Maximum entropy production and ecosystems

Roderick Dewar

The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

International Atomic Energy Agency

SMR 1655 - 13

WORKSHOP ON QUANTITATIVE ECOLOGY
9 to 20 May 2005

Maximum entropy production and ecosystems

Roderick C. DEWAR
Unit Functioning Ecology and Environmental Physics
INRA Bordeaux
France

These are preliminary lecture notes, intended only for distribution to participants.

Maximum entropy production and ecosystems

Roderick C Dewar

Unit of Functional Ecology and

Environmental Physics INRA Bordeaux

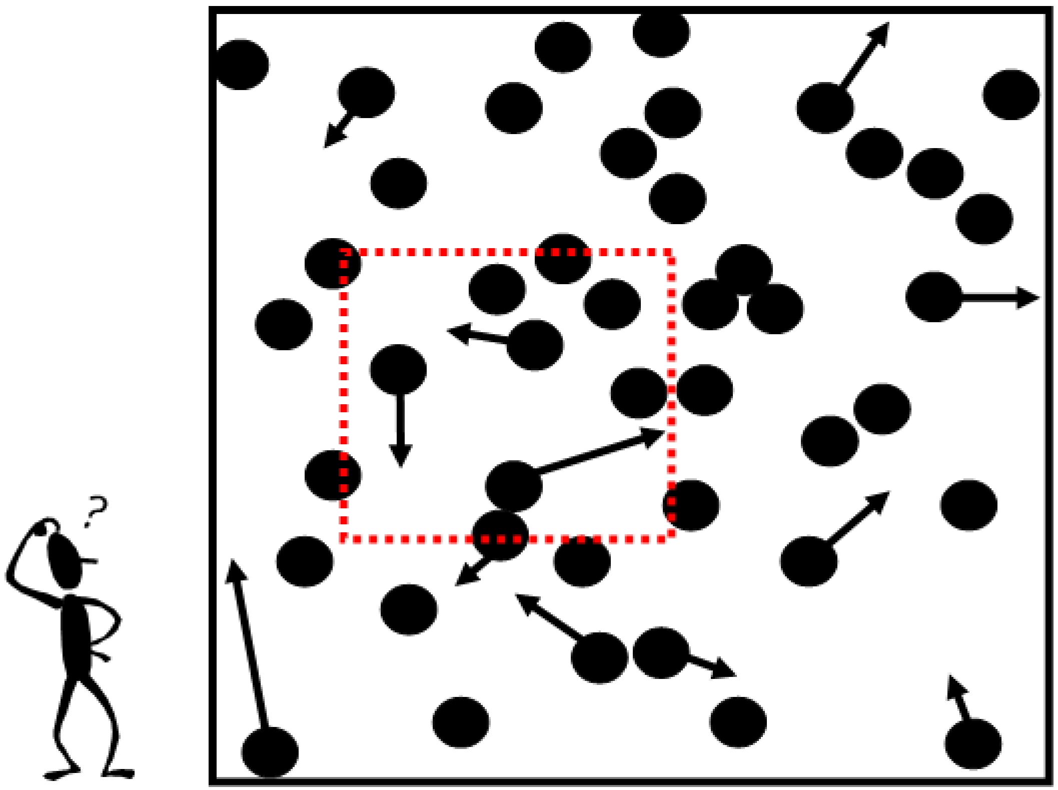
France

Workshop on Quantitative Ecology, Abdus Salam ICTP Trieste, 9-20 May 2005

- Natural selection and diversity in physics
- MaxEnt and maximum entropy production
- Natural selection and diversity in ecology

- Natural selection and diversity in physics
- MaxEnt and maximum entropy production
- Natural selection and diversity in ecology

Why is there such a diversity of molecular positions and velocities ?



