

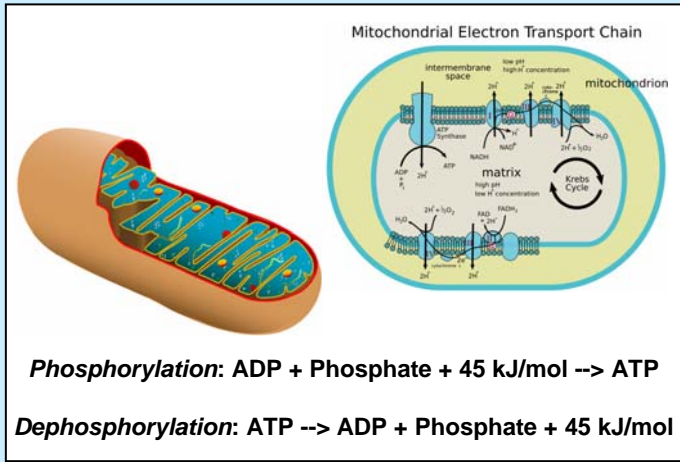


Visualizing and Analyzing Large Systems of Differential Equations

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1. Modeling Biochemical Reactions

Mental Model



This is a model of a mitochondrion which fuels the cell by producing ATP, the universal energy currency of the cell. Once synthesized, ATP is essential for providing the energy for a large number of chemical reactions inside the living cell.

ODE-System

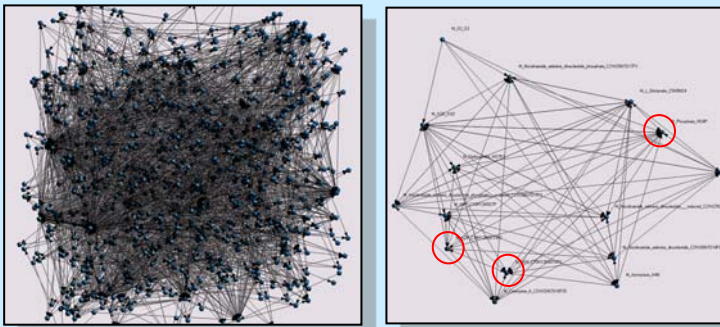
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dPDK001.g/dt=(1/(1))*((-1)*RXN9+(-1)*RXN49+RXN31+RXN113)
dCRK001.g/dt=(1/(1))*((-1)*RXN34)
dFRS2001.g/dt=(1/(1))*((-1)*RXN35+(-1)*RXN70+(-1)*RXN77+(-1)*RXN109+RXN33+RXN46+RXN80+RXN84)
dSHC001.g/dt=(1/(1))*((-1)*RXN13+(-1)*RXN68+(-1)*RXN72+(-1)*RXN105+RXN19+RXN30+RXN32+RXN82+...
dPSOS_01.g/dt=(1/(1))*((-1)*RXN12+RXN5+RXN49+RXN114)
dGRAP1_01.g/dt=(1/(1))*((-1)*RXN61+RXN60+RXN112+RXN121)
dMEX0001.g/dt=(1/(1))*((-1)*RXN115+(-1)*RXN122+(-1)*RXN126+(-1)*RXN130+RXN55)
dMEX3001.g/dt=(1/(1))*((-1)*RXN147+(-1)*RXN148+RXN149+RXN150)
dPSHC_01.g/dt=(1/(1))*((-1)*RXN10+(-1)*RXN25+RXN8+RXN14)
dDPEGF01.g/dt=(1/(1))*((-1)*RXN15+(-1)*RXN27+(-1)*RXN105+(-1)*RXN106+(-1)*RXN109+(-1)*RXN110+...
dC_RAF01.g/dt=(1/(1))*((-1)*RXN121+(-1)*RXN130+(-1)*RXN131+(-1)*RXN132+(-1)*RXN133+RXN52+...
dPSHC_02.g/dt=(1/(1))*((-1)*RXN20+(-1)*RXN107+RXN10+RXN22+RXN106)
dPFRS201.g/dt=(1/(1))*((-1)*RXN41+(-1)*RXN44+RXN40+RXN43+RXN110)
dSHC_D01.g/dt=(1/(1))*((-1)*RXN14+(-1)*RXN17+RXN13)
dC_CBL01.g/dt=(1/(1))*((-1)*RXN7+(-1)*RXN10+(-1)*RXN17+(-1)*RXN26+(-1)*RXN39+(-1)*RXN40+(-1)*...
dRAGS001.g/dt=(1/(1))*((-1)*RXN48)
dC_RAF01.g/dt=(1/(1))*((-1)*RXN5+RXN19)
dC_RAF02.g/dt=(1/(1))*((-1)*RXN52+(-1)*RXN53+RXN120+RXN121)
dHRK001.g/dt=(1/(1))*((-1)*RXN115+(-1)*RXN116+(-1)*RXN117+RXN149+RXN150)

