5
1.4	128.9	24.7	95.9	153.6	249.5
1.5	123.3	23.2	103.1	146.4	249.5
1.6	118.2	21.5	109.8	139.7	249.5



$$\frac{dS}{dt} = -\beta SI \qquad \frac{dI}{dt} = \beta SI - \alpha I \qquad \frac{dD}{dt} = \alpha I$$

$$\frac{dS}{dt} = -\beta SI$$

$$\frac{dI}{dt} = \beta SI - \alpha I$$

$$\frac{dD}{dt} = \alpha I$$

Leonhard Euler
1707-1783

Euler numerical *iterative* solution scheme

$$\alpha = 2.894, \quad \beta = \frac{\alpha}{163.3}$$

$$t_0 = 0, \ S_0 = 235, \ I_0 = 14.5, \ D_0 = 0$$

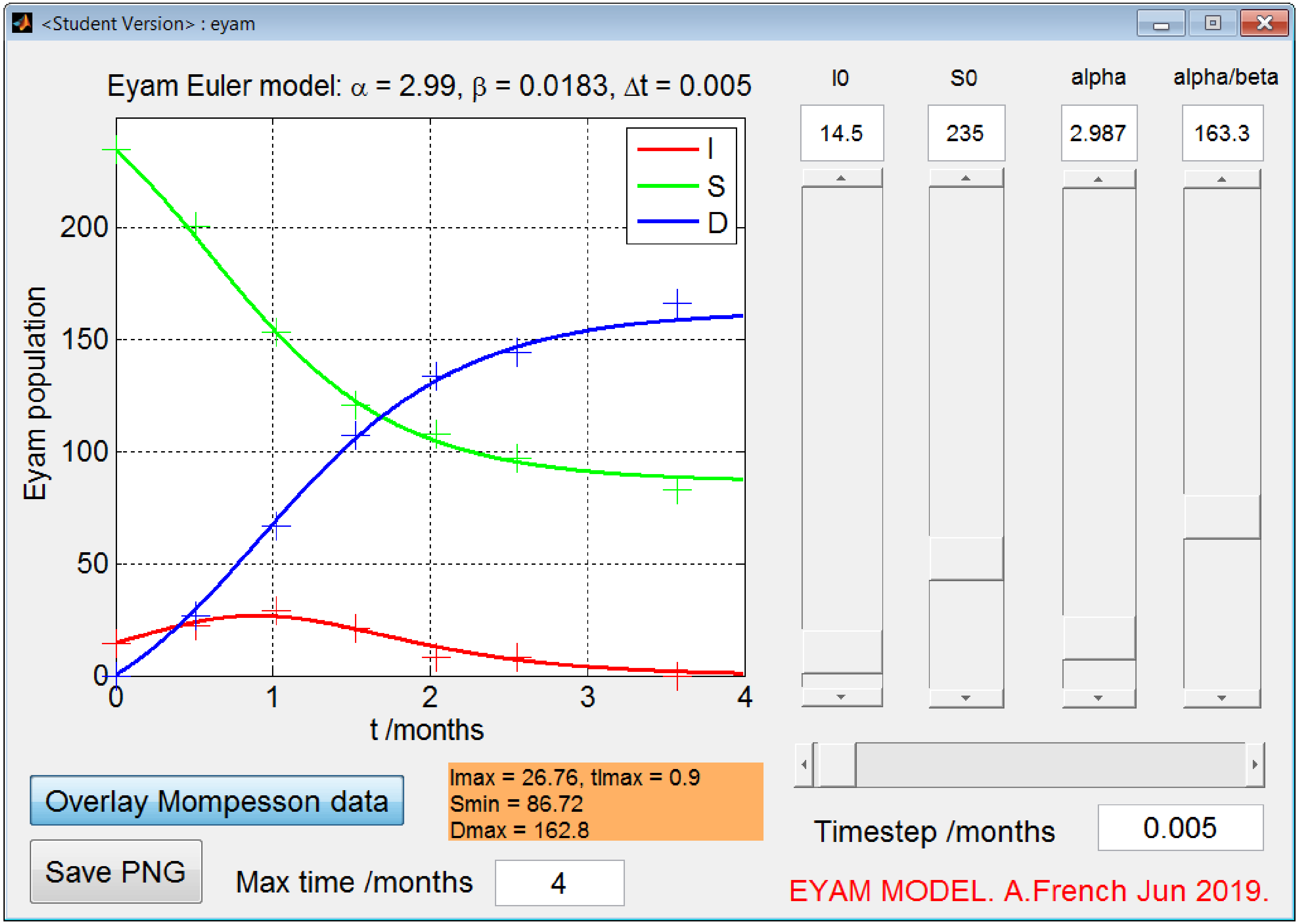
$$t_{n+1} = t_n + \Delta t$$

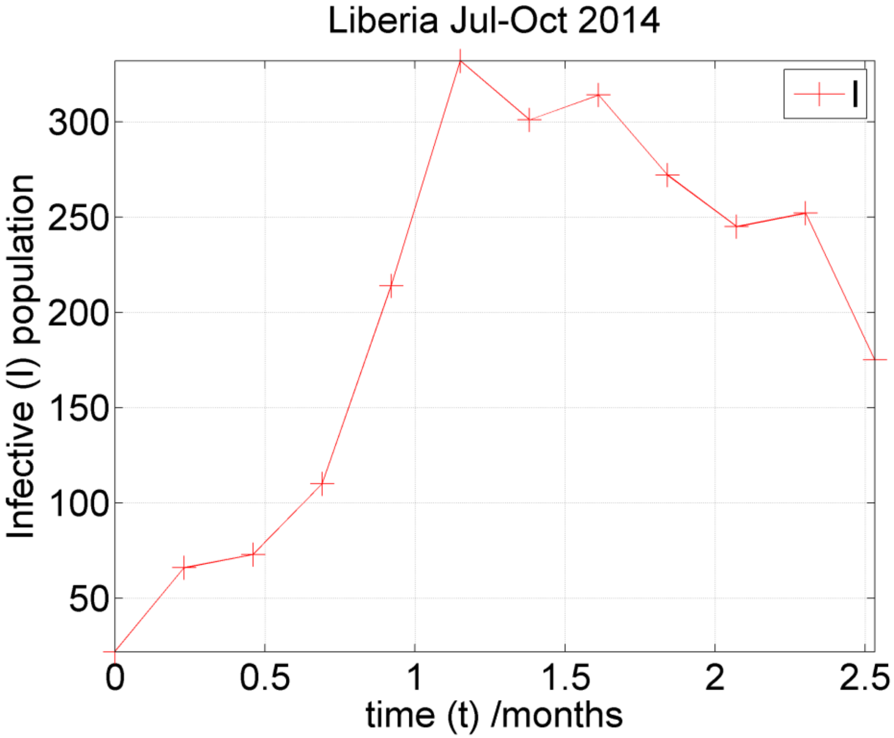
$$S_{n+1} = S_n - \beta S_n I_n \Delta t$$

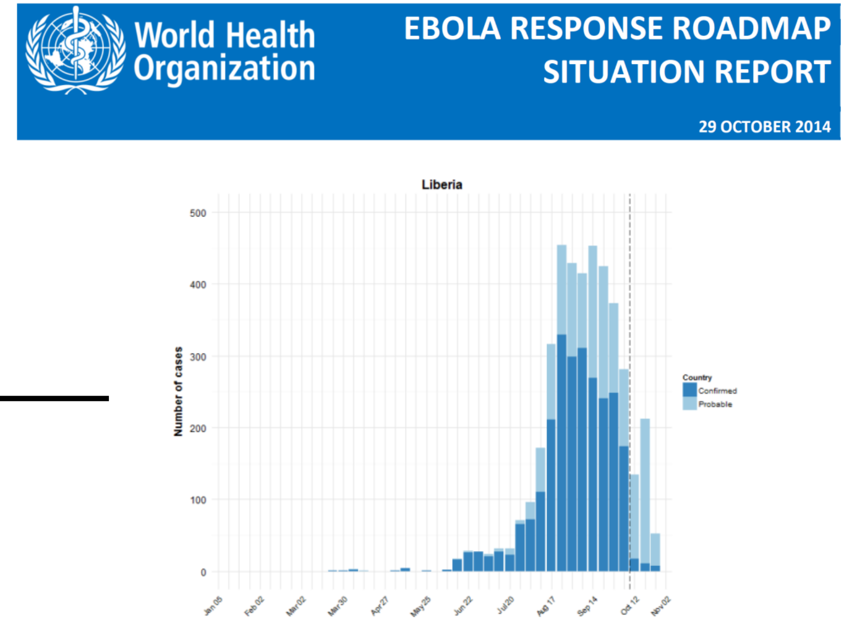
$$I_{n+1} = I_n + \left(\beta S_n I_n - \alpha I_n\right)\Delta t$$

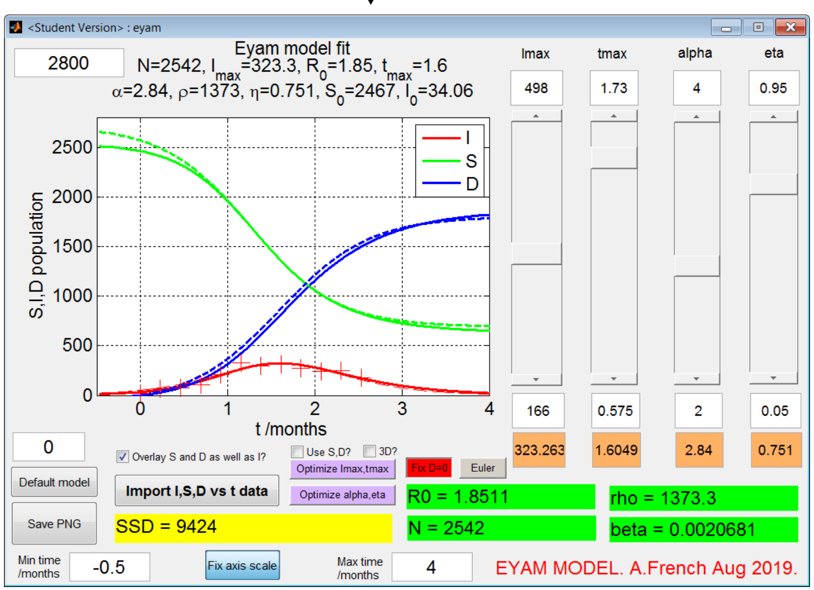
$$D_{n+1} = D_n + \alpha I_n \Delta t$$

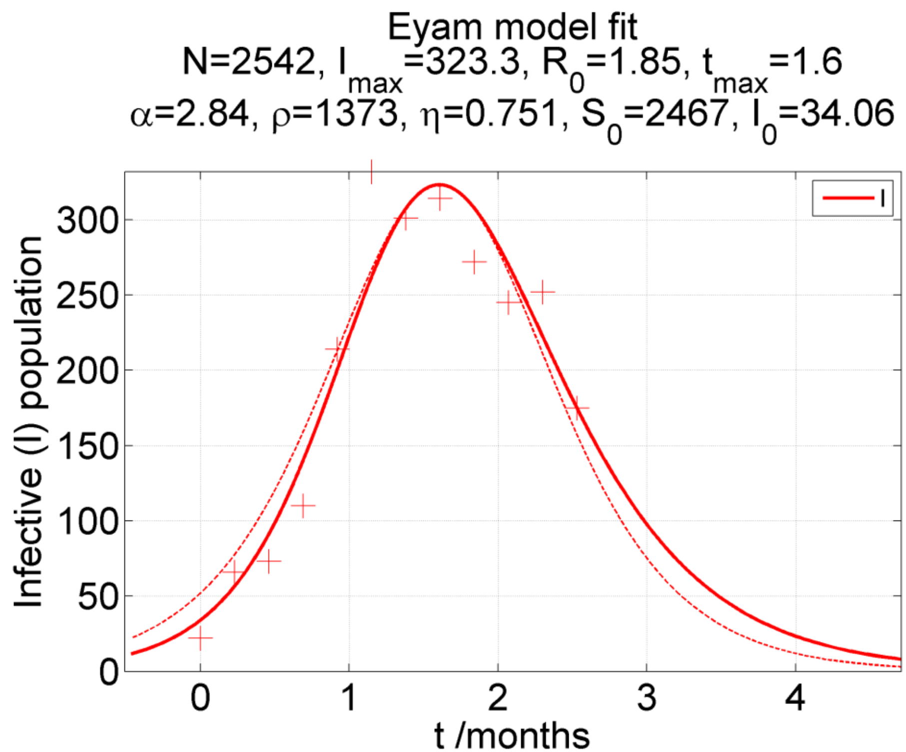
Euler Eyam solver implemented in MATLAB with a Graphical User Interface (GUI).
Change the inputs via the sliders or edit boxes, and the curves are computed automatically.

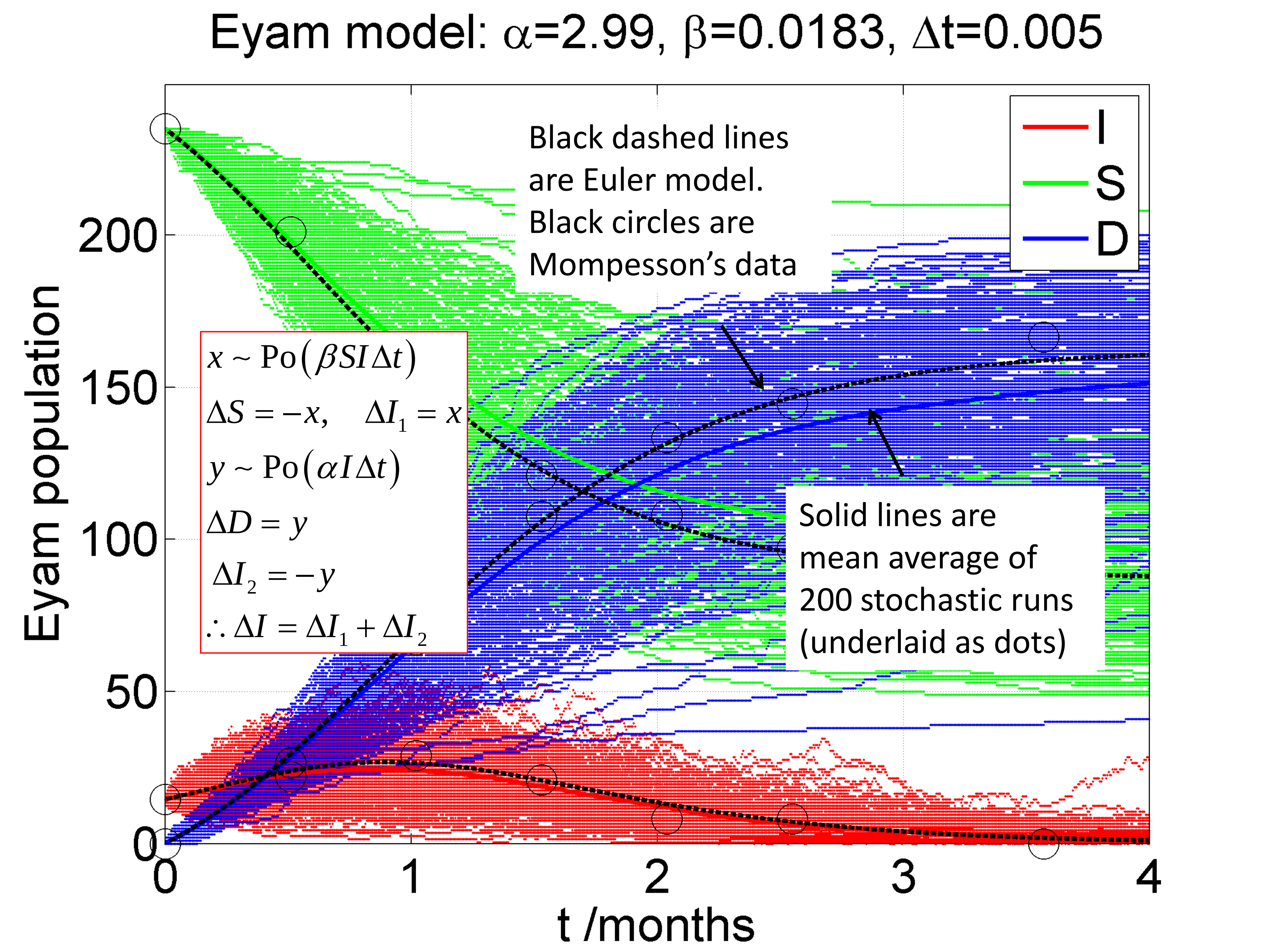



Liberia Jul-Oct 2014
Infective (I) population
time (t) /months
I
300
250
200
150
100
50
0
0.5
1
1.5
2
2.5

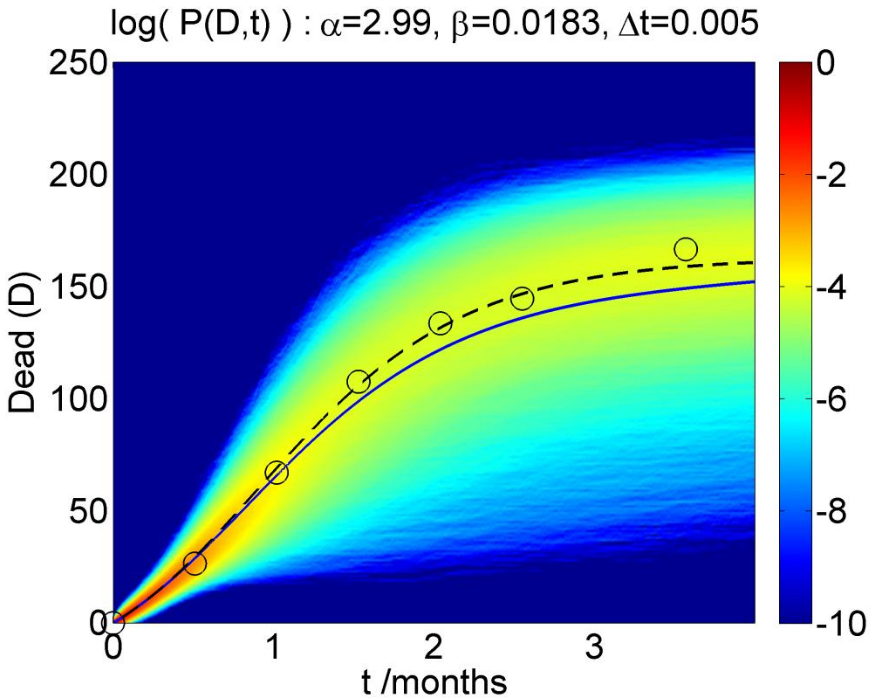

World Health Organization
EBOLA RESPONSE ROADMAP
SITUATION REPORT
29 OCTOBER 2014
Liberia
Number of cases
Country
Confirmed
Probable

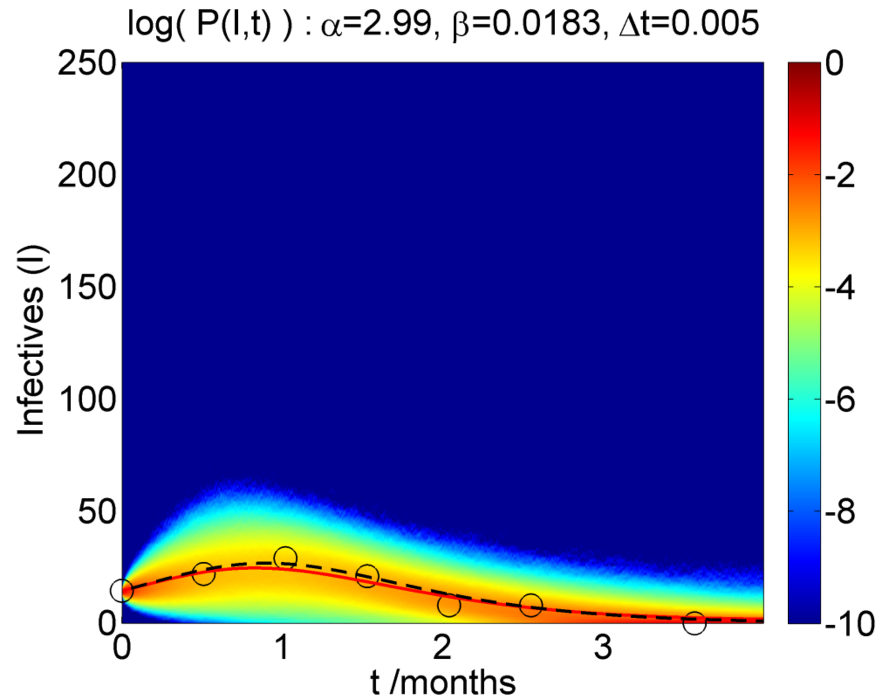

<Student Version> : eyam
Eyam model fit
N=2542, Imax=323.3, R0=1.85, tmax=1.6
α=2.84, ρ=1373, η=0.751, S0=2467, I0=34.06
2800
Imax
tmax
alpha
eta
498
1.73
4
0.95
166
0.575
2
0.05
323.263
1.6049
2.84
0.751
S,I,D population
t /months
I
S
D
0
Default model
Save PNG
Overlay S and D as well as I?
Use S,D?
3D?
Optimize Imax,tmax
Optimize alpha,eta
Fix D=0
Euler
Import I,S,D vs t data
SSD = 9424
R0 = 1.8511
N = 2542
rho = 1373.3
beta = 0.0020681
Min time /months
-0.5
Fix axis scale
Max time /months
4
EYAM MODEL. A.French Aug 2019.

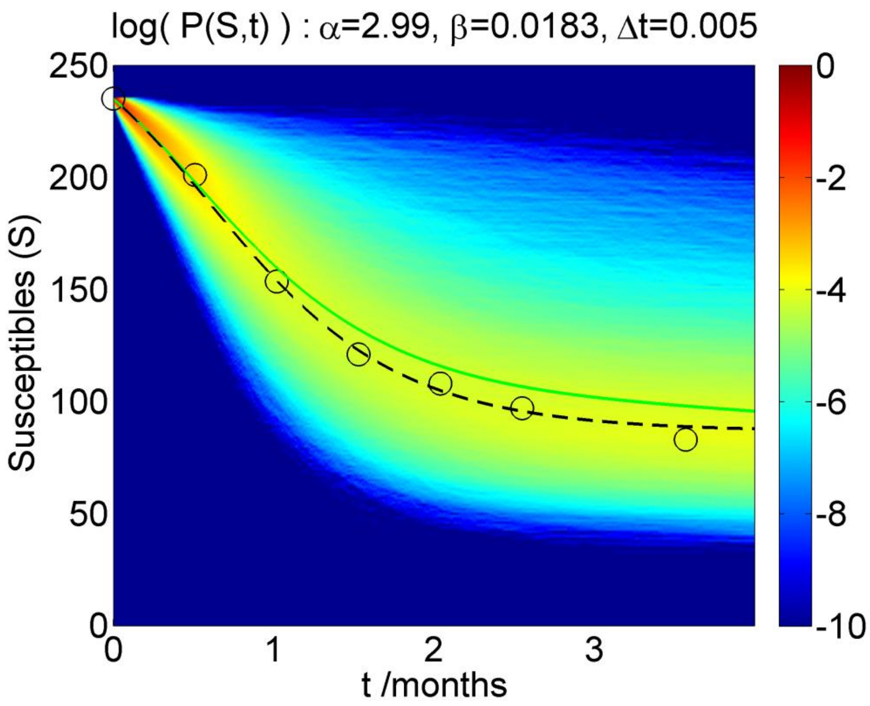

Eyam model fit
N=2542, Imax=323.3, R0=1.85, tmax=1.6
α=2.84, ρ=1373, η=0.751, S0=2467, I0=34.06
Infective (I) population
t /months
I



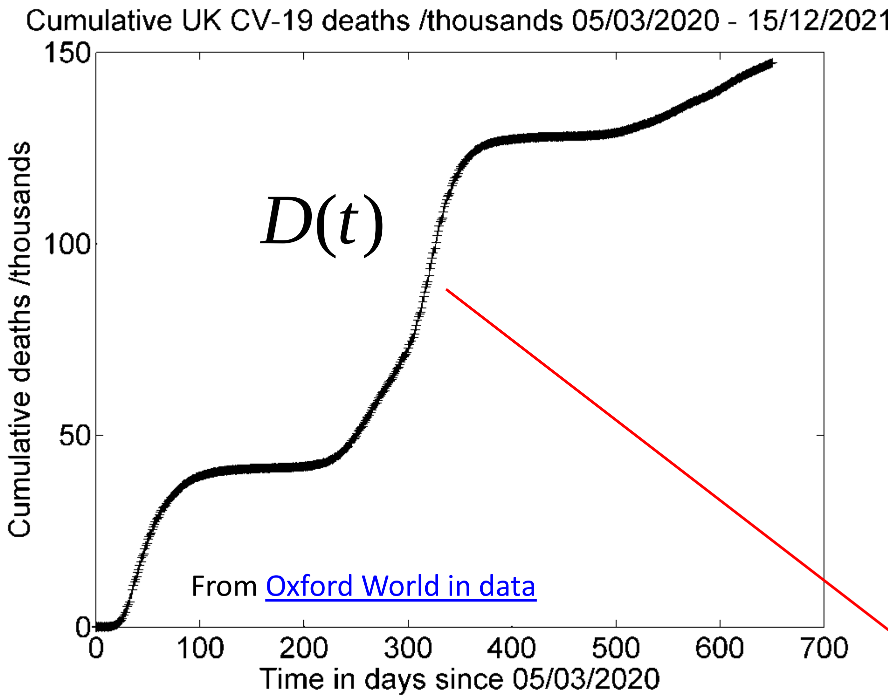
Eyam model: α=2.99, β=0.0183, Δt=0.005
Eyam population
t /months
0
50
100
150
200
0
1
2
3
4
I
S
D
Black dashed lines are Euler model. Black circles are Mompesson's data
$x \sim \mathrm{Po}(\beta S I \Delta t)$
$\Delta S = -x, \quad \Delta I_1 = x$
$y \sim \mathrm{Po}(\alpha I \Delta t)$
$\Delta D = y$
$\Delta I_2 = -y$
$\therefore \Delta I = \Delta I_1 + \Delta I_2$
Solid lines are mean average of 200 stochastic runs (underlaid as dots)



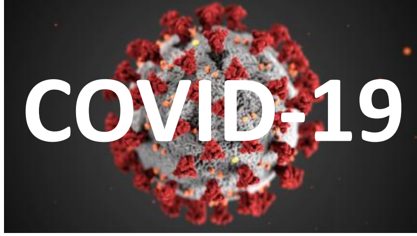




Probability map, computed from 50,000 iterations. Black circles are Mompesson data and black dashed lines correspond to the Euler model.