$\langle N_s \rangle$, $\langle E_s \rangle$, V_s fixed

N, E, V fixed

Macroscopic description *A*

spatial distribution of molecules in box

S_A = entropy of *A*

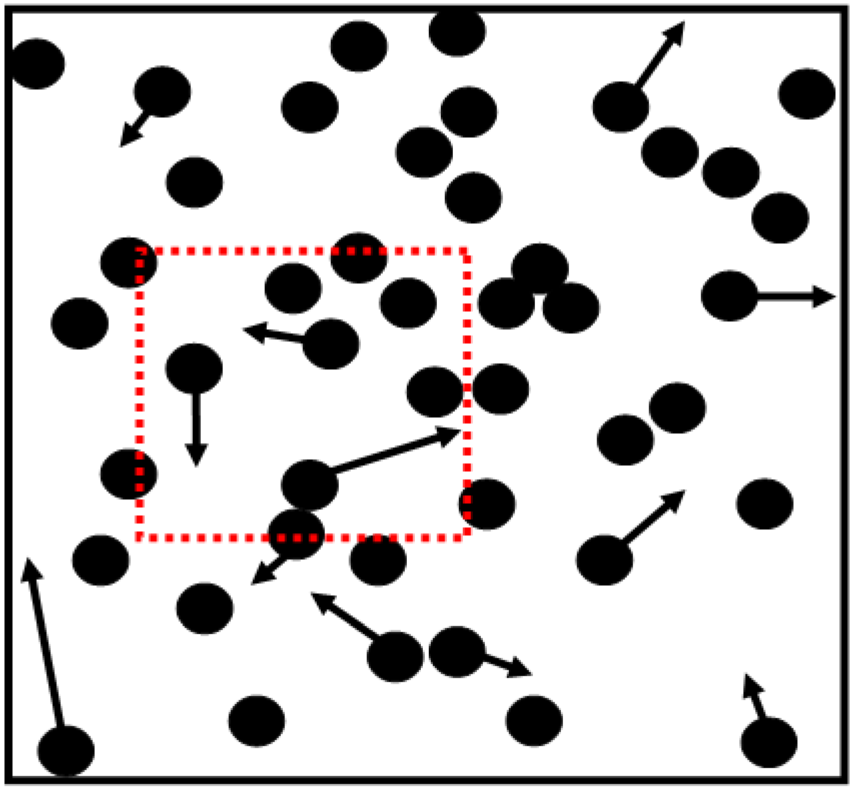
Ludwig Boltzmann
(1844 - 1906)

Microscopic description *i*

individual positions of every molecule

W_A = number of ways *A* can be realized microscopically

Diverse (spread-out) distributions are more probable (W is bigger)



