DEB 2025

Dynamic Energy Budget models in Ecotoxicology II. Links across levels of biological organization

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University of Crete, Heraklion, Greece

DEB 2025

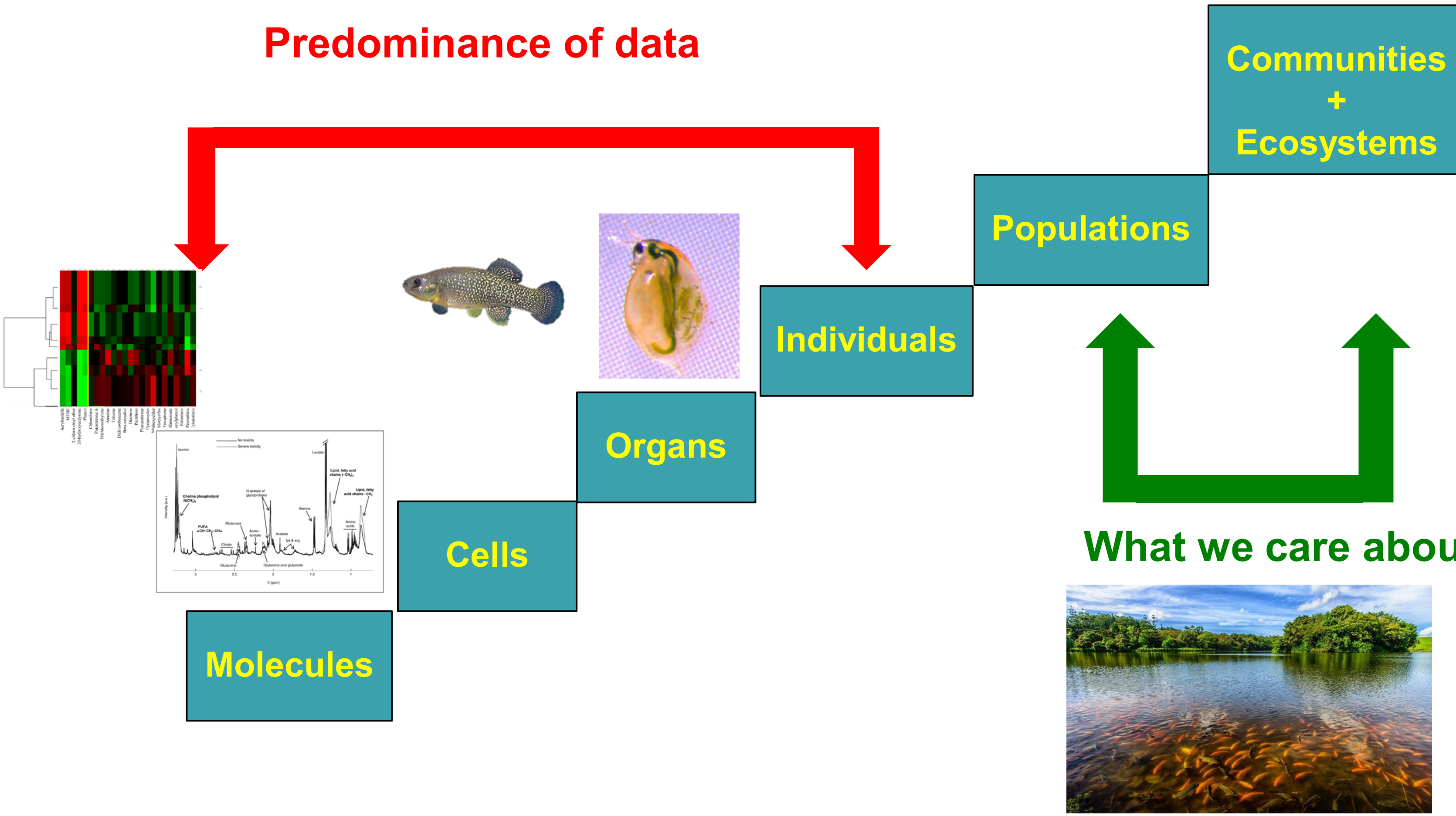
Ecotox Lecture 2: Linking levels of biological organization (and linking species)

- Levels of biological organization – individual as a pivot
- Individual to population
  - well established modeling techniques (e.g. papers by Andre de Roos)
  - conceptually simplest approach uses Individual-Based Models (IBMs)
  - Case study: effect of a contaminant on food limited *Daphnia* populations
  - Feedback via abiotic environment (phytoplankton and silver naonparticles)
- Suborganismal to individual
  - Use damage variable (example: ROS and MDA)
  - adverse outcome pathways (AOPs) – key events and DEB damage variable
  - gene expression from mRNA – links to pathways and DEB fluxes
  - Case study: killifish and dioxin-like compounds