One can *estimate* the number of CV-19 **infectives** from the cumulative deaths:

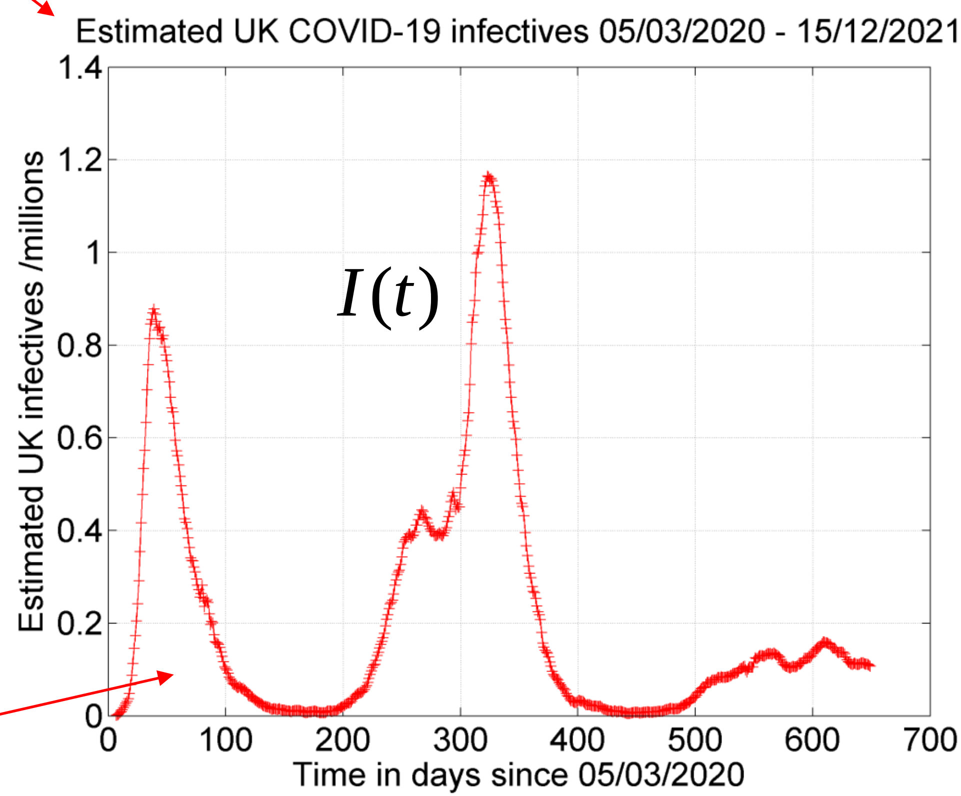


$$I_n = \frac{1}{k\alpha}\frac{dD}{dt} \approx \frac{1}{k\alpha}\frac{D_{n+1} - D_{n-1}}{t_{n+1} - t_{n-1}}$$

Find the gradient and scale by:

$$k\alpha = 0.01 \times \tfrac{1}{9.32} \text{ days}^{-1}$$

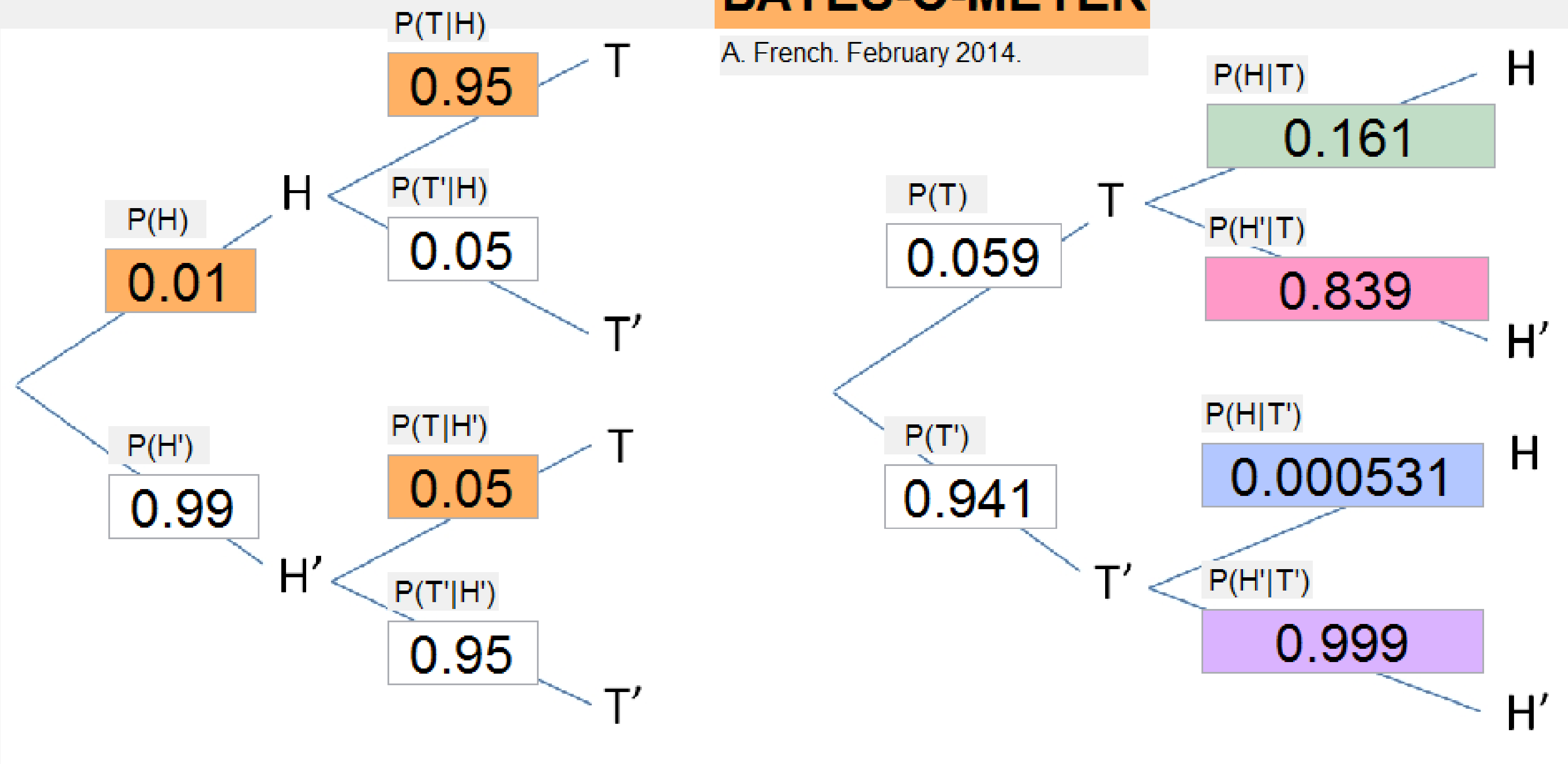
Note *mortality fraction k* and *disease time constant* α may vary considerably within a population and indeed post-vaccination – so treat with caution!



Note: as per the 'daily death rate' graphs in *World in Data*, we also apply a **seven-day moving average** to smooth the numerical derivative.

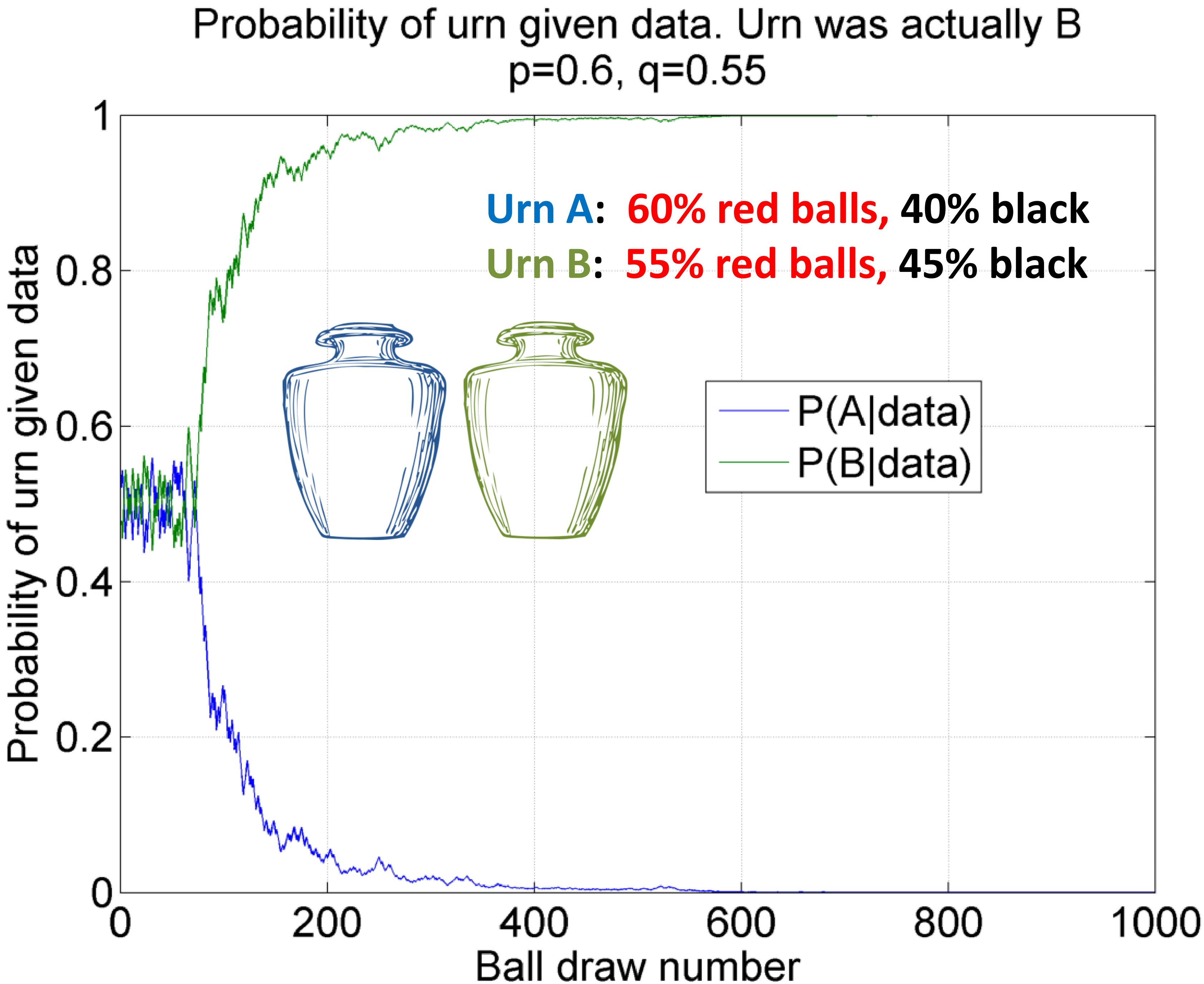
BAYES-O-METER

A. French. February 2014.

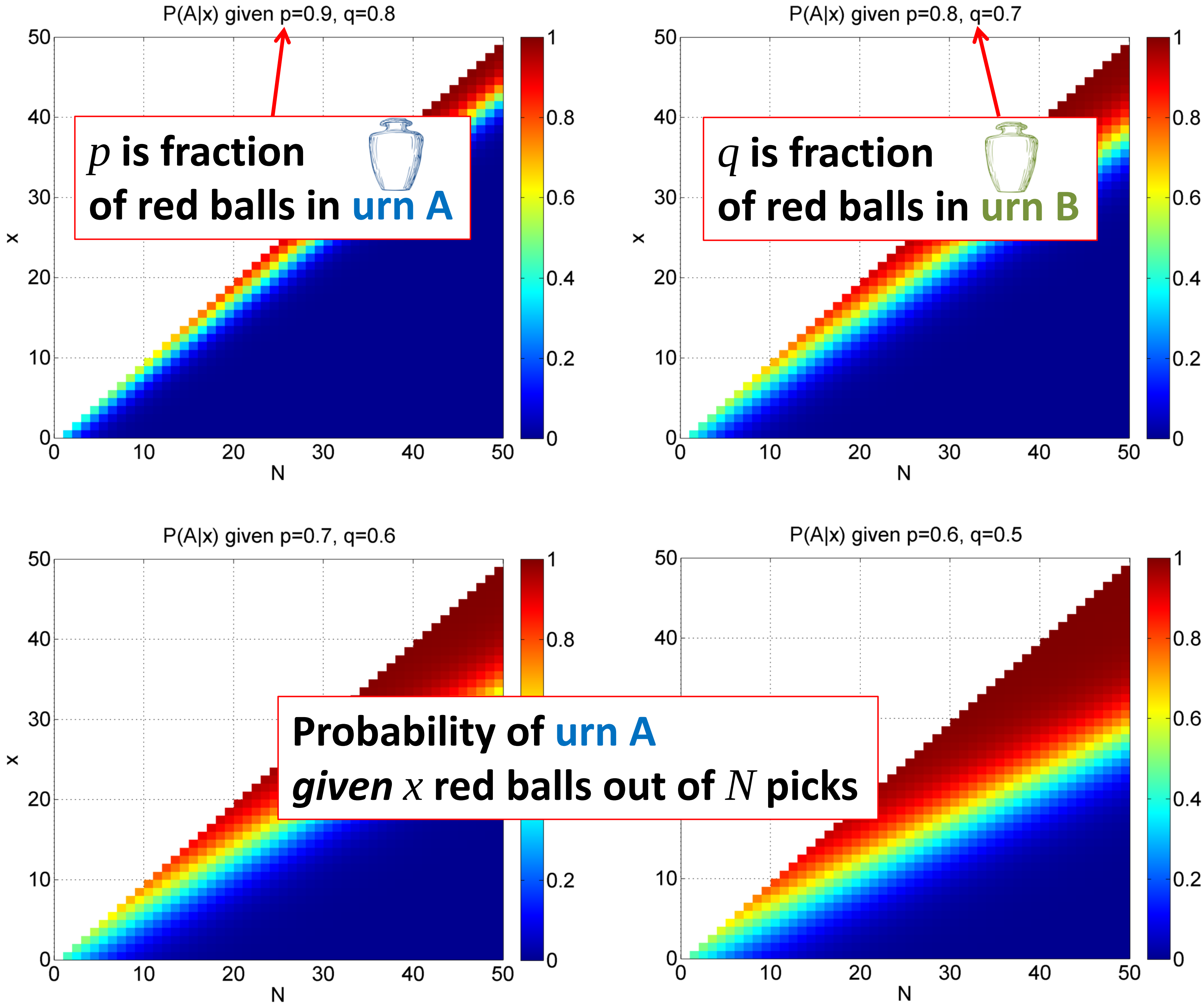


P(H|T) Probability of hypothesis true given pass of test	0.161
P(H'|T) (False positive) Probability of hypothesis false given pass of test	0.839
P(H|T') (False negative) Probability of hypothesis true given fail of test	0.000531
P(H'|T') Probability of hypothesis false given fail of test	0.999

Thomas Bayes
1701-1761

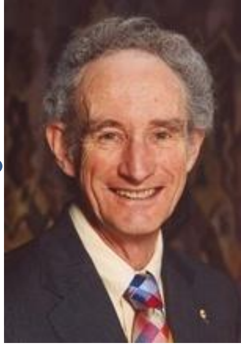


Probability of urn given data. Urn was actually B
p=0.6, q=0.55
Urn A: 60% red balls, 40% black
Urn B: 55% red balls, 45% black
P(A|data)
P(B|data)
Probability of urn given data
Ball draw number
0
0.2
0.4
0.6
0.8
1
0
200
400
600
800
1000


P(A|x) given p=0.9, q=0.8
P(A|x) given p=0.8, q=0.7
P(A|x) given p=0.7, q=0.6
P(A|x) given p=0.6, q=0.5
x
N
p is fraction of red balls in urn A
q is fraction of red balls in urn B
Probability of urn A given x red balls out of N picks

May’s Chaotic Bunnies

I published this model in 1976



Robert May
1936-

Assume an ecosystem can support a maximum number of rabbits. Let x be the fraction of this maximum at year n.

To account for **reproduction**, next year’s population is proportional to the previous.

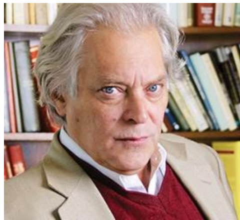
To account for **starvation**, next year’s population is *also proportional* to the fraction of the maximum population as yet unfilled.

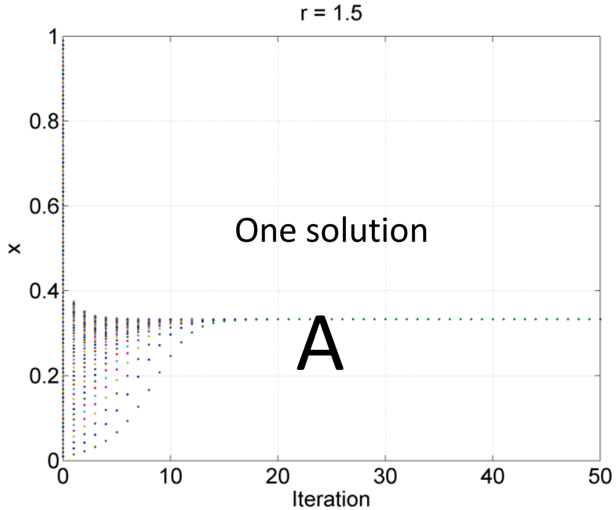
$$x_{n+1} = r x_n \left(1 - x_n\right)$$

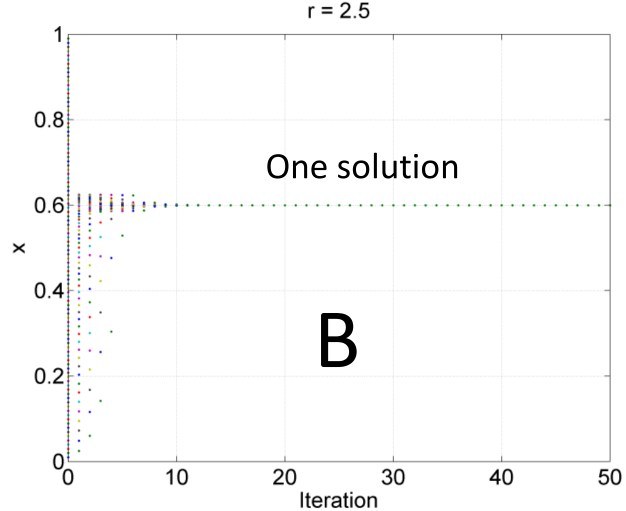
Growth parameter

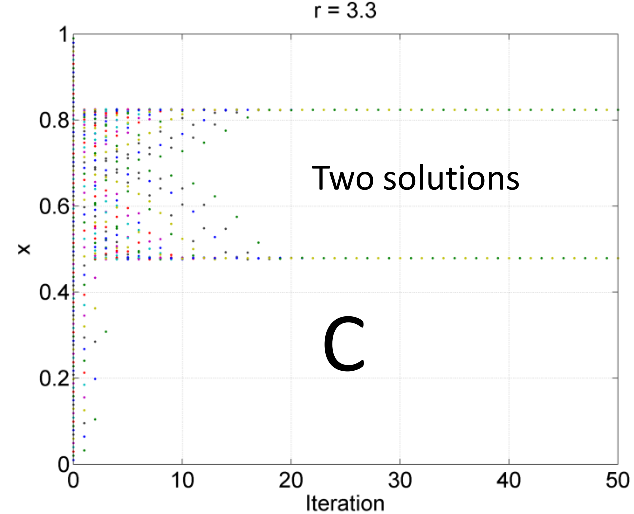
The population next year is predicted using this **iterative equation** called a **logistic map**

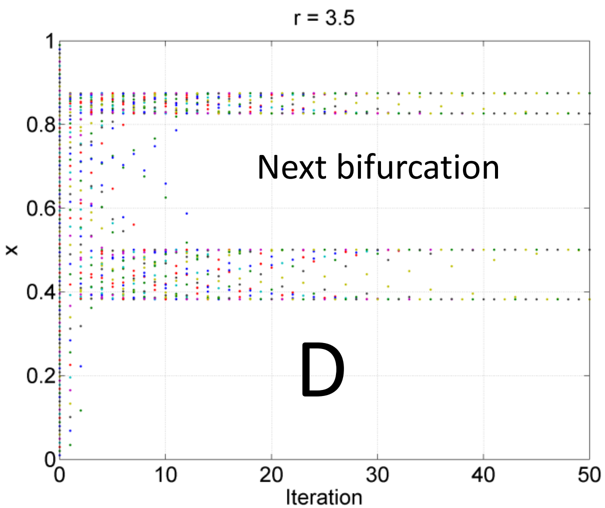
The pattern of x values with n is not always simple .....

