Title: Astrobiology, homochirality, and the origin of life

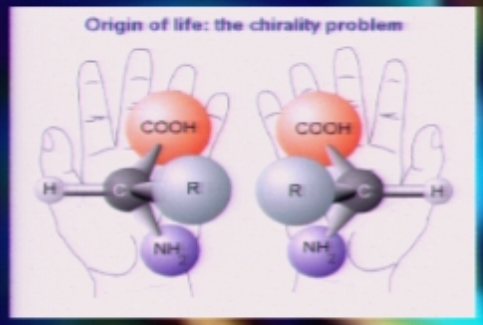
Date: Jun 01, 2005 02:00 PM

URL: http://pirsa.org/05060055

Abstract:

Astrobiology, homochirality, and the origin of life

Axel Brandenburg, Anja Andersen, Susanne Höfner, Martin Nilsson, Tuomas Multamäki
(all at *Nordita*)



If prerequisite for life:

Due to polarized light, electroweak force, magnetic fields, …

If consequence of life:

Must have emerged during polymerization of first replicating molecules

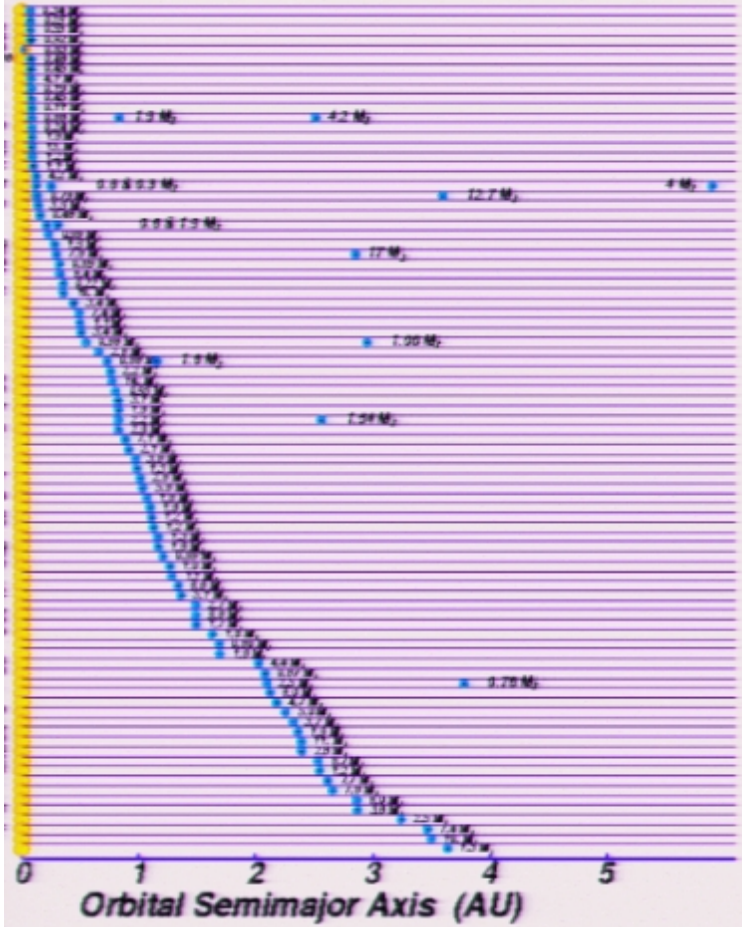
Different at different places on Earth??

Reaction-diffusion-advection equation

Int. J. Astrobio. 3, 209 (2004), Orig. Life Evol. Biosph. (2005a,b), Astrobiology (2005), see also arXiv: q-bio.BM/0401036, 0502008, 0505040, 0505041

Exoplanets and Extremophiles

By now 136 exoplanets…



CO

ETHANE

FORMIC ACID

ACETO-

RNA

ACETYLENE

Mars 3-4 Gyr ago? Europa, etc

me line

10^{10} yr after Big Bang

10^4 yr — planetesimals

10^6 yr — Sun ignites

10^8 yr — All gas gone

10^9 yr — First life

Remaining dust settles

lest
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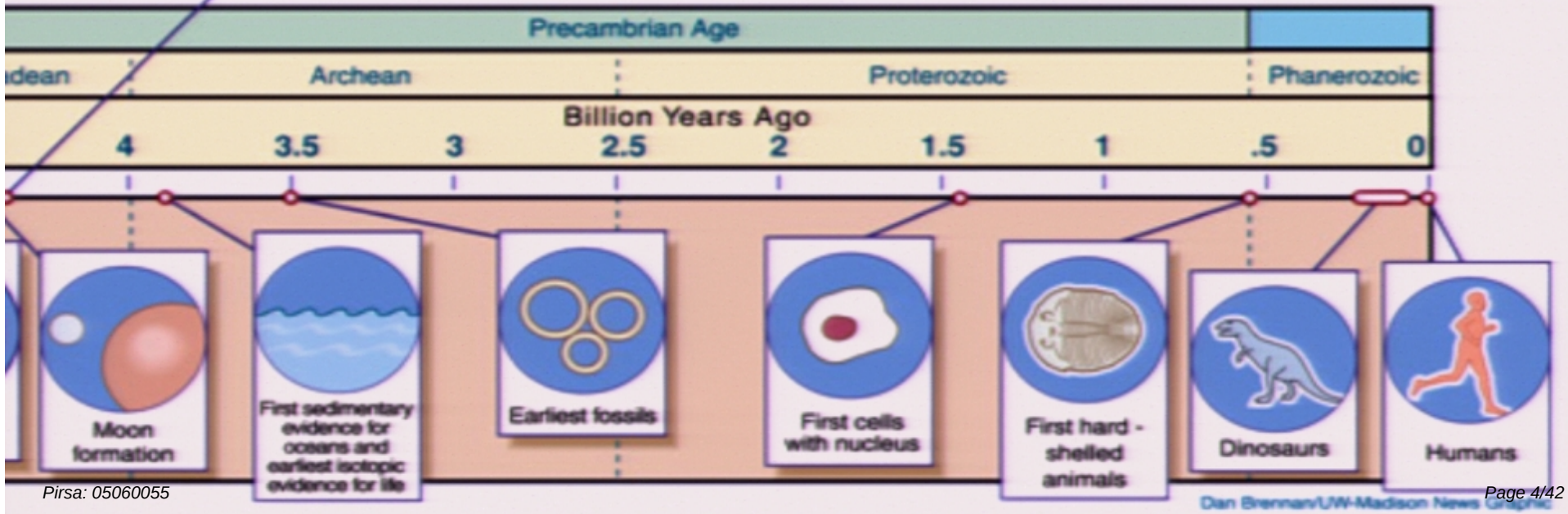
spitable
rly Earth

Newly discovered zircon crystal is the world's oldest known sample of a terrestrial material at an estimated 4.4 billion years old.

Chemical and isotopic analysis of this crystal suggest the presence of rocks formed at low temperatures and that the infant Earth cooled much faster after formation of the Moon than previously believed. Instead of being covered by a magma ocean, as conventional wisdom holds, the early Earth may instead have had continents, oceans, and a hydrosphere, all the conditions necessary for life.



Dan Brennan/UW-Madison News Graphic

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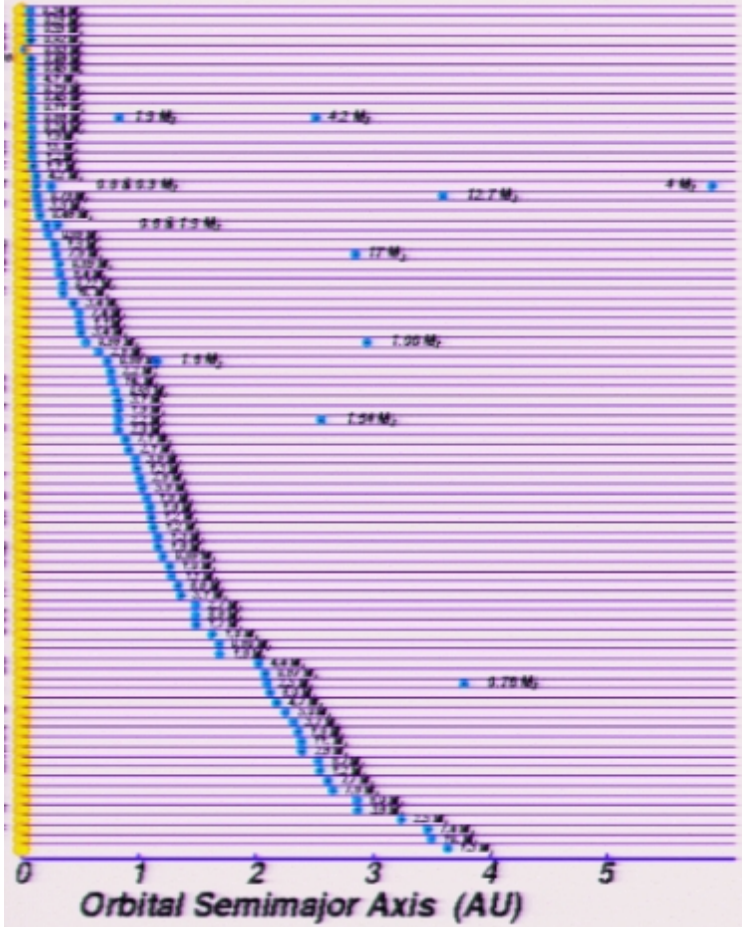

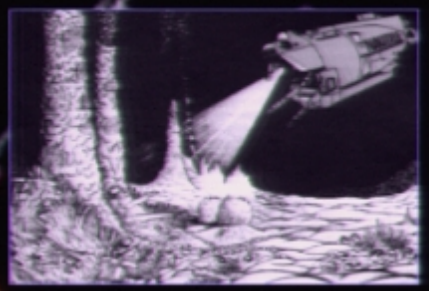

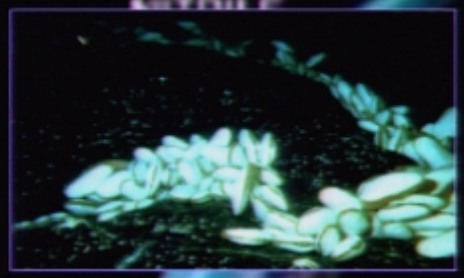

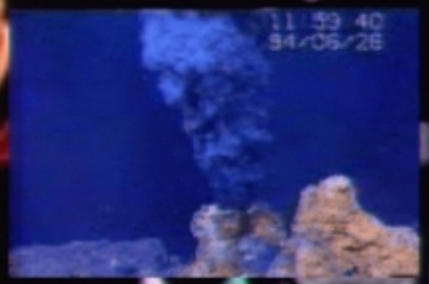

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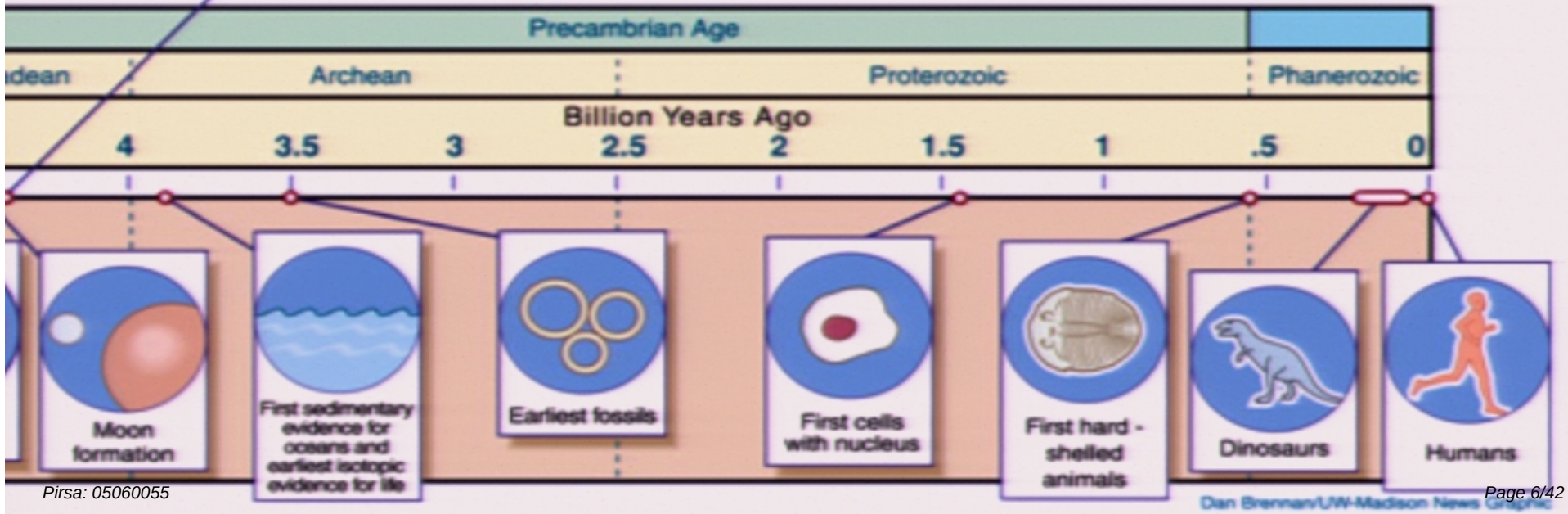
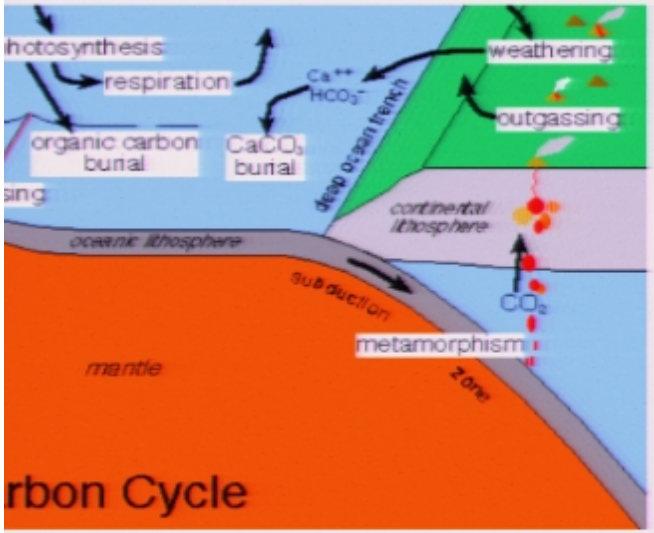
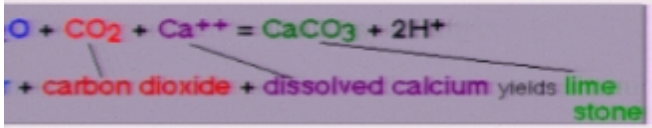