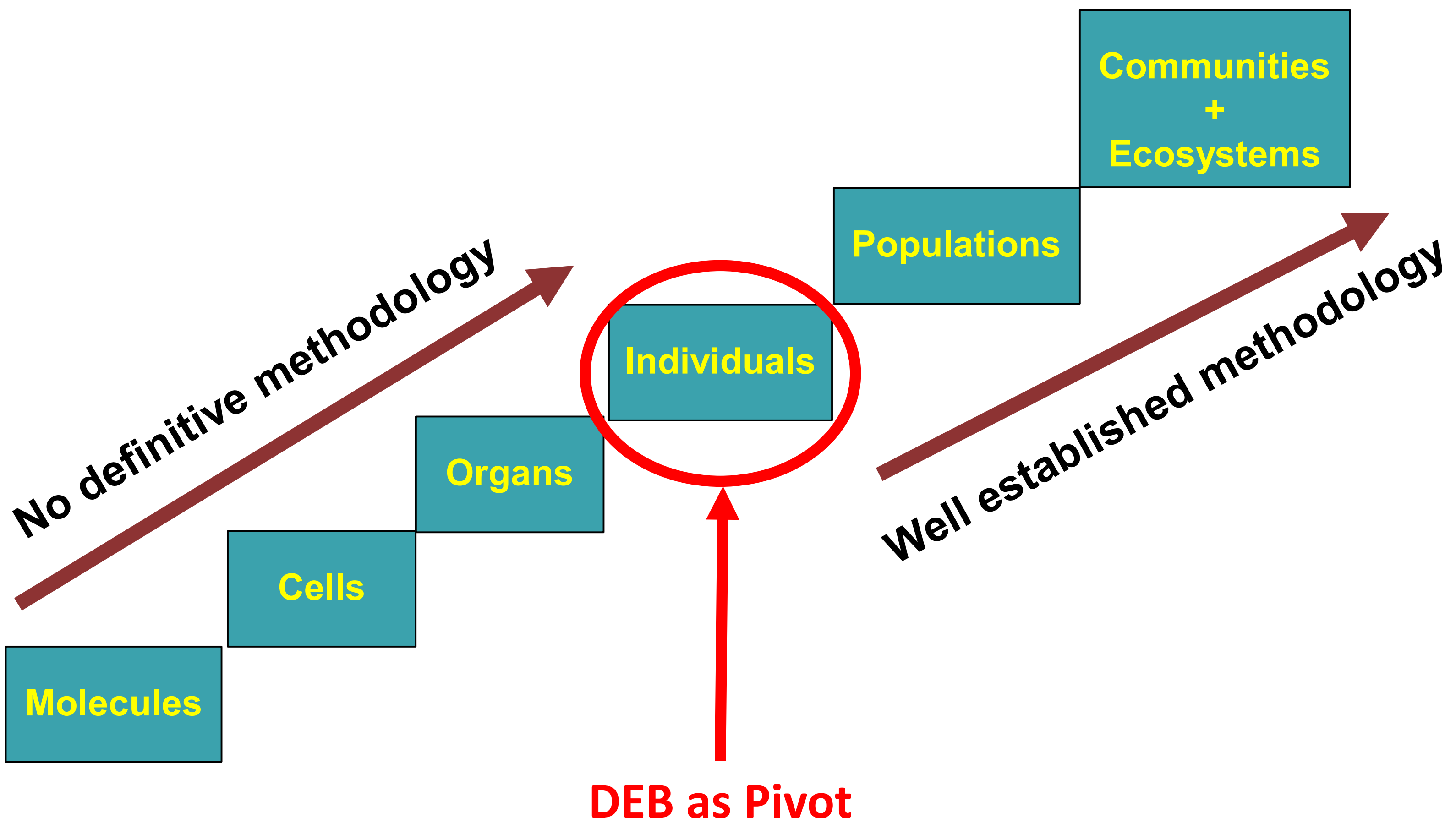
Reference:

- C.A. Murphy et al (2018) *Integrated Environmental Assessment and Management* https://doi.org/10.1002/ieam.4063.

Ecological risk across levels of organization: mismatch of data to societal concerns

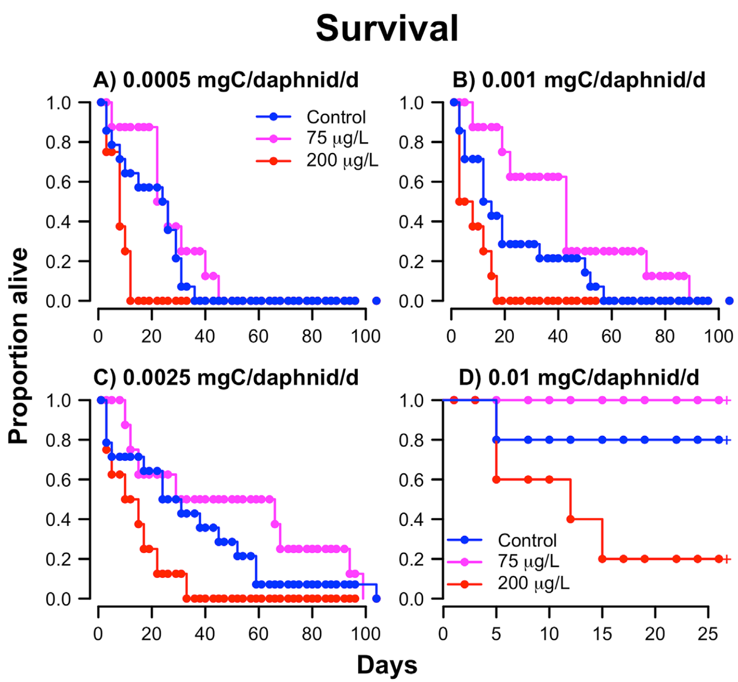


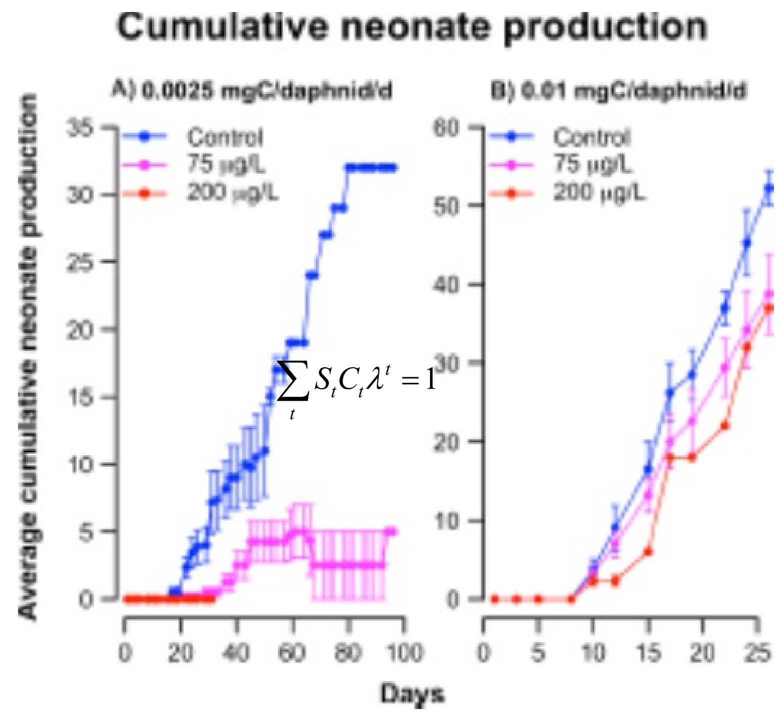
Theory connecting levels of biological organization