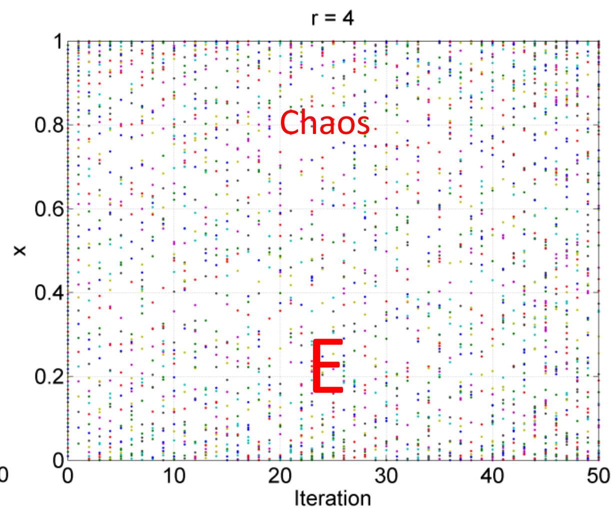




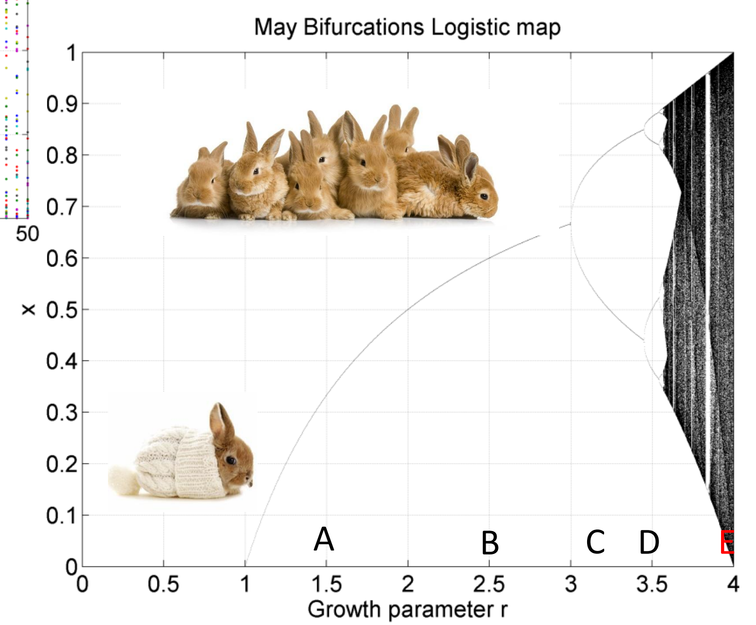






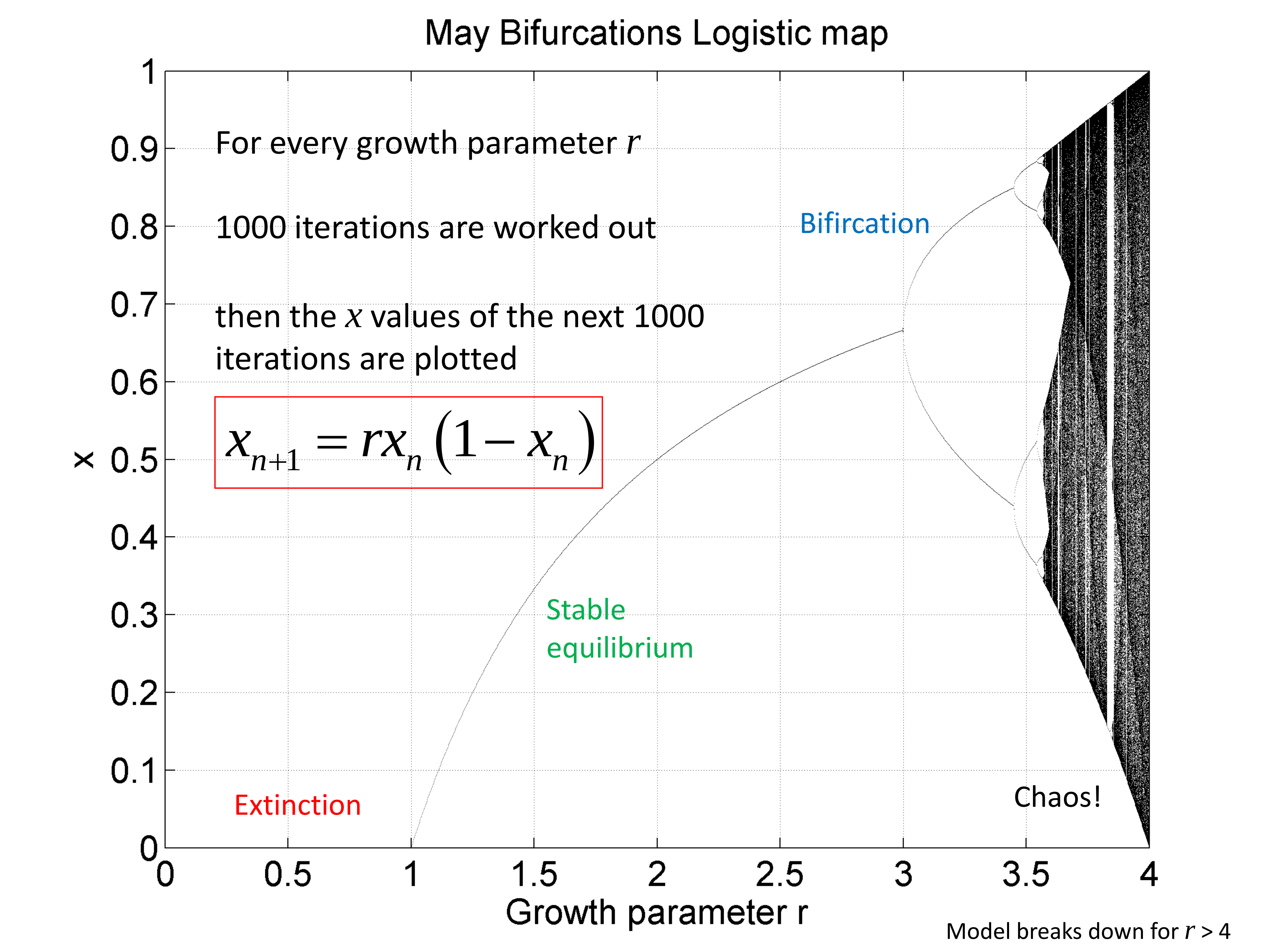


$$x_{n+1} = rx_n\left(1 - x_n\right)$$

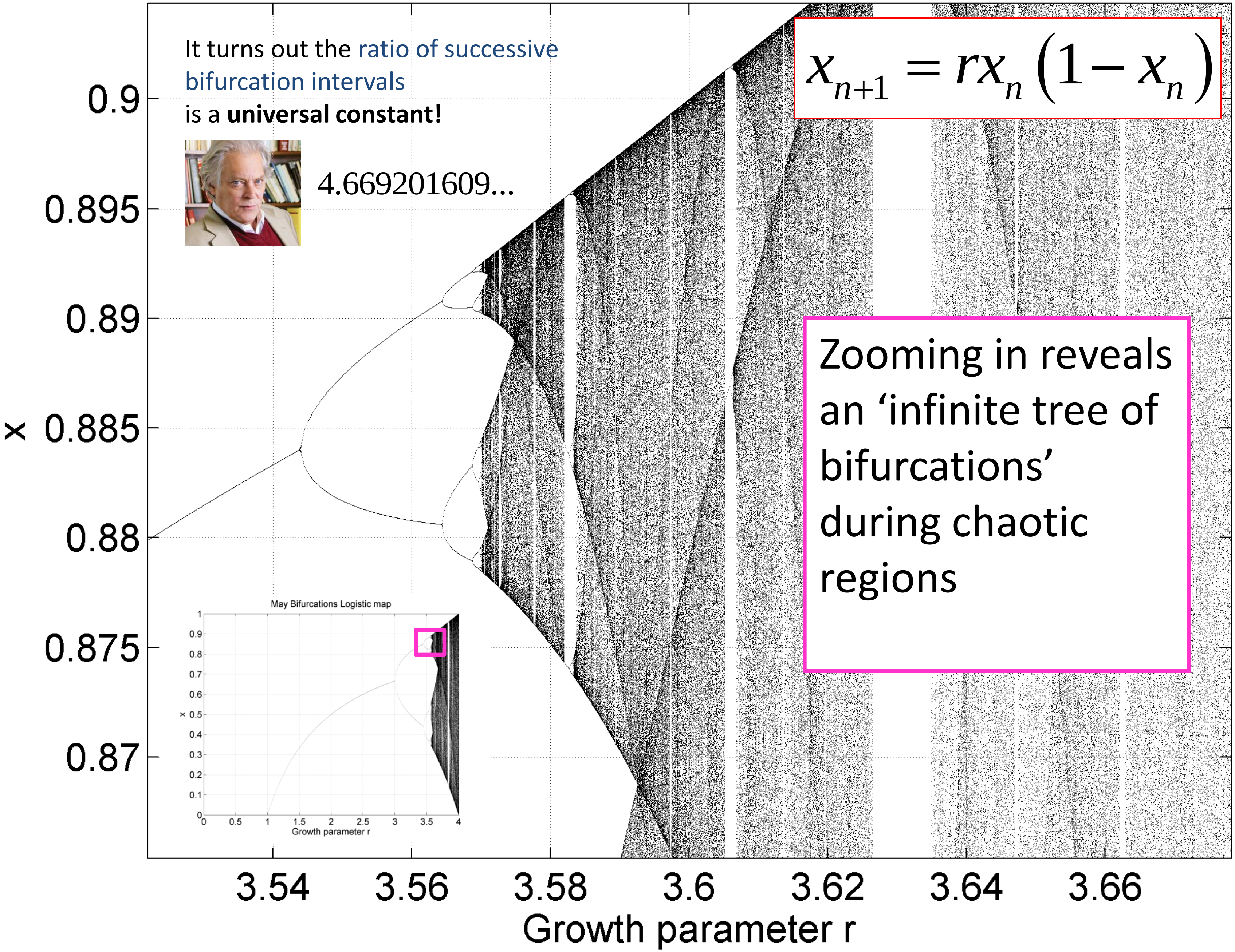


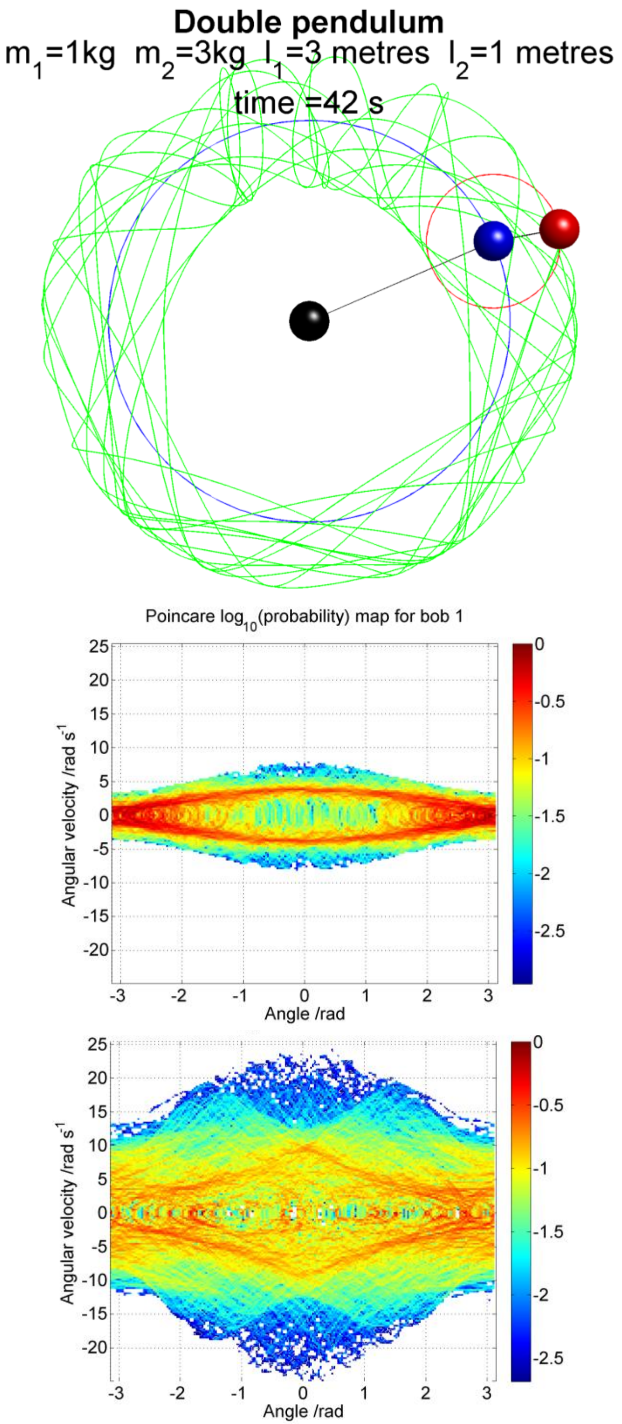
Tracking the bifurcations maps the ‘road to chaos’. The ratio of successive bifurcation intervals is a **universal constant!**

4.669201609…

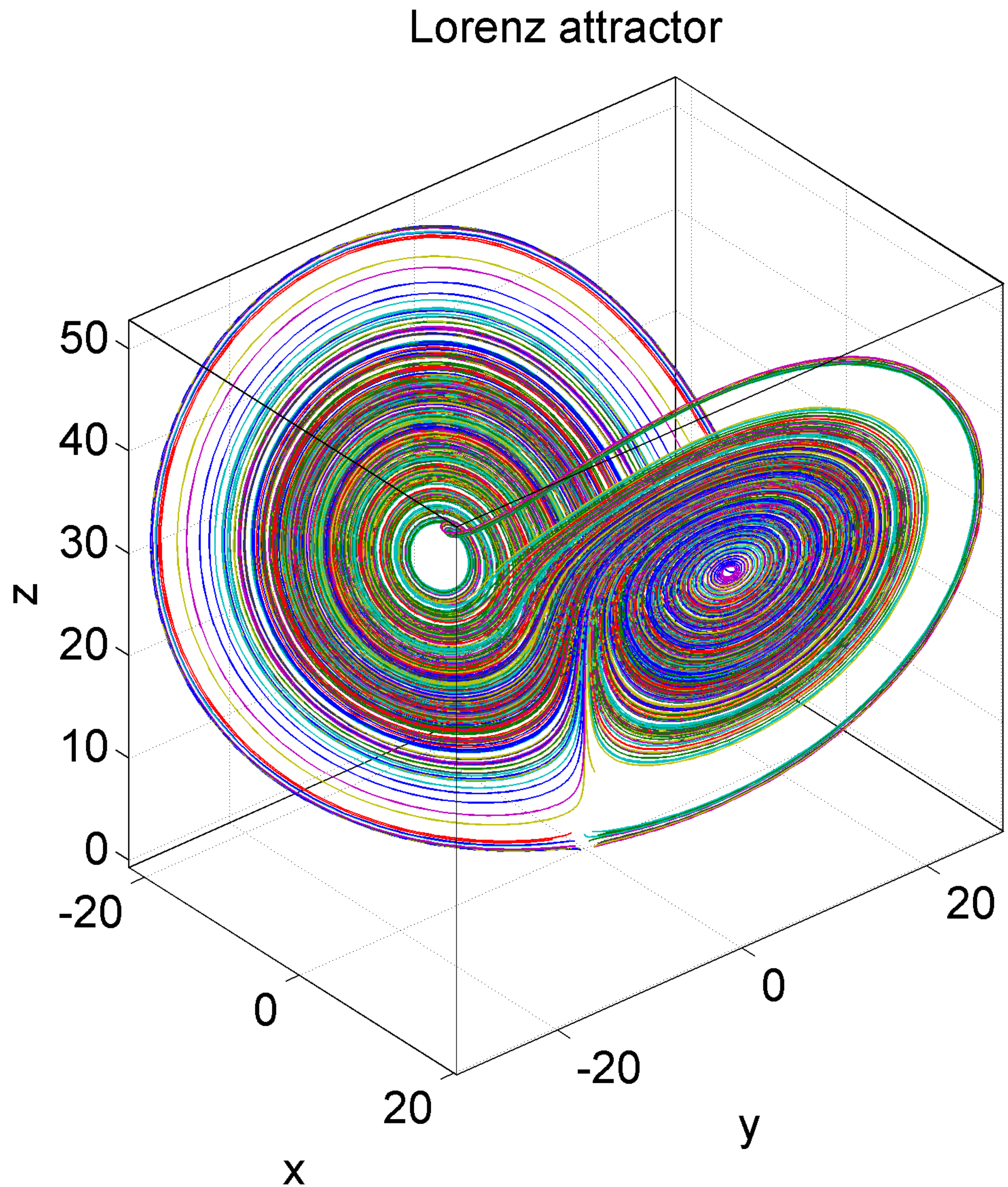

May Bifurcations Logistic map
For every growth parameter r
1000 iterations are worked out
then the x values of the next 1000 iterations are plotted
$$x_{n+1} = r x_n (1 - x_n)$$
Bifircation
Stable equilibrium
Extinction
Chaos!
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.5
1
1.5
2
2.5
3
3.5
4
Growth parameter r
Model breaks down for $r > 4$

May Bifurcations Logistic map





Double pendulum
m1=1kg m2=3kg l1=3 metres l2=1 metres
time =42 s
Poincare log10(probability) map for bob 1
Angular velocity /rad s-1
Angle /rad
25
20
15
10
5
0
-5
-10
-15
-20
-3
-2
-1
0
1
2
3
-0.5
-1
-1.5
-2
-2.5
Angular velocity /rad s-1
Angle /rad



Lorenz attractor
z
x
y
50
40
30
20
10
0
-20
0
20
-20
0
20

Lorenz and Rössler **strange attractors**

Edward Lorenz was using a Royal McBee LGP-30 computer in 1961 to model weather patterns. He accidentally fed in 3 digit precision numbers into the model from a printout rather than the 6 digits used by the computer. These tiny errors created a hugely different weather forecast....

Lorenz's weather model was *very* sensitive to initial conditions.

His equations looked a bit like these:

$$\frac{dx}{dt} = s(y - x)$$

$$\frac{dy}{dt} = x(r - z) - y$$

$$\frac{dz}{dt} = xy - bz$$

$$s = 10$$

$$r = 28$$

$$b = \frac{8}{3}$$

Edward Lorenz
1917-2008

Although x,y,z trajectories are **chaotic**, they tend to *gravitate towards a particular region.*

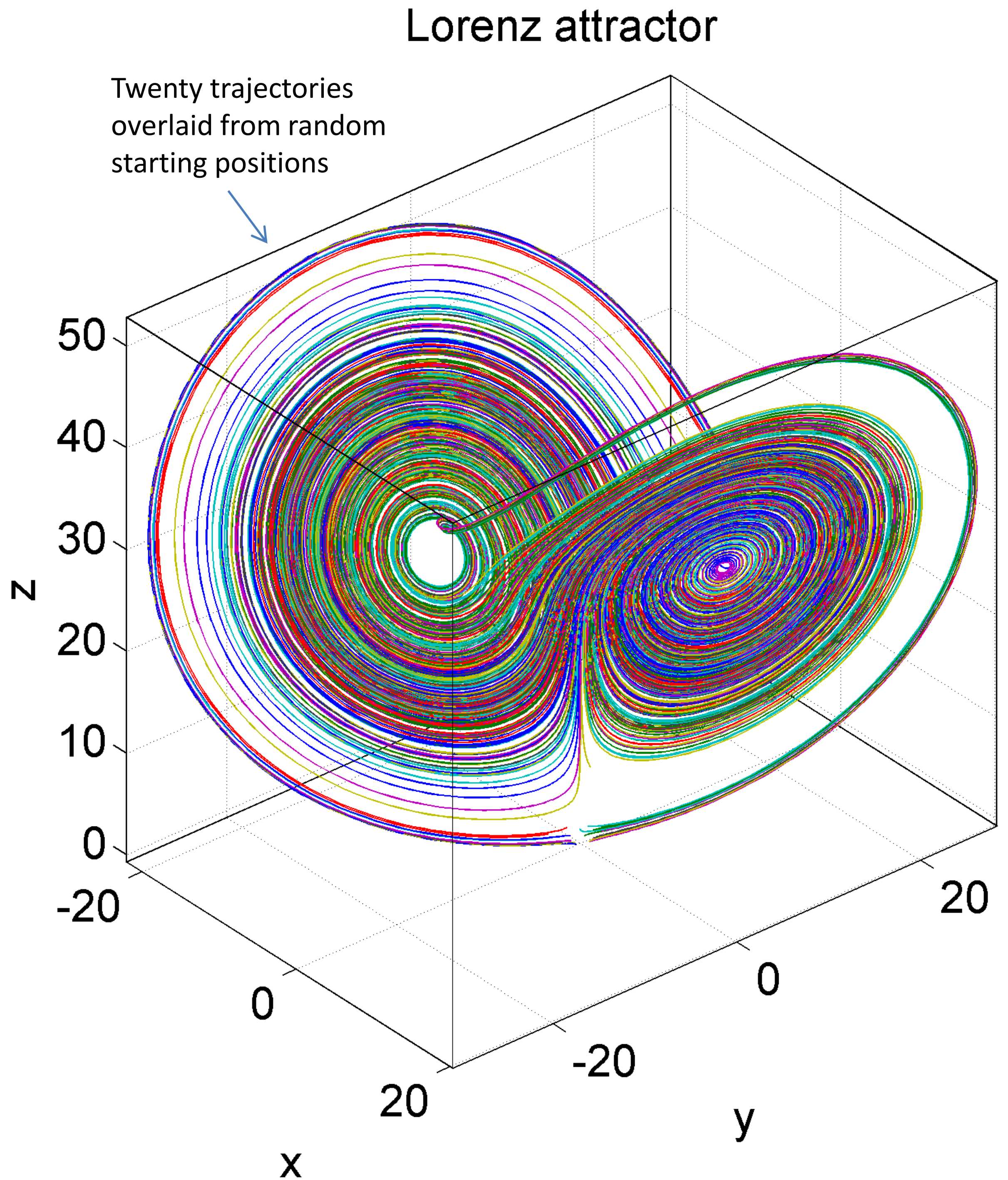
This region is called a **Strange Attractor**

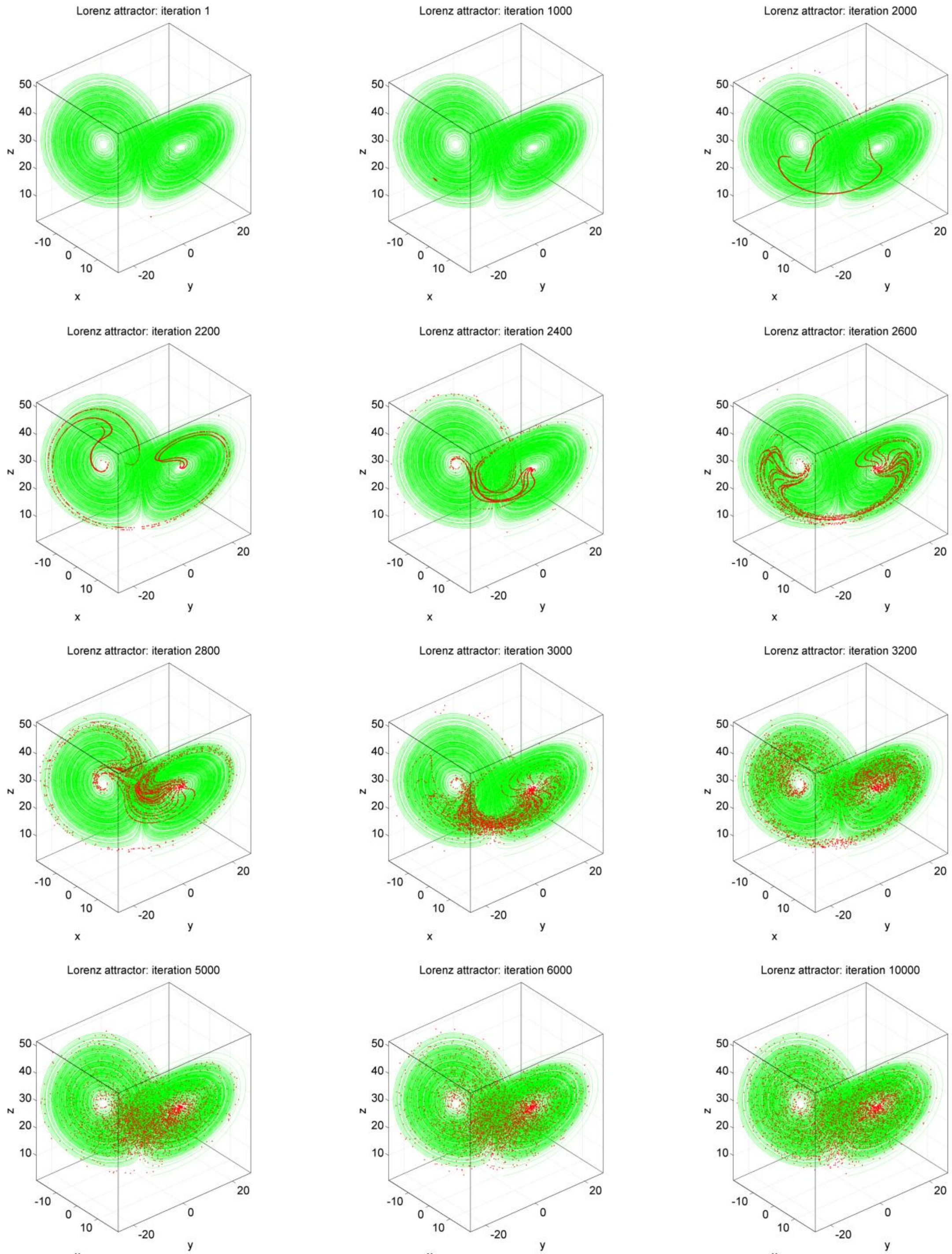
$$\frac{dx}{dt} = s(y - x)$$

$$\frac{dy}{dt} = x(r - z) - y$$

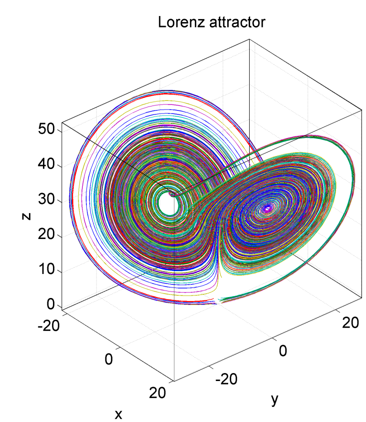
$$\frac{dz}{dt} = xy - bz$$

$$s = 10 \quad r = 28 \quad b = \tfrac{8}{3}$$



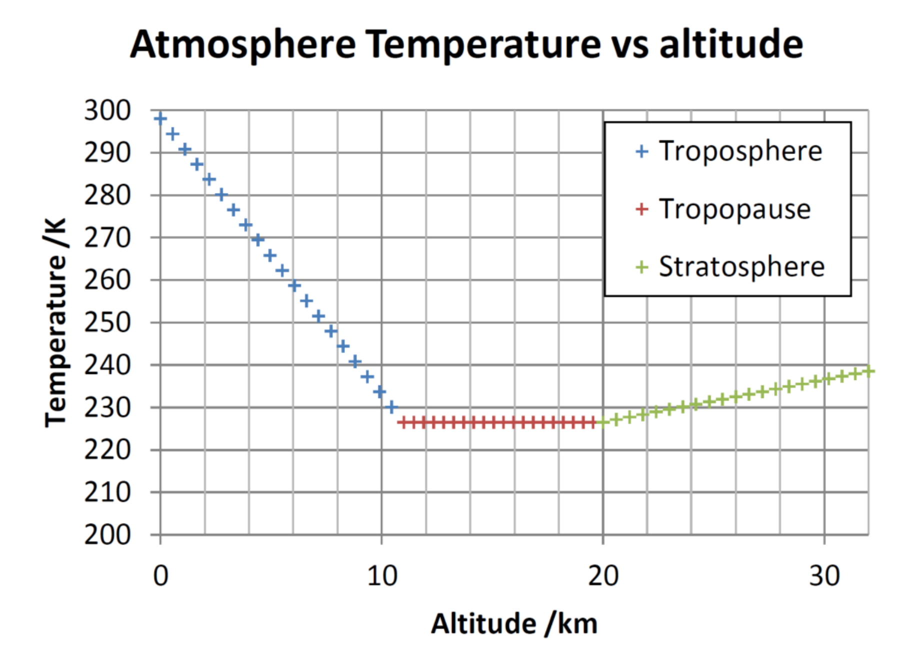


Applying the Lorenz equations, a cluster of initial x,y,z values separated by a *tiny* random deviation will eventually **spread out evenly throughout the strange attractor.**

