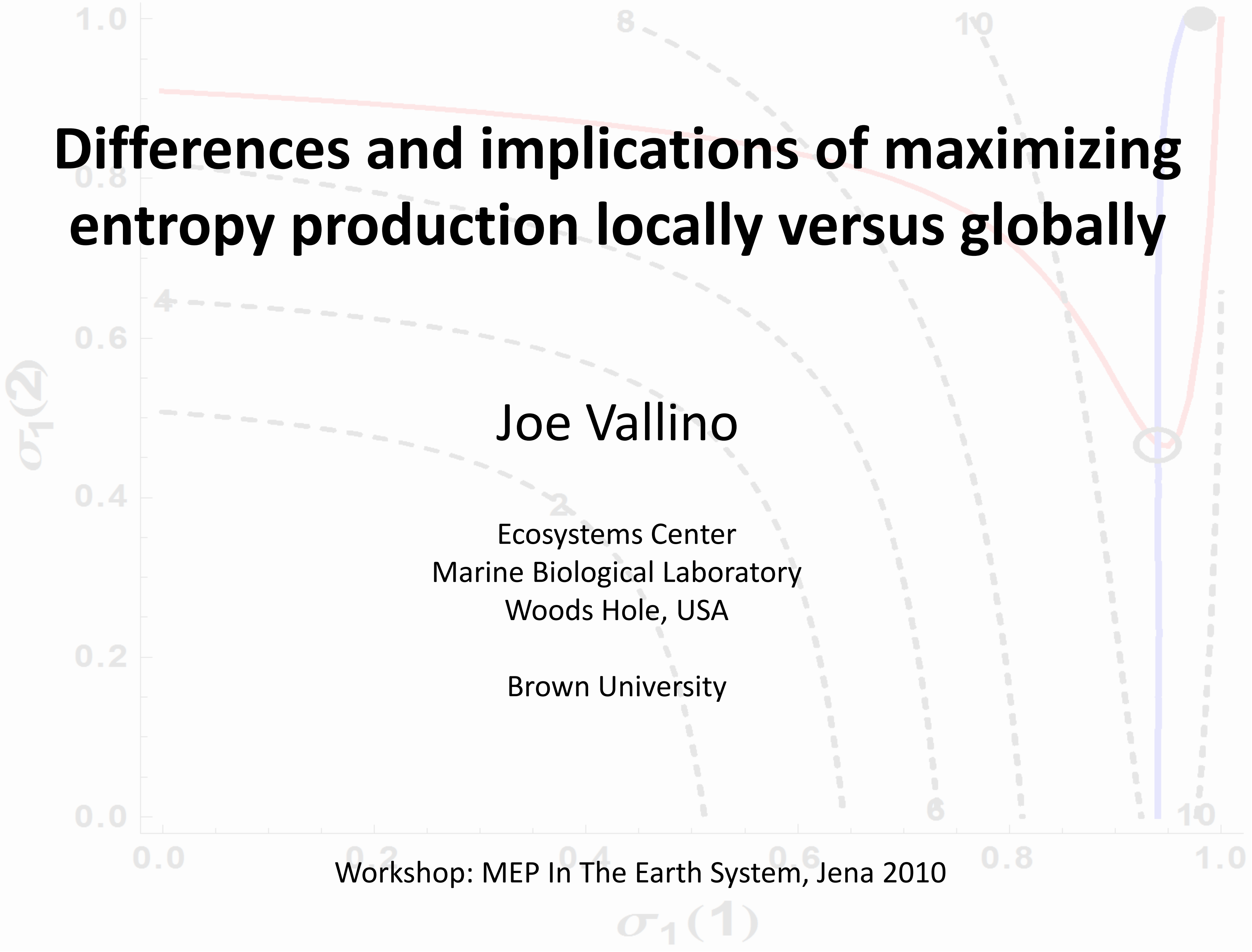

Differences and implications of maximizing entropy production locally versus globally

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Objectives

- Develop a biogeochemistry (BGC) model based on the maximum entropy production (MEP) principle.
- *Hypothesis*: Models based on fundamental principles will have better predictive capabilities than those based on empirical relationships.
- *Alt-Hypothesis*: Forecast length will be greater with MEP-based models because model details are not needed.
- Demonstrate: Compare MEP-BGC and classic-BGC models to observations to test hypothesis.
- Longer term: Integrate MEP-BGC model into larger scale BGC models.

Today focus on: MEP and spatial scale

Emergent Systems Approach

Propose living systems organize around a dynamical attractor

- Concept attributable to at least Lotka (1922): maximum power

MEP as the dynamical attractor has many advantages

- Dewar (2003, 2005), and others, theoretical support
- Natural extension to classic equilibrium thermodynamics
- Thermodynamic entropy, S, is a well defined state variable:

$$r: \quad A + B \rightarrow C + D \qquad \frac{dS}{dt} = -\frac{\Delta G_r \, r(t)}{T}$$

Constant P and T
No mechanical energy storage

MEP paraphrasing:

If internal ordered structures facilitate energy dissipation, then the probability of a system with them is greater than a system without them.