Dan Brennan/UW-Madison News Graphic

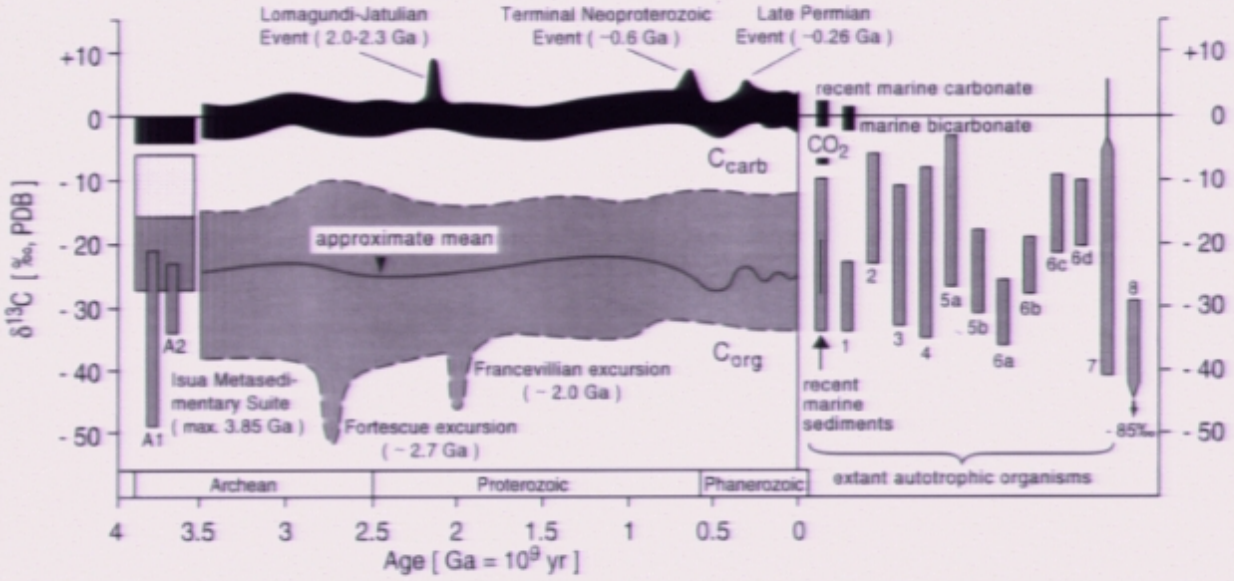
Carbon cycle → Source of the atmosphere

Carbonic and organic carbon





$$6CO_2 \xrightarrow{\text{chem.}} C_6H_{12}O_6 + 6O_2$$



Photosynthesis: 270 mW/m²
Internal energy: 80 mW/m²
Solar energy: 340 W/m²

(Rosing 2005)

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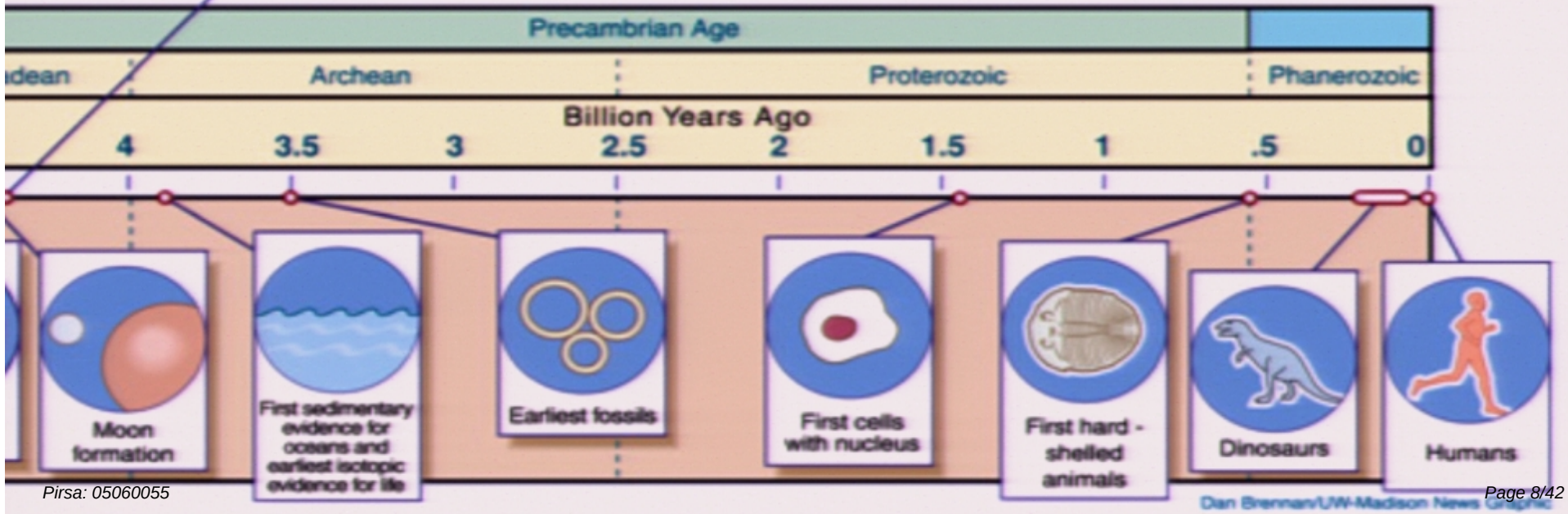

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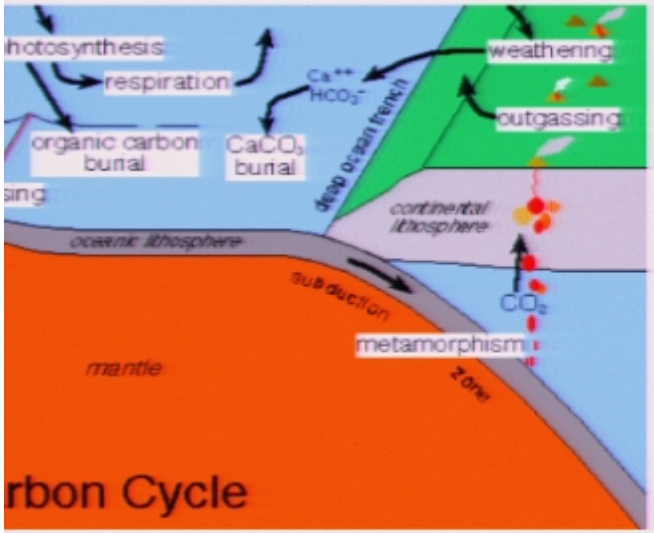

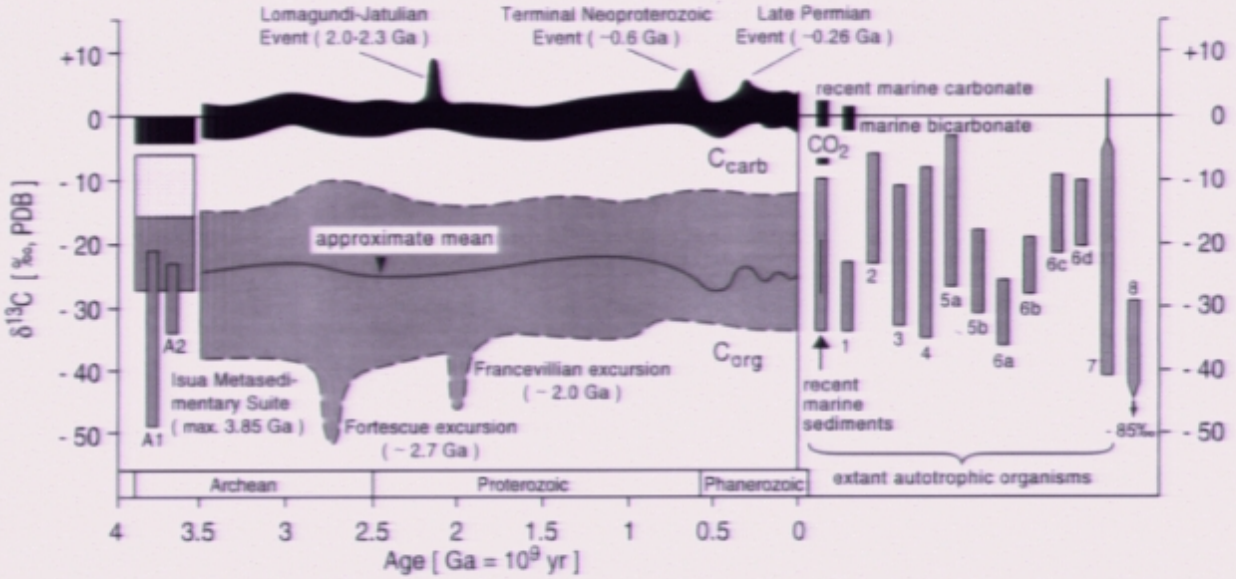

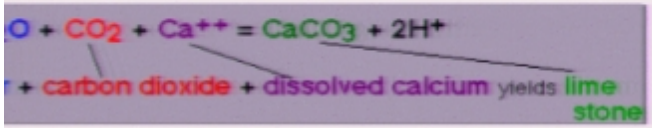

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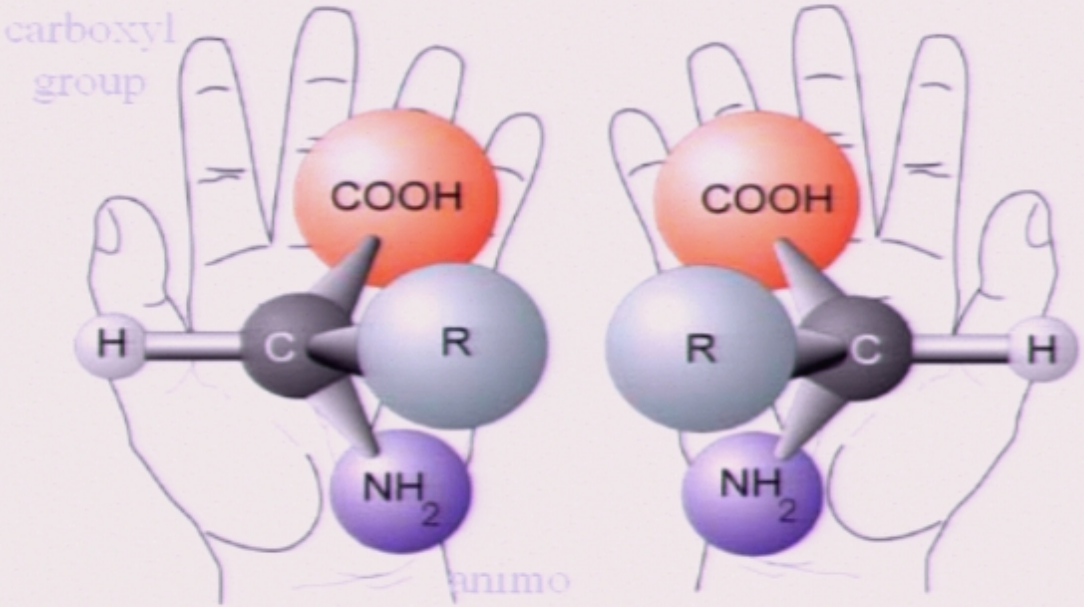
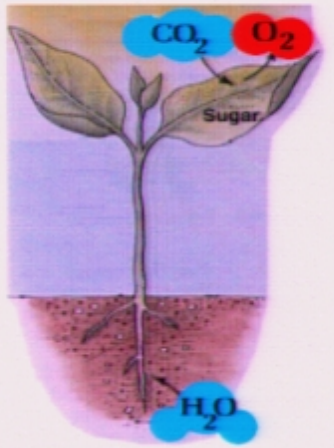
Aminoacids in proteins: left-handed
ugars in DNA and RNA: right-handed

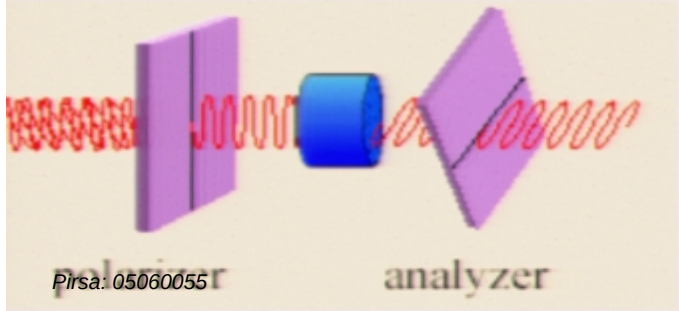
is Pasteur
22-1895)

Origin of life: the chirality problem



Is chirality:
(i) prerequisite
(ii) consequence
of life?





chlorophyll

$$6H_2O + 6CO_2 \text{ ----------> } C_6H_{12}O_6 + 6O_2$$

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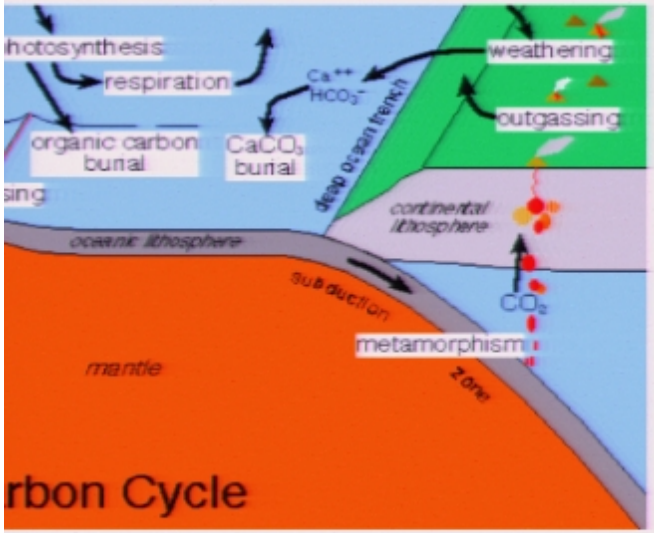

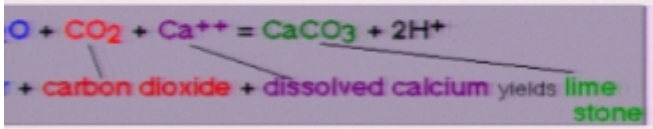

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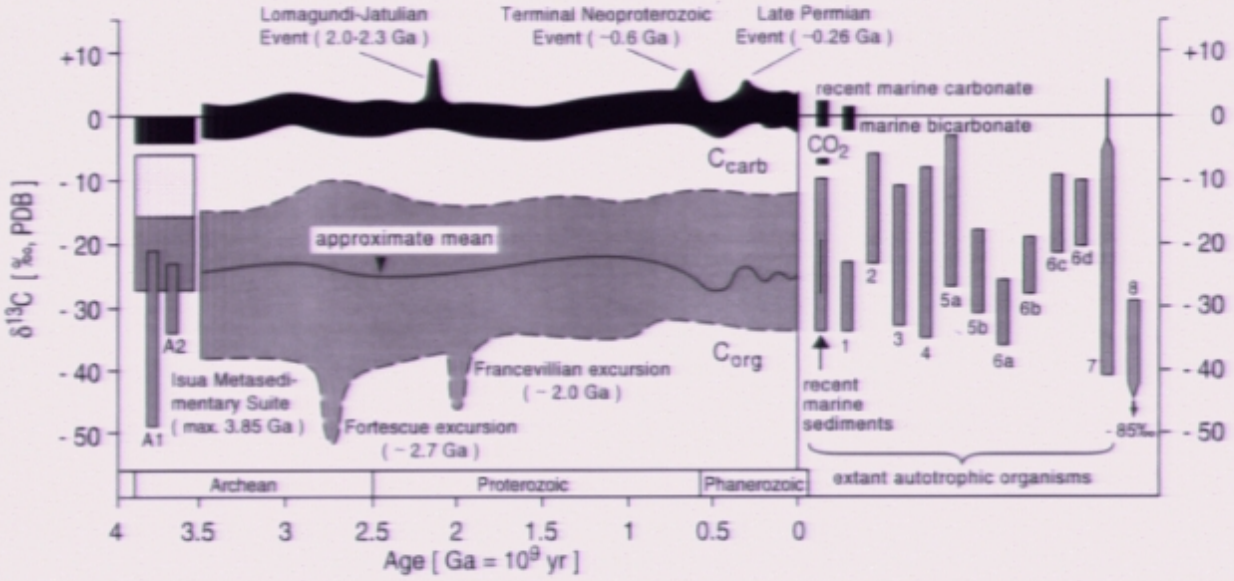