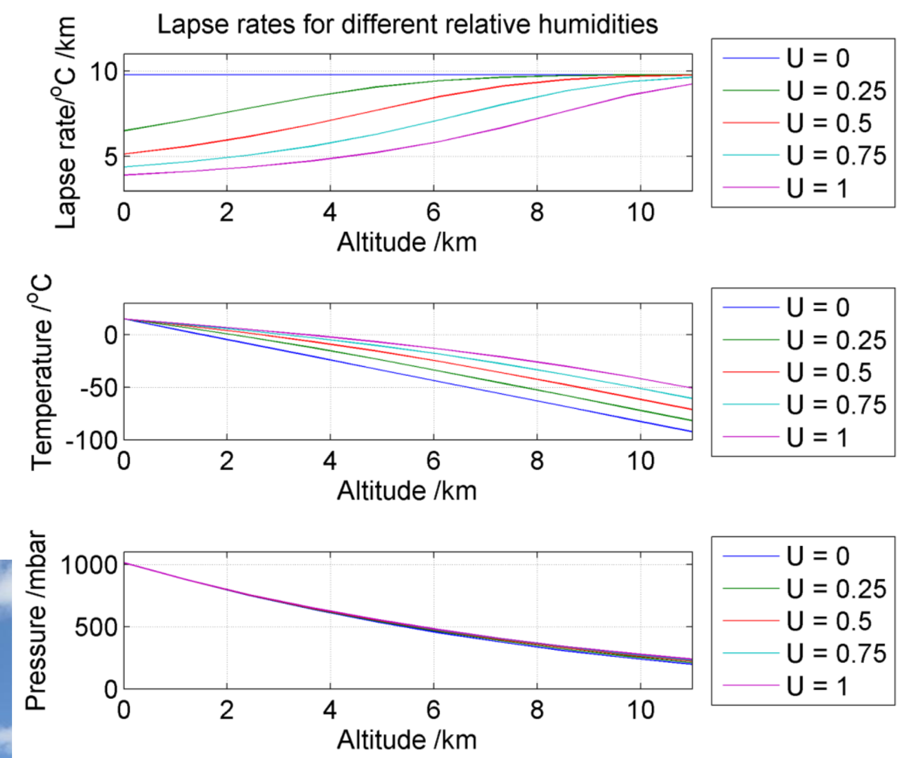


Based upon Shaw *et al*; “Chaos”, Scientific American 54:12 (1986) 46-57

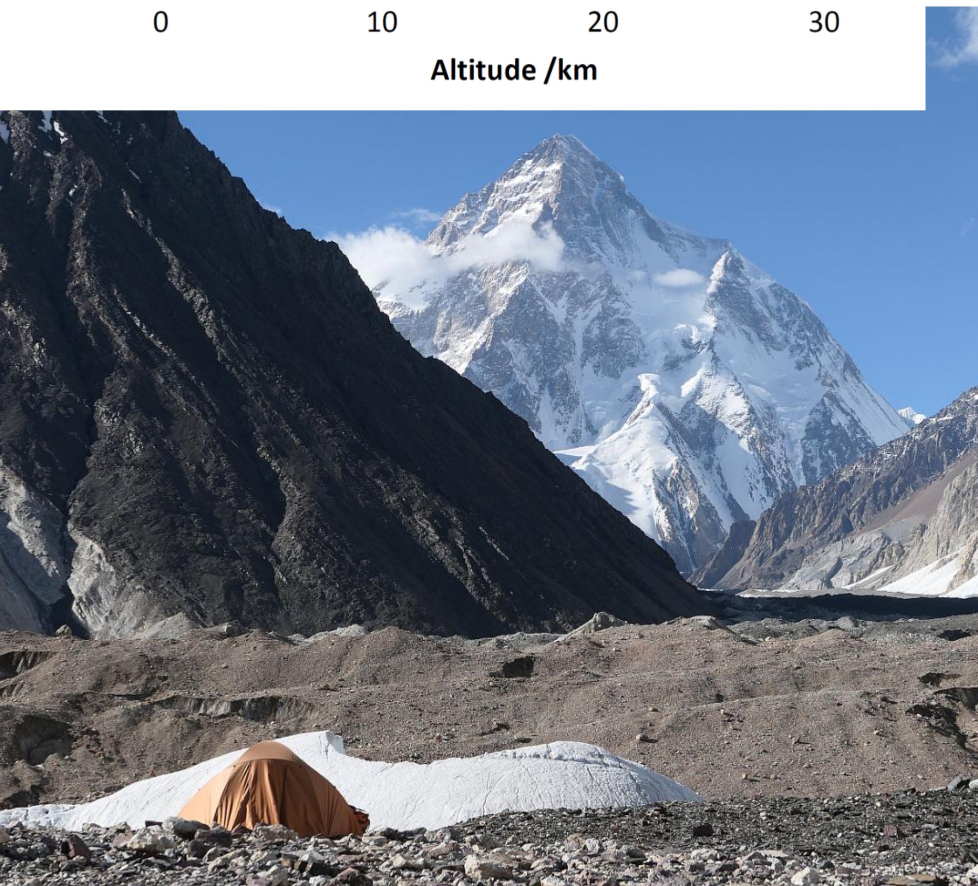

Computing
Super
Computer
summit
IBM
BBC Model B SRAM Elite
Master 128 Elite
6502 Second Processor Elite
ZX Spectrum
GAUNTLET
TVPaint
COMPUTERS, CHILDREN AND THE NATIONAL CURRICULUM
computing

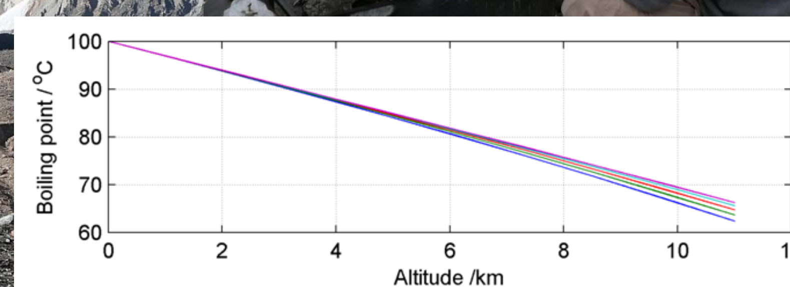


Atmosphere Temperature vs altitude
Temperature /K
Altitude /km
300
290
280
270
260
250
240
230
220
210
200
0
10
20
30
Troposphere
Tropopause
Stratosphere

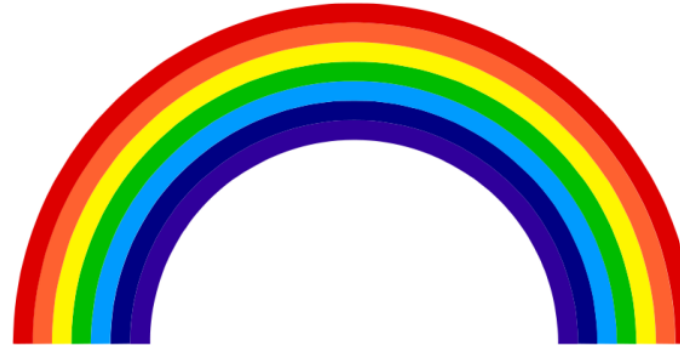


Lapse rates for different relative humidities
Lapse rate/°C /km
Altitude /km
10
5
0
2
4
6
8
10
U = 0
U = 0.25
U = 0.5
U = 0.75
U = 1
Temperature /°C
0
-50
-100
Altitude /km
U = 0
U = 0.25
U = 0.5
U = 0.75
U = 1
Pressure /mbar
1000
500
0
Altitude /km
U = 0
U = 0.25
U = 0.5
U = 0.75
U = 1

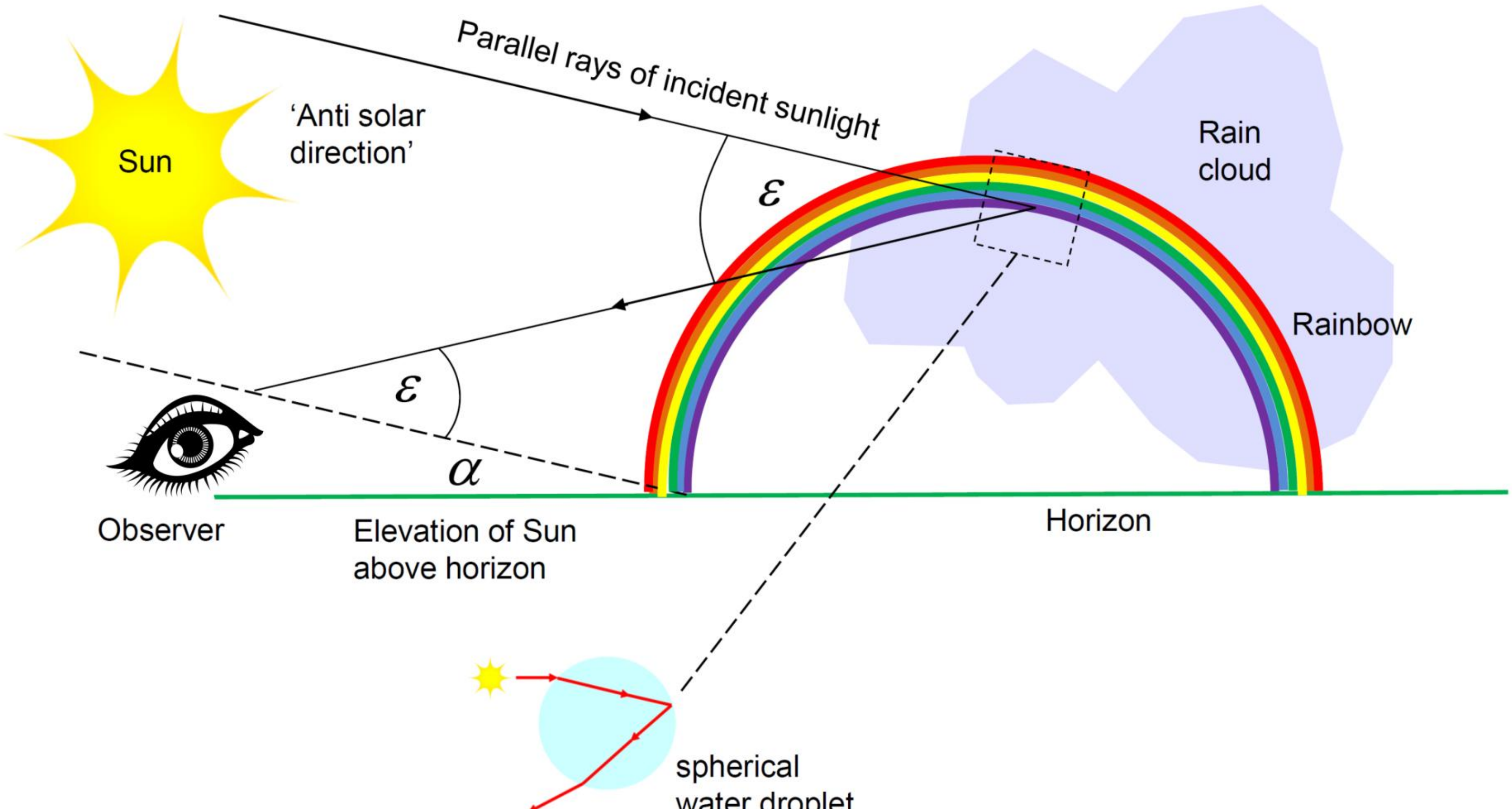


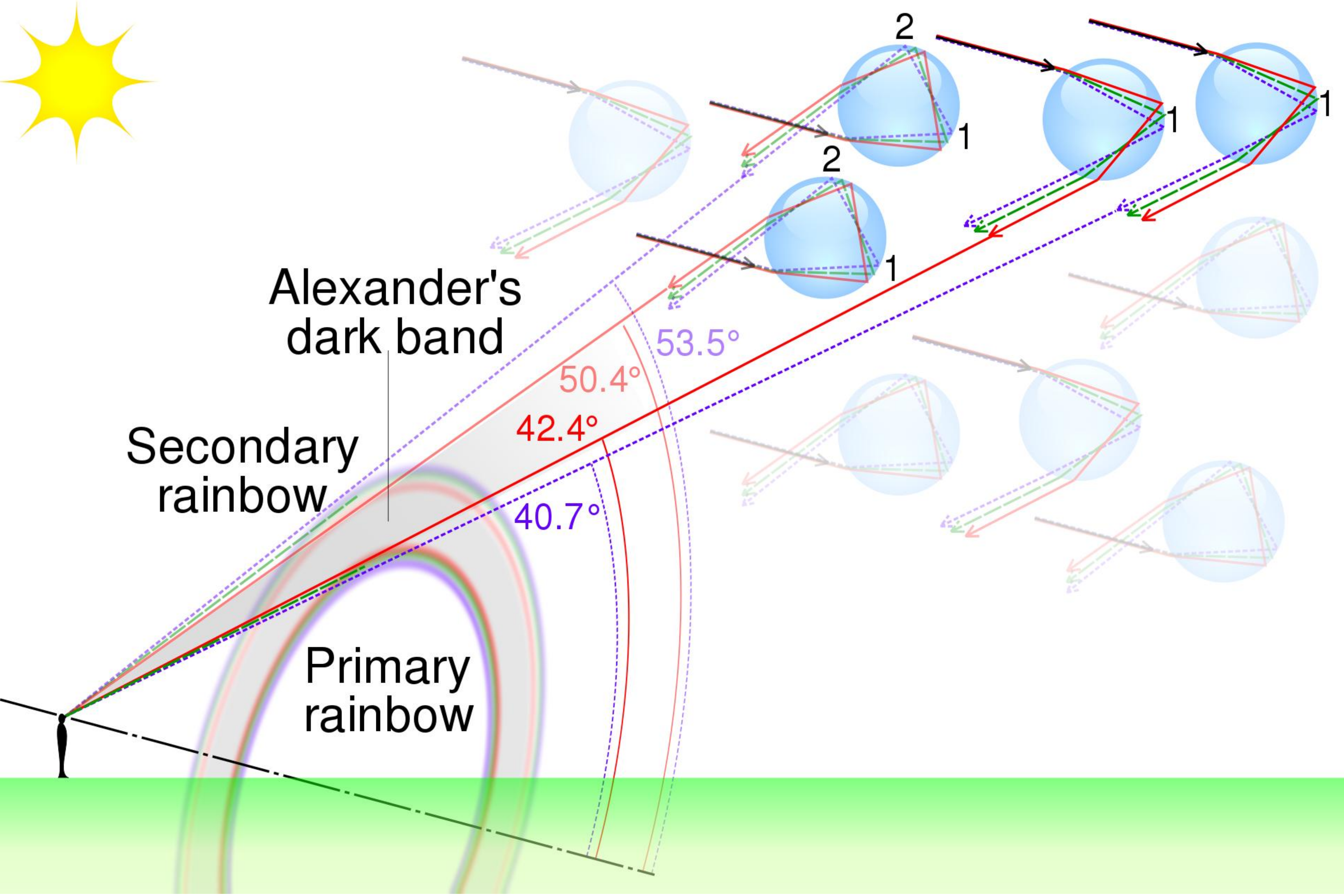


Boiling point / °C
100
90
80
70
60
0
2
4
6
8
10
12
Altitude /km

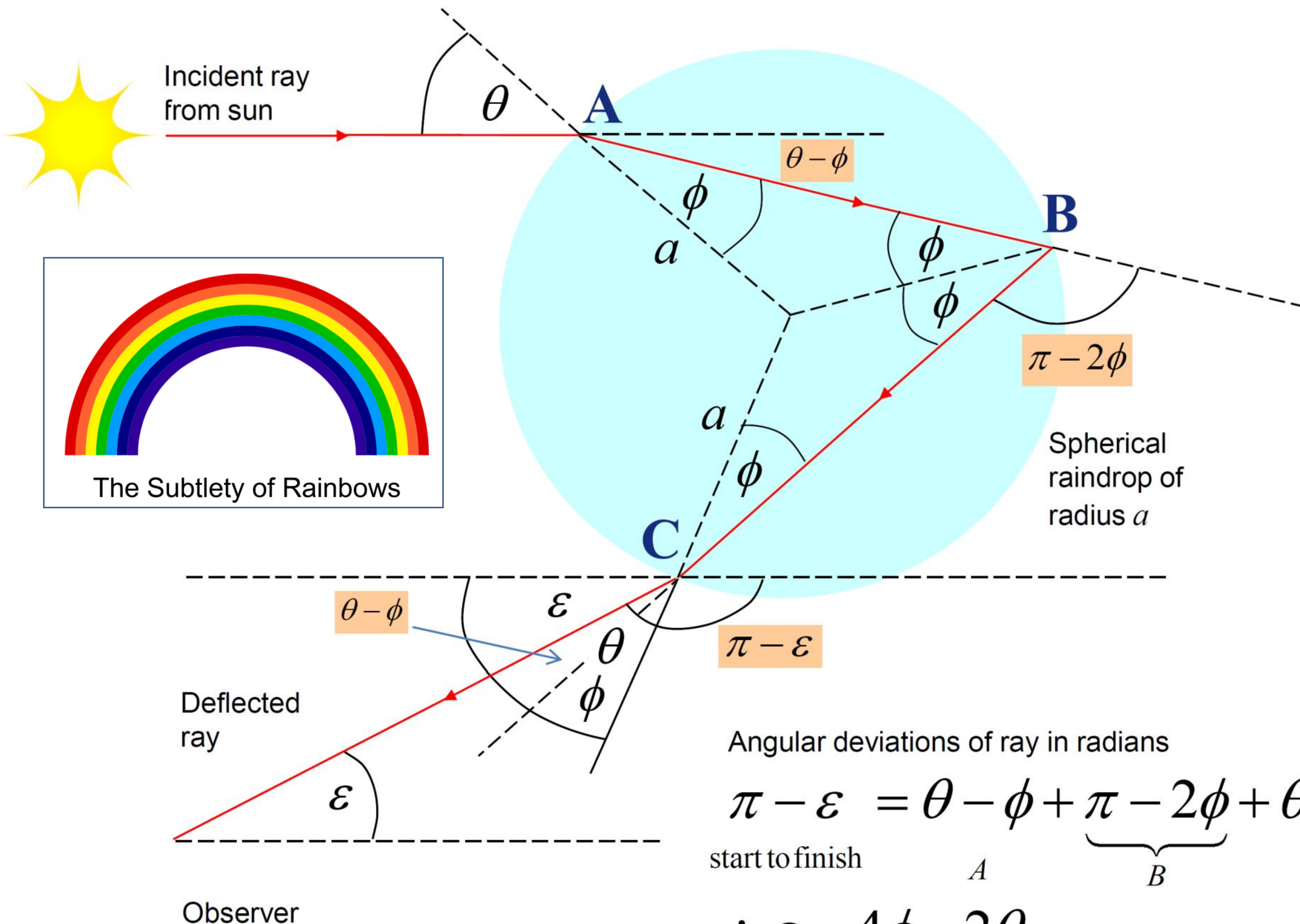


The Subtlety of Rainbows





https://en.wikipedia.org/wiki/Rainbow

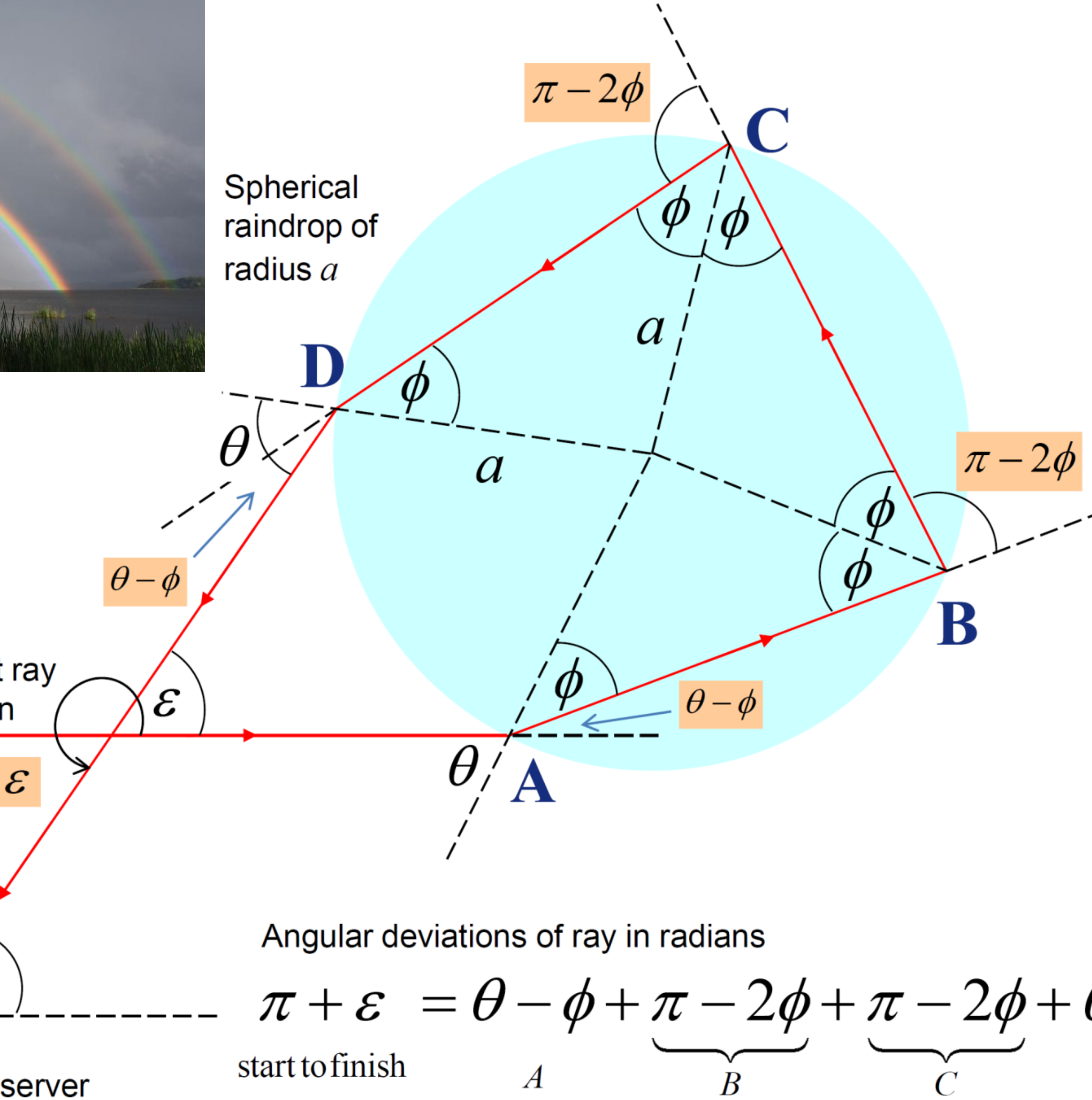


The Subtlety of Rainbows

Angular deviations of ray in radians

$$\underset{\text{start to finish}}{\pi - \varepsilon} = \underbrace{\theta - \phi}_{A} + \underbrace{\pi - 2\phi}_{B} + \underbrace{\theta - \phi}_{C}$$