Time and Space Considerations

Time*

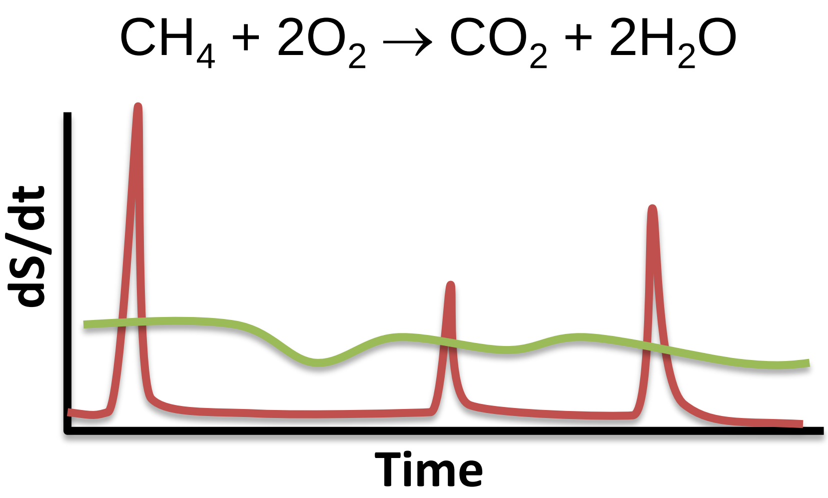
- Maximize entropy production *Instantaneously*?
- Maximize entropy production *Integrated Over Time*?

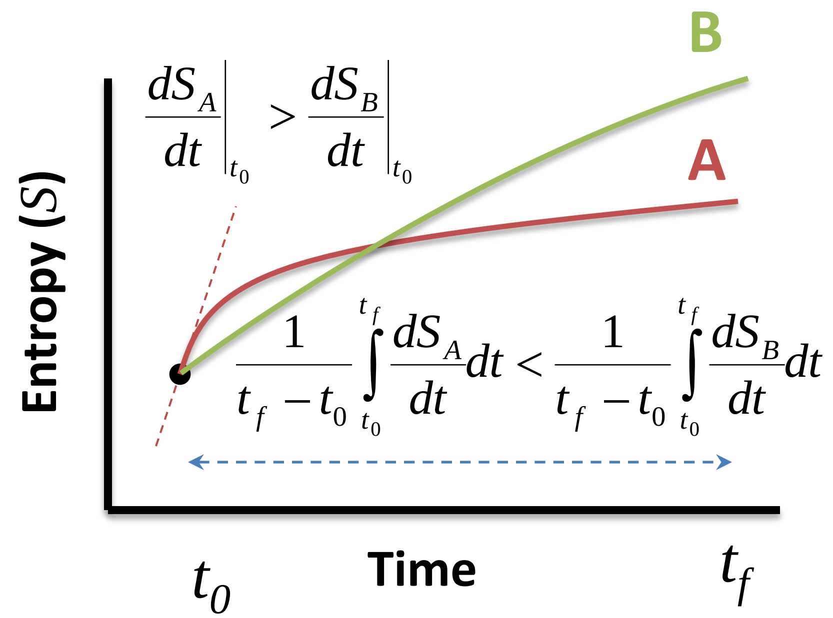
Space

- Maximize entropy production *At a Point*?
- Maximize entropy production *Integrated Over Space*?

*Vallino (2010) *Phil. Trans. R. Soc. B*

Average vs Instantaneous EP



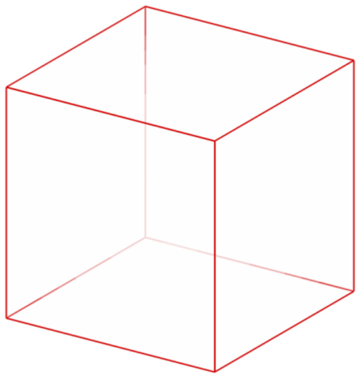


- "Useful information" stored in the metagenome allows living systems to predict future states and proceed along pathways that result in greater averaged entropy production than abiotic systems.
- **This is the only difference biotic systems and abiotic systems**
- However, pathways for maximal averaged entropy production may be flanked by pathways of steepest descent (e.g., forest fires, invasive species).

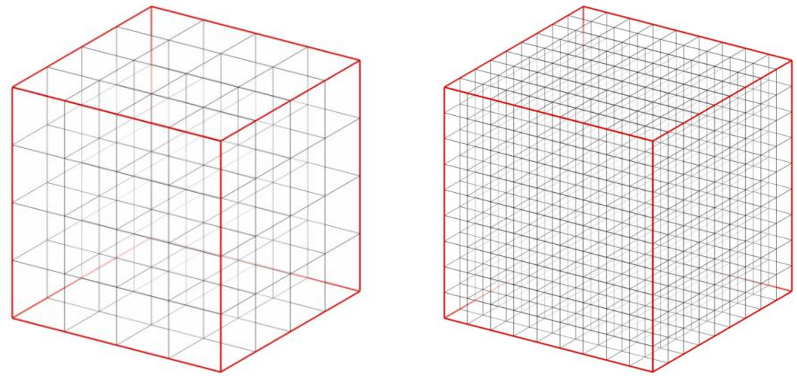
Entropy Production and Discretization?