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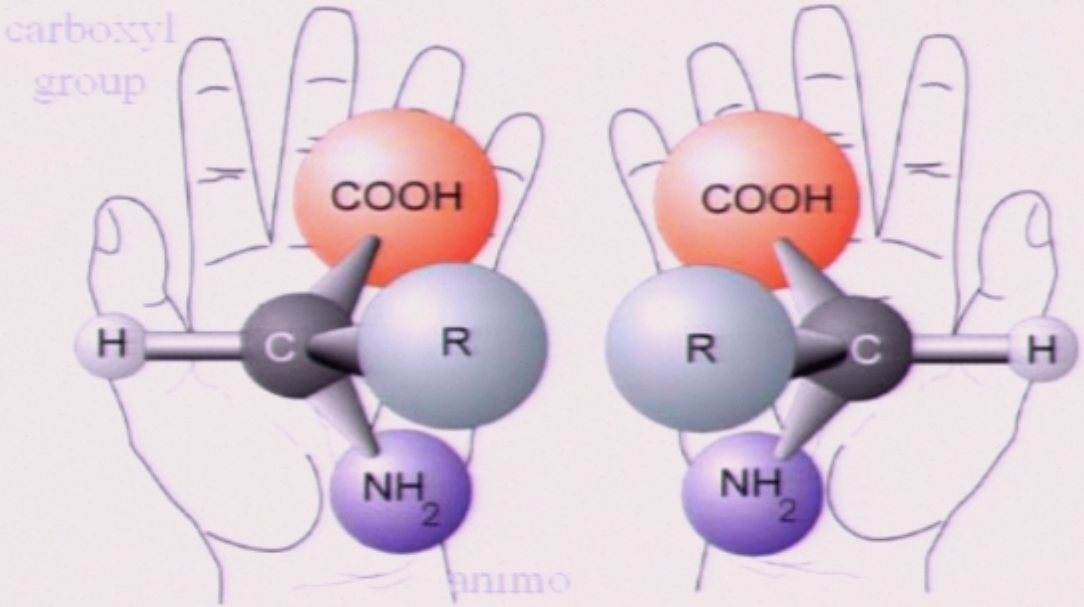

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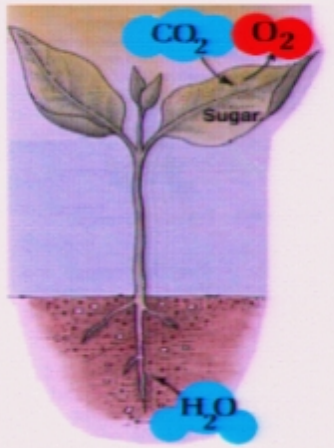

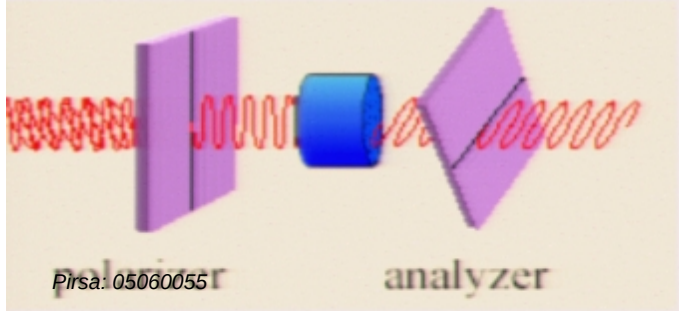

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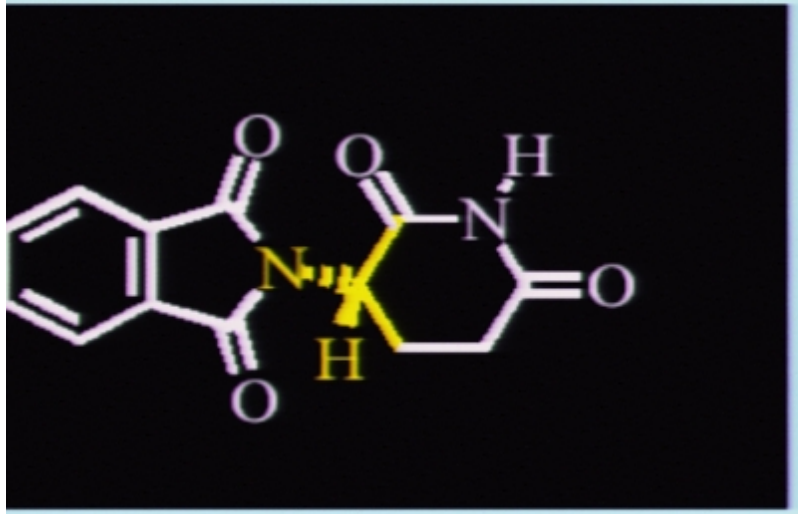
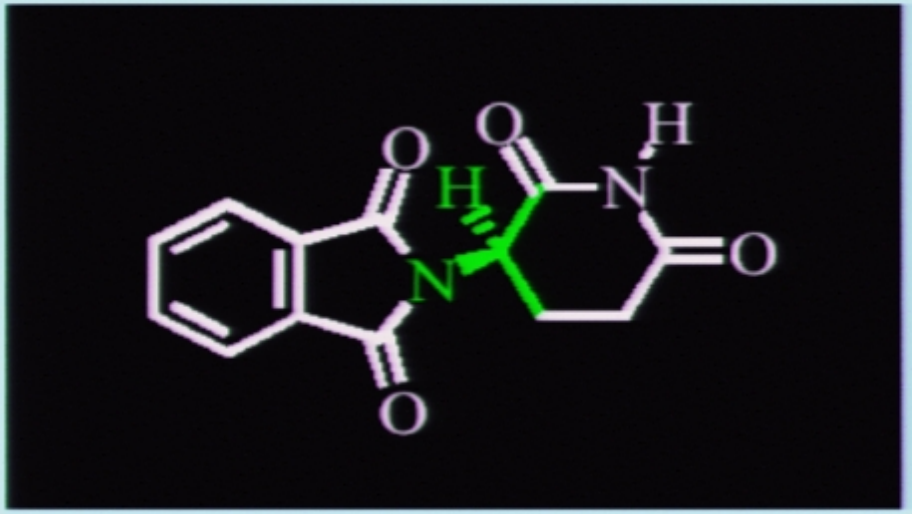
ontergan: was sold as racemic mixture

Thalidomid molecule



(S)-Contergan



(R)-Contergan

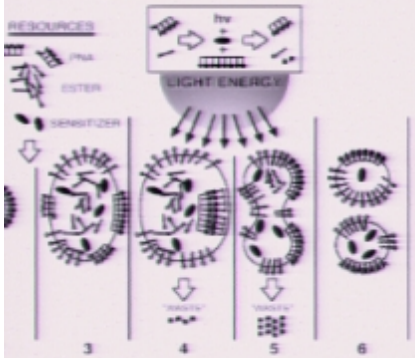
causes misformations

abandoned in December 1961)

Cures morning sickness
during pregnancy

Chirality selection during polymerization of the first replicating molecule?

lipid world

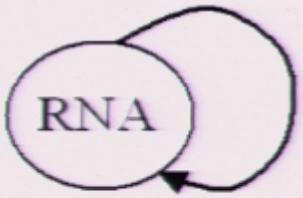


ıssen et al (2003
Life **9**, 269-316)

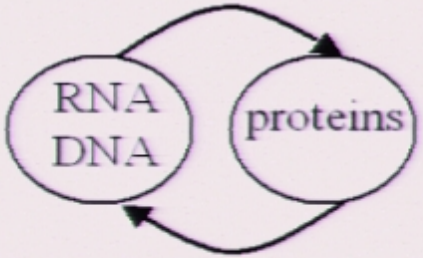
PNA world

achiral
↓
chiral

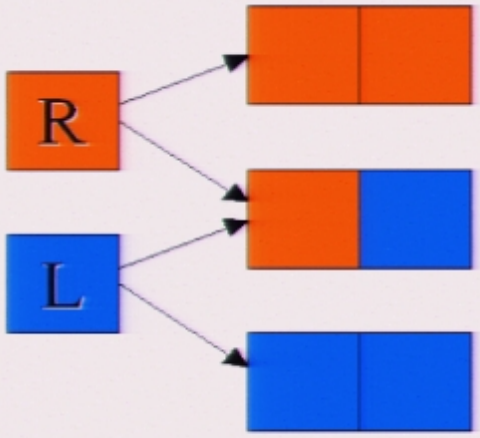
RNA world



dual world

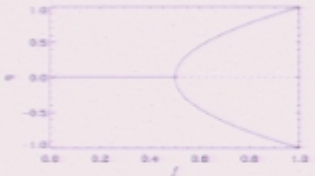


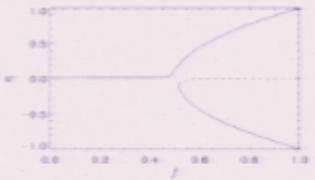
rization



Isotactic polymer
(same chirality)

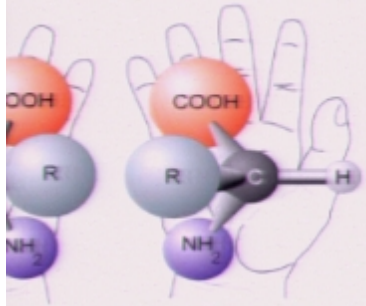
"waste"
(enantiomeric
cross-inhibition)



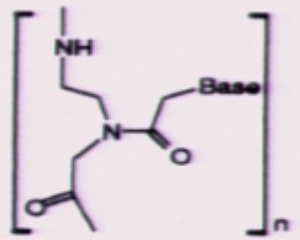


PNA world prior to RNA world

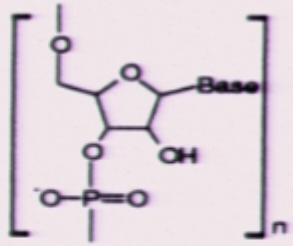
f life: the chirality problem



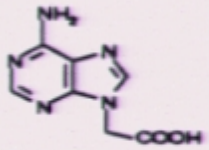
PE Nielsen (1993)



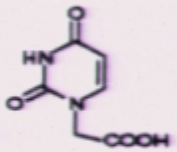
Peptide Nucleic Acid



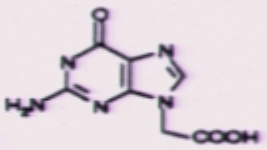
RNA



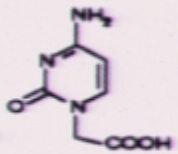
Adenine-N^9-acetic acid



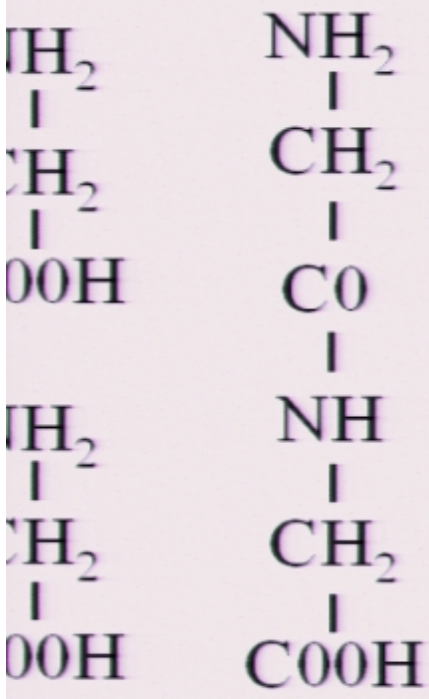
Uracil-N^1-acetic acid



Guanine-N^9-acetic acid

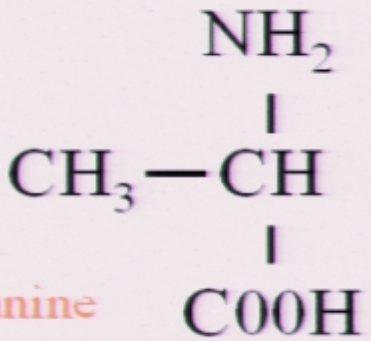


Cytosine-N^1-acetic acid



Peptide nucleotide

achiral

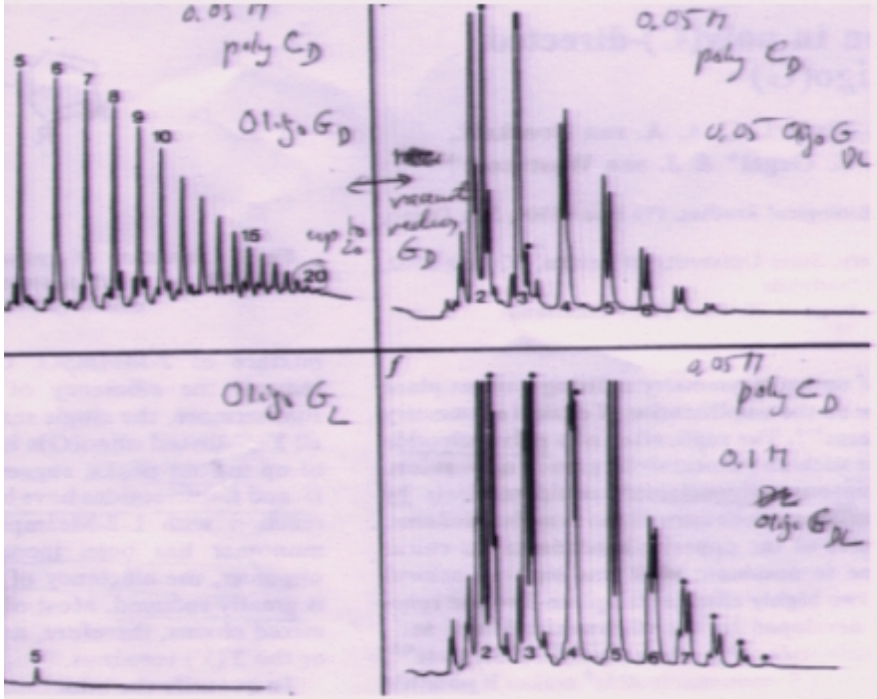


alanine

chiral

dipeptide

Relevant experiments: nucleotides



→ Mononucleotides with wrong chirality terminate chain growth

ok

poisoned

(using HPLC)

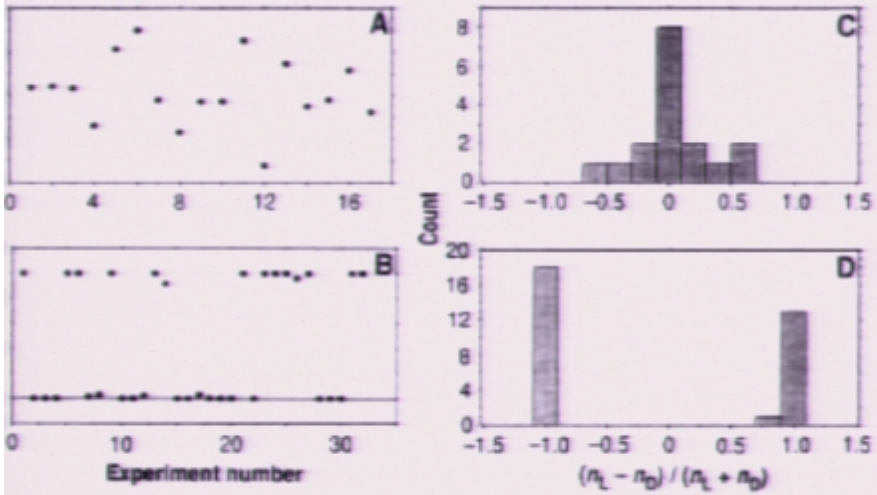
ate-directed oligomerization
poly (C_D) → oligo (G_D)

cytosine guanine

→ *enantiomeric cross-inhibition*

Joyce et al. (1984)