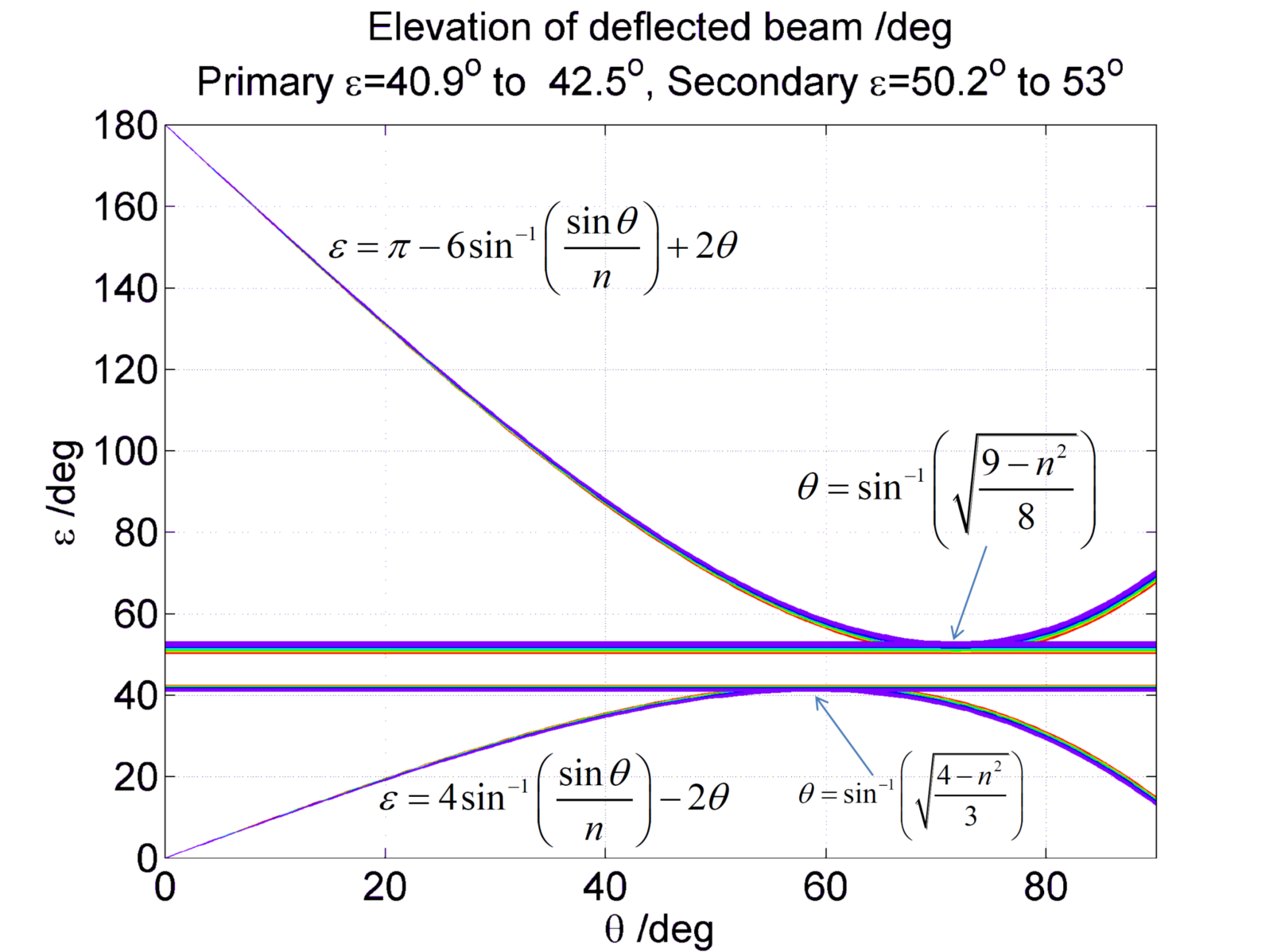
$$\therefore \varepsilon = 4\phi - 2\theta$$



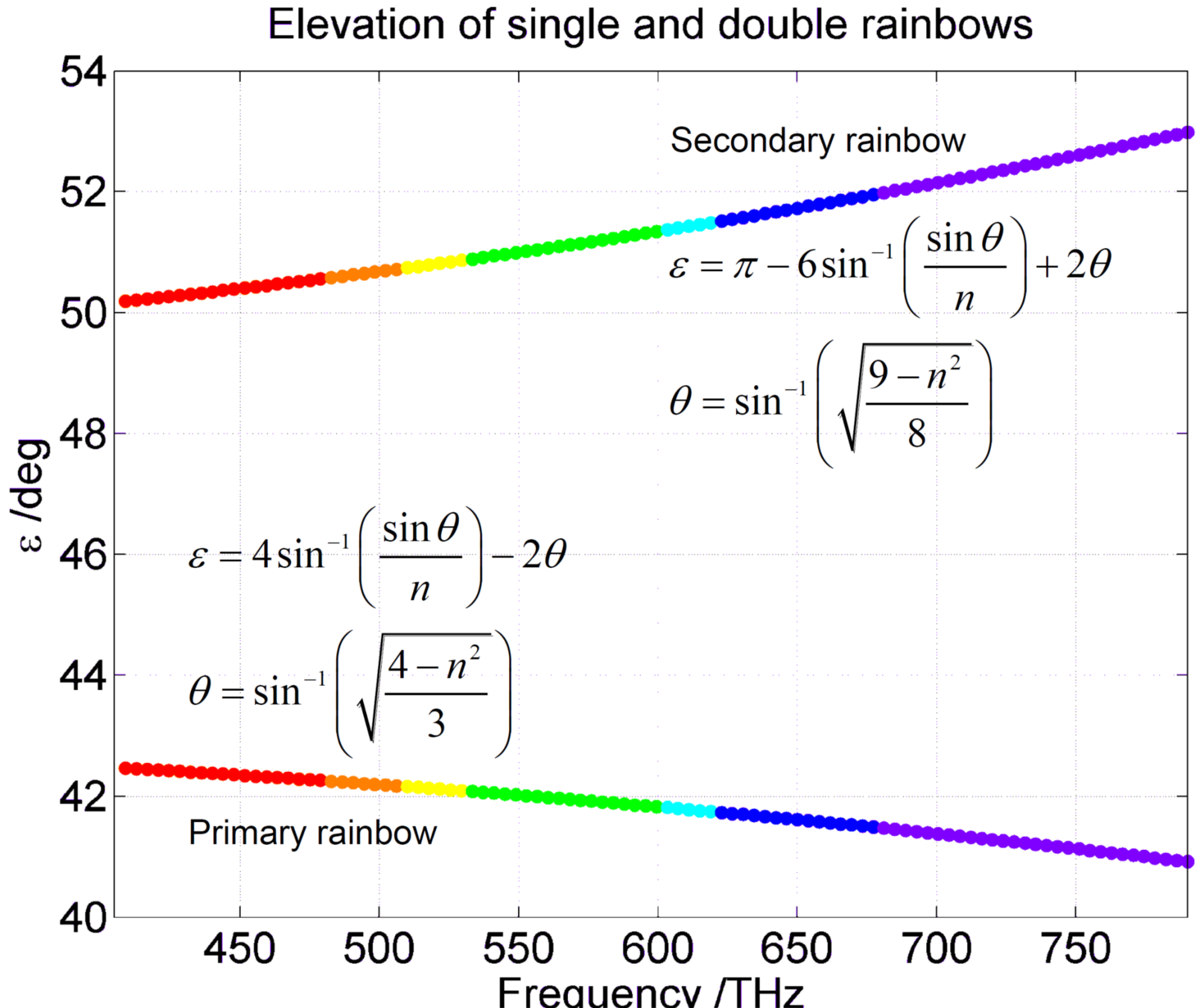
Angular deviations of ray in radians

$$\underset{\text{start to finish}}{\pi + \varepsilon} = \underset{A}{\theta - \phi} + \underbrace{\pi - 2\phi}_{B} + \underbrace{\pi - 2\phi}_{C} + \underset{D}{\theta - \phi}$$

$$\therefore \varepsilon = \pi - 6\phi + 2\theta$$



Elevation of deflected beam /deg
Primary ε=40.9° to 42.5°, Secondary ε=50.2° to 53°
$\varepsilon = \pi - 6\sin^{-1}\left(\frac{\sin\theta}{n}\right) + 2\theta$
$\theta = \sin^{-1}\left(\sqrt{\frac{9-n^2}{8}}\right)$
$\varepsilon = 4\sin^{-1}\left(\frac{\sin\theta}{n}\right) - 2\theta$
$\theta = \sin^{-1}\left(\sqrt{\frac{4-n^2}{3}}\right)$
ε /deg
θ /deg
0
20
40
60
80
100
120
140
160
180


Elevation of single and double rainbows
Secondary rainbow
$\varepsilon = \pi - 6\sin^{-1}\left(\frac{\sin\theta}{n}\right) + 2\theta$
$\theta = \sin^{-1}\left(\sqrt{\frac{9-n^2}{8}}\right)$
$\varepsilon = 4\sin^{-1}\left(\frac{\sin\theta}{n}\right) - 2\theta$
$\theta = \sin^{-1}\left(\sqrt{\frac{4-n^2}{3}}\right)$
Primary rainbow
ε /deg
54
52
50
48
46
44
42
40
450
500
550
600
650
700
750
Frequency /THz

Mandlebrot transformations of **complex numbers**

$$i^2 = -1$$

$$z = x + iy$$

$$x = \mathrm{Re}(z)$$

$$y = \mathrm{Im}(z)$$

$$|z| = \sqrt{x^2 + y^2}$$

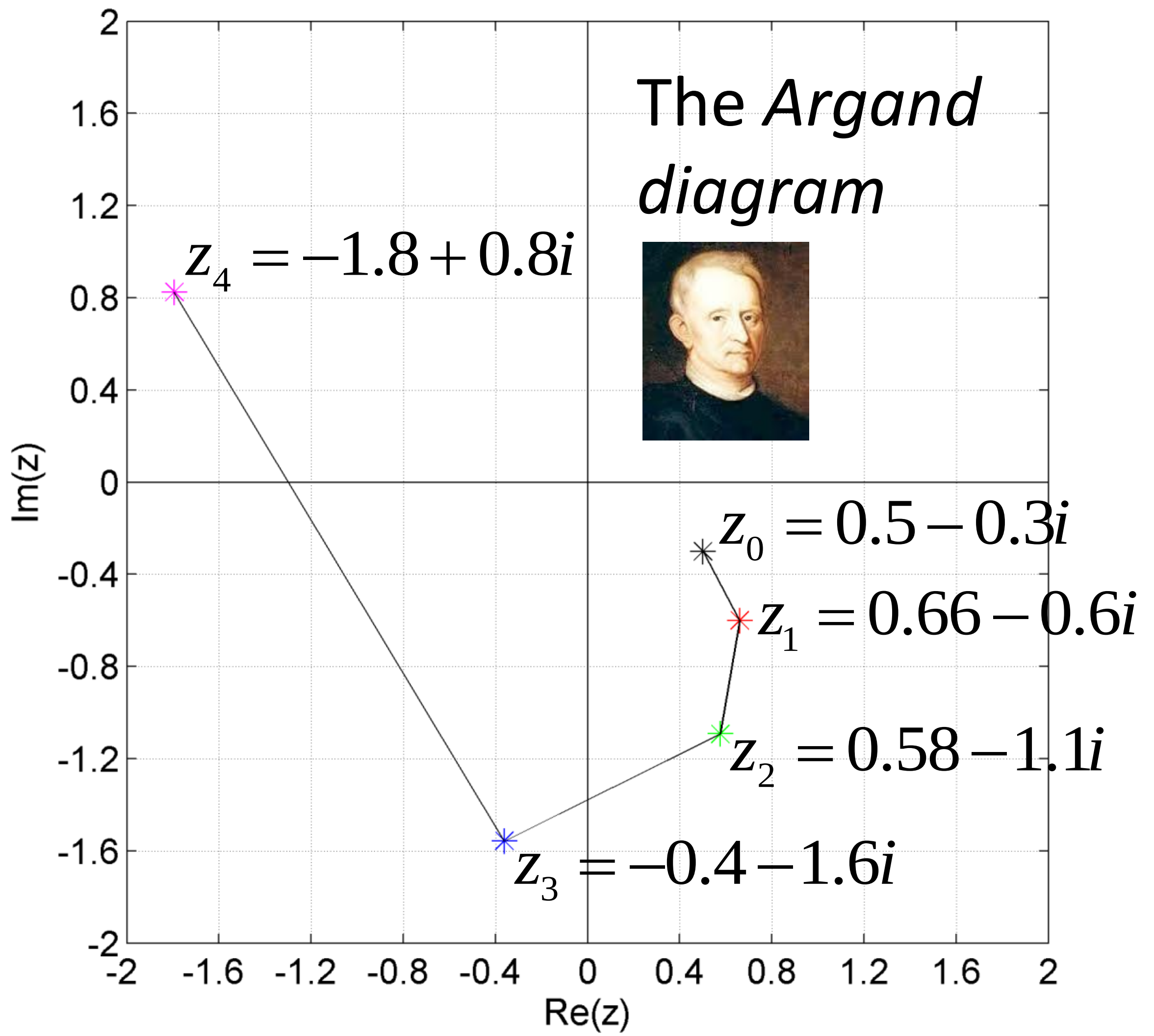
$$(1+i)(1+i)$$

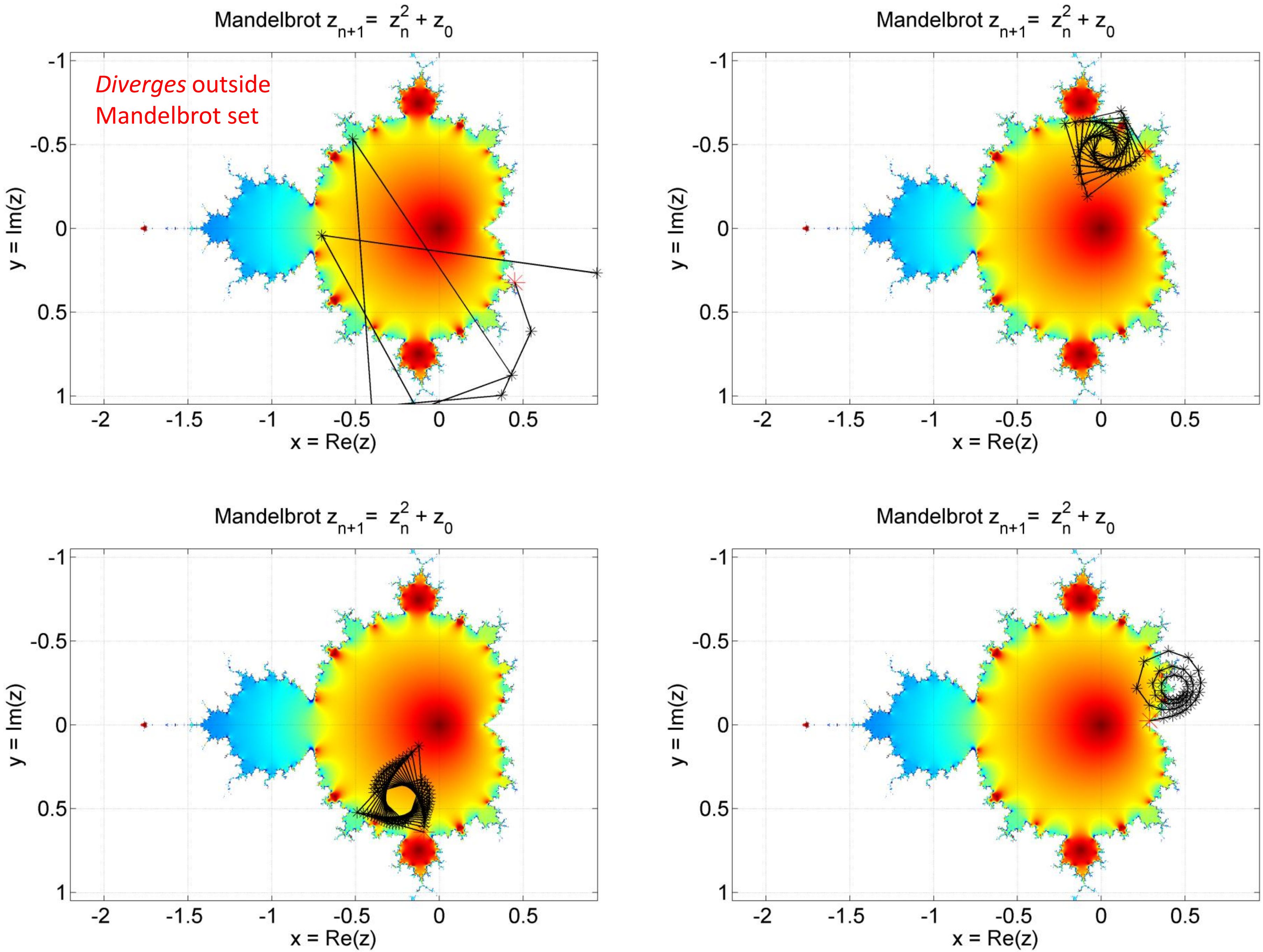
$$= 1 + 2i + i^2$$

$$= 1 + 2i - 1$$

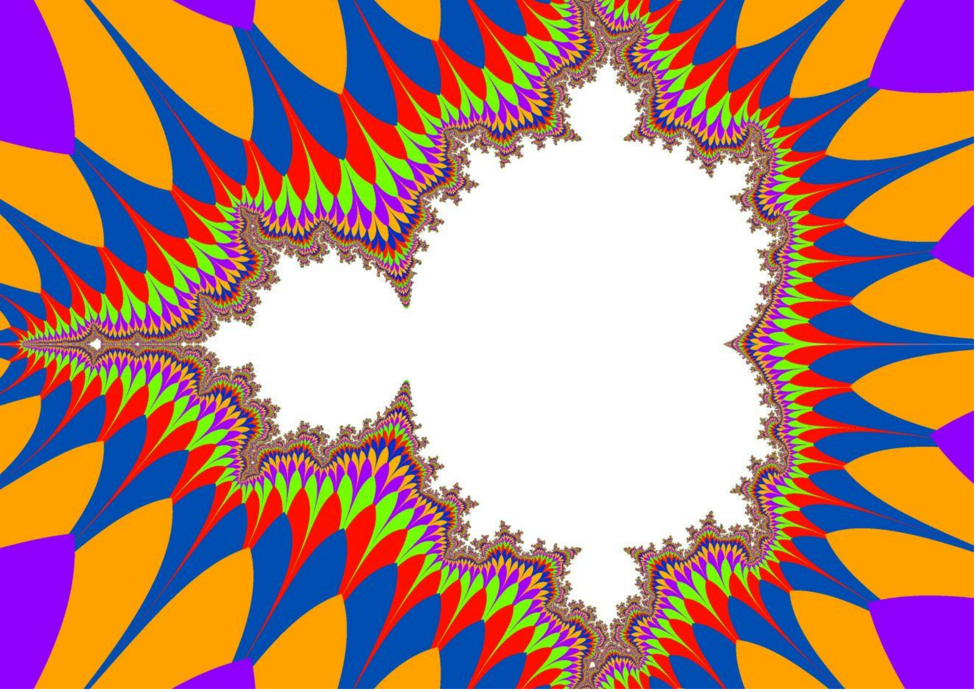
$$= 2i$$

$$z_{n+1} = z_n^2 + z_0$$





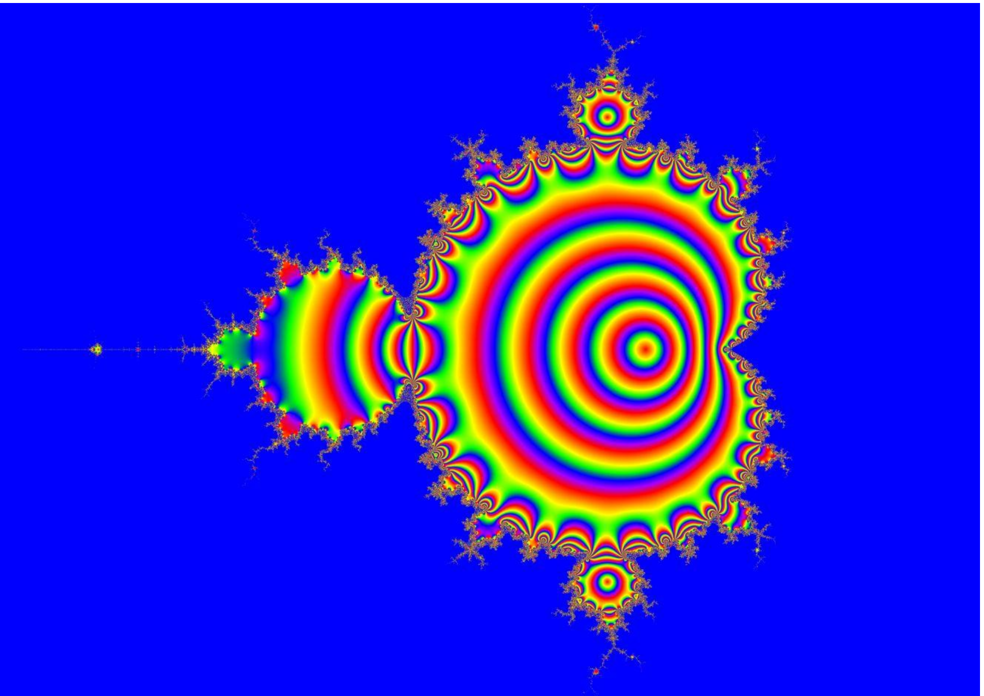
Mandelbrot $z_{n+1} = z_n^2 + z_0$
Diverges outside
Mandelbrot set
y = Im(z)
x = Re(z)
Mandelbrot $z_{n+1} = z_n^2 + z_0$
y = Im(z)
x = Re(z)
Mandelbrot $z_{n+1} = z_n^2 + z_0$
y = Im(z)
x = Re(z)
Mandelbrot $z_{n+1} = z_n^2 + z_0$
y = Im(z)
x = Re(z)



`julia.m` plot option `abs diverge`

Plot a surface with height *h(x,y)*. This is the *iteration number* when $|z|$ exceeds a certain value e.g. 4

In this case *colours* indicate height *h(x,y)*. It is a 'colour-map'.