Individual to Population

Individual to Population
Simplest approach



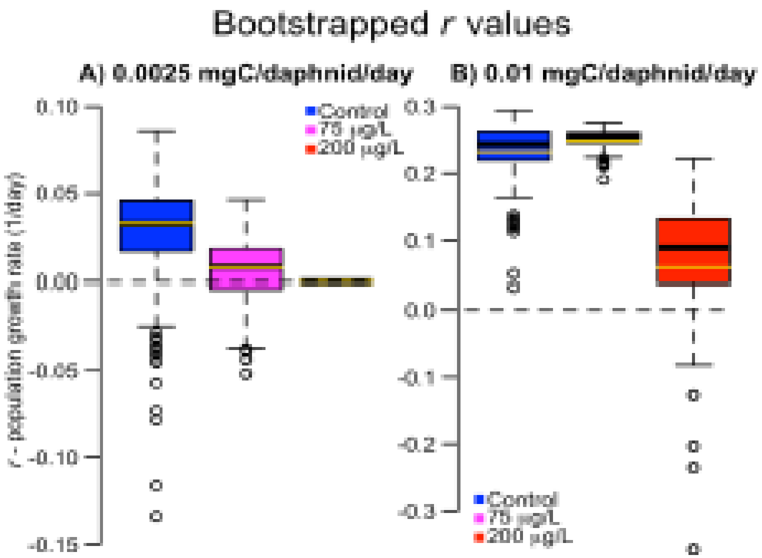


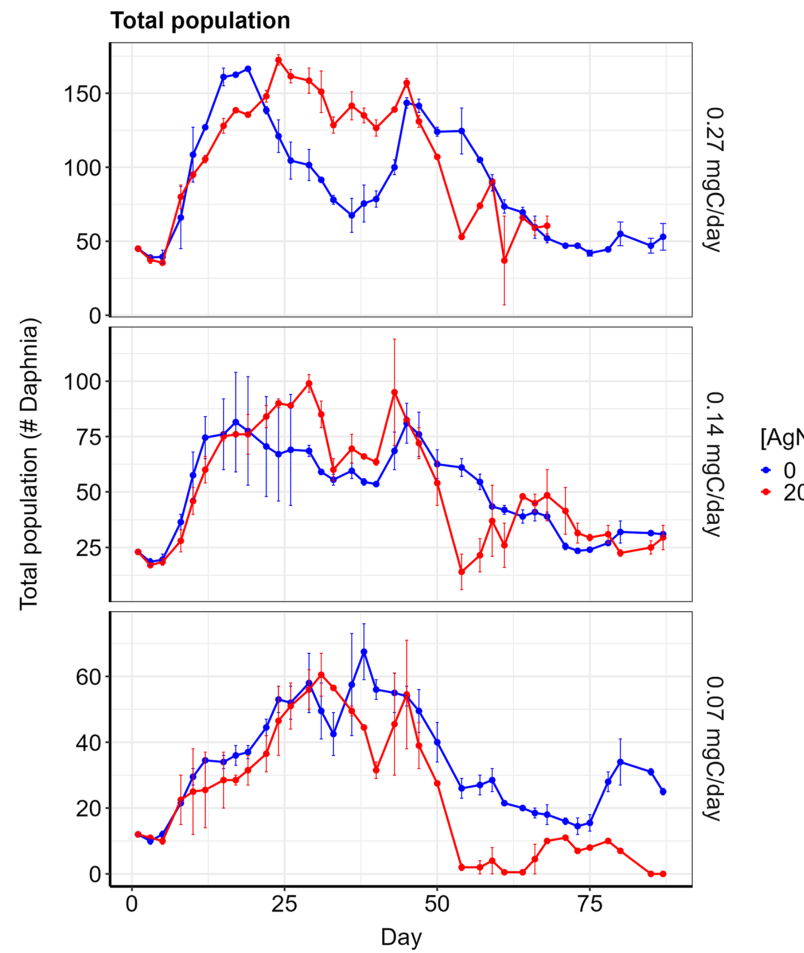
$$\sum_t S_t C_t \lambda^t = 1$$

Calculate long run growth rate, r, from Lotka equation

Stevenson et al. *Environmental Toxicology and Chemistry* 2017