Relevant experiments: crystals

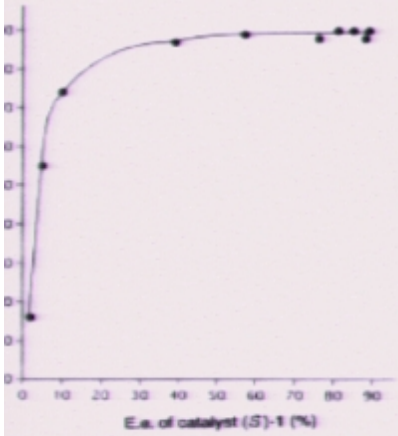


Crystal growth, many different nucleation sites: racemic mixture

Crystal growth with stirring: primary nucleation suppressed

Kondepudi et al. (1990)

→ *competition important*



Alkanol with 2% e.e. treated with carboxylaldehyde

Soai et al. (1995)

→ autocatalytic self-amplification

Frank (1953), Goldanskii & Kuzmin (1989), …

alkynylzine-catalyzed reaction (Blackmond 2004)

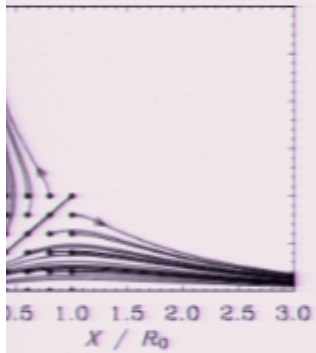
Simplistic models: trial and error?

ank (1953)

$$= kR(1-L)$$

$$= kL(1-R)$$

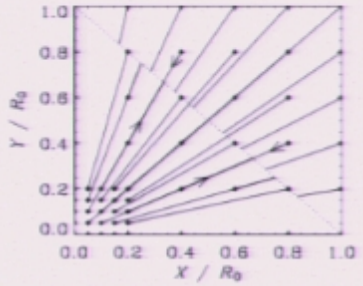
st — anti-catalyst



unspecific quenching

$$\frac{dR}{dt} = kR(1-R-L)$$

$$\frac{dL}{dt} = kL(1-R-L)$$

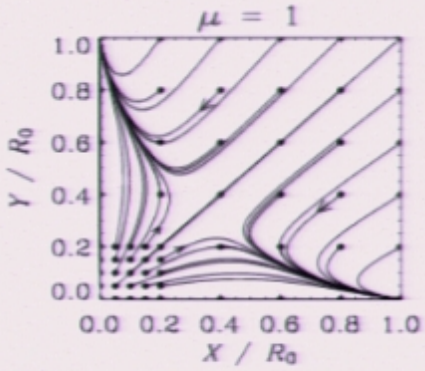


chemically unrealistic (Blackmond 2002)

Specific antagonism

$$\frac{dR}{dt} = kR(1-R-L) - \mu RL$$

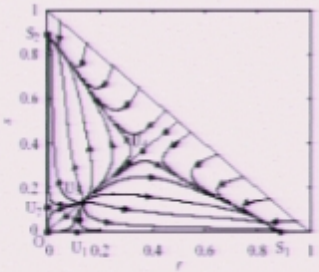
$$\frac{dL}{dt} = kL(1-R-L) - \mu RL$$



aito & Hyuga (2004)

$$= kR^2(1-R-L) - \mu R$$

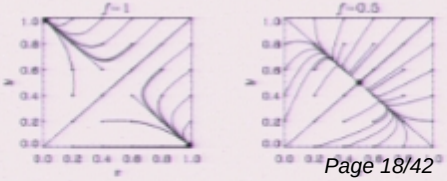
$$= kL^2(1-R-L) - \mu L$$



our model (BAHN 2005)

$$\frac{dR}{dt} = \frac{R^2}{R^2+L^2} - (L+R)R$$

$$\frac{dL}{dt} = \frac{L^2}{R^2+L^2} - (L+R)L$$



Polymerization model of Sandars

Orig. Life Evol. Biosph. **33**, 575-587 (2003)

ction for left-handed monomers

$$L_{n-1} + L_1 \xrightarrow{2k_S} L_n$$

$$\frac{d}{dt}[L_n] = 2k_S[L_{n-1}][L_1]$$

s term for each constituent

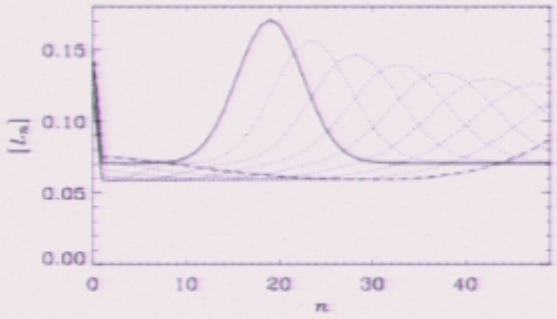
$$\frac{d}{dt}[L_{n-1}] = -2k_S[L_{n-1}][L_1]$$

$$\frac{d}{dt}[L_1] = -2k_S[L_{n-1}][L_1]$$

Combined equations

$$\frac{d}{dt}[L_n] = -2k_S[L_1]([L_n] - [L_{n-1}])$$

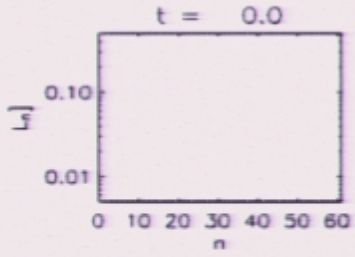
$$\frac{d}{dt}[L_1] = Q_L - 2k_S[L_1]\sum_{n=1}^{N}[L_n]$$



umber of left-handed
Building blocks const

$$\sum_{n=1}^{N} n[L_n] = \text{const}$$

(if Q_L=0)



Coupling to substrate S

ource of L_1 monomers Q_L

$$\frac{d}{dt}[L_1] = Q_L - 2k_S[L_1]\sum_{n=1}^{N}[L_n]$$

acts as a sink of substrate S

$$\frac{d}{dt}[S] = Q - (Q_L + Q_R)$$

-catalytic properties of polymers

$$Q_L = k_C[S][L_N]$$
$$Q_R = k_C[S][R_N]$$

Refinements

finite fidelity f

$$Q_L = k_C[S]\{\tfrac{1}{2}(1+f)C_L + \tfrac{1}{2}(1-f)C_R\}$$
$$Q_R = k_C[S]\{\tfrac{1}{2}(1+f)C_R + \tfrac{1}{2}(1-f)C_L\}$$

Possible proposals for C_L (or C_R)

$$C_L = \begin{cases} [L_N] & \text{(Sandars 2003)} \\ [L_M] & \text{(another possibility)} \\ \sum[L_n] & \text{(Wattis \& Coveney 2004)} \\ \sum n[L_n] & \text{(our work)} \end{cases}$$

ncluding enantiomeric cross-inhibition

oss term for each constituent

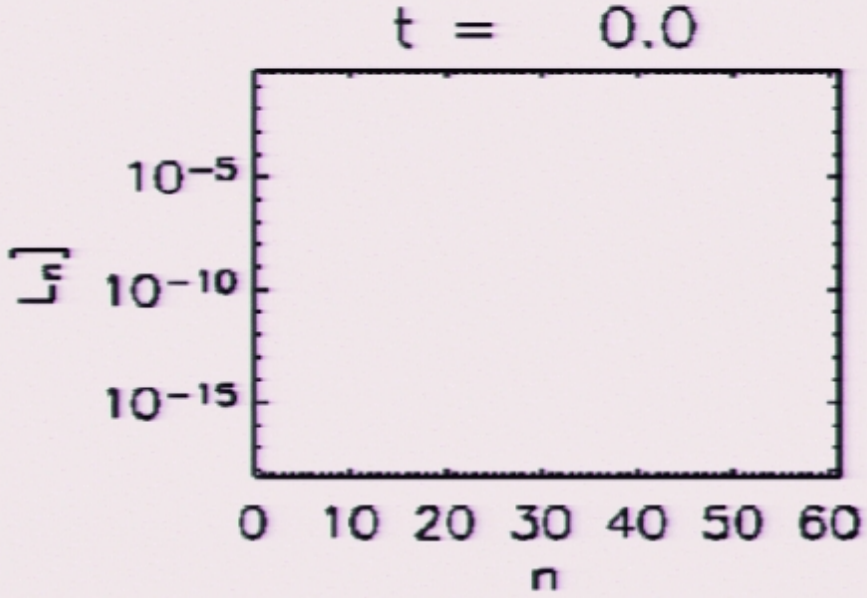
$$_n + R_1 \xrightarrow{2k_I} L_n R_1$$

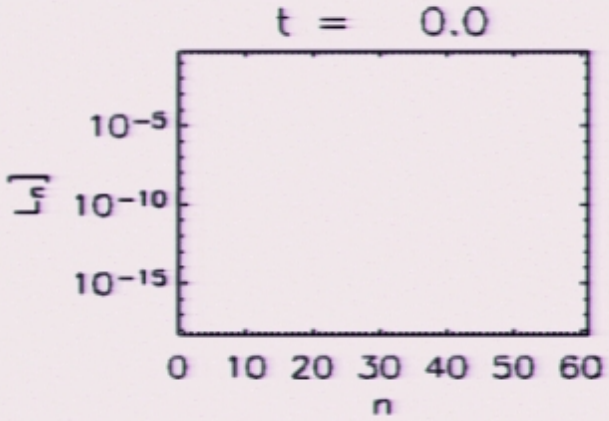
$$\frac{d}{t}[L_n R_1] = 2k_I[L_n][R_1]$$

$$_n R_1] = \ldots - 2k_I[R_1]([L_n R_1] - [L_{n-1} R_1])$$

$$_1] = \ldots - 2k_S[R_1]\sum_{n=1}^{N}[L_n R_1]$$

Racemic solution ~2^{1-n}





Stability

ncluding enantiomeric cross-inhibition

oss term for each constituent

$$_n + R_1 \xrightarrow{2k_I} L_n R_1$$

$$\frac{d}{t}[L_n R_1] = 2k_I[L_n][R_1]$$

$$_n R_1] = \ldots - 2k_I[R_1]([L_n R_1] - [L_{n-1} R_1])$$

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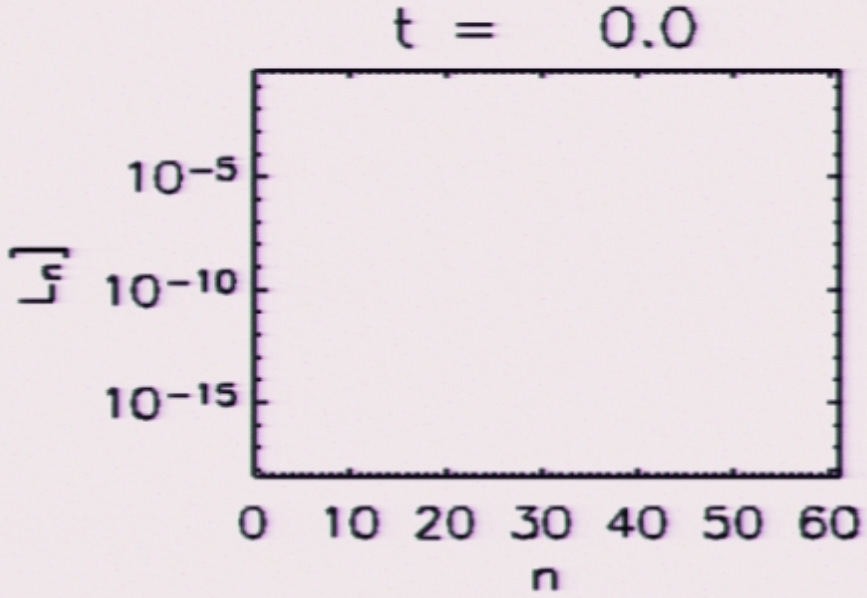
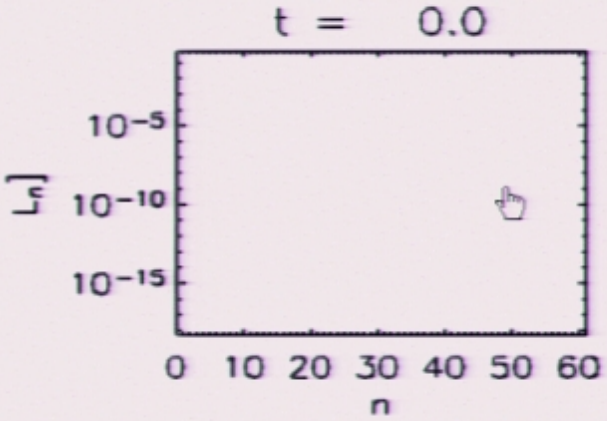
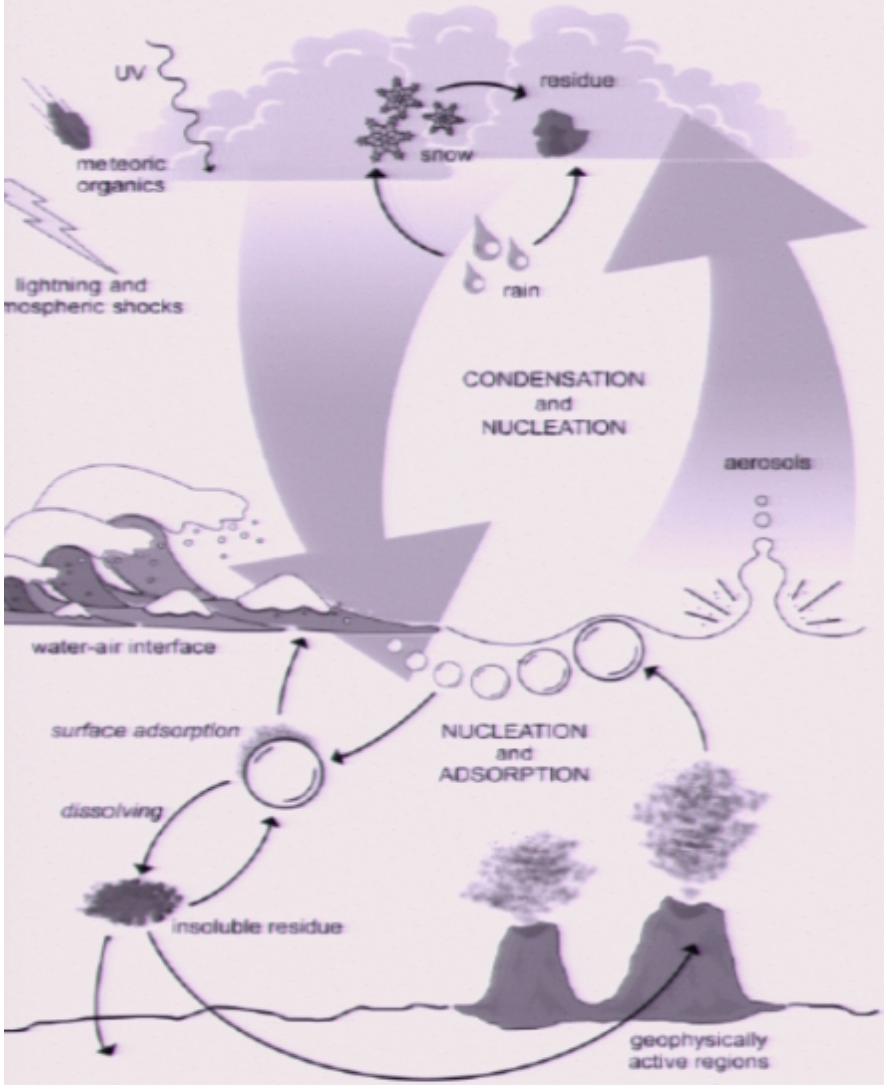
Racemic solution ~2^{1-n}