$\langle N_s \rangle$, $\langle E_s \rangle$, V_s fixed

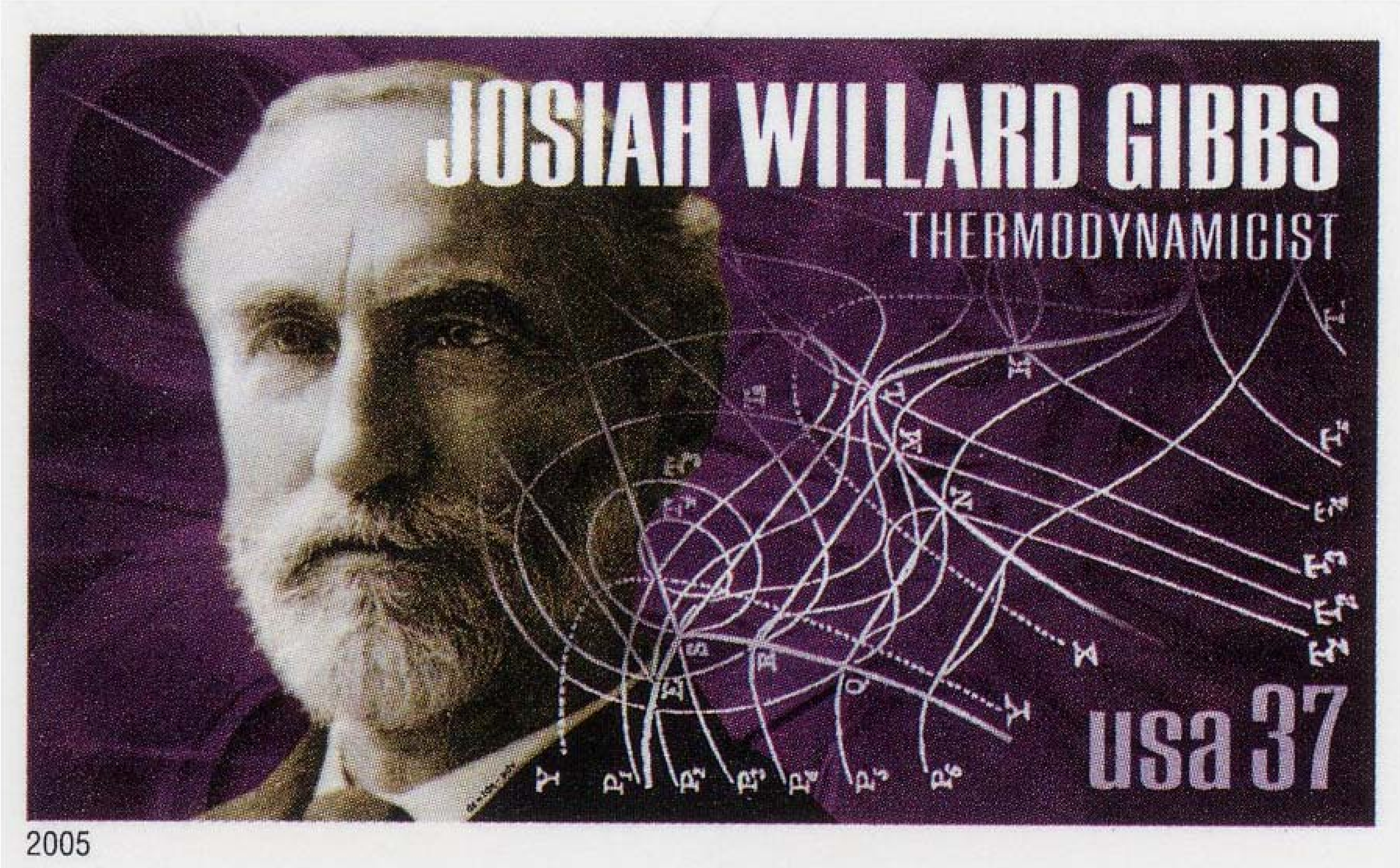
N, E, V fixed

- Natural selection and diversity in physics
- MaxEnt and maximum entropy production
- Natural selection and diversity in ecology

Summary

- Under given constraints (N, E, V), nature selects the most diverse (spread-out) distribution simply because it is the most probable one (max S = max log$W$)