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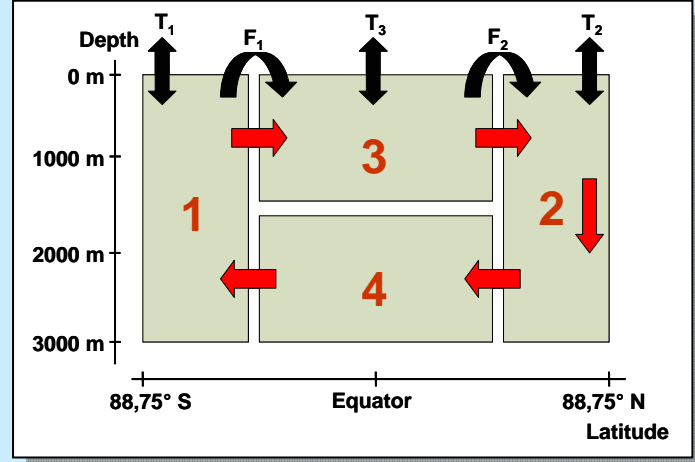
This ODE-system describes a number of biochemical reactions inside the baker's yeast cell [1]. Only a small part the model containing 1.266 ODEs is actually shown here. Realistic models of a cell's metabolism consist of 1.000 to 15.000 ODEs [2].

Visualization



To explore and understand such a vast model, we propose to use a graph-based visualization of the ODE-system, where each node corresponds to a variable and an edge between two nodes is introduced iff one variable depends upon the other in at least one equation. Interactively reducing the nodes from a complex view (left) to only those with a very high node degree (right) reveals the strong dependency of the entire metabolism on the (De-)Phosphorylation of ATP.

2. Modeling the Climate

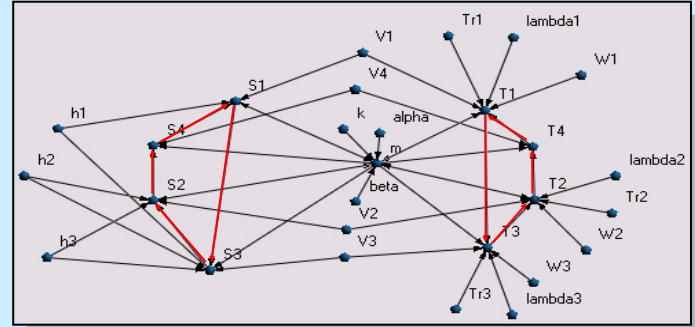


This simple model of the thermohaline stream in the Atlantic ocean [3] is used in climate simulations. Besides the interdependency between the atmosphere and the ocean (black arrows), it also very clearly shows the cyclic nature of the stream itself (red arrows).

$$\begin{aligned}
S_1'(t) &= \frac{m(t)}{V_1}(S_1(t) - S_1(t)) - \frac{h_1(t)}{V_1} \\
S_2'(t) &= \frac{m(t)}{V_2}(S_2(t) - S_2(t)) - \frac{h_2(t) + h_3(t)}{V_2} \\
S_3'(t) &= \frac{m(t)}{V_3}(S_3(t) - S_3(t)) - \frac{h_1(t) - h_2(t) - h_3(t)}{V_3} \\
S_4'(t) &= \frac{m(t)}{V_4}(S_4(t) - S_4(t)) \\
T_1'(t) &= \frac{m(t)}{V_1}(T_1(t) - T_1(t)) + \lambda_1(T_1 + W_1(t) - T_1(t)) \\
T_2'(t) &= \frac{m(t)}{V_2}(T_2(t) - T_2(t)) + \lambda_2(T_2 + W_2(t) - T_2(t)) \\
T_3'(t) &= \frac{m(t)}{V_3}(T_3(t) - T_3(t)) + \lambda_3(T_3 + W_3(t) - T_3(t)) \\
T_4'(t) &= \frac{m(t)}{V_4}(T_4(t) - T_4(t))
\end{aligned}$$

$$m(t) = k(\beta(S_2(t) - S_1(t)) - \alpha(T_2(t) - T_1(t)))$$

This ODE-system describes the above model mathematically. While it is not as large as the ODE-systems that model biochemical reaction networks, it is on the other hand not as homogenous and thus not as self-explanatory as these.



Such a visualization of the above ODE-system enables the users to quickly reveal the cyclic nature of the thermohaline stream even if they are not familiar with the mental model. The software system used for the combined graph analysis and visualization is our research group's own development Colossus [4].

REFERENCES

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[3] K. Zickfeld, T. Slawig, S. Rahmstorf: A low-order model for the response of the Atlantic thermohaline circulation to climate change. *Ocean Dynamics*, Vol.54, p.8-26, 2004

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