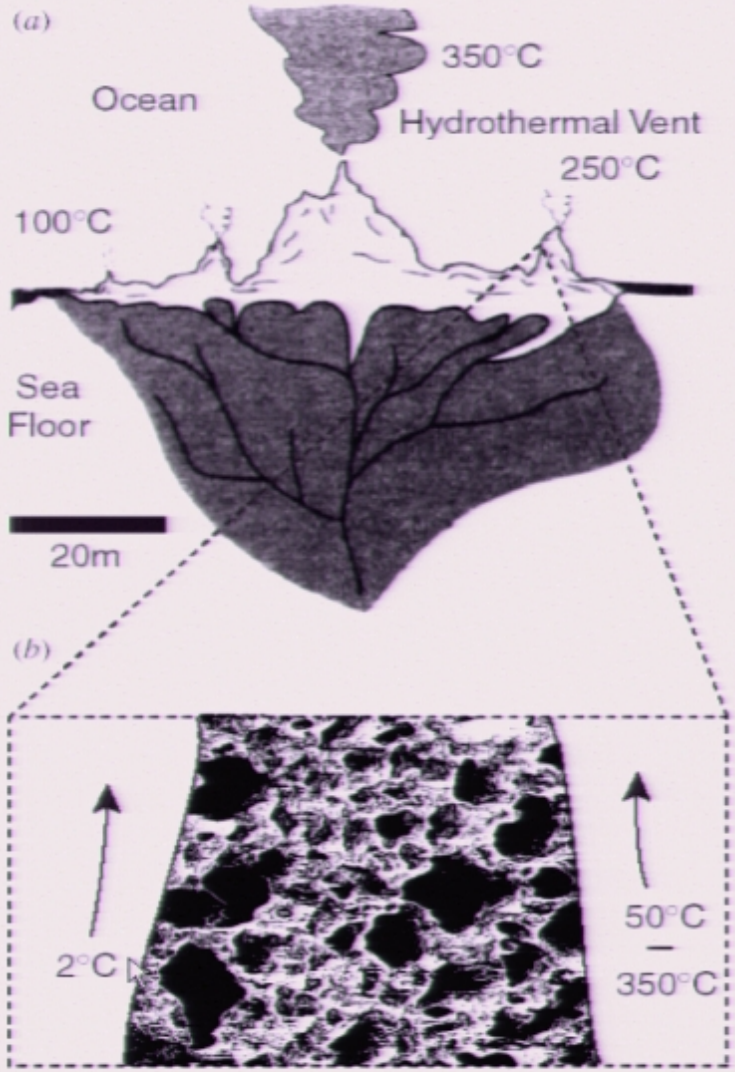


Stability

Where could this work?



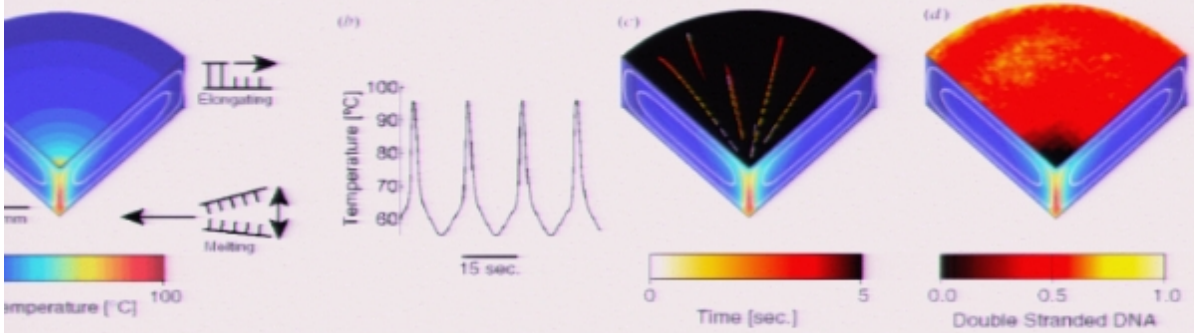
Lerman & Teng (2005)

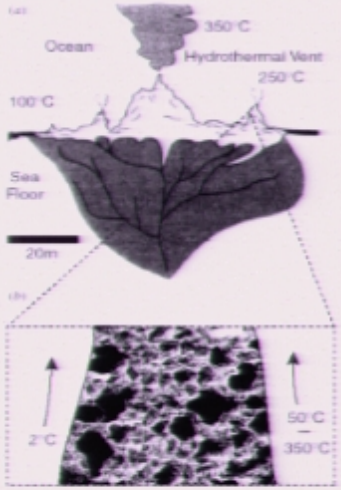


Braun & Libchaber (2003)

How to drive the system?

drothermal vents





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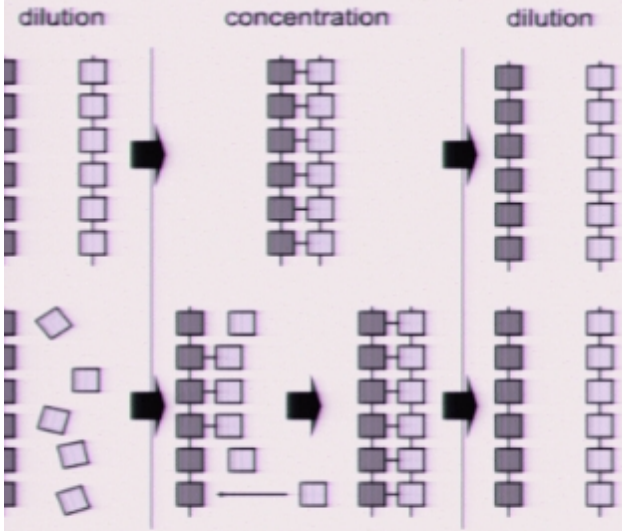
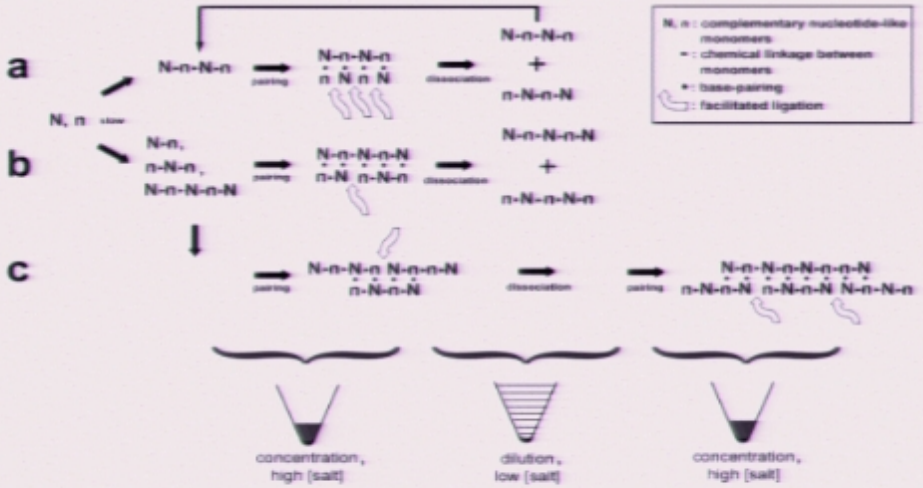
des





Lathe (2003)

Reduced equations

2-mode reduction

$$\frac{d}{dt}[L_2] = -2k_S[L_1]([L_2]-[L_1])$$

Adiabatic elimination
rapidly adjusting variables

$$0 = -2k_S[L_1]([L_2]-[L_1])$$

Quantitatively close to full model

$$\frac{dR}{dt} = \frac{R^2}{R^2+L^2} - (L+R)R$$

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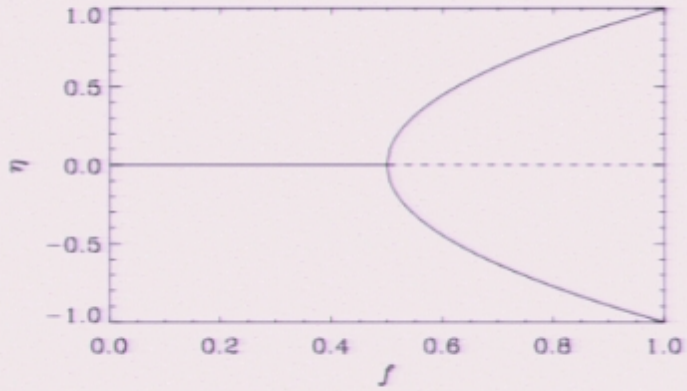
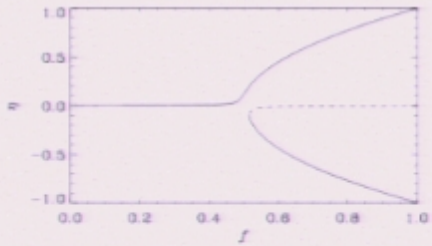
BAHN (Orig. Life Evol. Biosph. 2005)



Initial bias →



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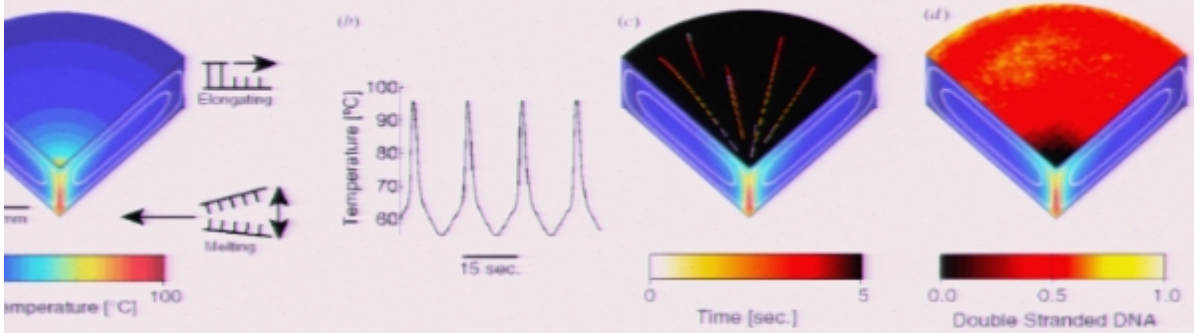
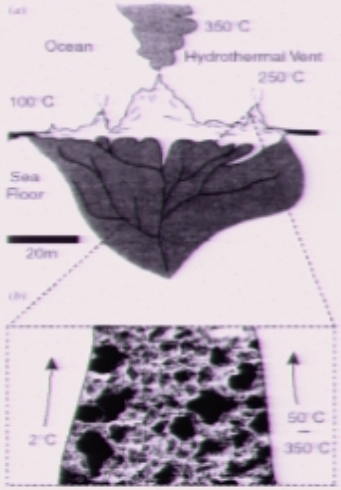
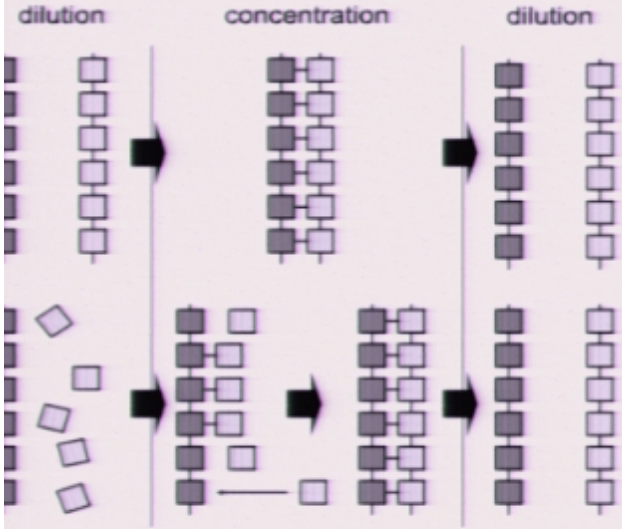
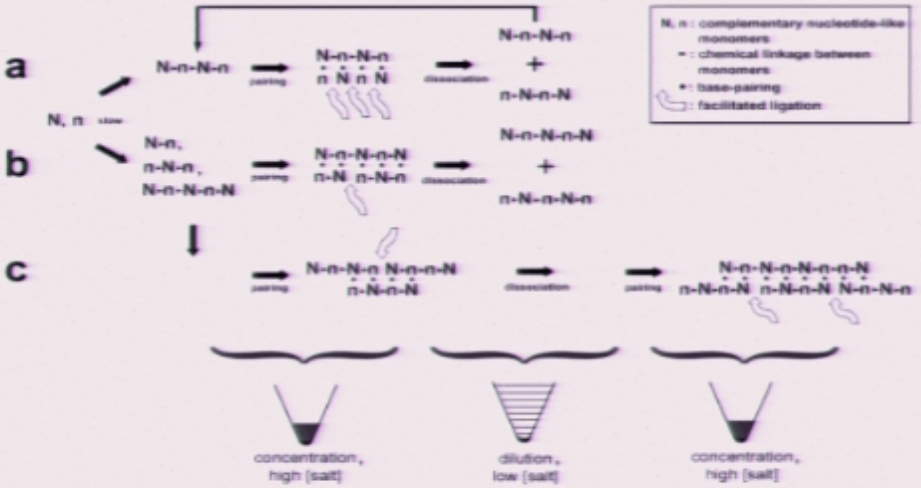




Braun & Libchaber (2003)

des





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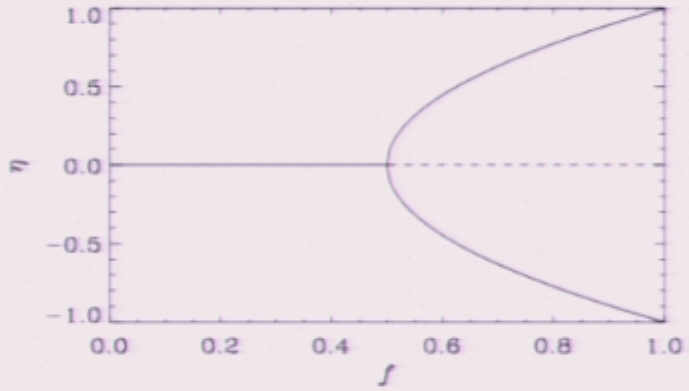

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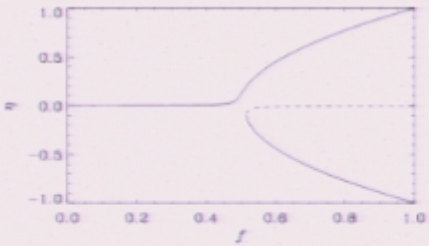