Individual to Population
Direct approach

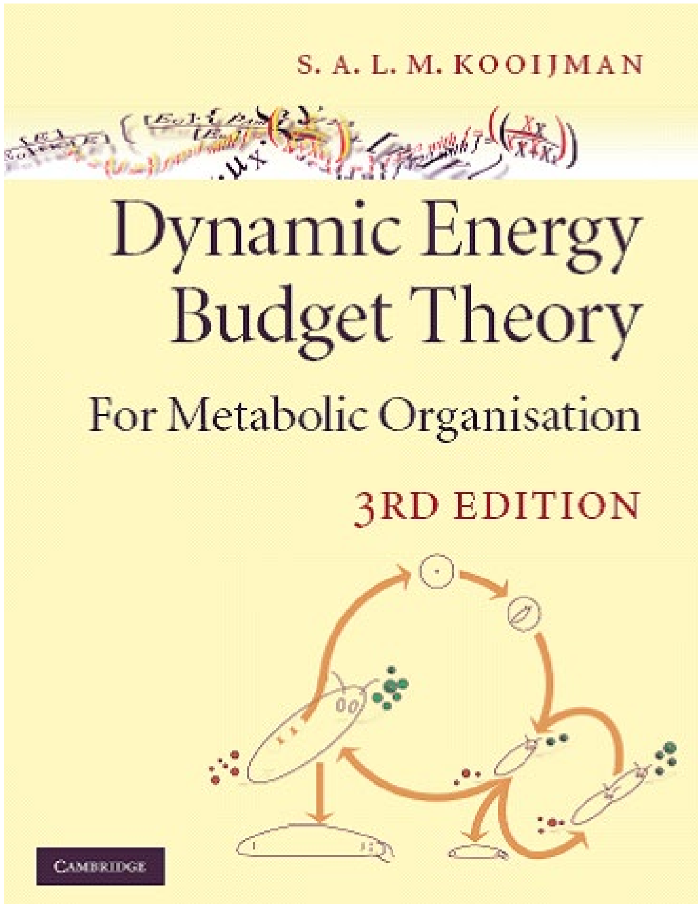


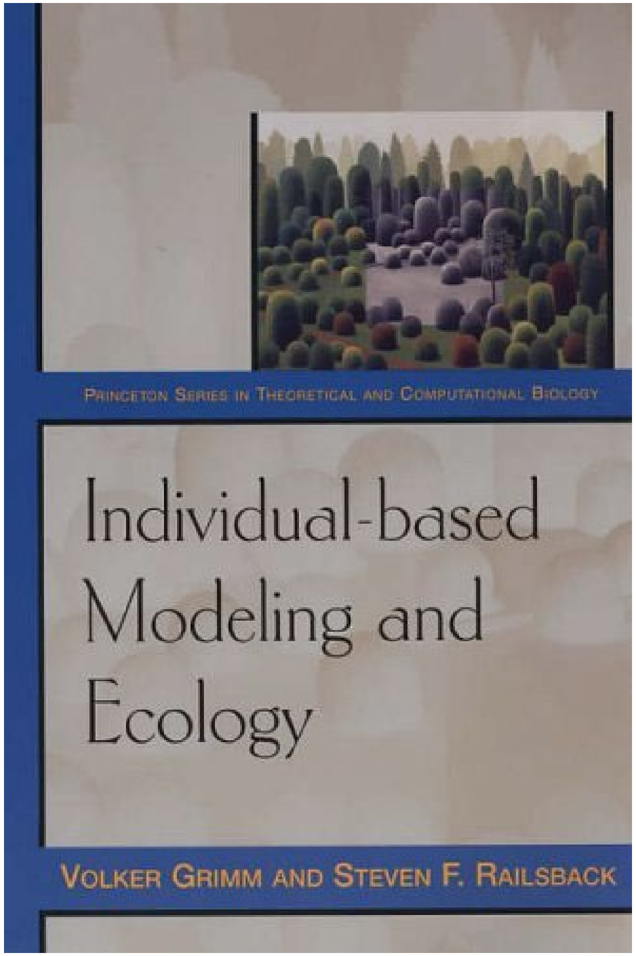


- 2 of 3 replicate populations extinct by time 85 at high exposure.
- No extinction in controls

Stevenson et al, 2023

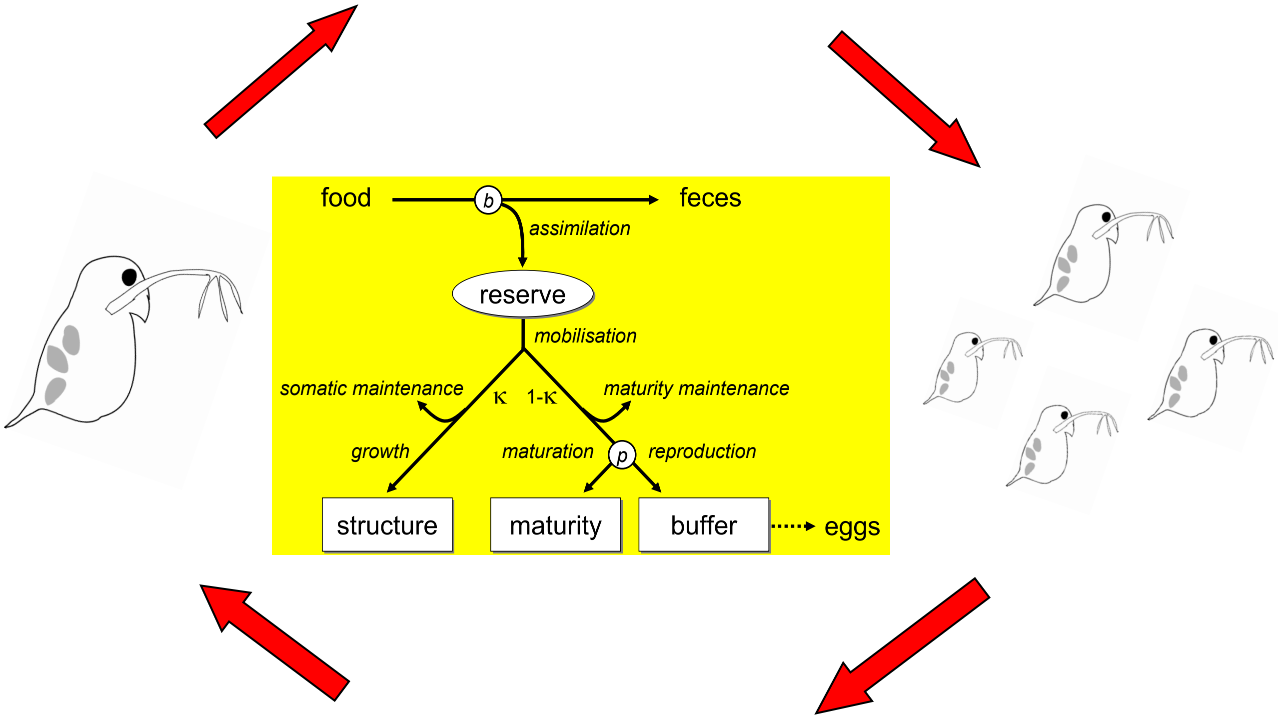
Individual to Population
DEB – based IBM