`julia.m` plot option `plot z`

Plot a surface with height *h(x,y)*

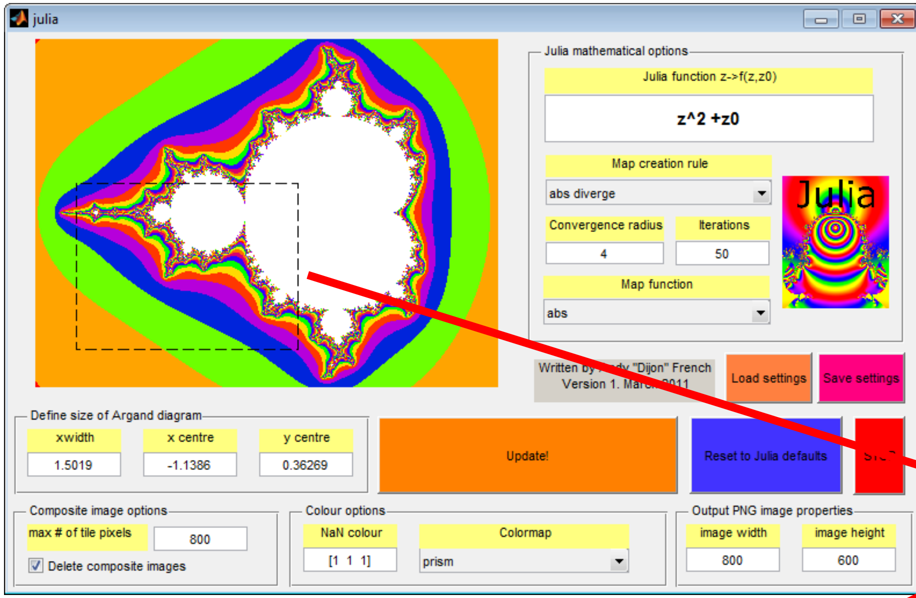
$$x = \mathrm{Re}(z), \quad y = \mathrm{Im}(z)$$

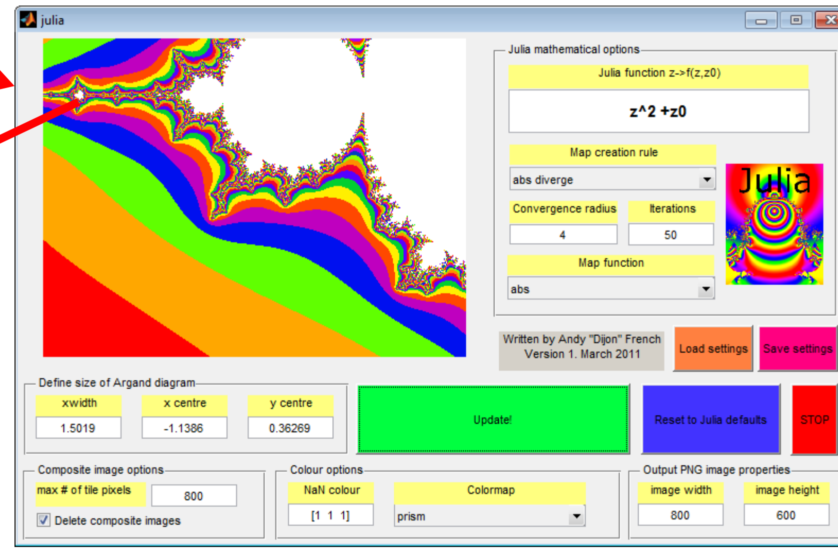
$$h(x,y) = e^{-\sqrt{x^2+y^2}}$$

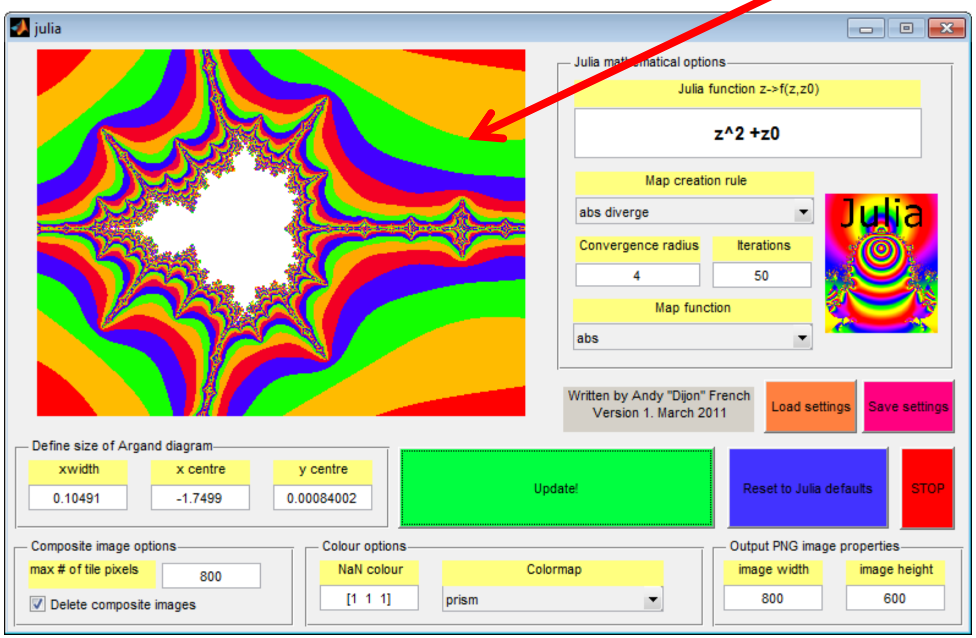
Mandlebrot, complex numbers and iteration

The *Mandlebrot Set* has infinite complexity!

... But a recursive *fractal* geometry

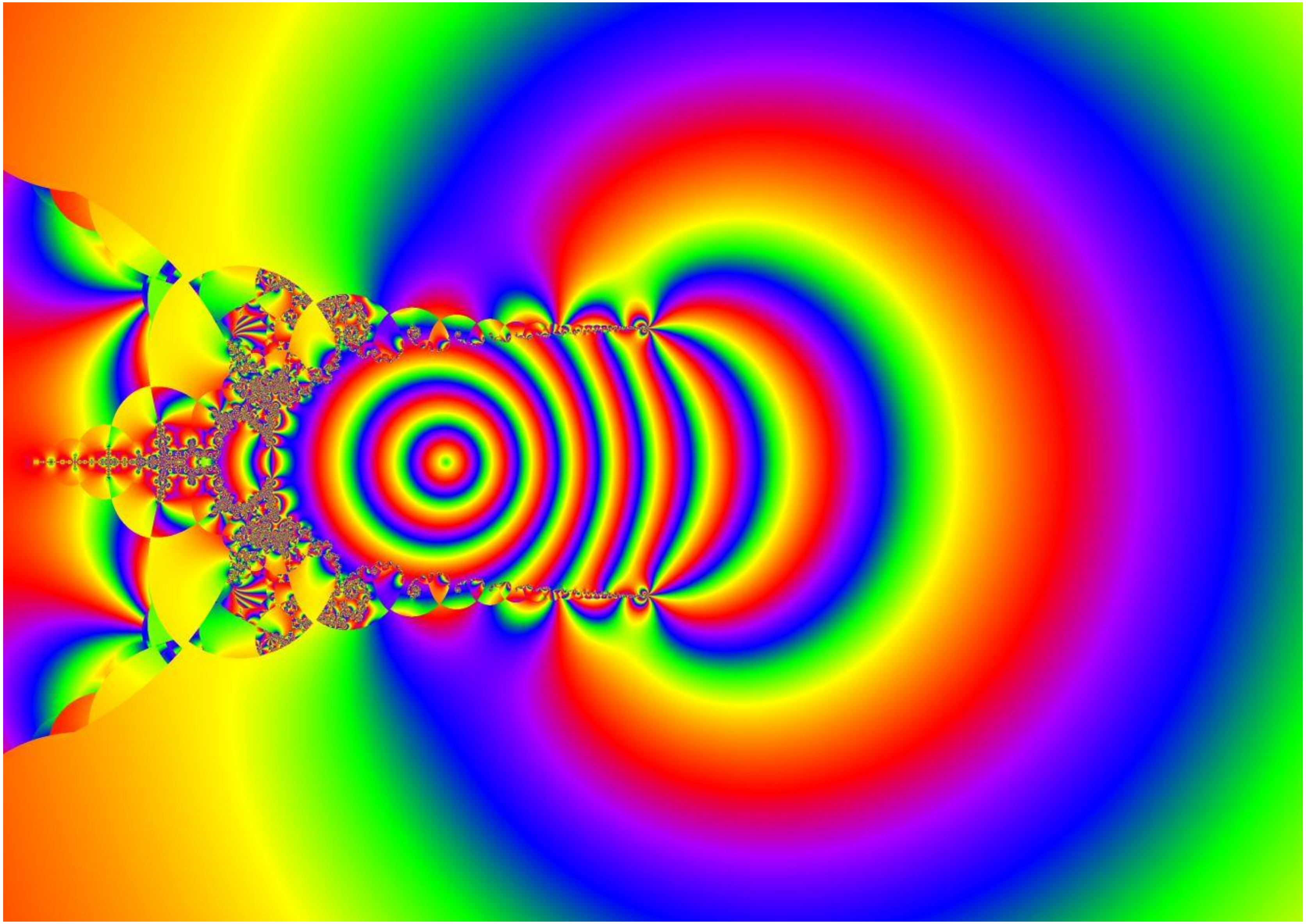






Benoit Mandlebrot (1924-2010)

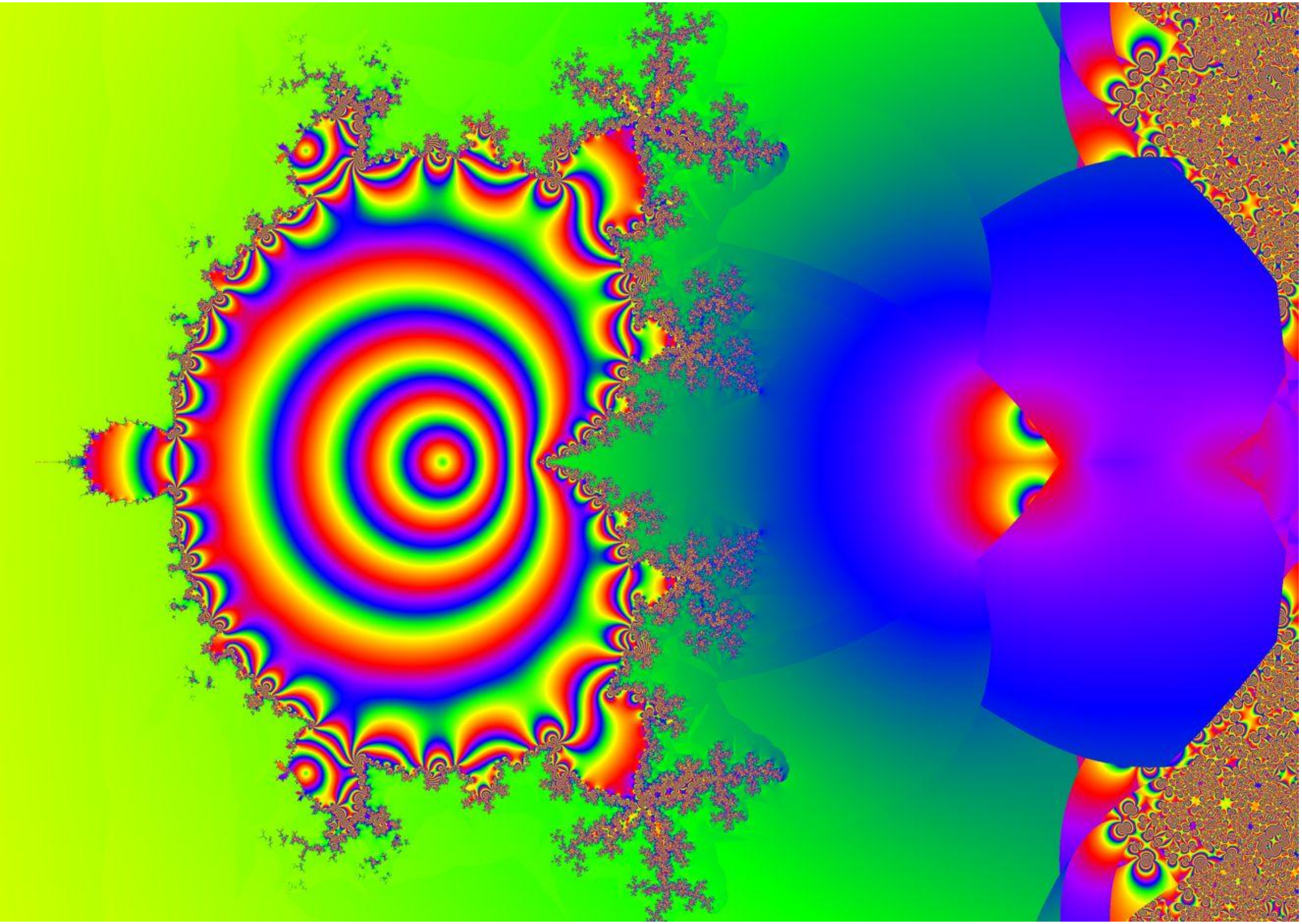

The
Mandlebrot
Variations



The light bulb

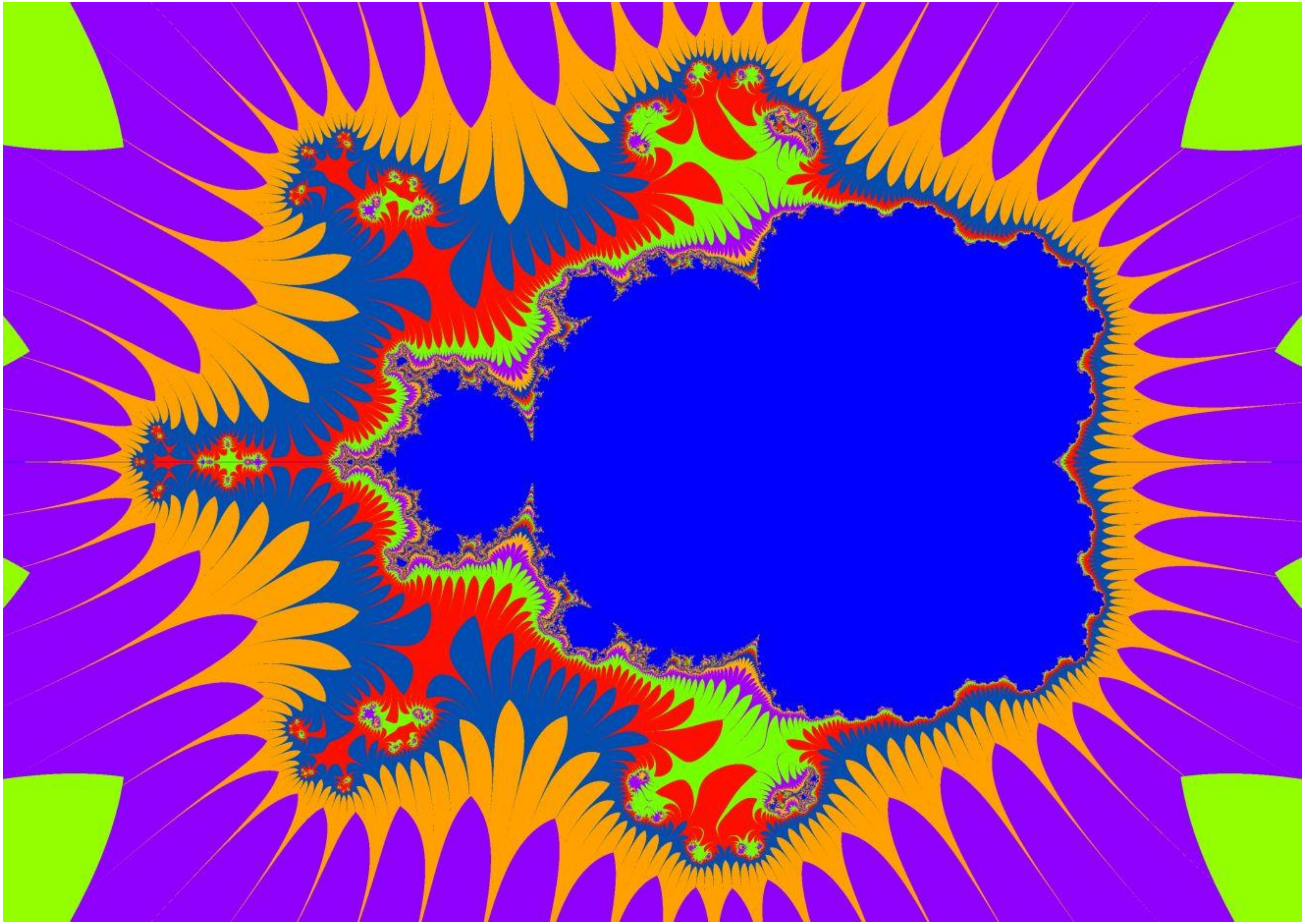
$$z_{n+1} = \log\left(z_n^2 + z_0\right)$$

7 steps to enlightenment $$z_{n+1} = \tan^{-1}\left(z_n^2 + z_0\right)$$



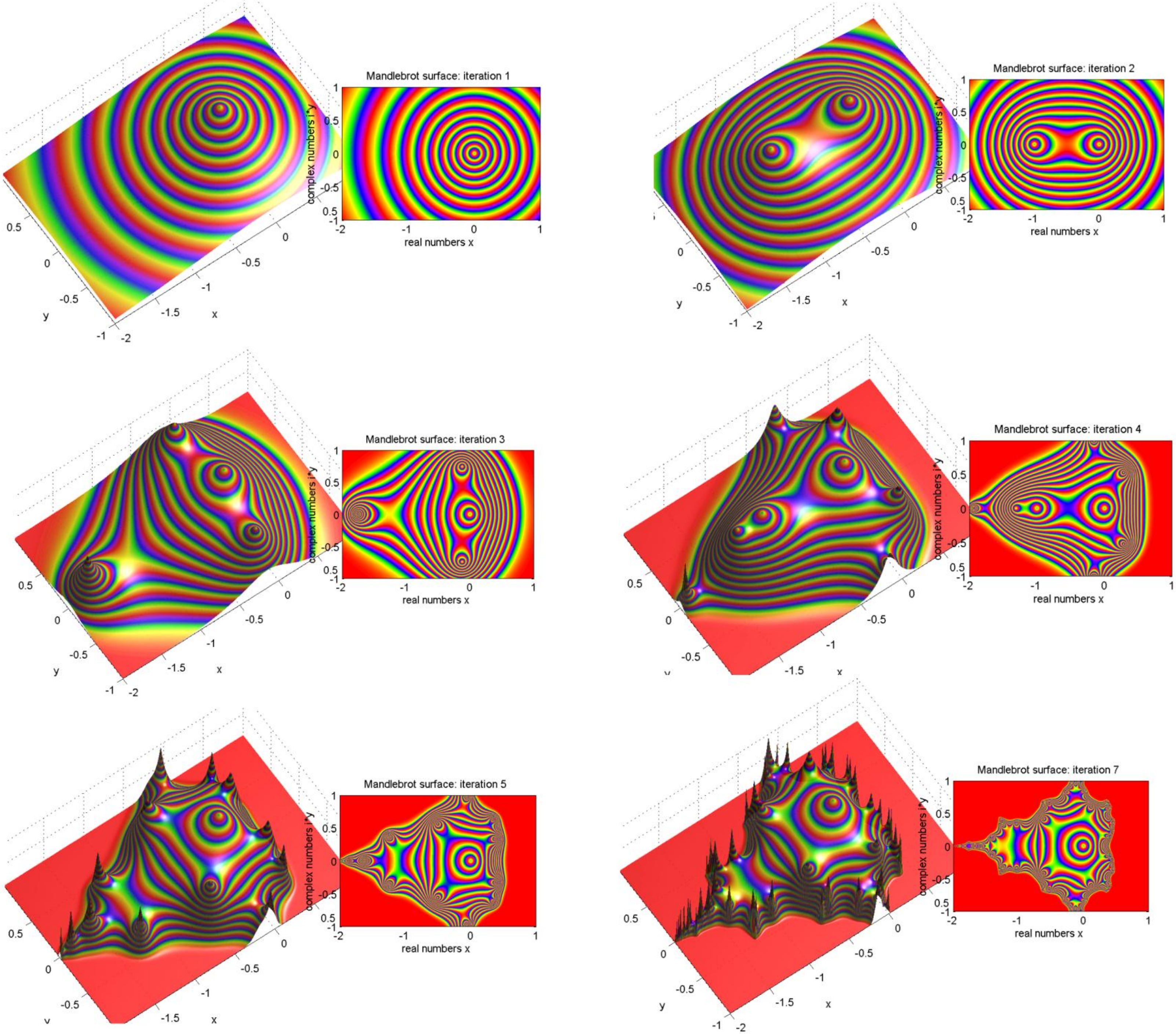
The Mandlerocket!

$$z_{n+1} = \sin^{-1}\left(z_n^2 + z_0\right)$$

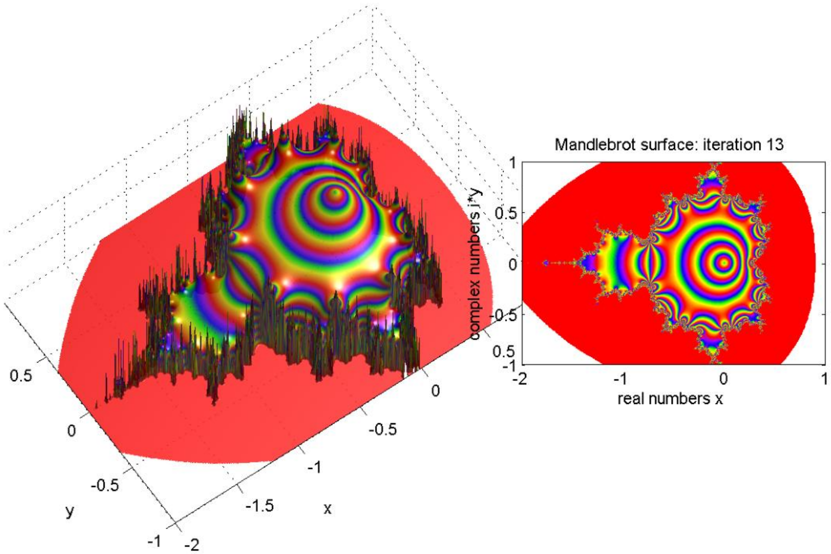


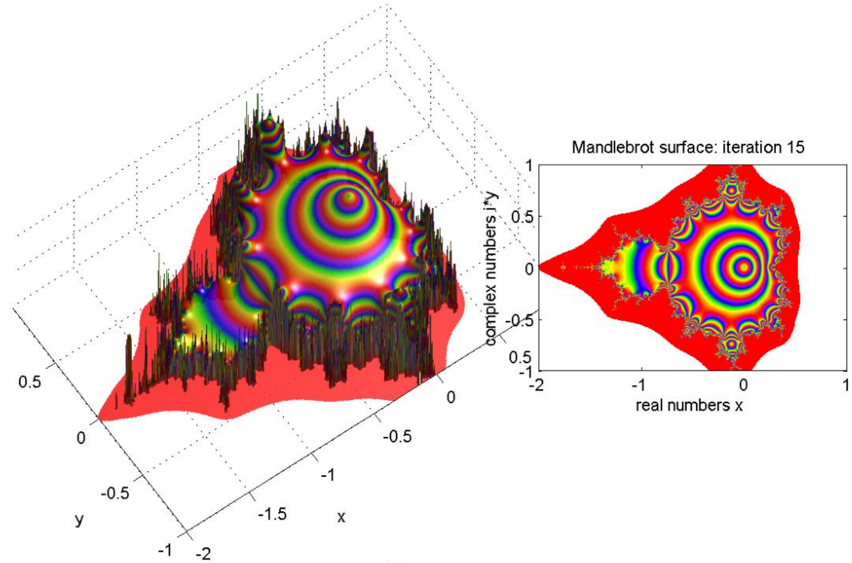
Micro mandlebeast

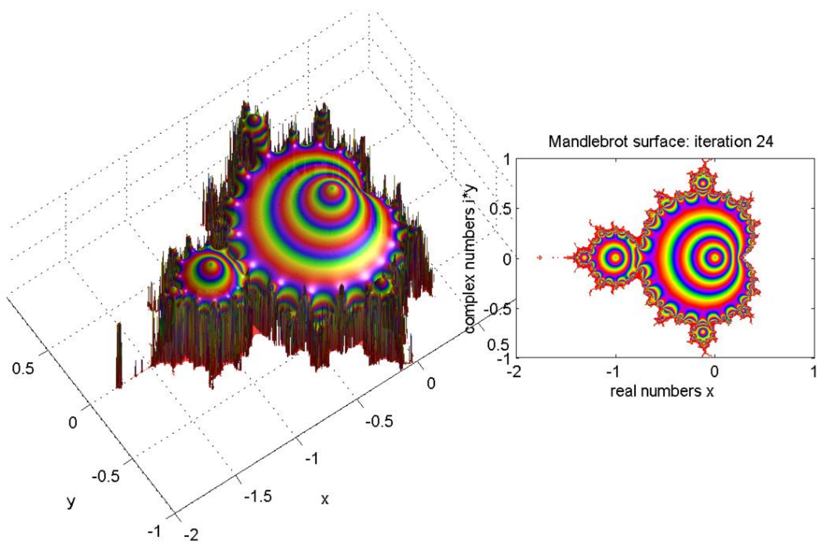
$$z_{n+1} = \left(z_n^2 + z_0 \right)^2$$