Spatially extended model

with Tuomas Multamäki, Int. J. Astrobio. 3, 209 (2004)

eaction-diffusion equation

$$\frac{dR}{dt} = \frac{R^2}{R^2+L^2} - (L+R)R + \kappa\nabla^2 R$$

$$\frac{dL}{dt} = \frac{L^2}{R^2+L^2} - (L+R)L + \kappa\nabla^2 L$$

roto type: Fisher's equation

$$\dot{X} = X(1-X) + \kappa X''$$

agating front solutions

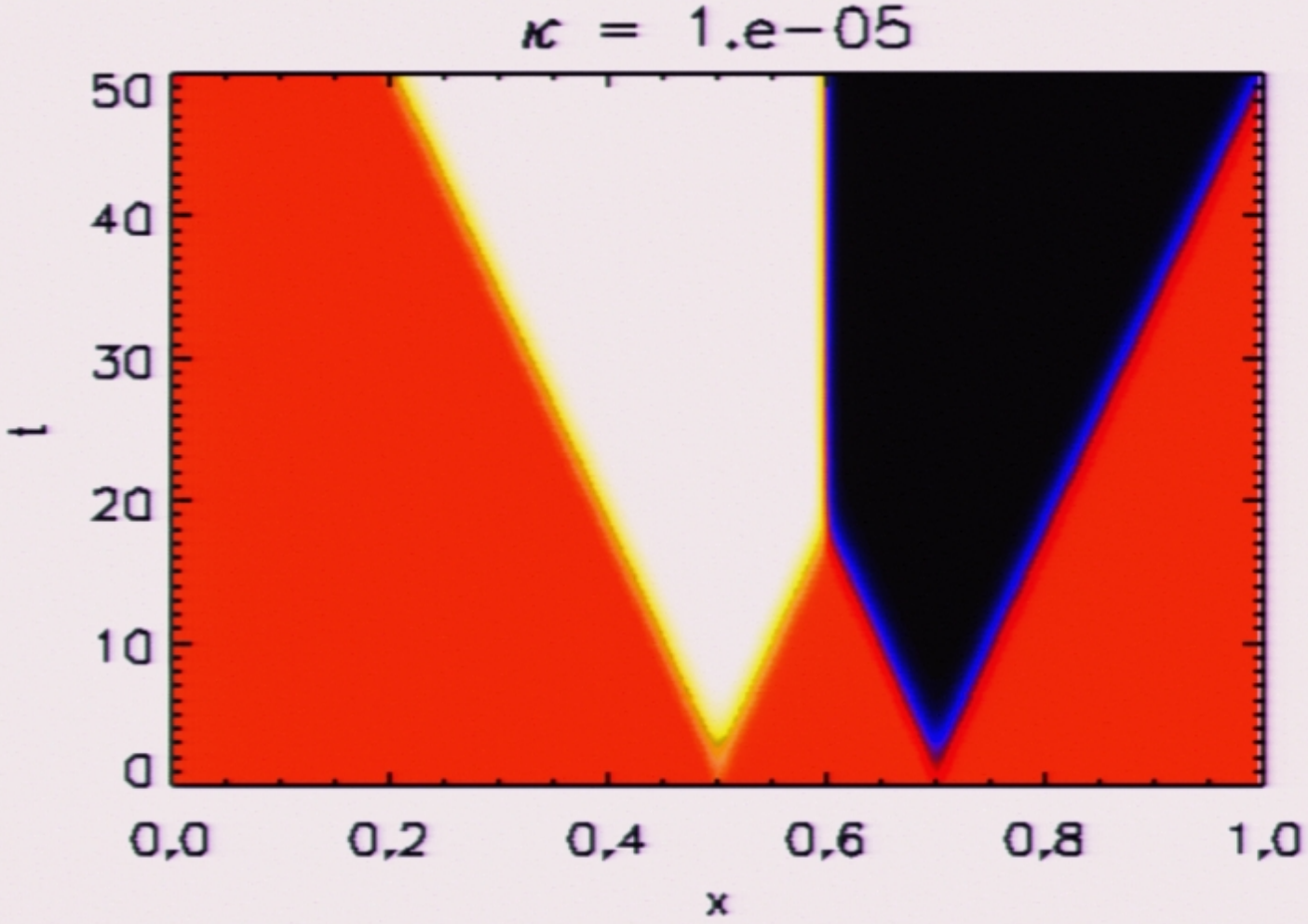
$$= f(x-ct)$$

wave speed

$$c \geq 2\sqrt{\lambda\kappa}$$

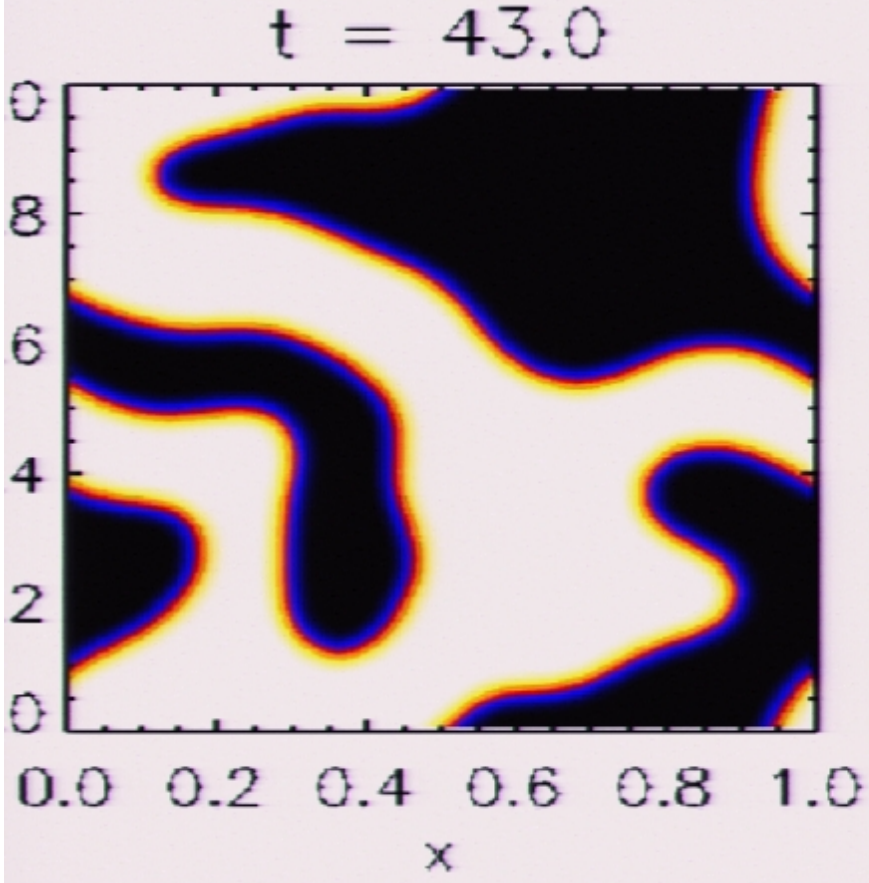
Spread of the black death

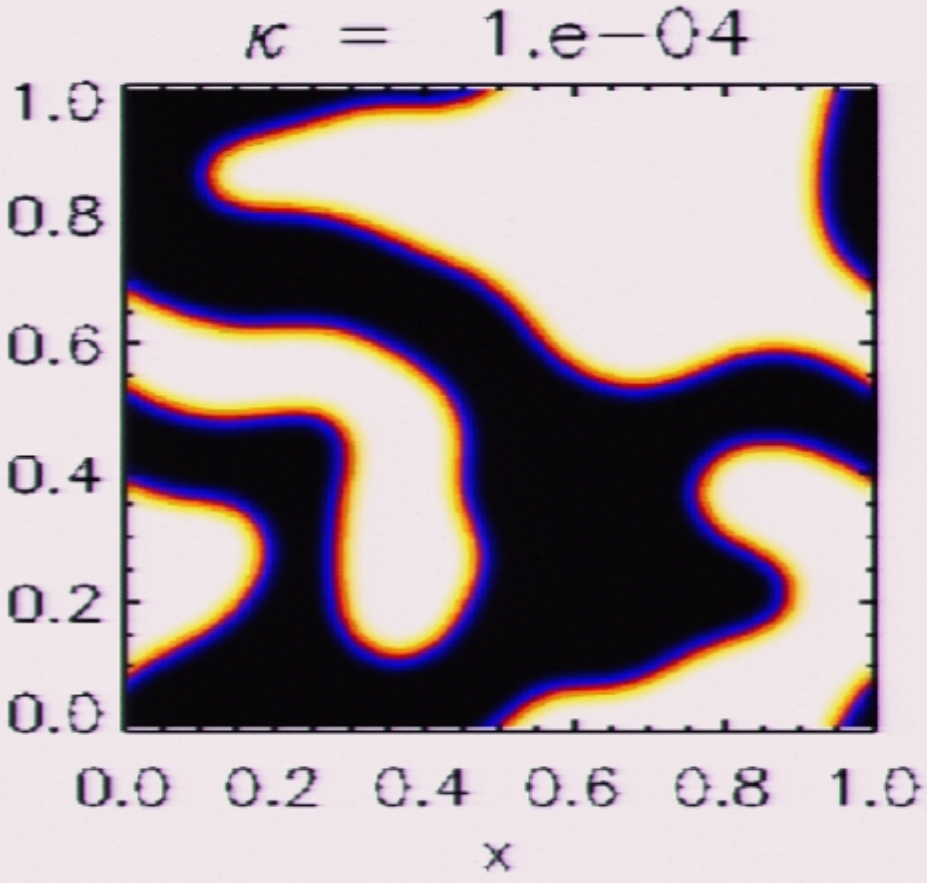
D model (reaction-diffusion equation)



Propagation into racemic environment

D model (reaction-diffusion equation)

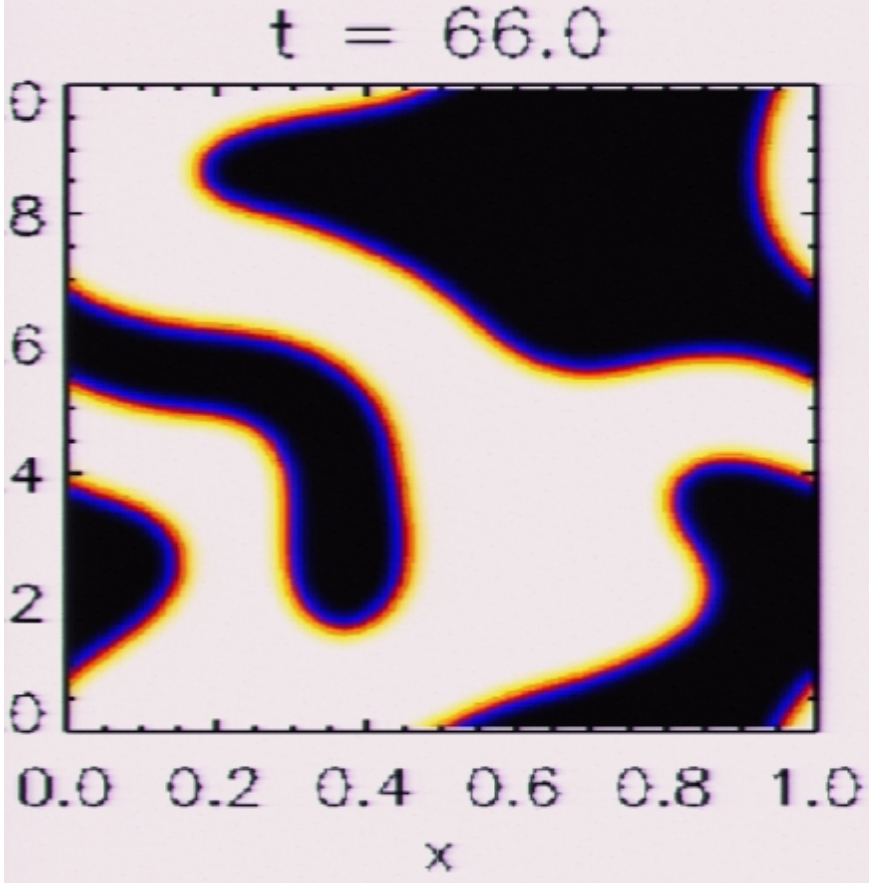


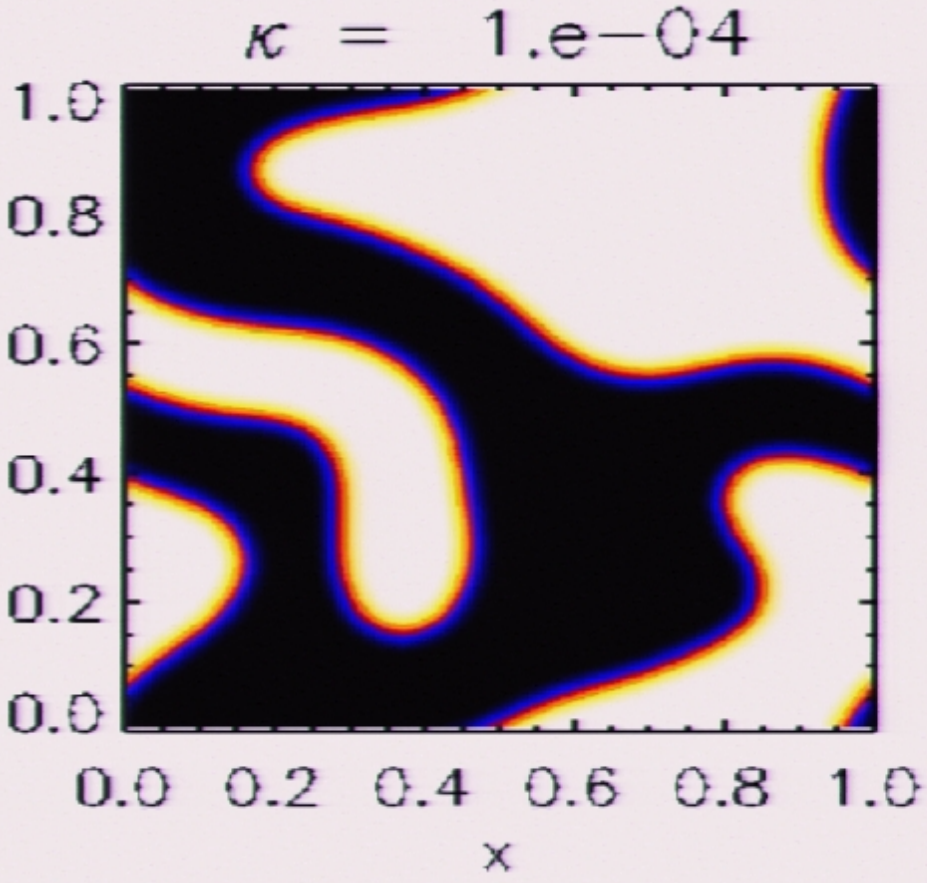


R L

short run

D model (reaction-diffusion equation)