How should domain be discretized?

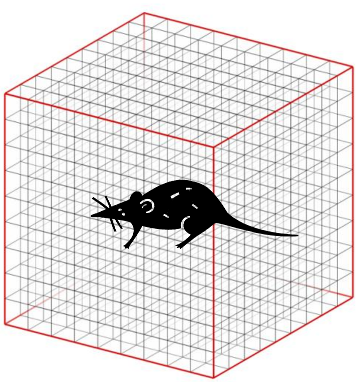
$$\iiint_{\Omega} \frac{dS}{dt}\, d\boldsymbol{\Omega}$$



The standard approach for fluids:



How about if "Organized Structures" are in domain; Discretize them too?



If yes, discretize how?

- Into small cubes?
- Molecule?
- Cellular organelle?
- Cell?
- Whole organism?
- Community, Ecosystem?

Maximize Entropy How?

Locally $$\sum_i \max\left(\frac{dS_i}{dt}\right)$$

or

Globally $$\max\left(\sum_i \frac{dS_i}{dt}\right)$$

Example: “Two Layer Ocean”

Metabolic Network:

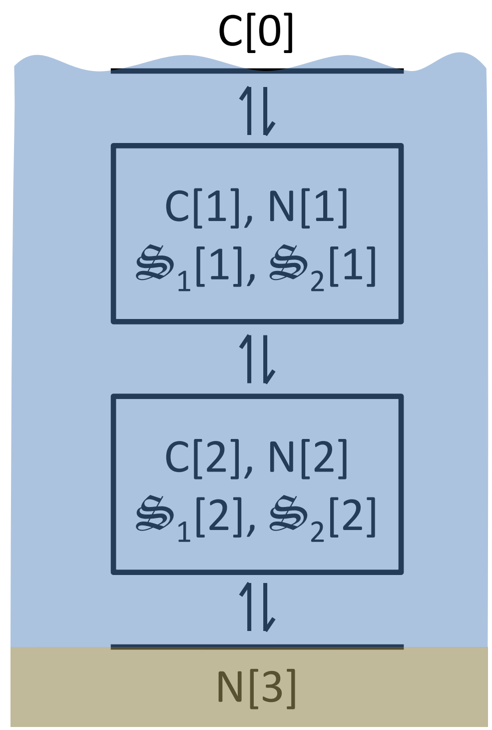
$$r_1: \quad CH_2O + (1-\varepsilon)O_2 + \varepsilon\rho NH_4^+ \xrightarrow{\mathfrak{S}_1} \varepsilon\left(\sigma_1\mathfrak{S}_1 + \sigma_2\mathfrak{S}_2\right) + (1-\varepsilon)(CO_2 + H_2O)$$

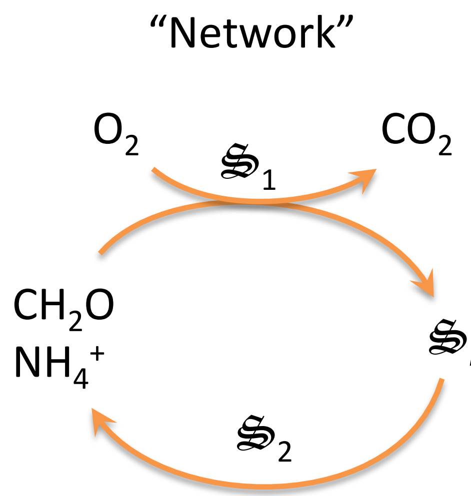
$$r_2: \quad \left(\delta_1\mathfrak{S}_1 + \delta_2\mathfrak{S}_2\right) \xrightarrow{\mathfrak{S}_2} CH_2O + \rho NH_4^+$$

Kinetics:

$$r_1[j] = \nu_1\mathfrak{S}_1[j]\frac{C[j]}{C[j]+k_{C,\mathfrak{S}}}\frac{N[j]}{N[j]+k_{N,\mathfrak{S}}}$$

$$r_2[j] = \nu_2\mathfrak{S}_2[j]\frac{\mathfrak{S}_T[j]}{\mathfrak{S}_T[j]+k_{\mathfrak{S},CN}}$$





Oxygen and other elements in excess

Example: State Equations

Surface layer: [1]

$$\frac{dC[1]}{dt} = \frac{D}{\ell^2}\big((C[0]-C[1])-(C[1]-C[2])\big)-r_1[1]+r_2[1]$$

$$\frac{dN[1]}{dt} = -\frac{D}{\ell^2}(N[1]-N[2])-\varepsilon\rho r_1[1]+\rho r_2[1]$$

$$\frac{d\mathfrak{S}_1[1]}{dt} = -\frac{D}{\ell^2}(\mathfrak{S}_1[1]-\mathfrak{S}_1[2])+\varepsilon\sigma_1[1]r_1[1]-\delta_1[1]r_2[1]$$

$$\frac{d\mathfrak{S}_2[1]}{dt} = -\frac{D}{\ell^2}(\mathfrak{S}_2[1]-\mathfrak{S}_2[2])+\varepsilon\sigma_2[1]r_1[1]-\delta_2[1]r_2[1]$$