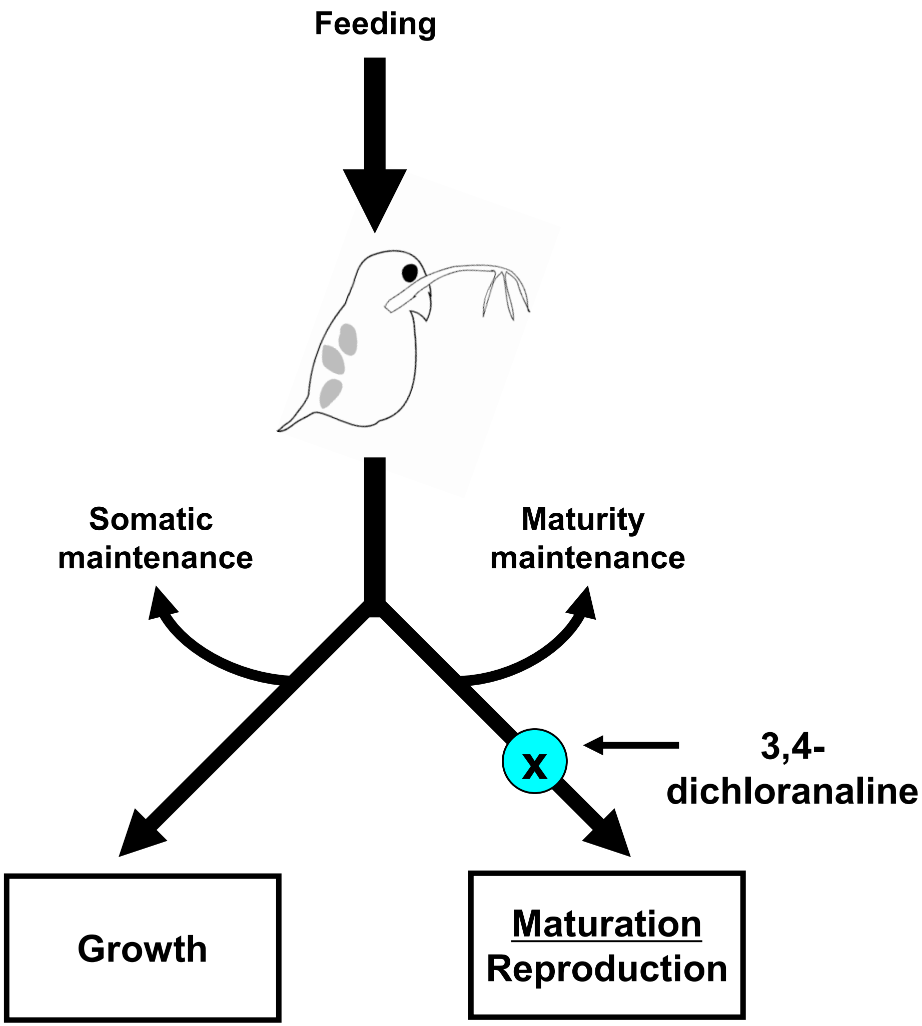
[*] B.T. Martin, E.I. Zimmer, V.Grimm and T. Jager (2012). *Methods in Ecology and Evolution* 3: 445-449

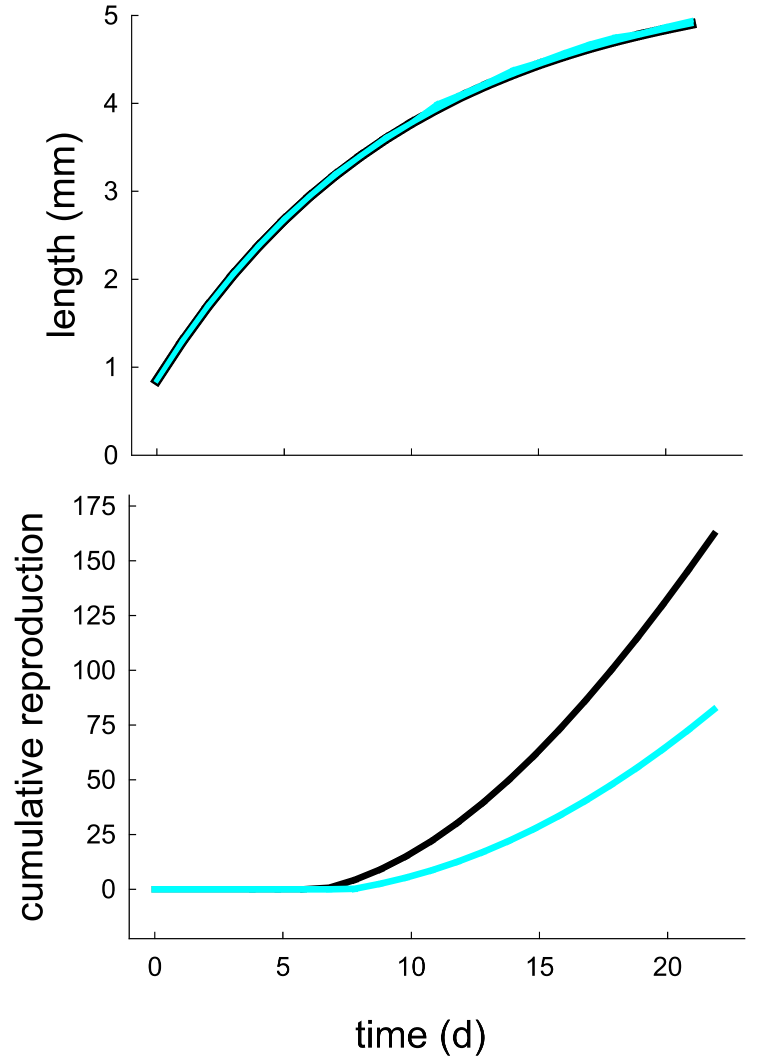
DEB-IBM



- Implemented in *Netlogo* (Free)
- Computes population dynamics in simple environments with minimal programming
- User manual with examples