- The maximum diversity (max S) attainable under given constraints increases as those constraints are removed

- Natural selection and diversity in physics
- MaxEnt and maximum entropy production
- Natural selection and diversity in ecology



(1839 - 1903)

The Gibbs algorithm (MaxEnt) ...

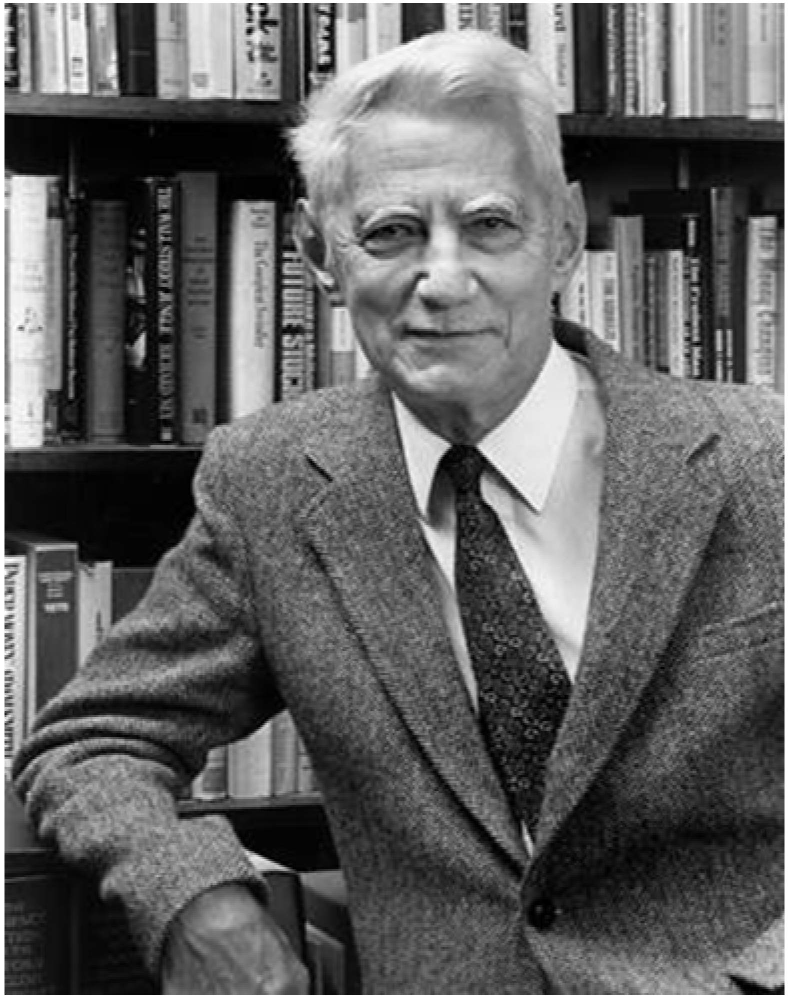
p_i : probability that the system is in microstate i
Given $\langle E \rangle$, what is p_i ?