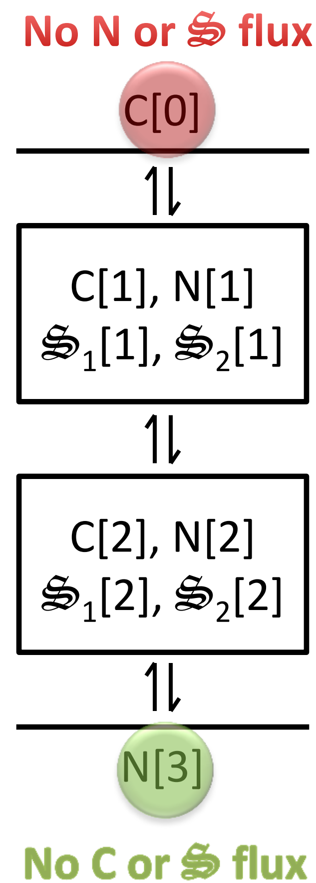
Deep layer: [2]

$$\frac{dC[2]}{dt} = \frac{D}{\ell^2}(C[1]-C[2])-r_1[2]+r_2[2]$$

$$\frac{dN[2]}{dt} = \frac{D}{\ell^2}\big((N[1]-N[2])-(N[2]-N[3])\big)-\varepsilon\rho r_1[2]+\rho r_2[2]$$

$$\frac{d\mathfrak{S}_1[2]}{dt} = \frac{D}{\ell^2}(\mathfrak{S}_1[1]-\mathfrak{S}_1[2])+\varepsilon\sigma_1[2]r_1[2]-\delta_1[2]r_2[2]$$

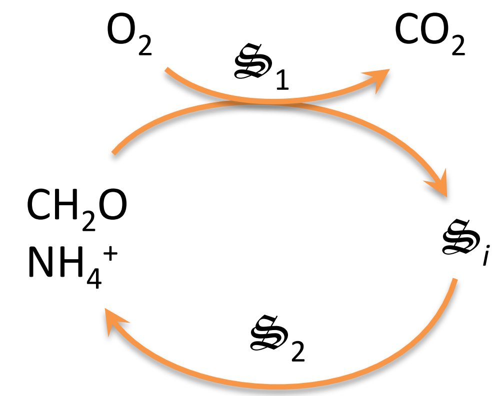
$$\frac{d\mathfrak{S}_2[2]}{dt} = \frac{D}{\ell^2}(\mathfrak{S}_2[1]-\mathfrak{S}_2[2])+\varepsilon\sigma_2[2]r_1[2]-\delta_2[2]r_2[2]$$



Example: Entropy Production

$$r_1 : \quad CH_2O + (1-\varepsilon)O_2 + \varepsilon\rho NH_4^+ \xrightarrow{\mathfrak{S}_1} \varepsilon\left(\sigma_1\mathfrak{S}_1 + \sigma_2\mathfrak{S}_2\right) + (1-\varepsilon)(CO_2 + H_2O)$$

$$r_2 : \quad (\delta_1\mathfrak{S}_1 + \delta_2\mathfrak{S}_2) \xrightarrow{\mathfrak{S}_2} CH_2O + \rho NH_4^+$$



Entropy Production:

$$\frac{dS}{dt} = -\frac{1}{T}(\Delta G_{r_1} r_1 + \Delta G_{r_2} r_2)$$

Free energy of biosynthesis is small

$$\Delta G_{r_1} = (1-\varepsilon)\Delta G^o_{CH_2Ox} + \cancelto{0}{\varepsilon\Delta G^o_{\mathfrak{S}}} + RT\ln\left(\frac{[H_2CO_3]^{(1-\varepsilon)}[\mathfrak{S}_T]^{\varepsilon}}{[CH_2O][O_2]^{(1-\varepsilon)}[NH_4^+]^{\varepsilon\rho}}\right)$$

$$\Delta G_{r_2} = -\cancelto{0}{\Delta G^o_{\mathfrak{S}}} + RT\ln\left(\frac{[CH_2O][NH_4^+]^{\rho}}{[\mathfrak{S}_T]}\right)$$

Example: Control Variables

$$r_1: \quad CH_2O + (1-\varepsilon)O_2 + \varepsilon\rho NH_4^+ \xrightarrow{\mathfrak{S}_1} \varepsilon\left(\sigma_1\mathfrak{S}_1 + \sigma_2\mathfrak{S}_2\right) + (1-\varepsilon)(CO_2 + H_2O)$$

$$r_2: \quad \left(\delta_1\mathfrak{S}_1 + \delta_2\mathfrak{S}_2\right) \xrightarrow{\mathfrak{S}_2} CH_2O + \rho NH_4^+$$

Parameters:

$$\varepsilon, \rho, \nu_1, \nu_2, k_{C,\mathfrak{S}}, k_{N,\mathfrak{S}}, k_{\mathfrak{S},CN}, D, \ell$$