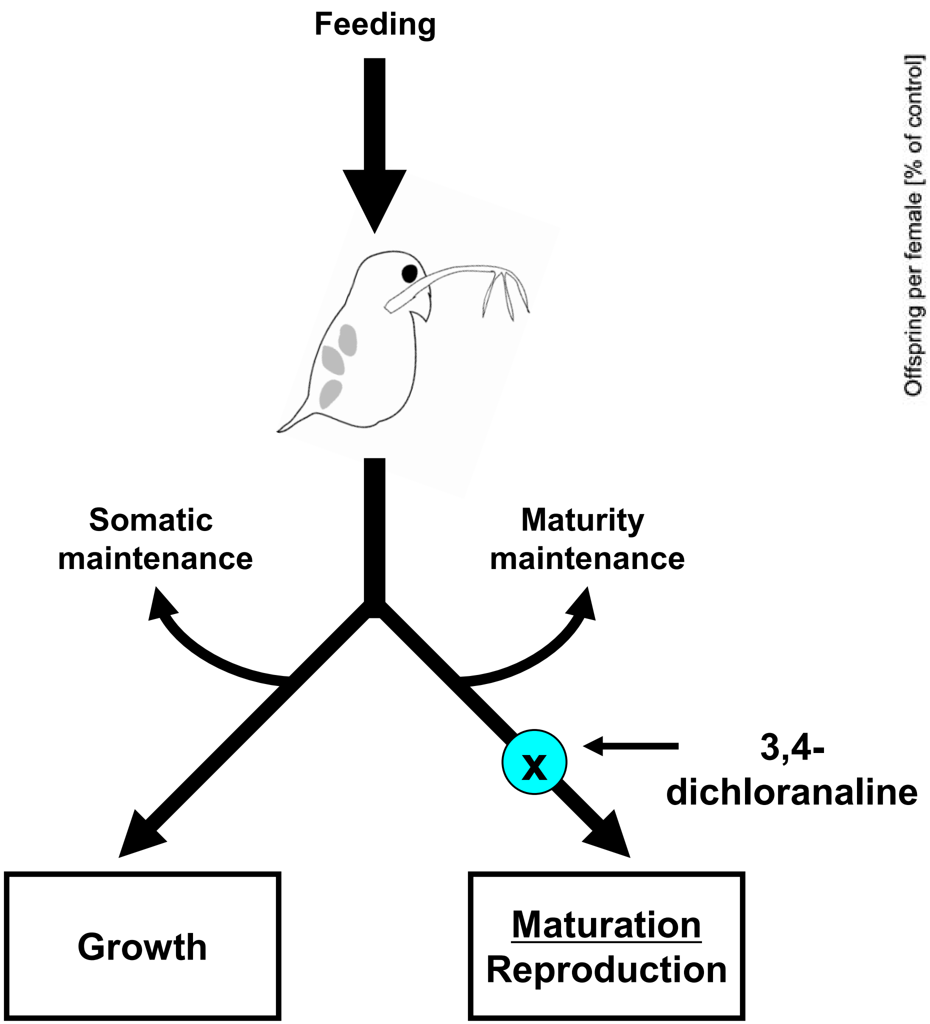
Effects of a contaminant on Daphnia populations

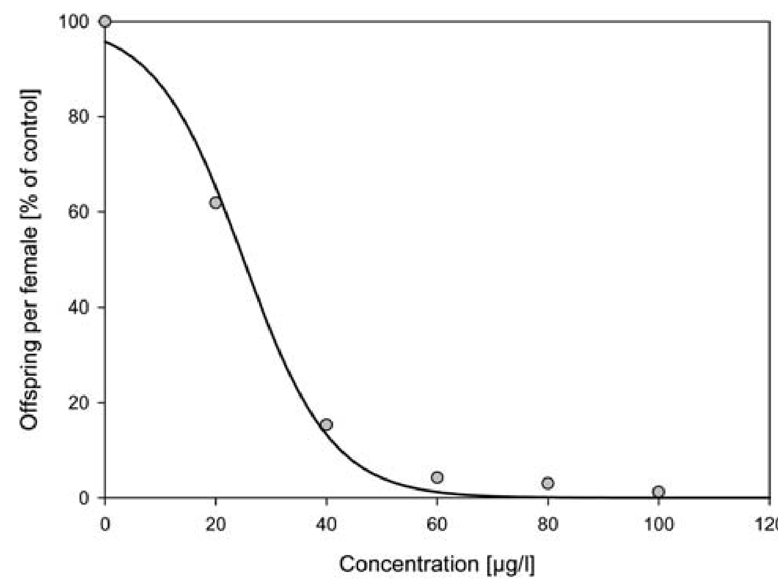




Data from T.G. Preuss et al. *J. Environmental Monitoring* 12: 2070-2079 (2010)
Modeling from B.T. Martin et al. *Ecotoxicology*, DOI 10.1007/s10646-013-1049-x (2013)

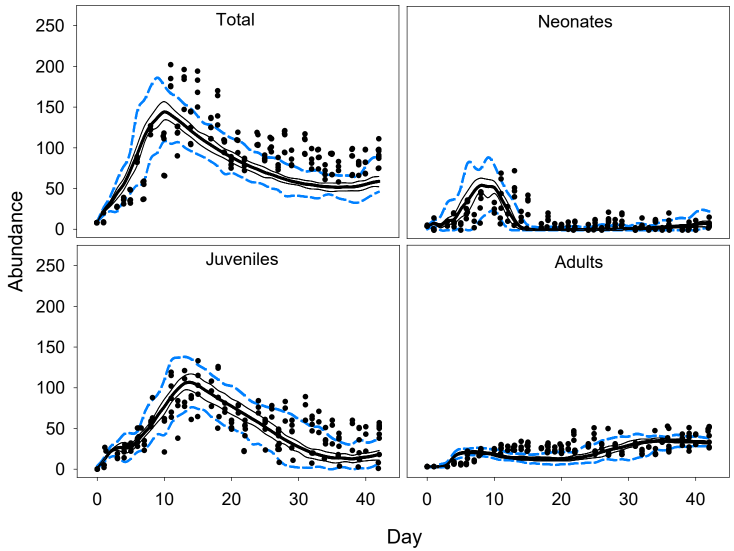
Effects of a contaminant on Daphnia populations