Maximise : $H = -\Sigma_i \, p_i \log p_i$

Subject to : $\Sigma_i \, p_i E_i = \langle E \rangle$ (given energy)
$\Sigma_i \, p_i = 1$ (normalisation)

Solution : $$p_i = \frac{1}{Z} \exp\left(-\frac{E_i}{kT} \right)$$ (= Boltzmann)

… it worked but what did it mean ?



Claude Shannon
(1916 - 2001)

$$H = -\Sigma_i \, p_i \log p_i$$

- H is a measure of the missing information about outcomes i
- (H = uncertainty)

- H is larger if p_i is more spread-out
- (H = diversity)

- $H \approx \log W$ where W is the number of outcomes i with $p_i > 0$
- ($H \approx$ Boltzmann entropy S)

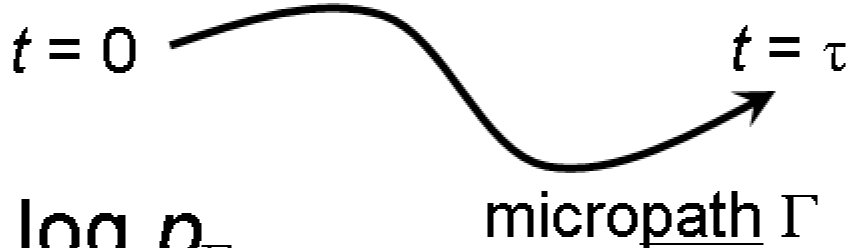
$\max H = -\Sigma_i \, p_i \log p_i$

- MaxEnt is a completely general algorithm for contructing p_i from known constraints C
- it works because it gives the most probable distribution under C (Gibbs ~ Boltzmann)
- it predicts the behaviour that is reproducibly selected under C
- it can be applied to non-equilibrium systems (e.g. climate, ecosystems ...)

Edwin Jaynes (1922 - 1998)

MaxEnt for non-equilibrium systems

J Phys A **36**, 631-641 (2003)
J Phys A **38**, L371-L381 (2005)



Maximise : $H_{\text{path}} = -\Sigma_\Gamma\, p_\Gamma \log p_\Gamma$

Subject to :

$\Sigma_\Gamma\, p_\Gamma J_\Gamma = \langle J \rangle$ (given energy flux)

$\Sigma_\Gamma\, p_\Gamma = 1$ (normalisation)

$\partial\rho_\Gamma / \partial t = -\nabla \cdot J_\Gamma$ (local continuity)

Solution :

$$p_\Gamma = \frac{1}{Z_{\text{path}}} \exp\left(\frac{\tau}{2k} \int_V J_\Gamma \nabla\left(\frac{1}{T}\right) \right)$$

entropy production (EP_Γ)

Two fundamental implications of the MaxEnt solution $p_\Gamma \propto \exp(\tau \mathrm{EP}_\Gamma / 2k)$

- *Maximum entropy production*
- *(or, sometimes, maximum flux) :*

The average entropy production $\langle \mathrm{EP} \rangle$ (or, sometimes the average flux $\langle \mathrm{F} \rangle$) takes its maximum possible value under the imposed constraints