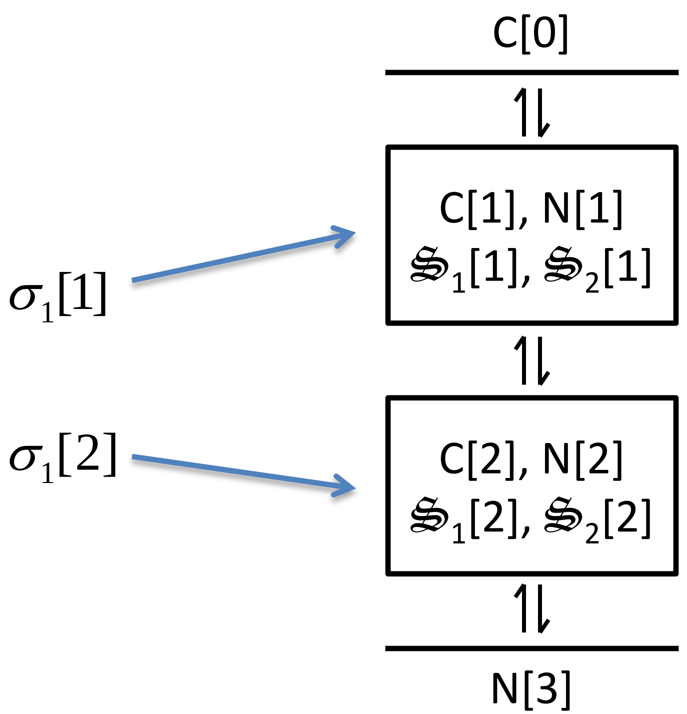
$$\delta_i[j] = \frac{\mathfrak{S}_i[j]}{\mathfrak{S}_1[j] + \mathfrak{S}_2[j]} = \frac{\mathfrak{S}_i[j]}{\mathfrak{S}_T[j]}$$

Control Variables:

$$\sigma_1[j], \quad \sigma_2[j], \quad j = 1, 2$$

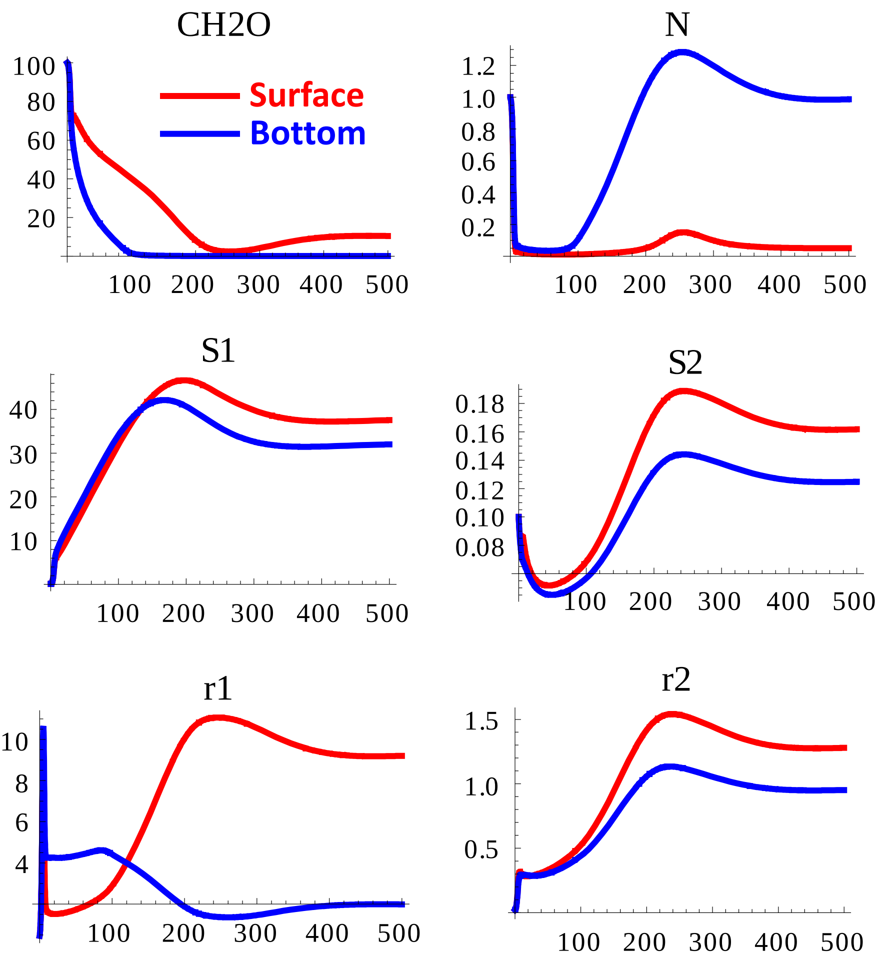
$$\sigma_1[j] + \sigma_2[j] = 1$$

$$\Rightarrow \quad \sigma_2[j] = (1 - \sigma_1[j])$$



Example: Transient Solutions

$\sigma_1[1] = 0.995, \ \sigma_1[2] = 1.0$

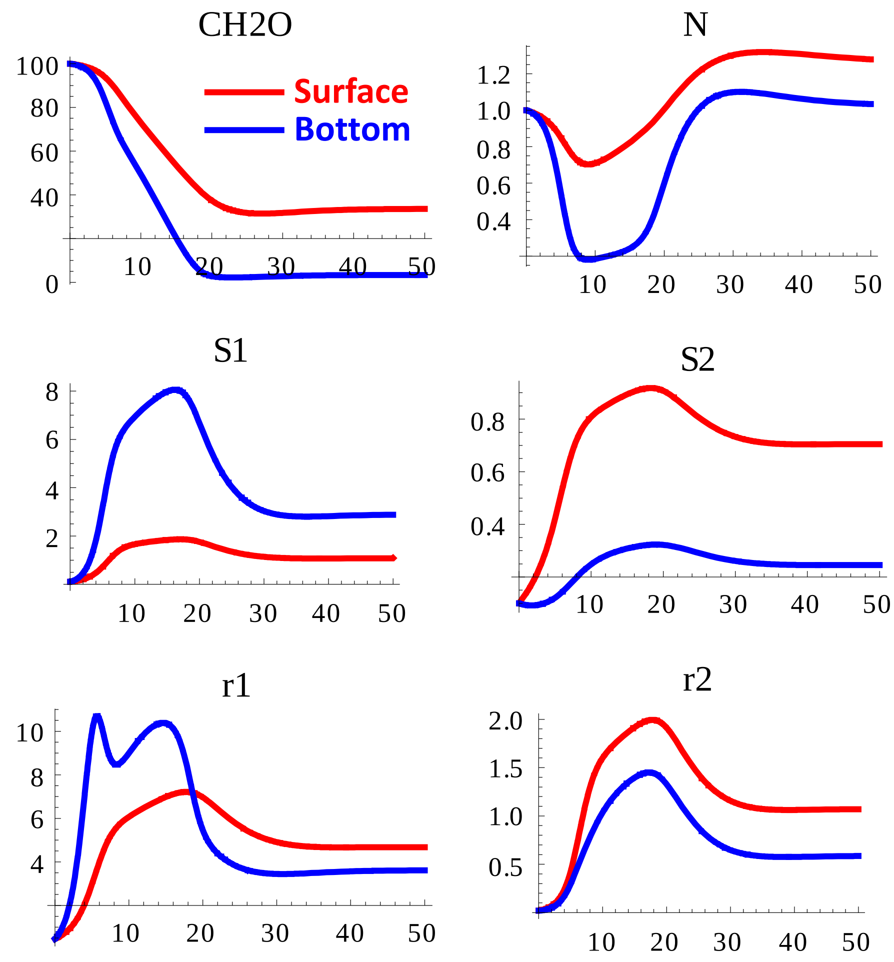


(mJ L^{-1} d^{-1} °K)

dSdt[1]	11.4734
dSdt[2]	2.45696
dSdt[1] + dSdt[2]	13.9304

Total N 12.68

$\sigma_1[1] = 0.5, \ \sigma_1[2] = 1.0$



(mJ L^{-1} d^{-1} °K)

dSdt[1]	5.87634
dSdt[2]	4.47857
dSdt[1] + dSdt[2]	10.3549

Total N 3.13137

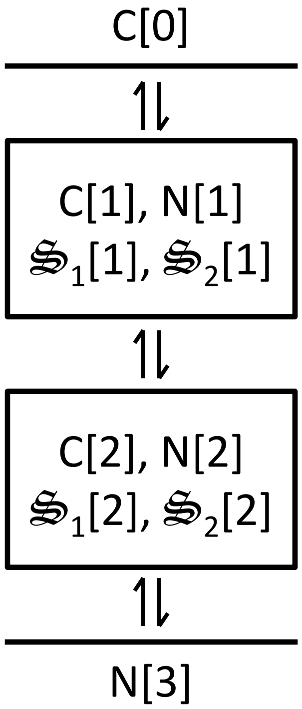
Example: Optimization

Local Optimization

$$\underset{\sigma_1[1]}{Max}\,\frac{dS[1]}{dt} \quad \text{and} \quad \underset{\sigma_1[2]}{Max}\,\frac{dS[2]}{dt}$$