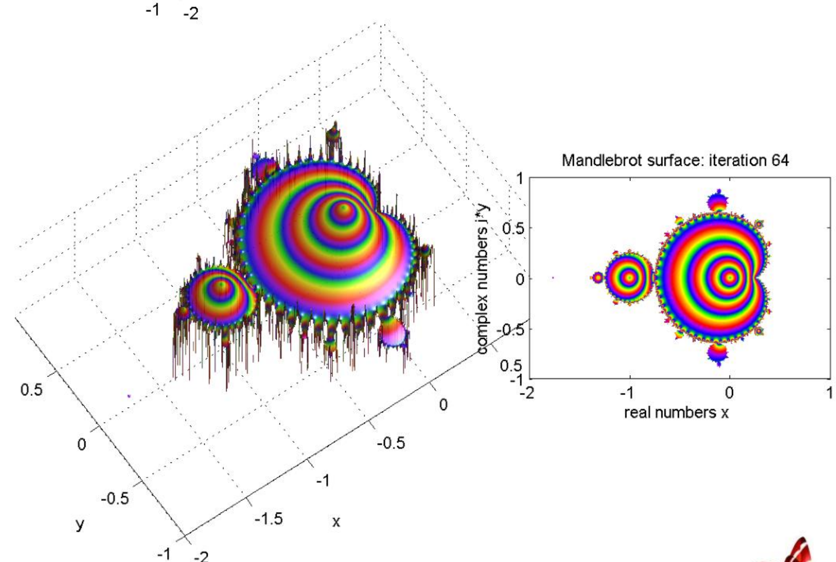


Mandlebrot surface: iteration 1
Mandlebrot surface: iteration 2
Mandlebrot surface: iteration 3
Mandlebrot surface: iteration 4
Mandlebrot surface: iteration 5
Mandlebrot surface: iteration 7
complex numbers i*y
real numbers x
x
y







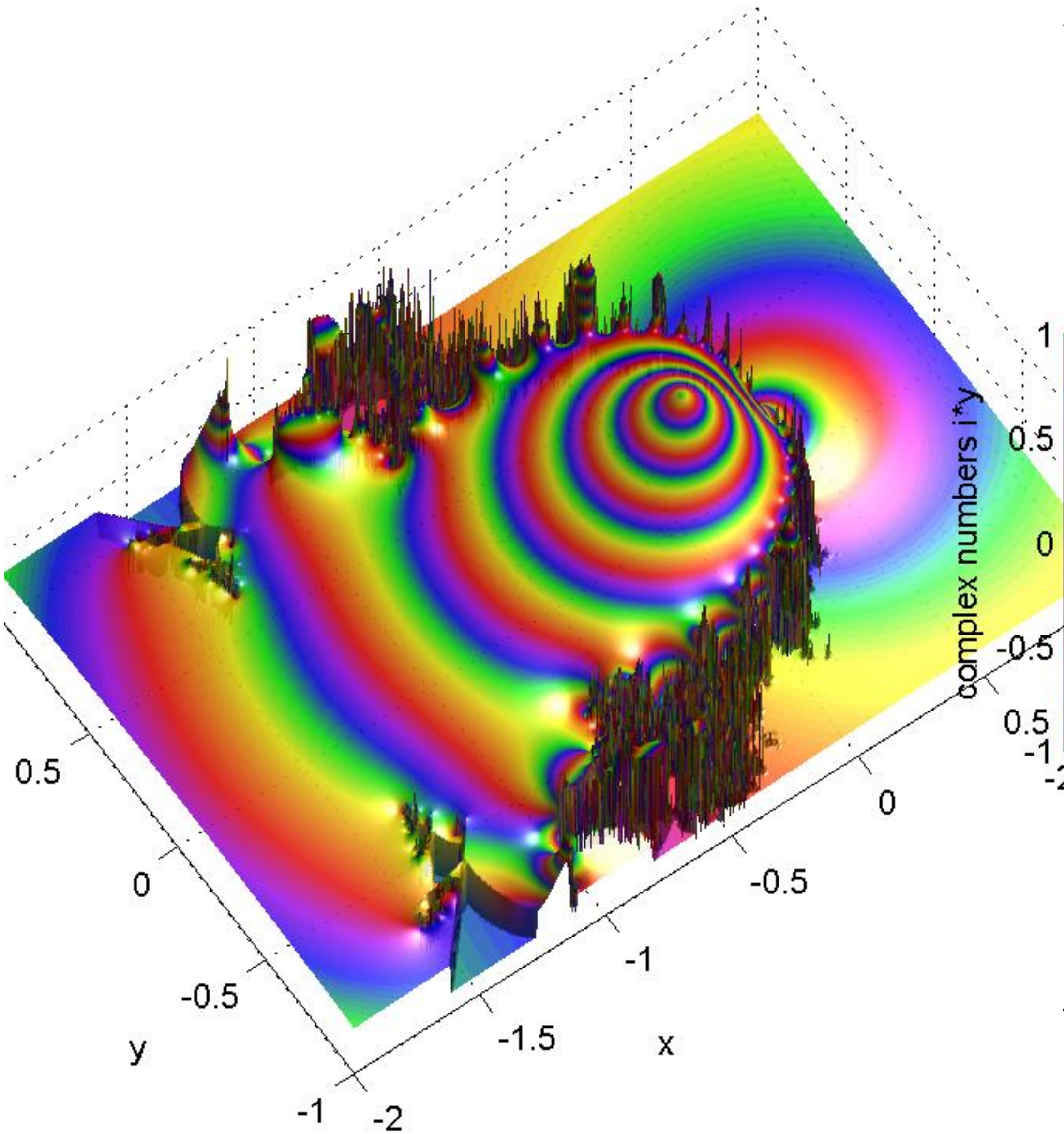


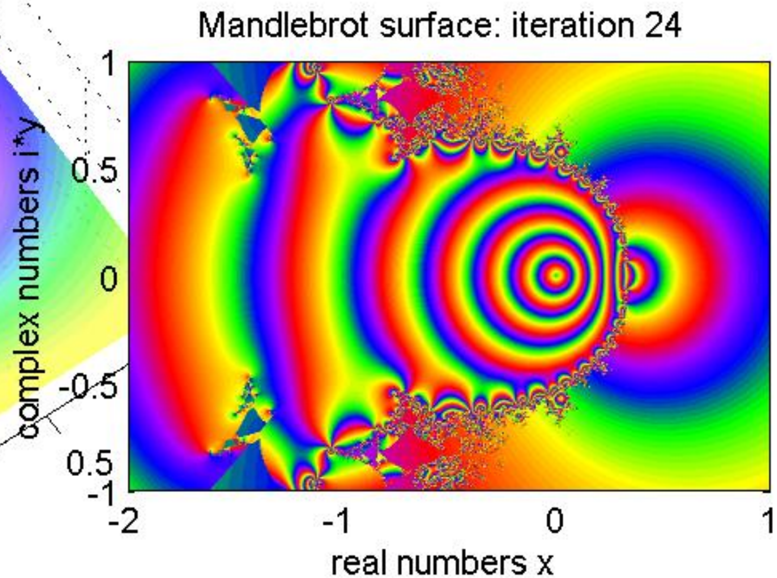
Selection from *Day of Julia.*
Mathematicon Exhibition, 2014

μathematicon

7 steps to enlightenment

$$z_{n+1} = \tan^{-1}\left(z_n^2 + z_0\right)$$



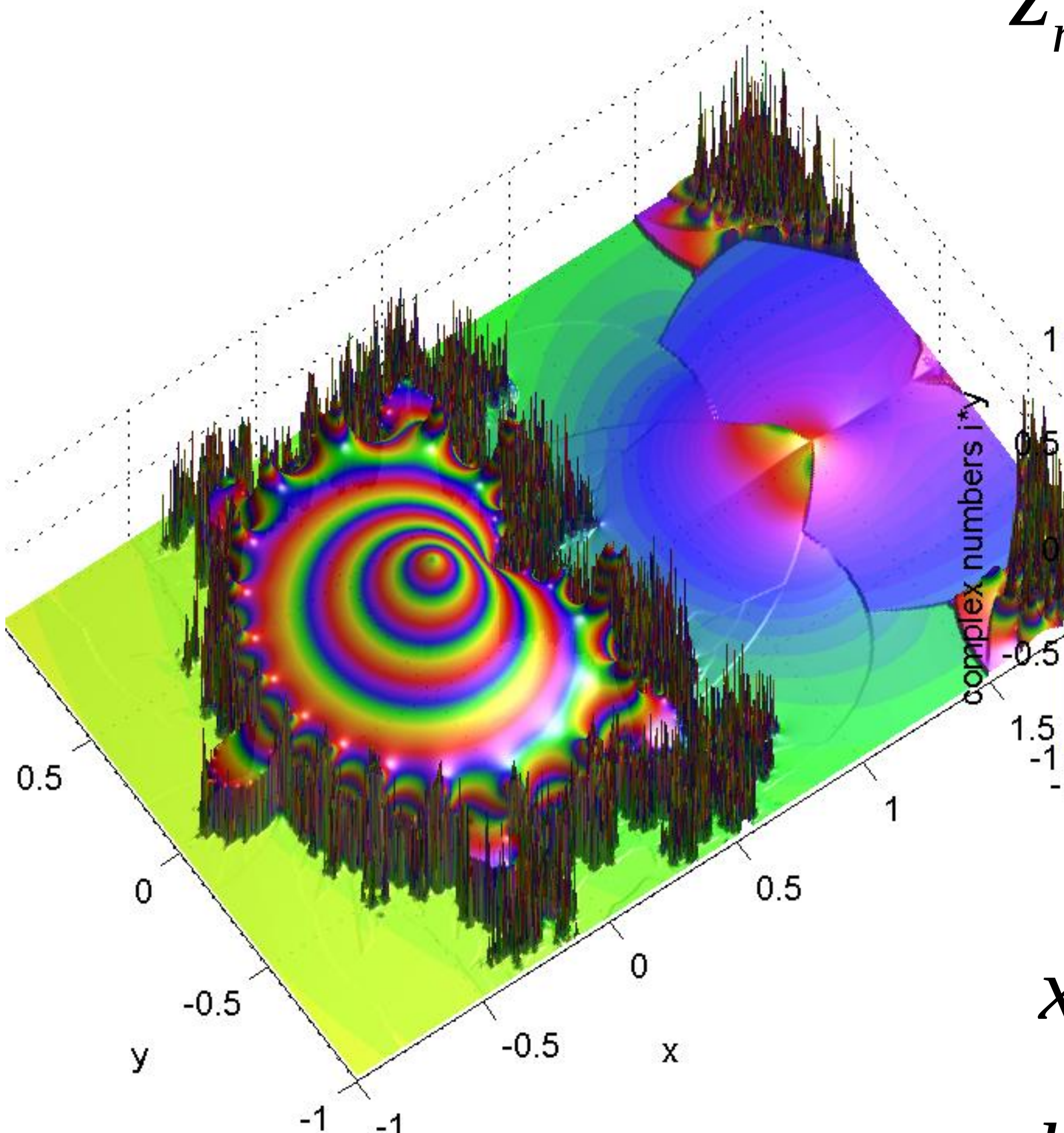


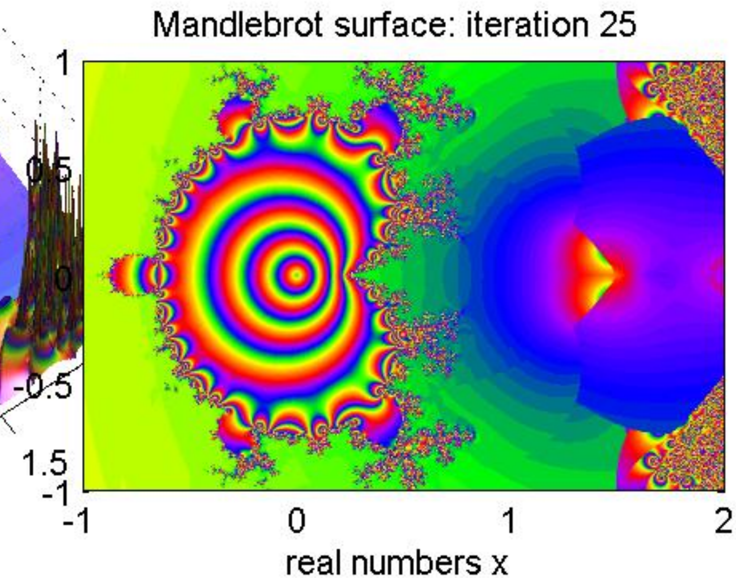
$$x = \mathrm{Re}(z), \quad y = \mathrm{Im}(z)$$

$$h(x, y) = e^{-\sqrt{x^2 + y^2}}$$

The Mandlerocket

$$z_{n+1} = \sin^{-1}\left(z_n^2 + z_0\right)$$



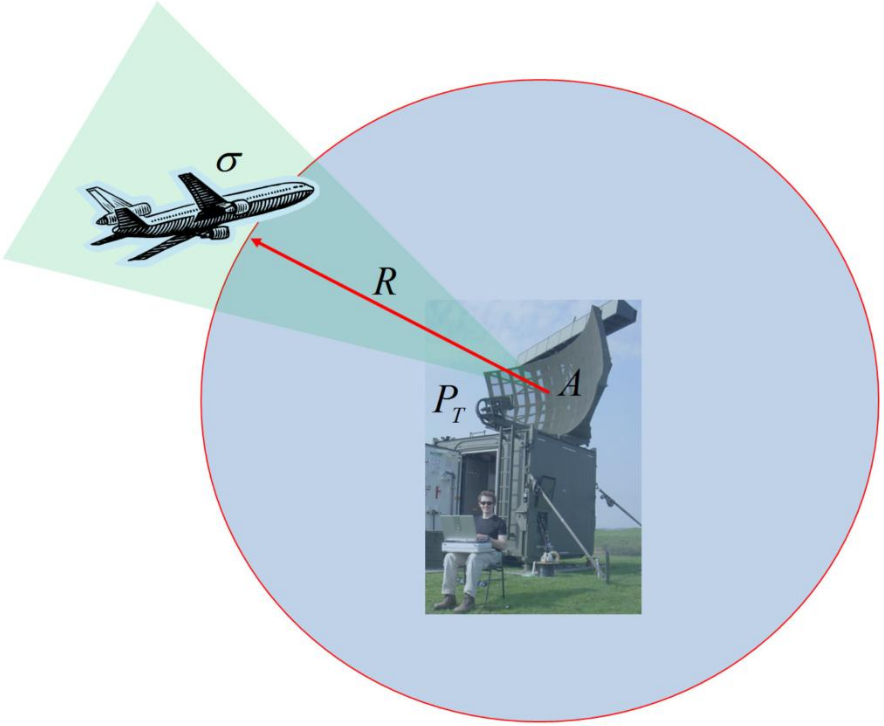


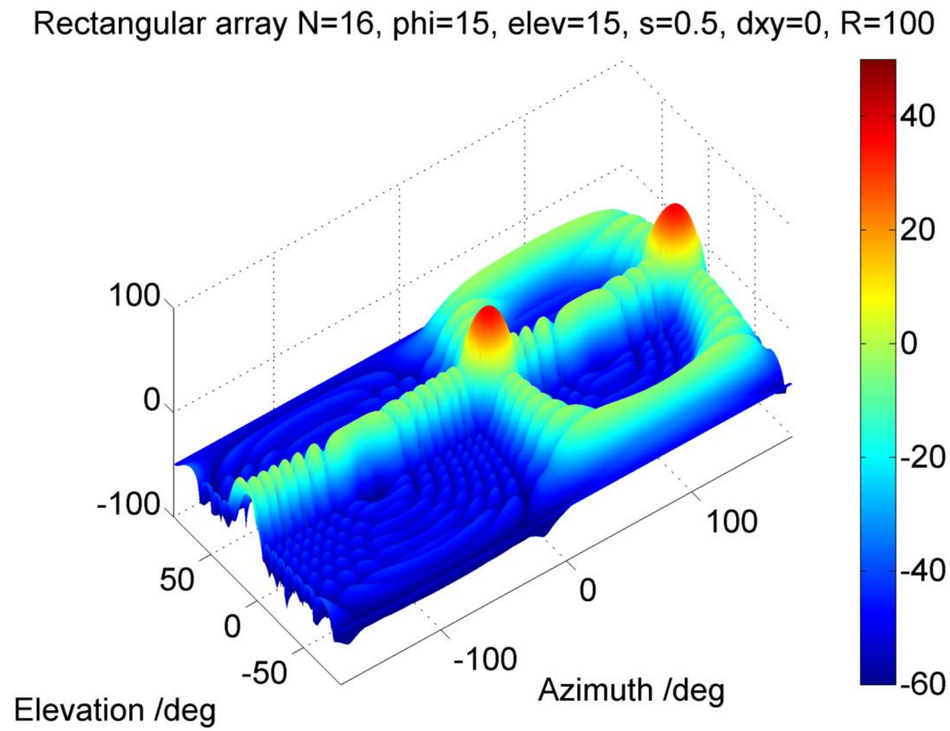
$$x = \mathrm{Re}(z), \quad y = \mathrm{Im}(z)$$

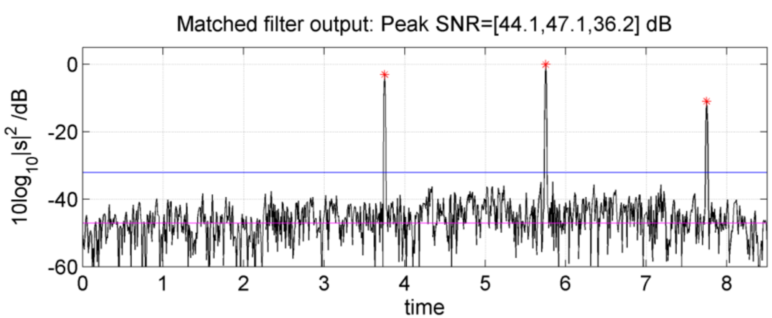
$$h(x, y) = e^{-\sqrt{x^2 + y^2}}$$

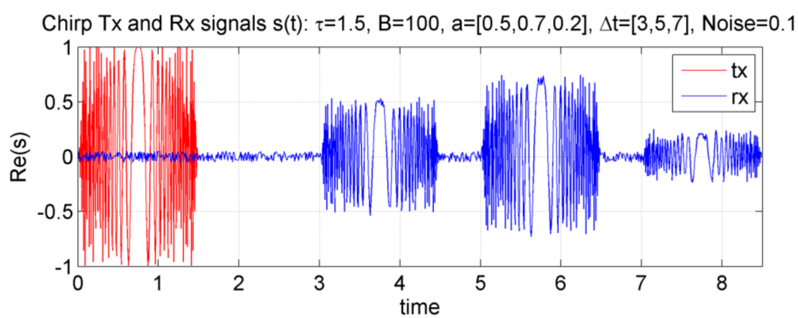
$$e^{i\pi} = -1$$

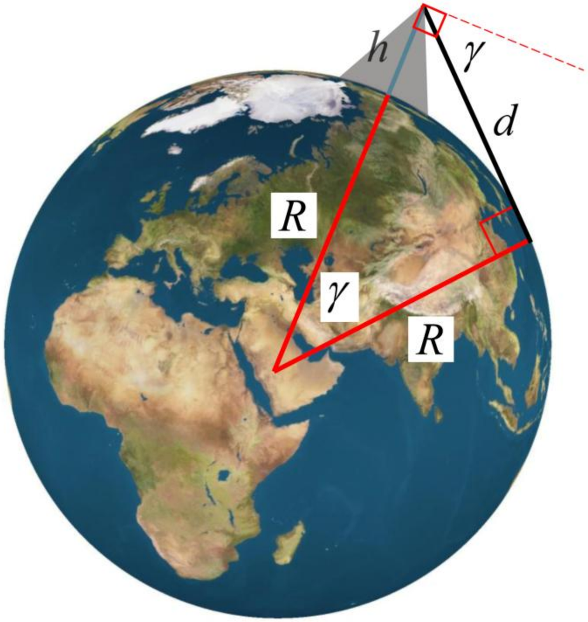
$$e^{i\theta} = \cos\theta + i\sin\theta$$

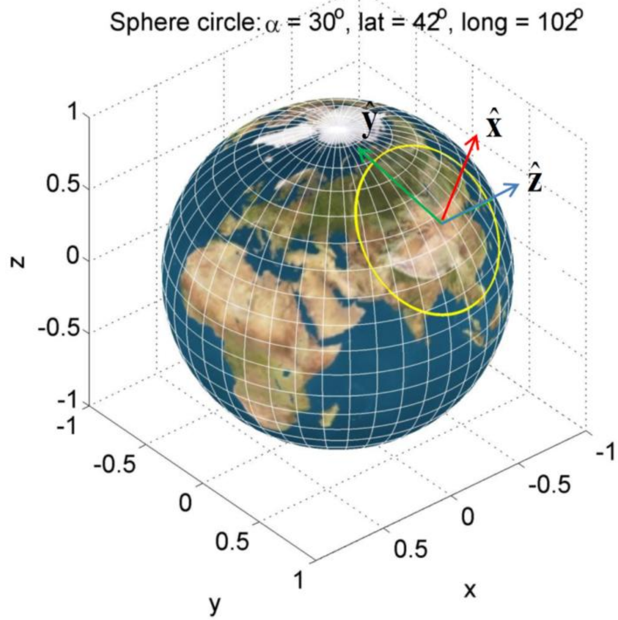

σ
R
P_T
A

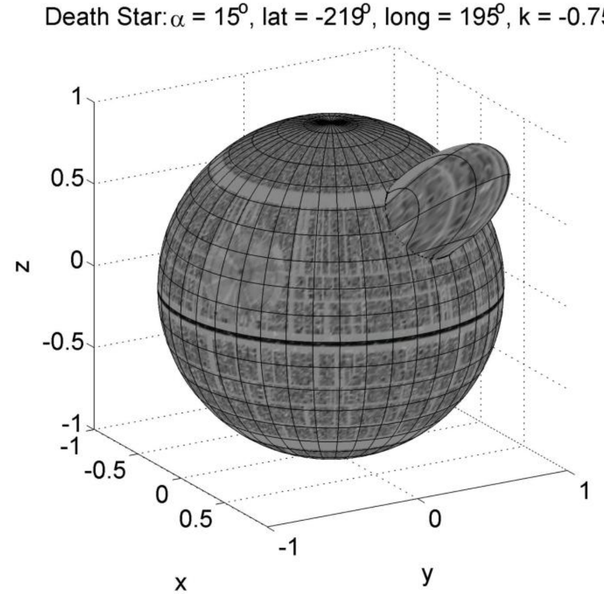

Rectangular array N=16, phi=15, elev=15, s=0.5, dxy=0, R=100
100
0
-100
50
0
-50
Elevation /deg
-100
0
100
Azimuth /deg
40
20
0
-20
-40
-60

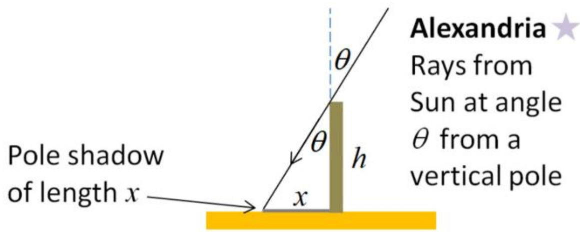

Matched filter output: Peak SNR=[44.1,47.1,36.2] dB
10log10|s|2 /dB
0
-20
-40
-60
0
1
2
3
4
5
6
7
8
time

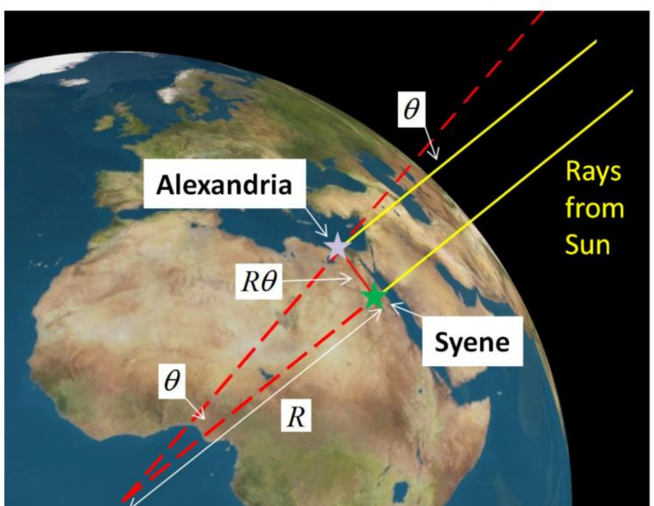

Chirp Tx and Rx signals s(t): τ=1.5, B=100, a=[0.5,0.7,0.2], Δt=[3,5,7], Noise=0.1
Re(s)
1
0.5
0
-0.5
-1
0
1
2
3
4
5
6
7
8
time
tx
rx