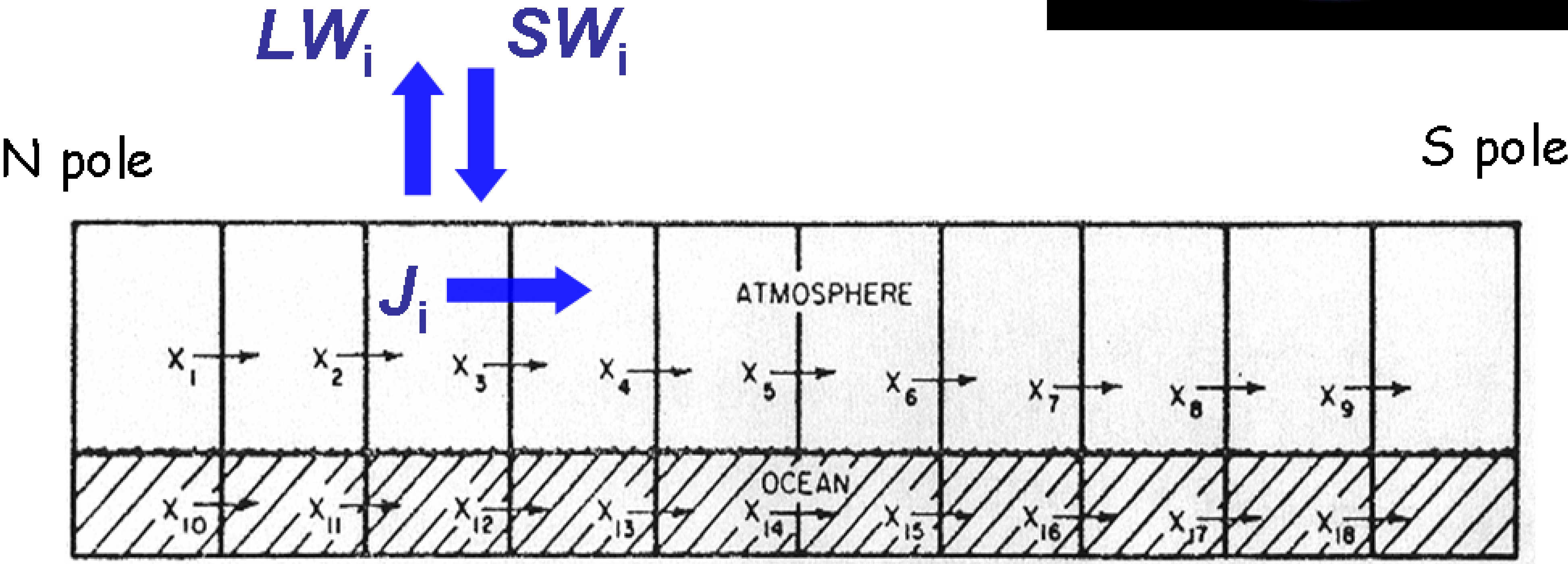
- *Fluctuation theorem :*

$\langle \mathrm{EP} \rangle = (\tau/2k)\,Var(\mathrm{EP})$

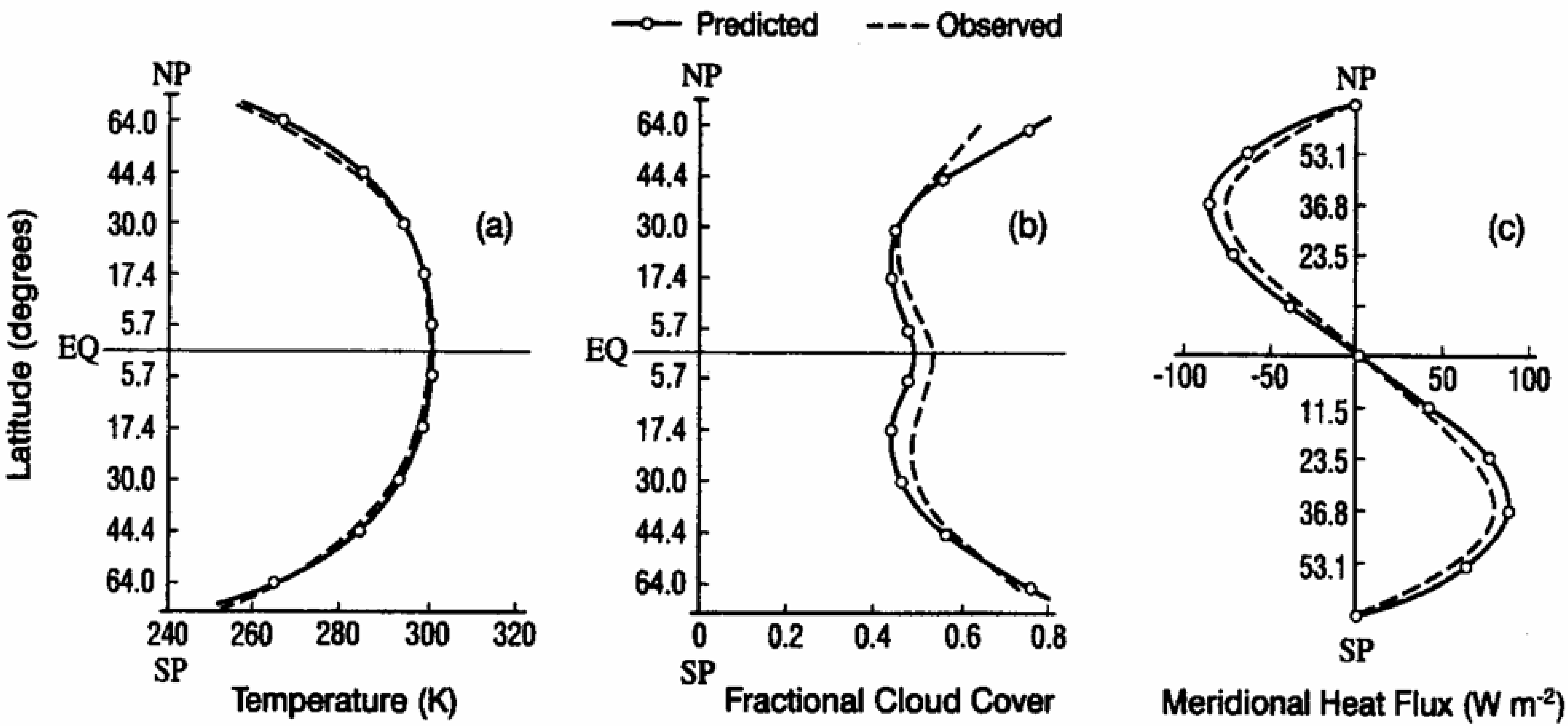
Paltridge (1978) :

10-zone climate model

$$EP_{planet} = \sum_{zone\ i=1}^{10} J_i \left(\frac{1}{T_{i+1}} - \frac{1}{T_i} \right)$$