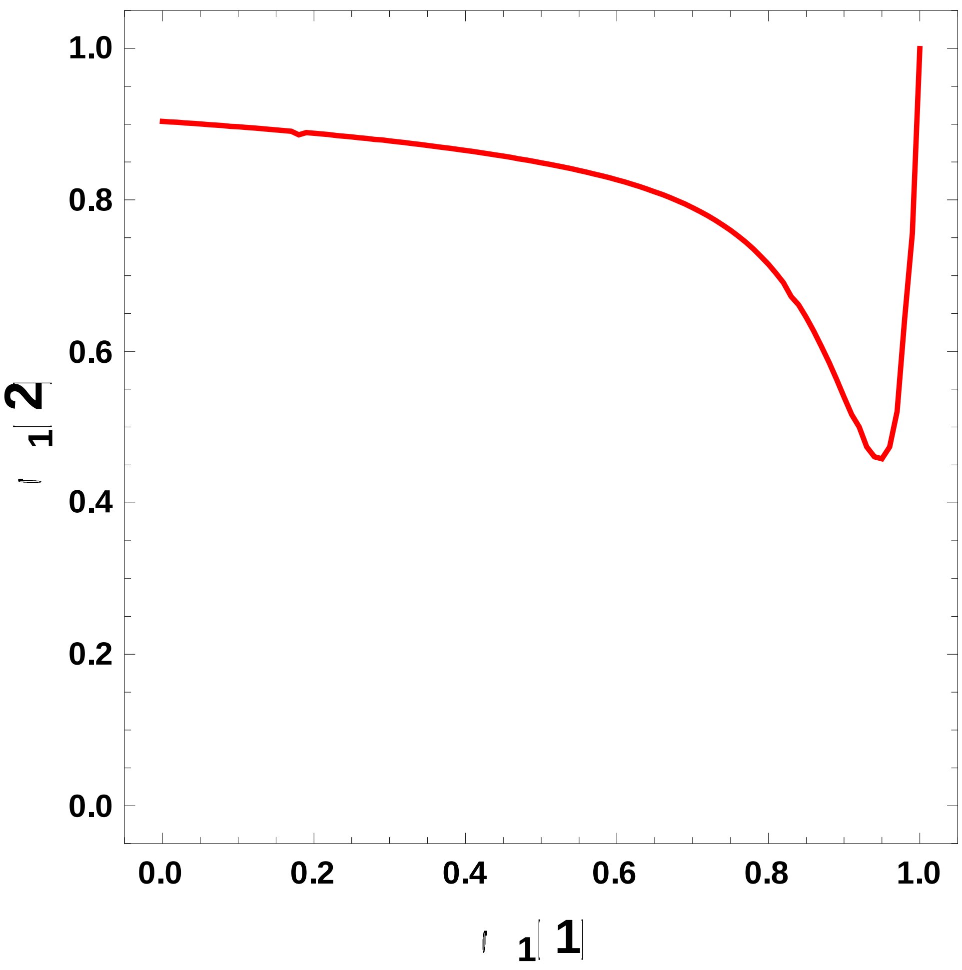
Global Optimization

$$\underset{\sigma_1[1],\sigma_1[2]}{Max}\,\frac{dS[1]}{dt}+\frac{dS[2]}{dt}$$



Example: Results, Local Optimum [2]

$$\underset{\sigma_1[2]}{Max} \frac{dS[2]}{dt}$$

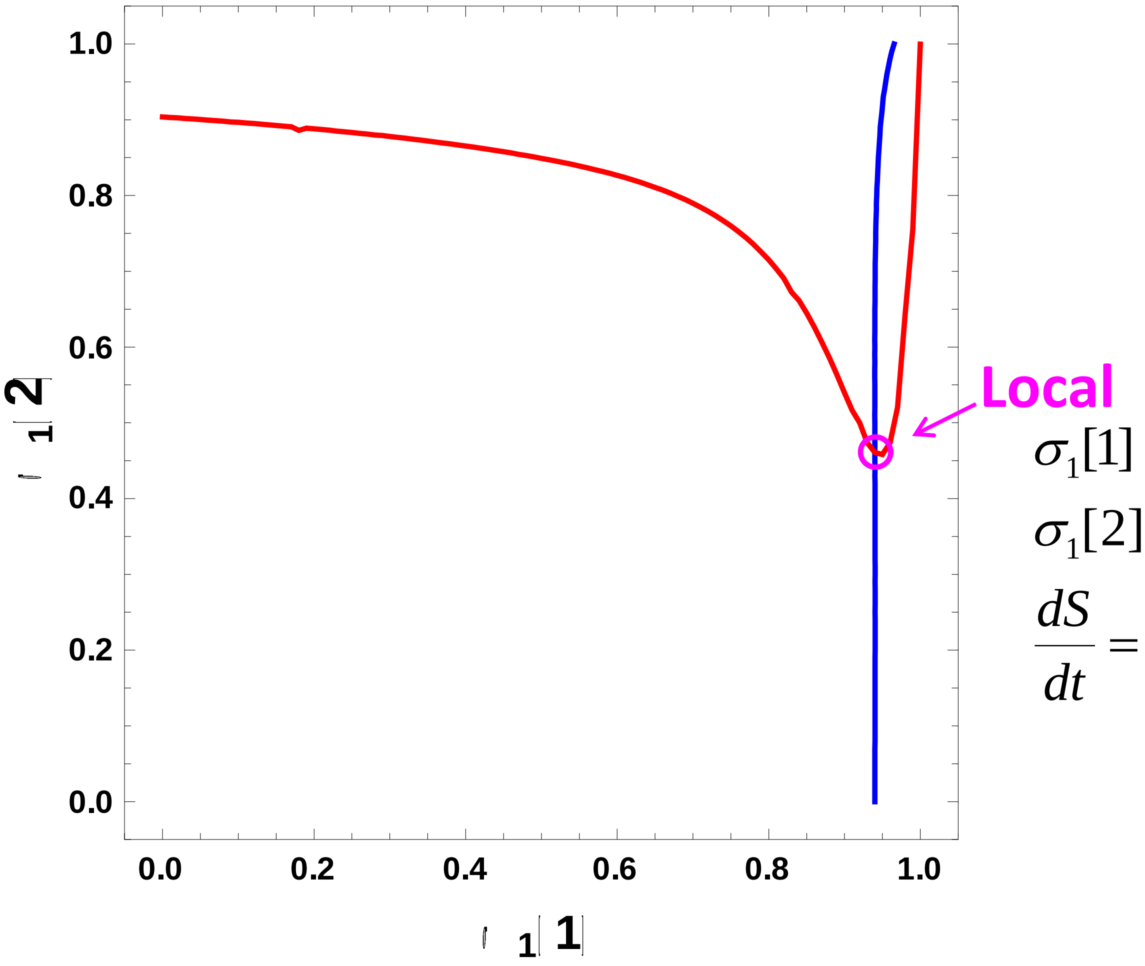


Example: Results, Local Optimum [2] and [1]