R L

short run

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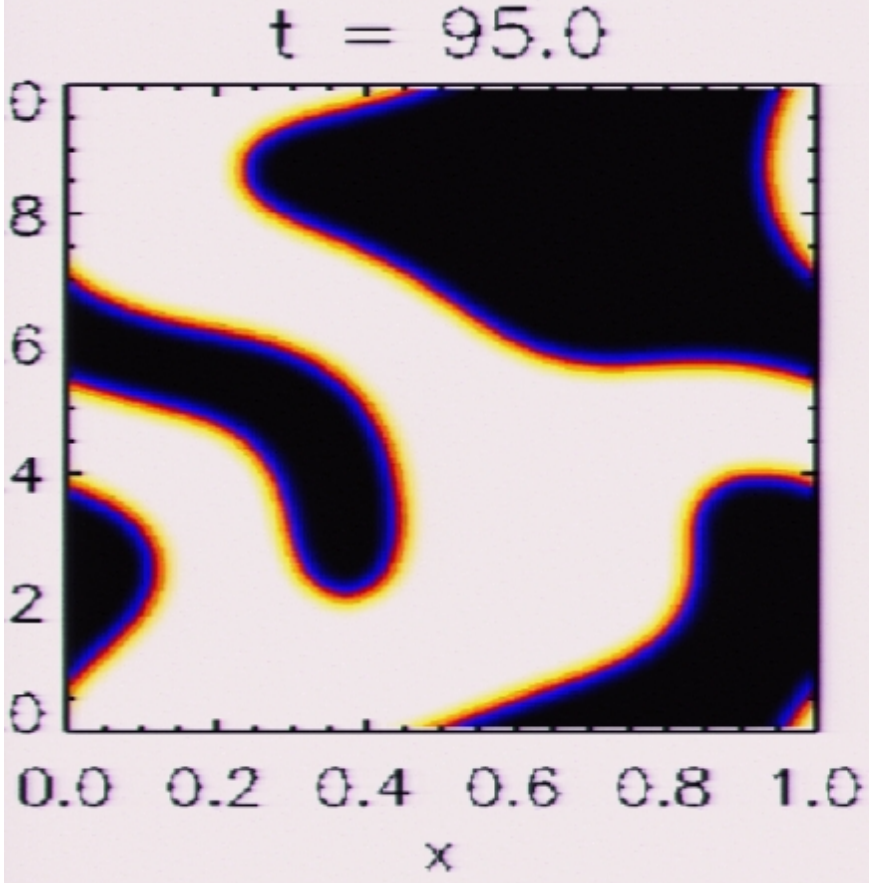
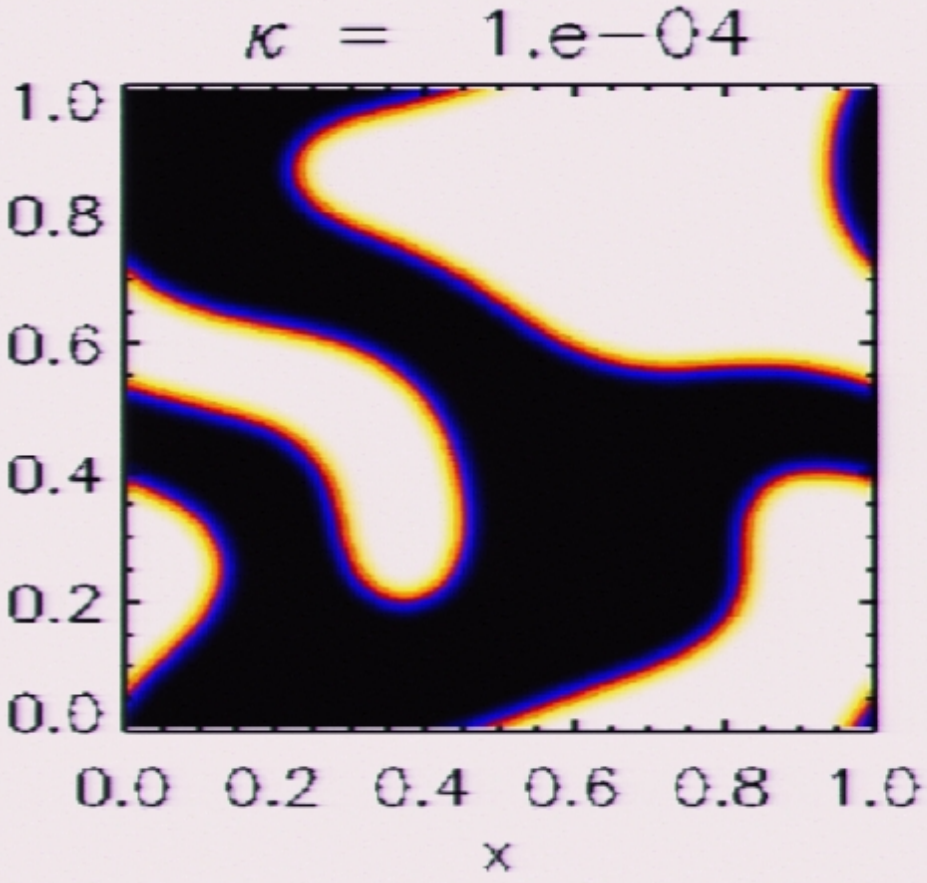
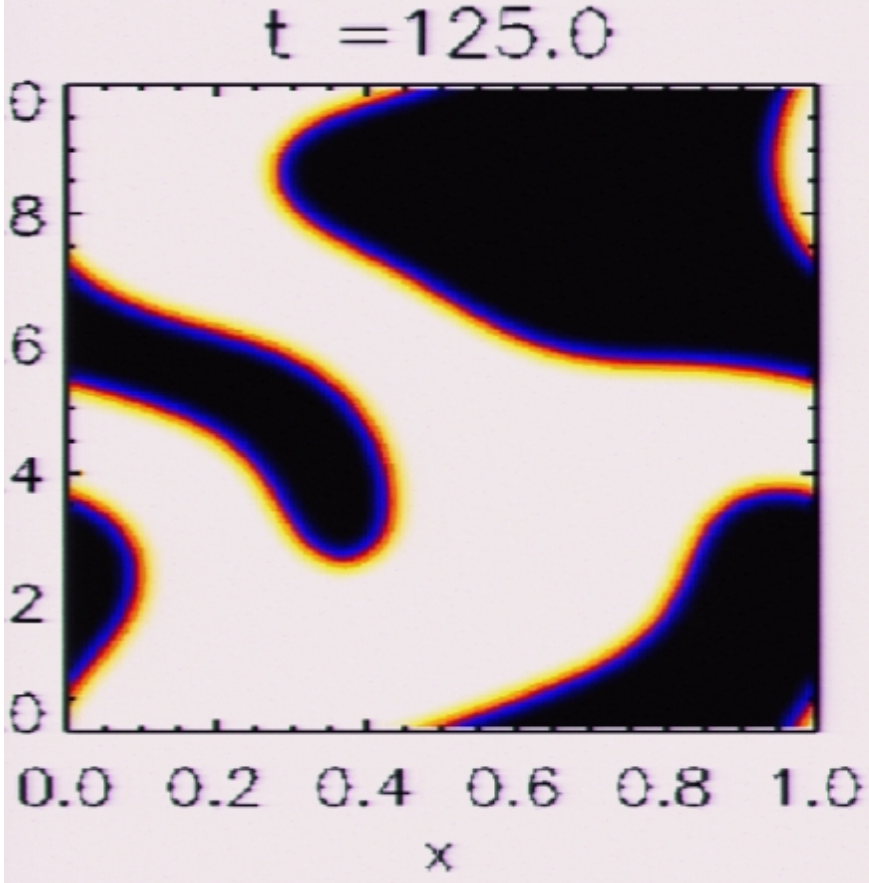


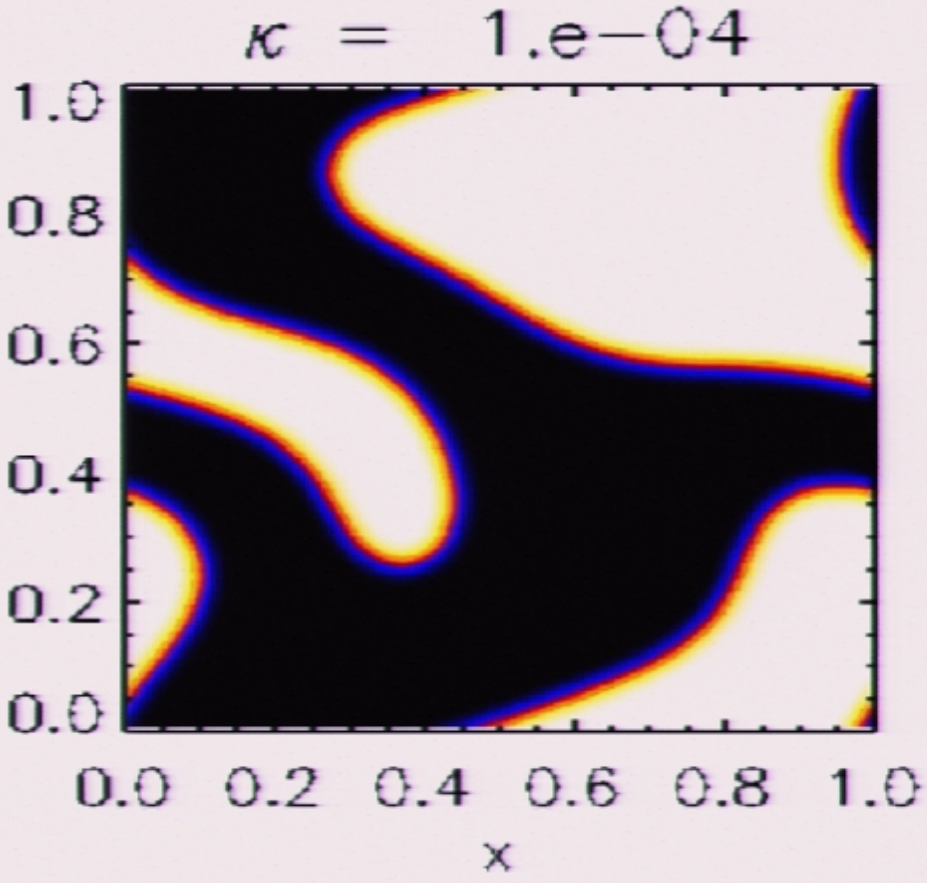


R L

short run

D model (reaction-diffusion equation)

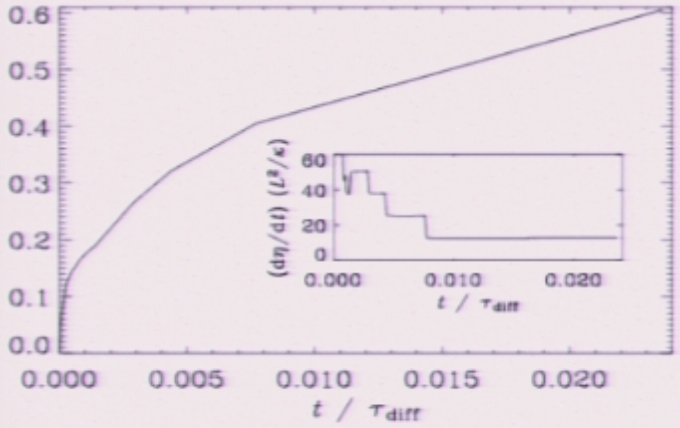


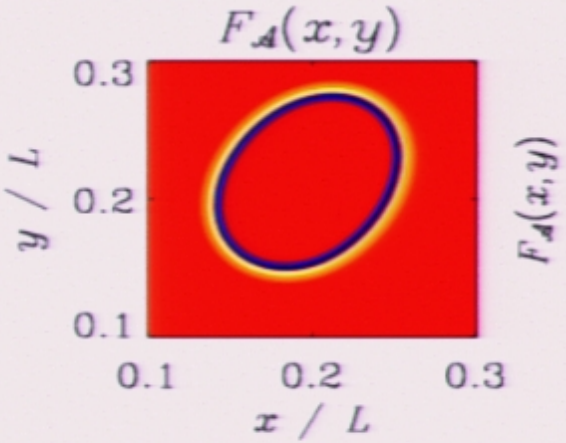


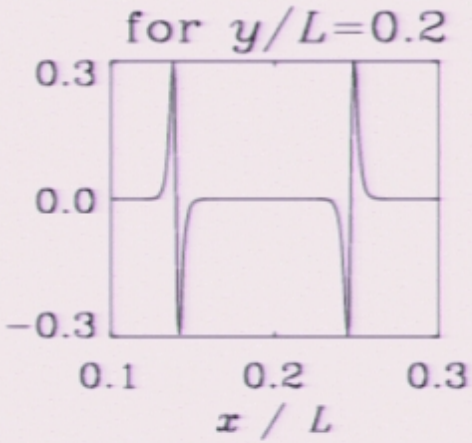
R L

short run

Piecewise linear increase







Reduced equations

$$\frac{dR}{dt} = \frac{R^2}{R^2+L^2} - (L+R)R$$

$$\frac{dL}{dt} = \frac{L^2}{R^2+L^2} - (L+R)L$$

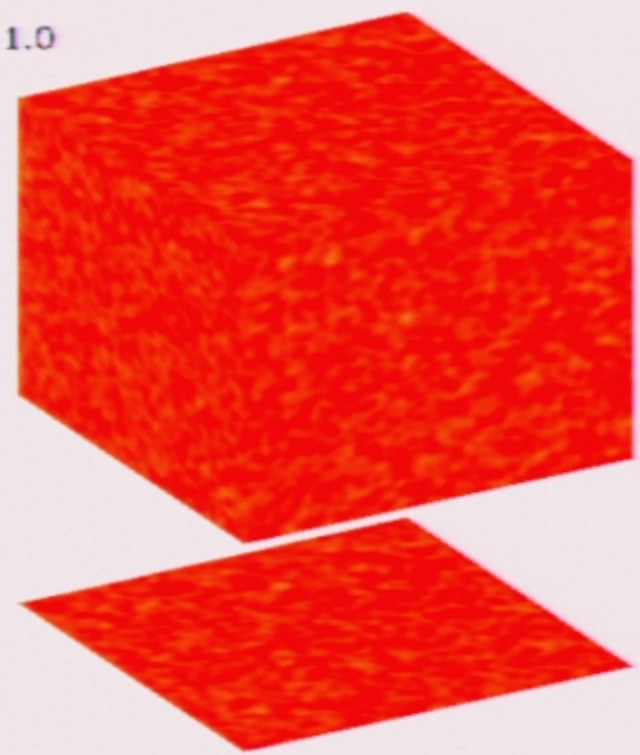
add/subtract:

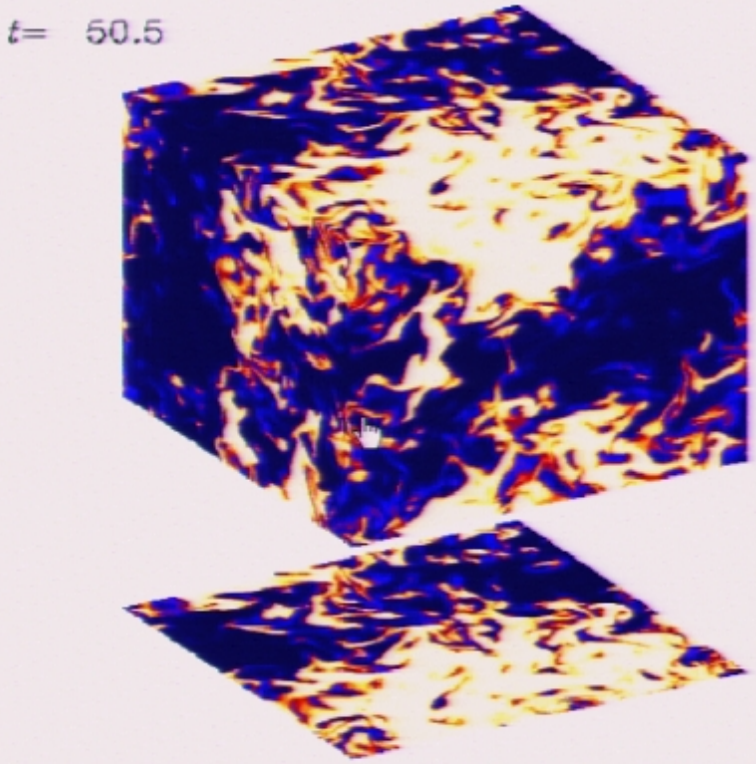
$$\dot{S} = 1 - S^2 + \kappa\nabla^2 S$$

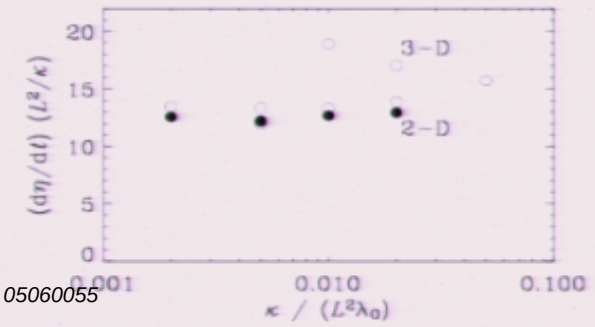
$$\dot{A} = \frac{2 - S^2 - A^2}{S^2 + A^2} SA + \kappa\nabla^2 A$$

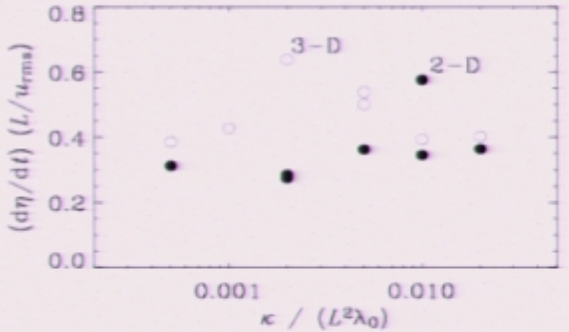
$$\Rightarrow \quad \frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = \int \frac{1-A^2}{1+A^2} A \, \mathrm{d}S$$