Paltridge (1978) : MEP predictions from a 10-zone climate model



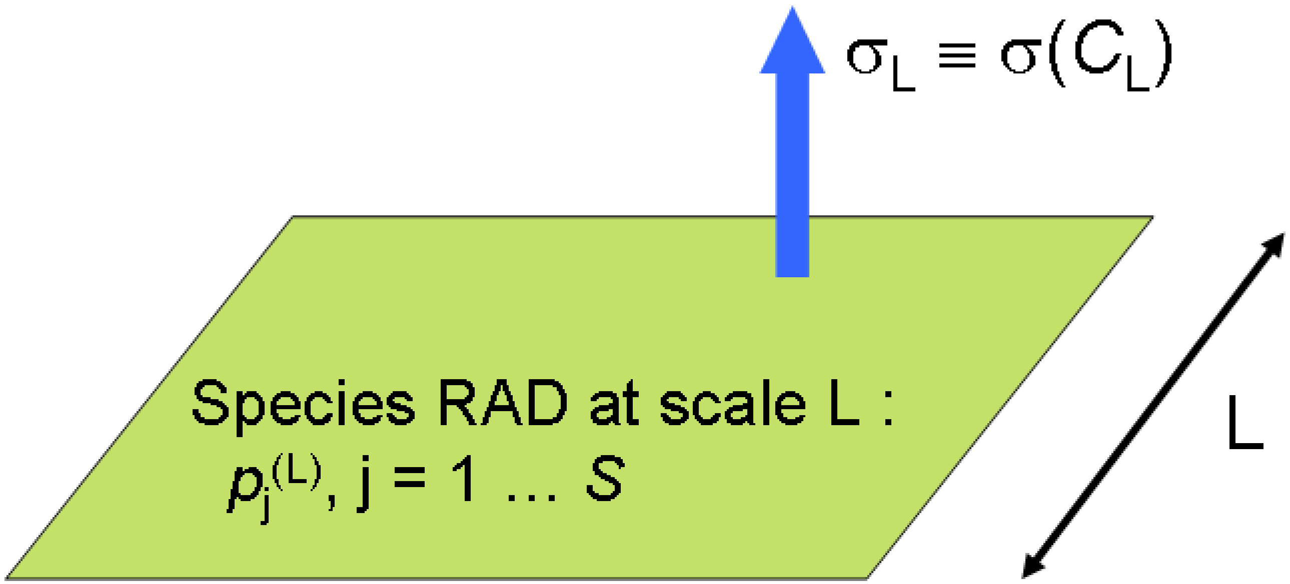
- Natural selection and diversity in physics
- **MaxEnt and maximum entropy production**
- Natural selection and diversity in ecology

Summary

- MaxEnt is a very general algorithm for predicting the behaviour which nature selects reproducibly under given constraints
- For non-equilibrium systems, MaxEnt predicts that nature selects the stationary state with the greatest entropy production
- Empirical evidence so far mainly from physics (planetary climates, thermal and shear turbulence, crystal growth ….)

- Natural selection and diversity in physics
- MaxEnt and maximum entropy production
- Natural selection and diversity in ecology

- C_L = constraints at scale L (J_{solar}, $J_{precipitation}$ …)
- Apply MaxEnt to p_Γ subject to C_L
- $\Rightarrow$ maximum $\langle EP_L \rangle$ at scale L = $\sigma(C_L)$



- What is the most probable RAD, $p_j^{(L)}$?
- Apply MaxEnt to $p_j^{(L)}$ subject to σ_L

Maximise :

$$H_L = -\sum_{j=1}^{S} p_j^{(L)} \log\left(p_j^{(L)}\right) \qquad \text{(log \# species)}$$

Subject to :

$$\sum_{j=1}^{S} p_j^{(L)} \sigma_j = \sigma_L \qquad \text{(given } \sigma_L \text{, } i.e.\ C_L\text{)}$$

$$\sum_{j=1}^{S} p_j^{(L)} = 1 \qquad \text{(normalisation)}$$

Solution :