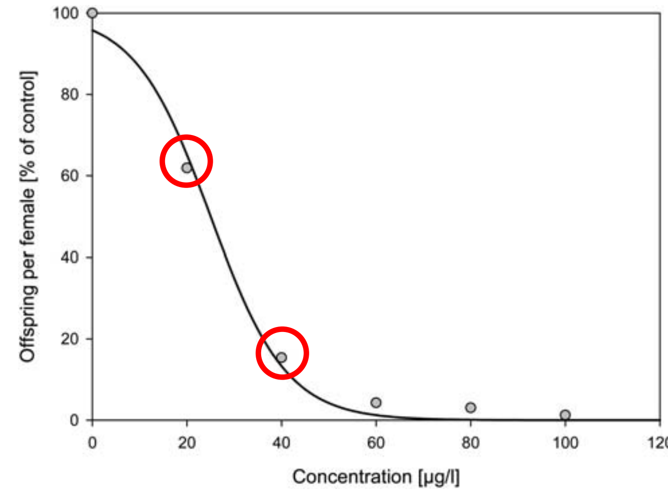


From Preuss et al 2010

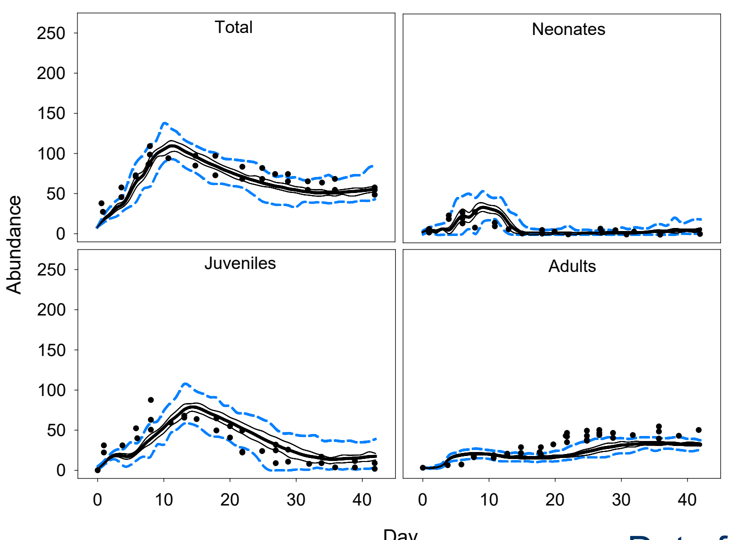
Control



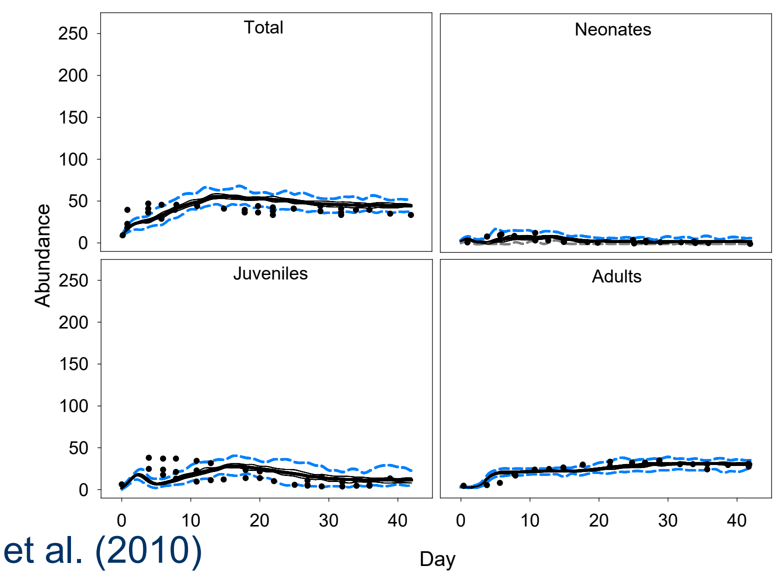
3,4 dichloroaniline



20 ug/l

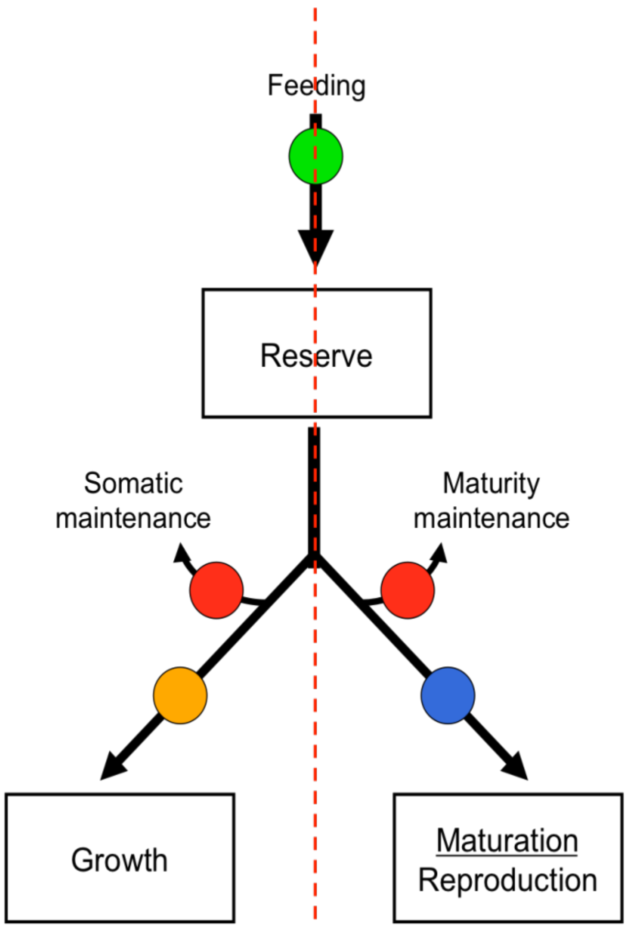


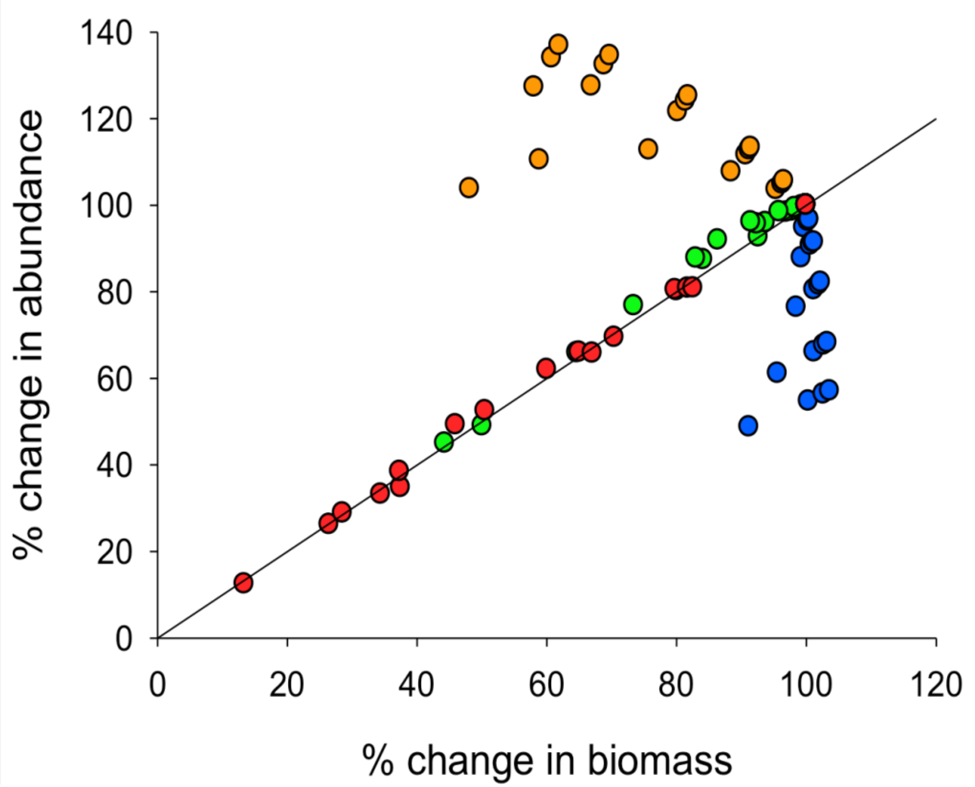
40 ug/l



Data from Preuss et al. (2010)

Ecological importance of pMoA*

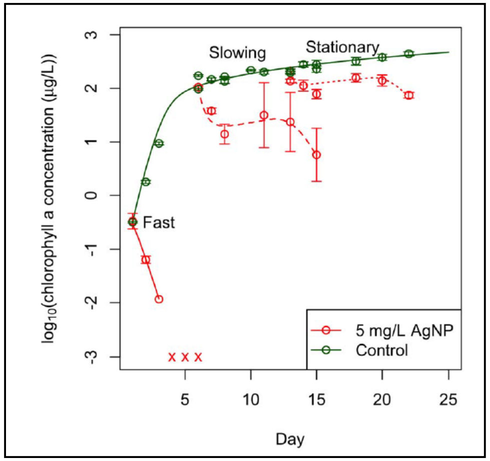


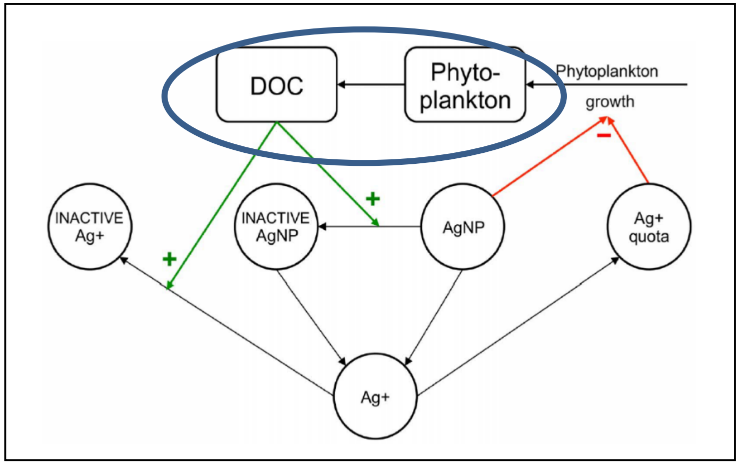


*Martin, B., Jager, T., Nisbet, R.M., Preuss, T.G., and Grimm, V: *Ecology Letters,* 2014