Effects of turbulence









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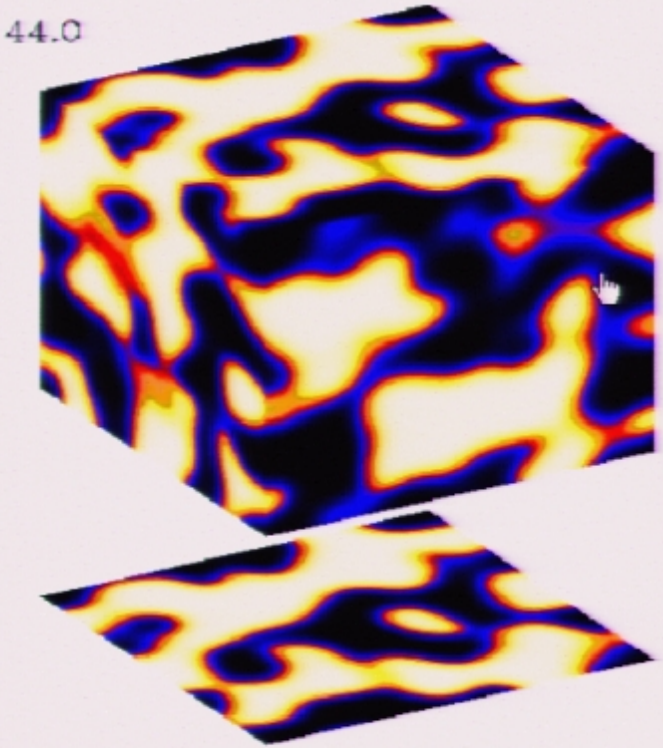
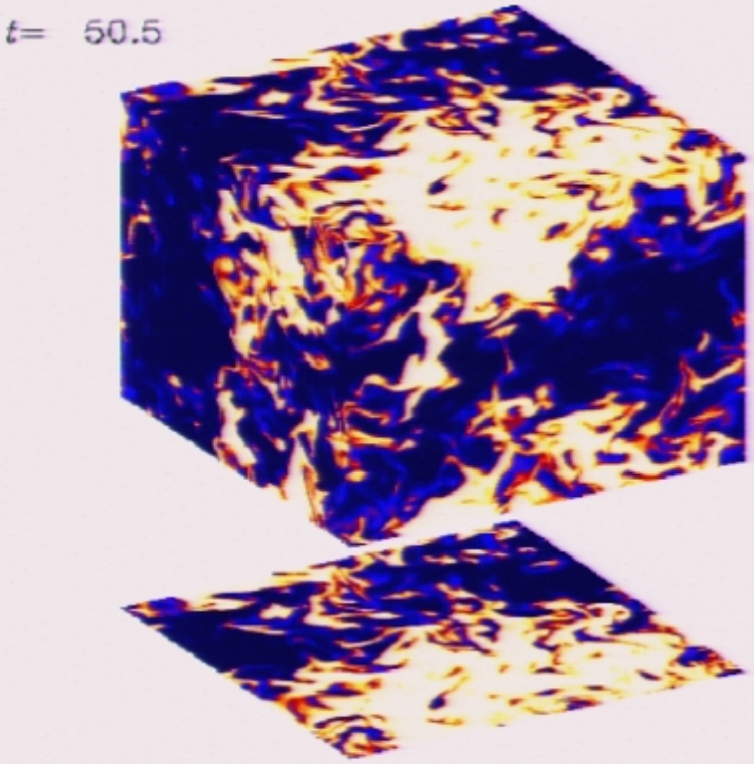
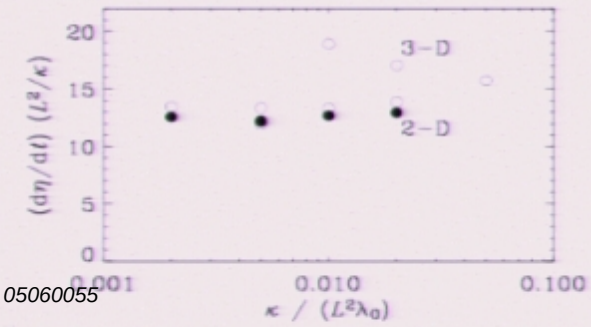
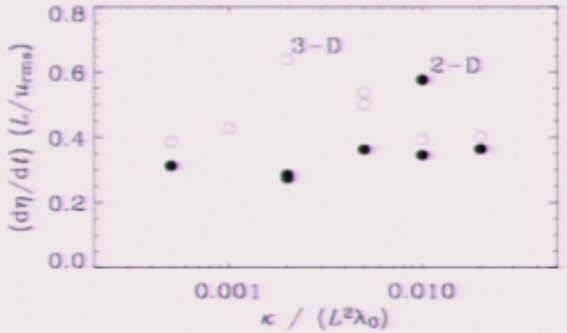








Pencil Code

Started in Sept. 2001 with Wolfgang Dobler

High order (6^{th} order in space, 3^{rd} order in time)

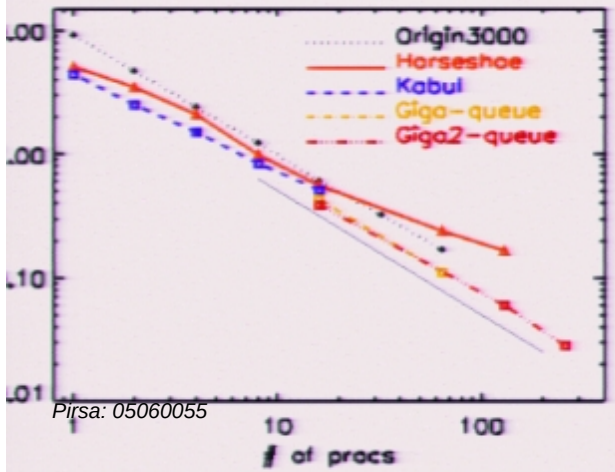
Cache & memory efficient

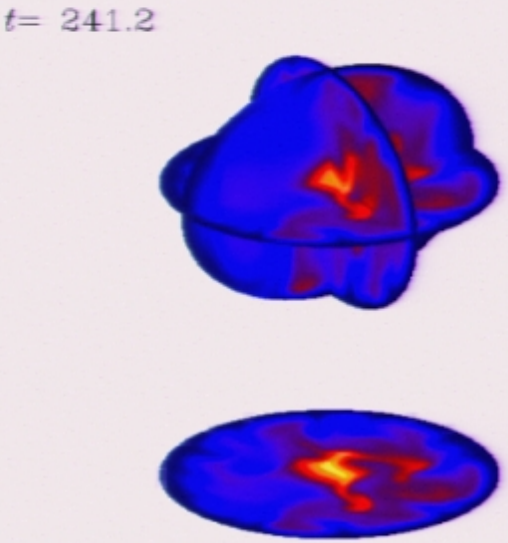
MPI, can run PacxMPI (across countries!)

Maintained/developed by ~20 people (CVS!)

Automatic validation (over night or any time)

Max resolution so far 1024^3, 256 procs

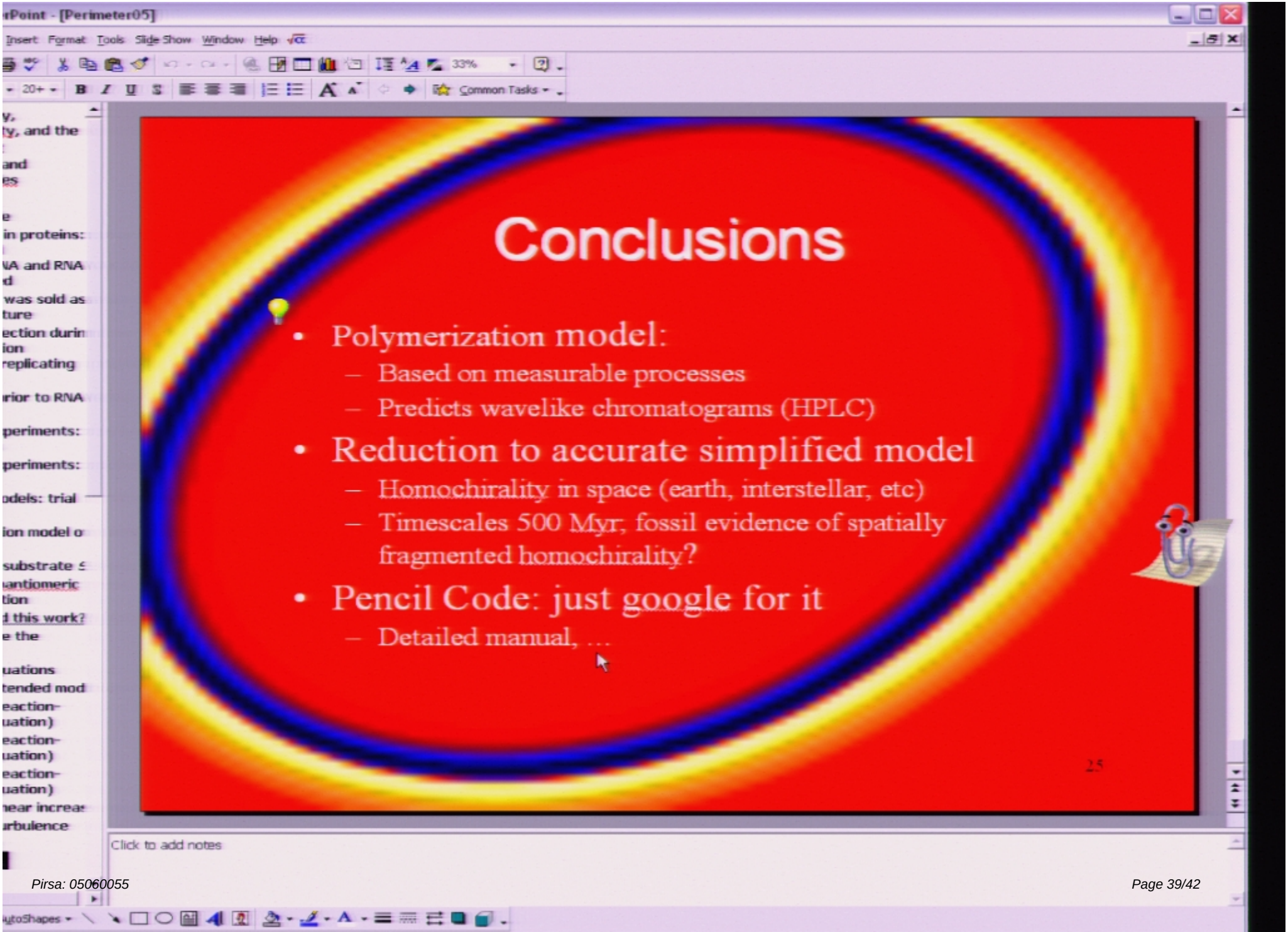




- Isotropic turbulence
  - MHD, passive scl, CR
- Stratified layers
  - Convection, radiation
- Shearing box
  - MRI, dust, interstellar
- Sphere embedded in box
  - Fully convective stars
  - geodynamo
- Other applications
  - Homochirality
  - Spherical coordinates

Conclusions

- Polymerization model:
  - Based on measurable processes
  - Predicts wavelike chromatograms (HPLC)
- Reduction to accurate simplified model
  - Homochirality in space (earth, interstellar, etc)
  - Timescales 500 Myr; fossil evidence of spatially fragmented homochirality?
- Pencil Code: just google for it
  - Detailed manual, …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Common Tasks
Conclusions
• Polymerization model:
– Based on measurable processes
– Predicts wavelike chromatograms (HPLC)
• Reduction to accurate simplified model
– Homochirality in space (earth, interstellar, etc)
– Timescales 500 Myr; fossil evidence of spatially fragmented homochirality?
• Pencil Code: just google for it
– Detailed manual, …
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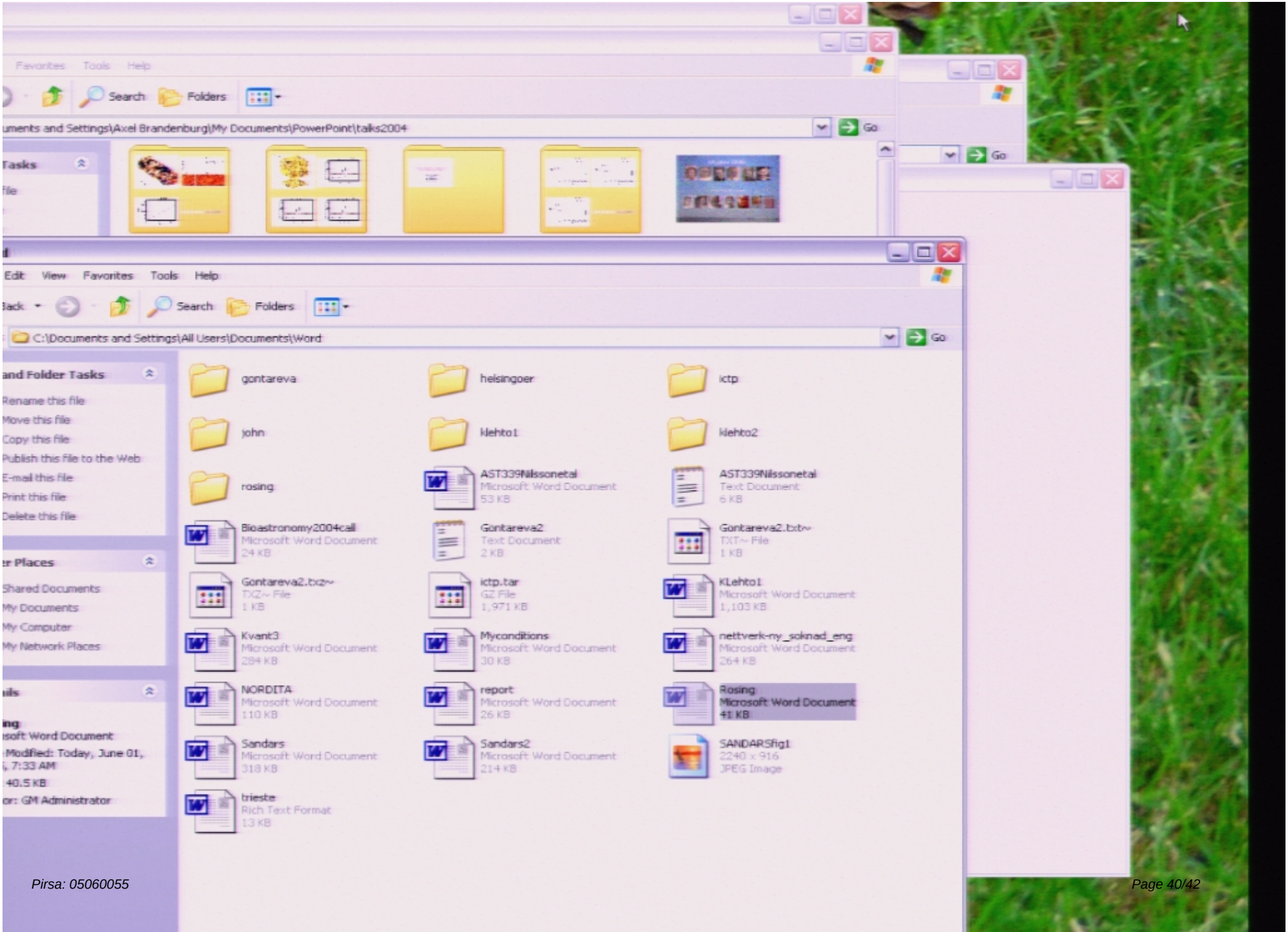
Click to add notes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