$$\underset{\sigma_1[2]}{Max}\frac{dS[2]}{dt}$$

and

$$\underset{\sigma_1[1]}{Max}\frac{dS[1]}{dt}$$



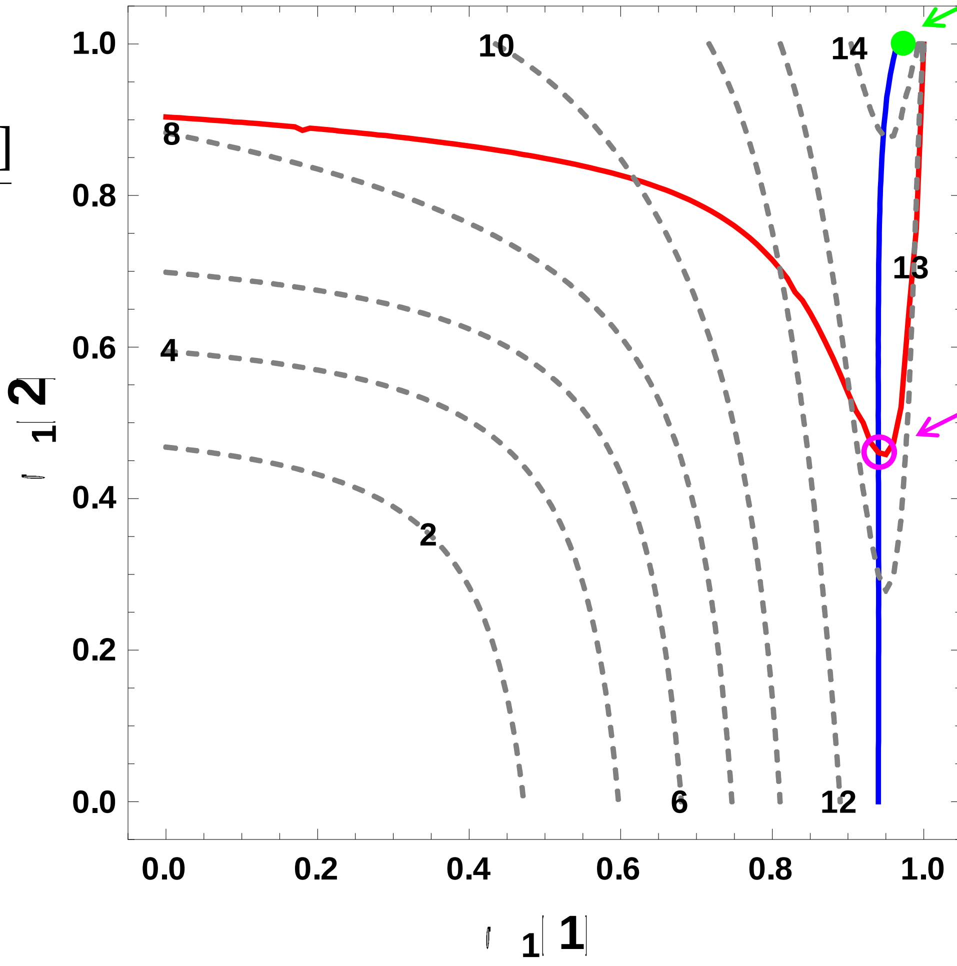
$\sigma_1[1] = 0.9401$

$\sigma_1[2] = 0.4607$

$\frac{dS}{dt} = 13.20$

Example: Results, Global Optimum

$$\underset{\sigma_1[1],\sigma_1[2]}{Max}\ \frac{dS[1]}{dt}+\frac{dS[2]}{dt}$$



Global

$\sigma_1[1]=0.9730$

$\sigma_1[2]=1.0000$

$\frac{dS}{dt}=14.52$

Local

$\sigma_1[1]=0.9401$

$\sigma_1[2]=0.4607$

$\frac{dS}{dt}=13.20$

CONCLUSIONS (CONJECTURES)

- Entropy production is greater when maximized globally rather than locally.
- Systems should organize/evolve to maximize entropy production globally then.
- Implies local "sacrifice" to maximize EP globally (altruism*).
- Systems must exhibit cooperation for entropy to be maximized globally.
- The extent of information exchange defines the domain of a system (extent of cooperation).
- Does information (aka Shannon entropy) facilitate thermodynamic entropy production over space and time?

*Ref: Wilson and Wilson (2008) *American Scientist*

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