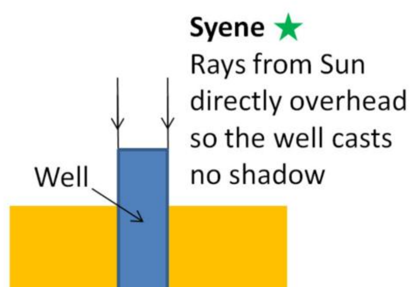

h
γ
d
R
γ
R

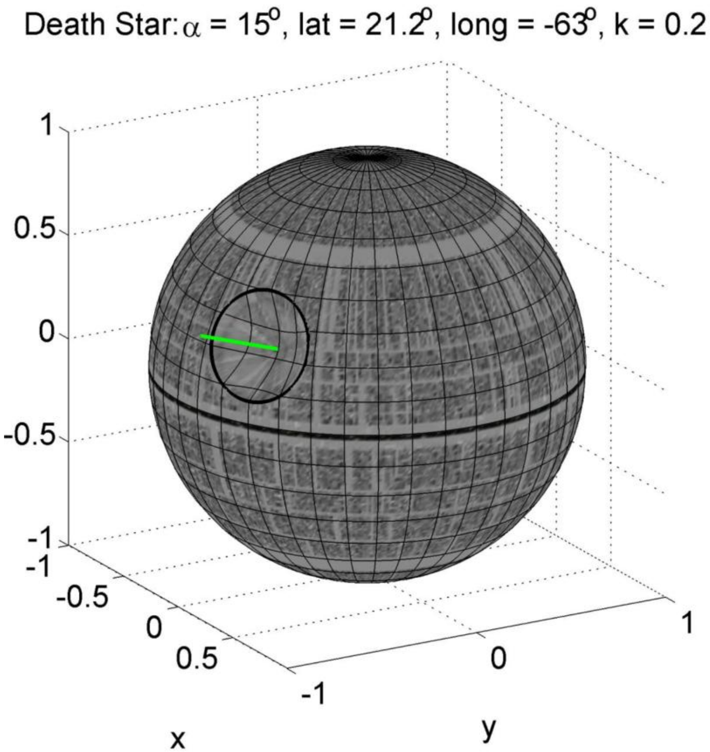

Sphere circle: α = 30°, lat = 42°, long = 102°
ŷ
x̂
ẑ
z
x
y

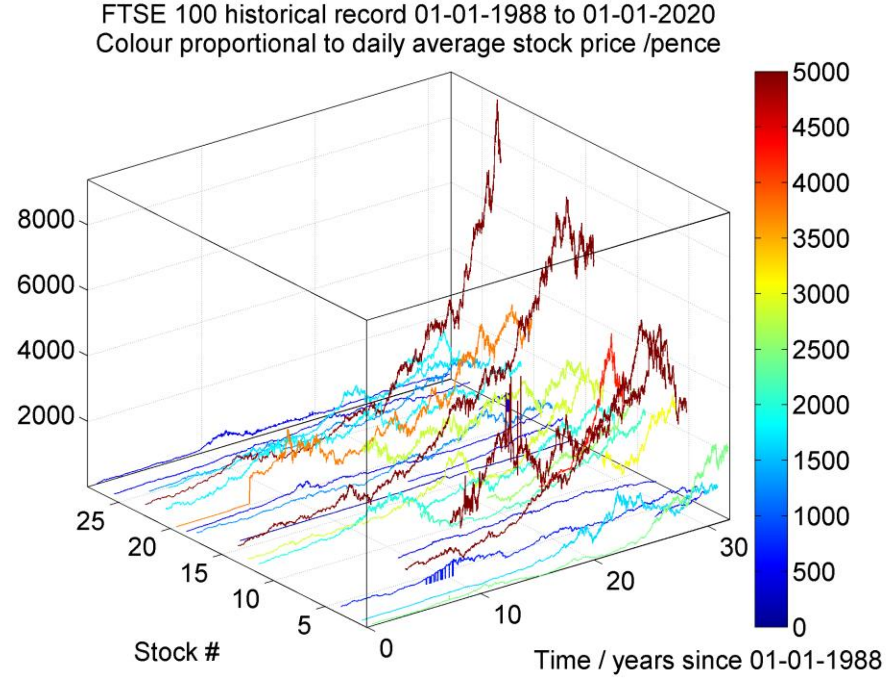

Death Star: α = 15°, lat = -219°, long = 195°, k = -0.75
z
x
y

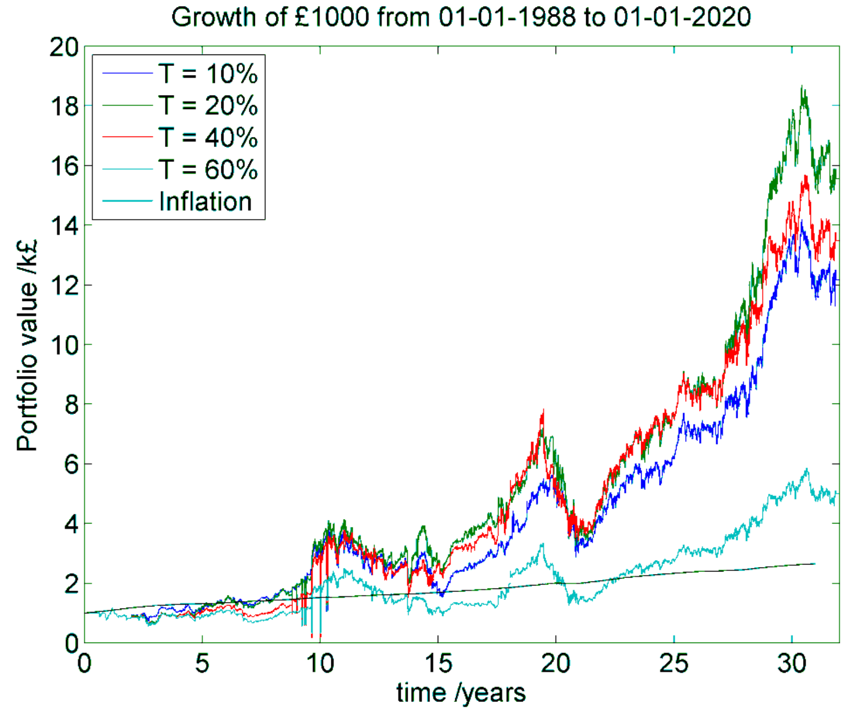

Alexandria
Rays from Sun at angle θ from a vertical pole
Pole shadow of length x
θ
θ
h
x

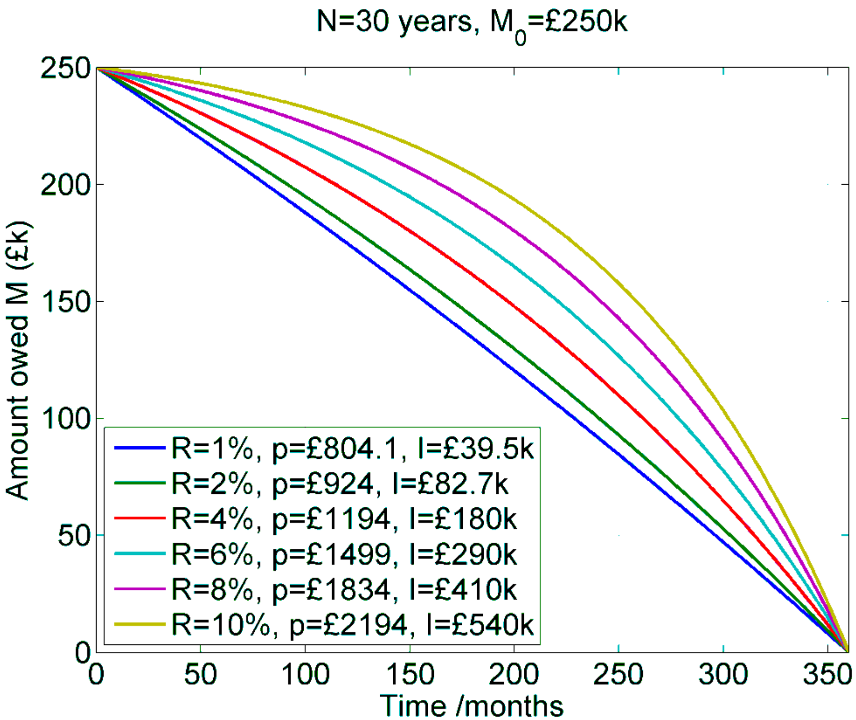

θ
Alexandria
Rays from Sun
Rθ
Syene
θ
R

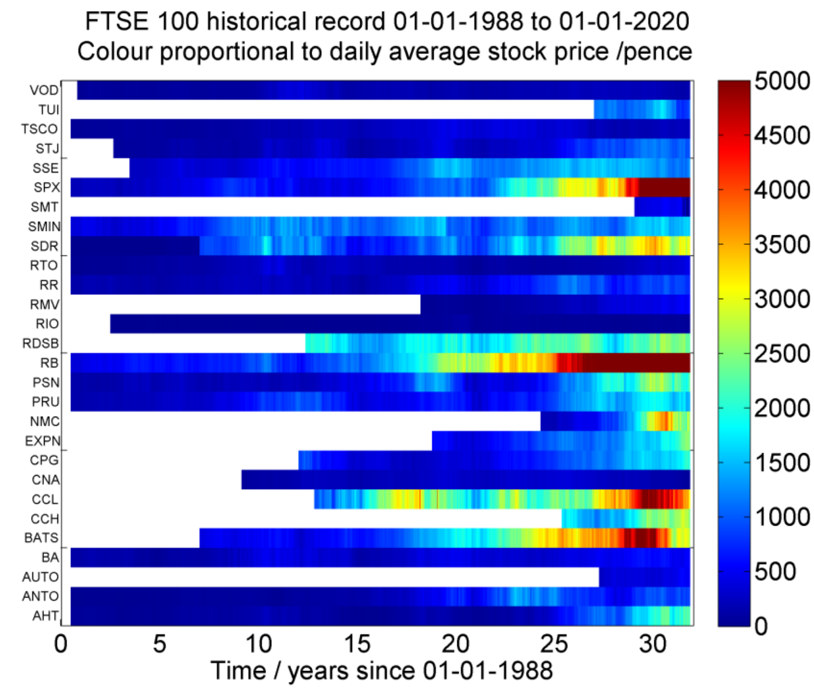

Syene
Rays from Sun directly overhead so the well casts no shadow
Well

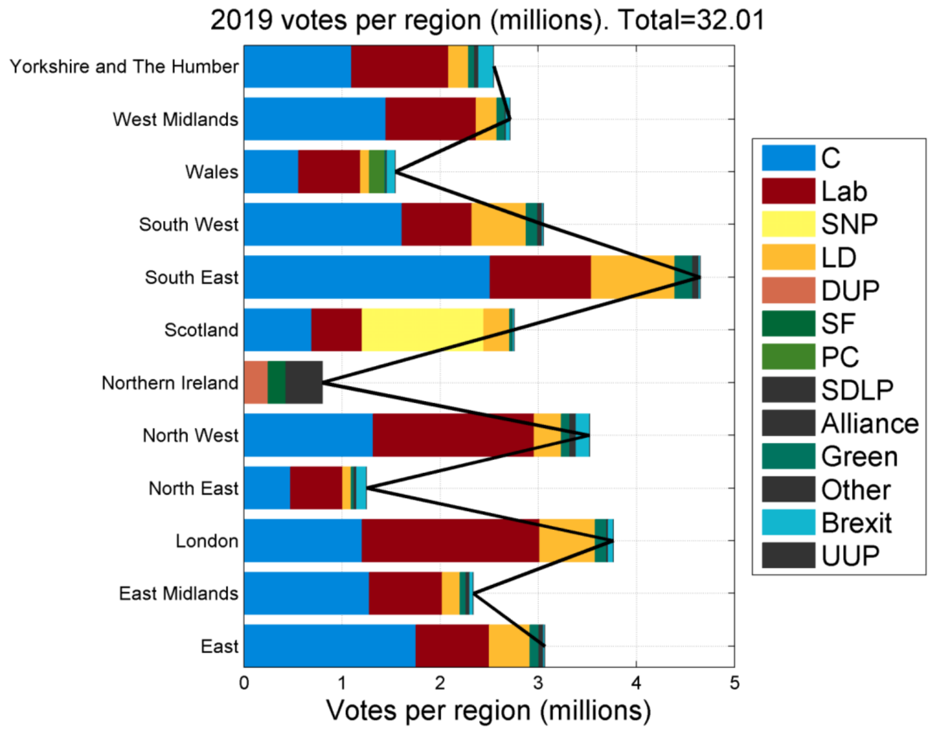

Death Star: α = 15°, lat = 21.2°, long = -63°, k = 0.2
x
y


FTSE 100 historical record 01-01-1988 to 01-01-2020
Colour proportional to daily average stock price /pence
Stock #
Time / years since 01-01-1988

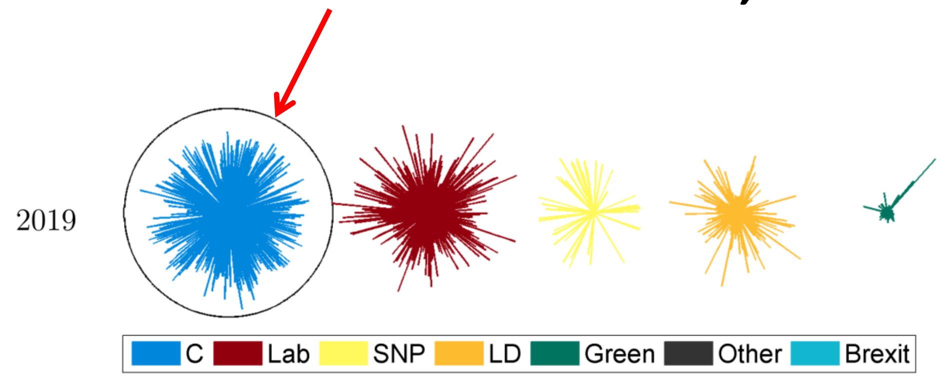

Growth of £1000 from 01-01-1988 to 01-01-2020
T = 10%
T = 20%
T = 40%
T = 60%
Inflation
Portfolio value /k£
time /years

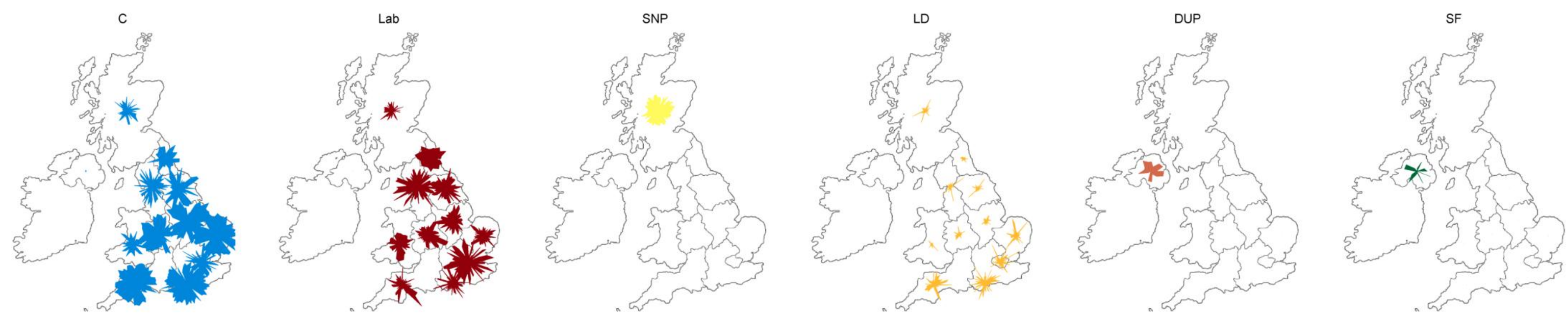

N=30 years, M0=£250k
Amount owed M (£k)
Time /months
R=1%, p=£804.1, I=£39.5k
R=2%, p=£924, I=£82.7k
R=4%, p=£1194, I=£180k
R=6%, p=£1499, I=£290k
R=8%, p=£1834, I=£410k
R=10%, p=£2194, I=£540k


FTSE 100 historical record 01-01-1988 to 01-01-2020
Colour proportional to daily average stock price /pence
VOD
TUI
TSCO
STJ
SSE
SPX
SMT
SMIN
SDR
RTO
RR
RMV
RIO
RDSB
RB
PSN
PRU
NMC
EXPN
CPG
CNA
CCL
CCH
BATS
BA
AUTO
ANTO
AHT
Time / years since 01-01-1988

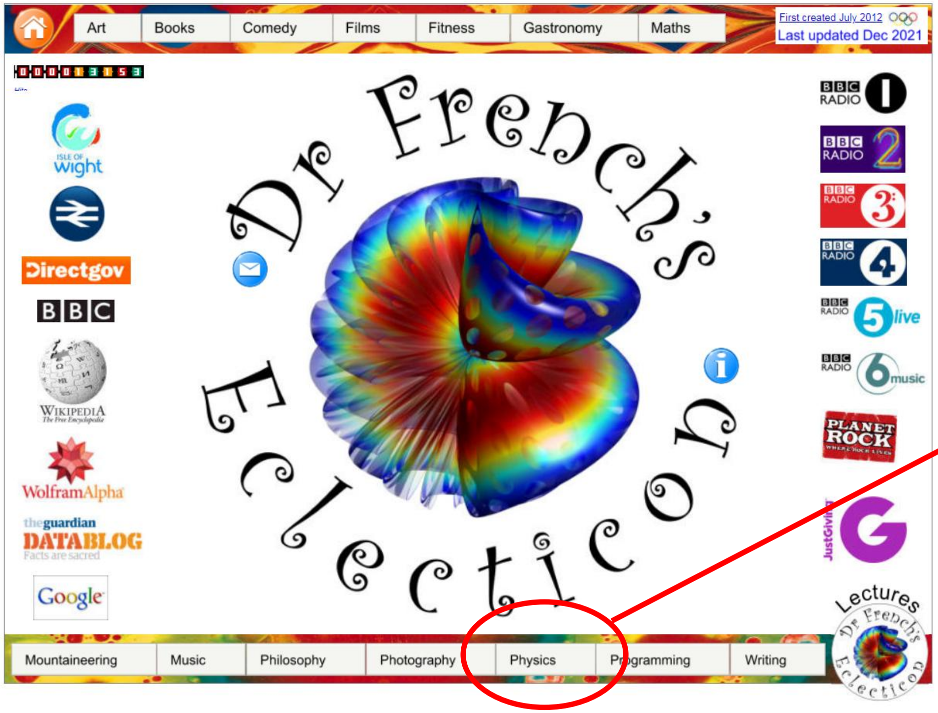


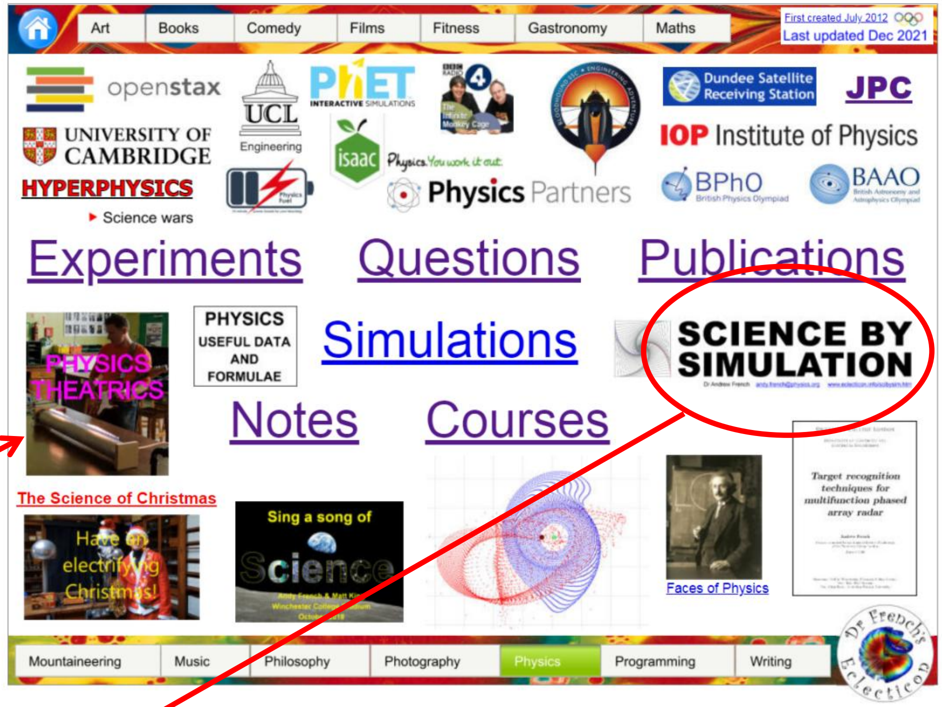
Votes per constituency circle radius = 48,000

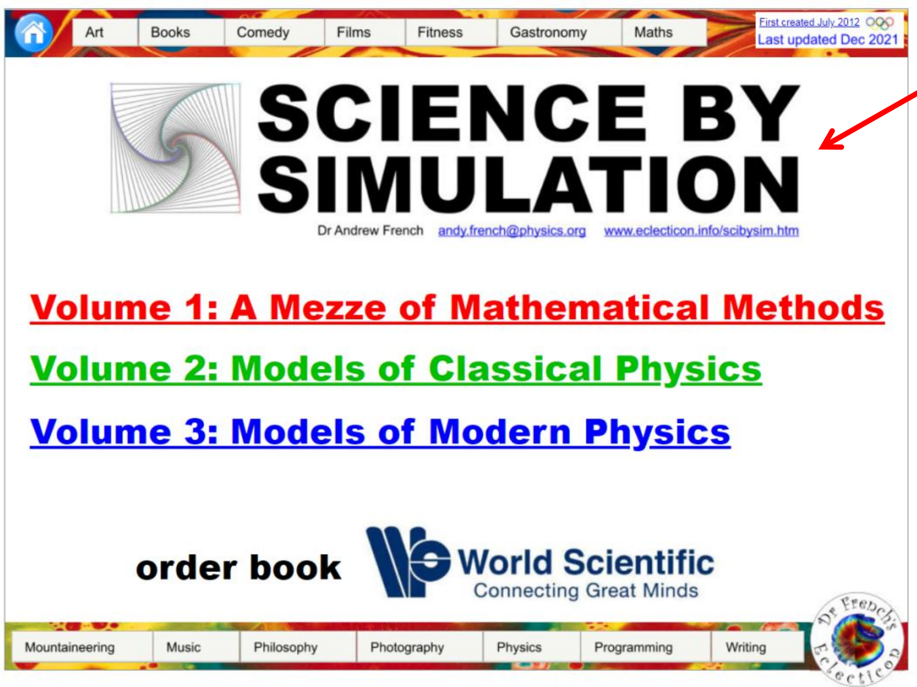




vote%	44%	32%	3.9%	12%	0.76%	0.57%
seats	365	202	48	11	8	7
PR	282	207	25	75	8	7







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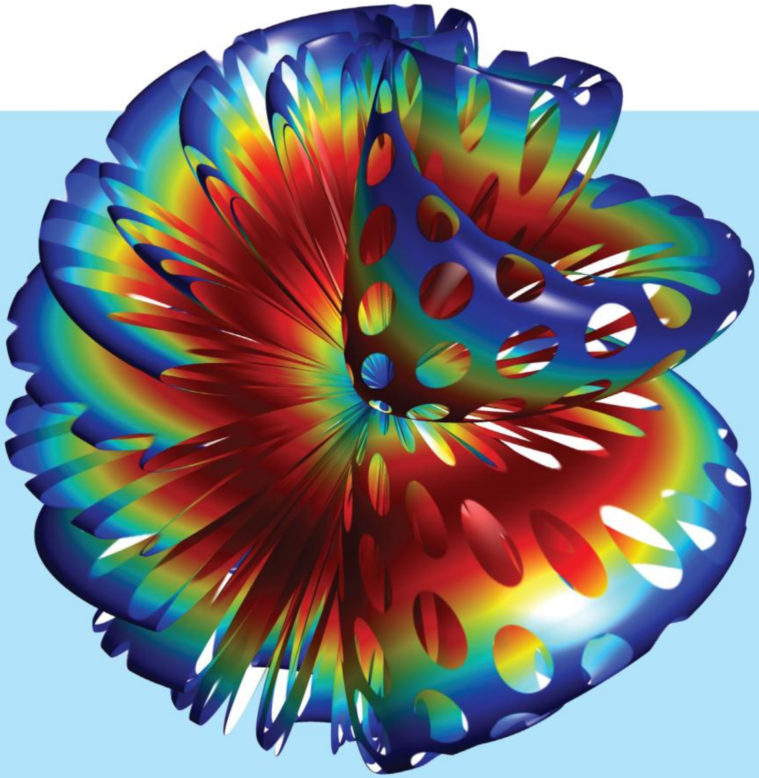

ANDREW FRENCH

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