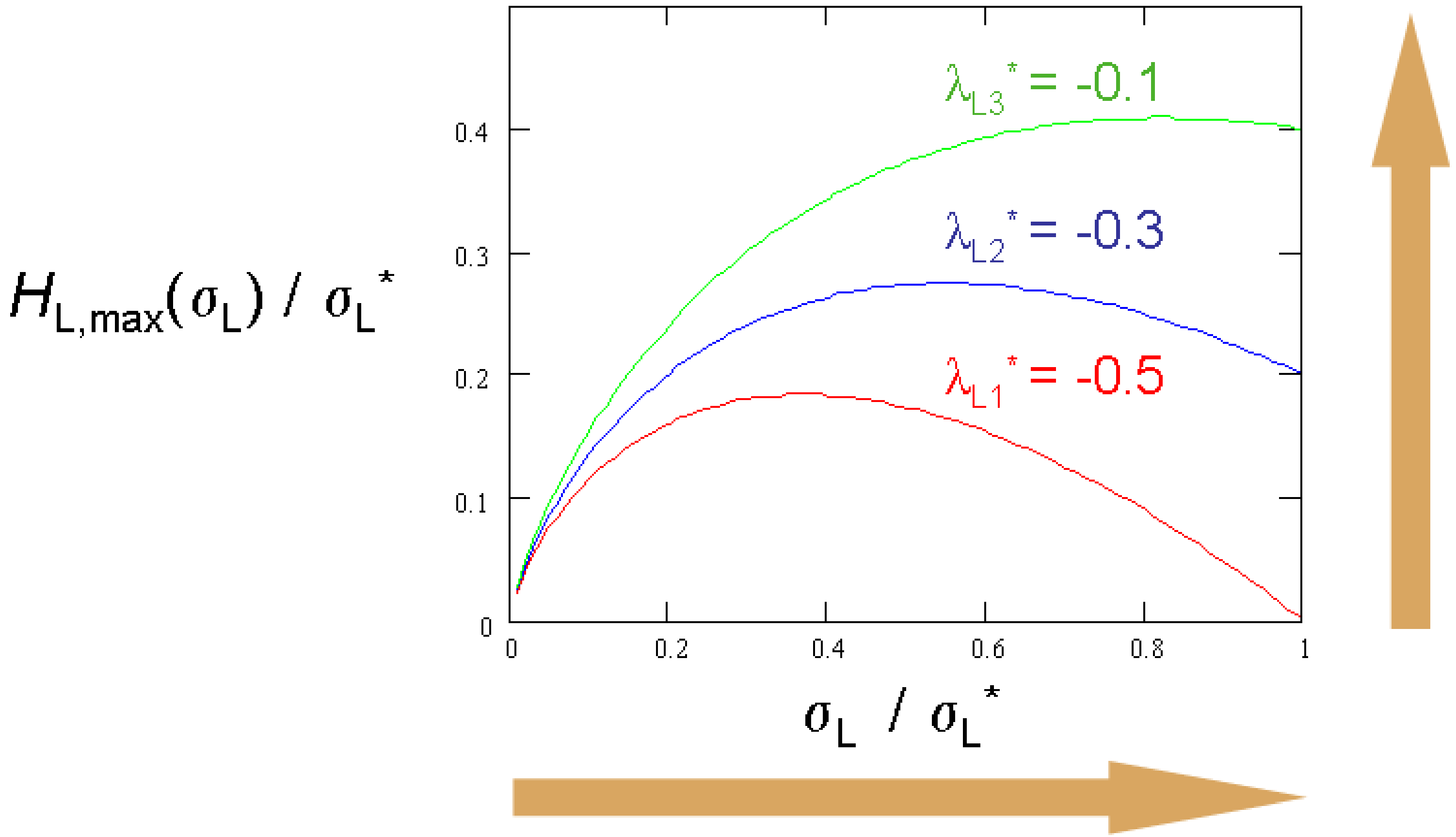
$$p_j^{(L)} = \frac{1}{Z_L} \exp\left(-\lambda_L \sigma_j\right) \qquad \text{where } \lambda_L = \lambda_L(\sigma_L)$$

$$\lambda_L(\sigma_L) = \frac{d H_{L,\max}(\sigma_L)}{d\sigma_L}$$

$$\frac{d\lambda_L}{d\sigma_L} = -\frac{1}{\mathrm{Var}(EP_L)} = -\frac{1}{2\sigma_L}$$

fluctuation theorem !

log (# species) vs. σ_L on different spatial scales



Increasing spatial scale L

$\lambda_L^* \equiv \lambda_L(\sigma_L^*)$
(model-specific)

Constraint C_L removed at fixed L
(*e.g.* increasing J_{solar})

Some other ongoing applications of maximum entropy production

Global climate patterns (G Paltridge, GD Farquhar)

Biosphere-climate feedbacks (A Kleidon, J Ogée, F Million)

Turbulent transport in atmospheric boundary layers (J-F Wang)

Leaf stomatal behaviour (S Delzon)

Optimal molecular structure of chloroplast ATP-synthase
(D Juretić, P Zupanović)

conclusions & conjectures

- MaxEnt is a general statistical method for predicting the most probable behaviour under given constraints

- For non-equilibrium systems, MaxEnt predicts that nature selects the stationary state with the greatest entropy production (MEP)

- Natural selection in both physics and biology
- = selection of the most probable ‘macroscopic’ state
- = selection of maximum ‘microscopic’ diversity

- Ecosystem diversity and functioning at different spatial scales reflects behaviour of maximum entropy production (σ_L) under scale-dependent changes in resources (C_L)