Feedback via abiotic environment*

Batch cultures of microalgae exposed to silver nanoparticles*





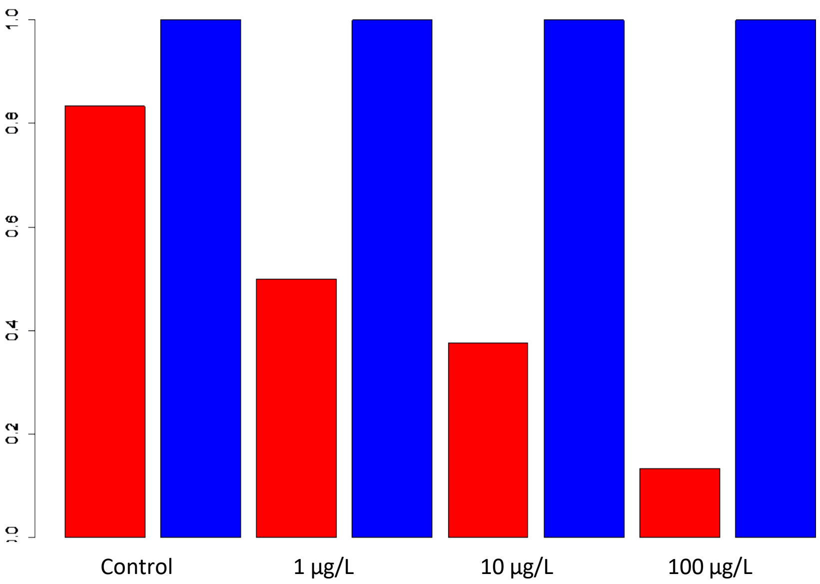
- Silver NPs were added to phytoplankton after 1, 6 and 13 days
- dynamic model included <u>DOC production</u>, <u>DOC-mediated inactivation</u> of nanoparticles and of ionic silver.

*Stevenson et al. (2013) PLOSone: https://doi.org/10.1371/journal.pone.0074456.

Impact on other species

Can algal-produced organic material protect other aquatic species?

Daphnia 48-hr survival when exposed to silver nanoparticles

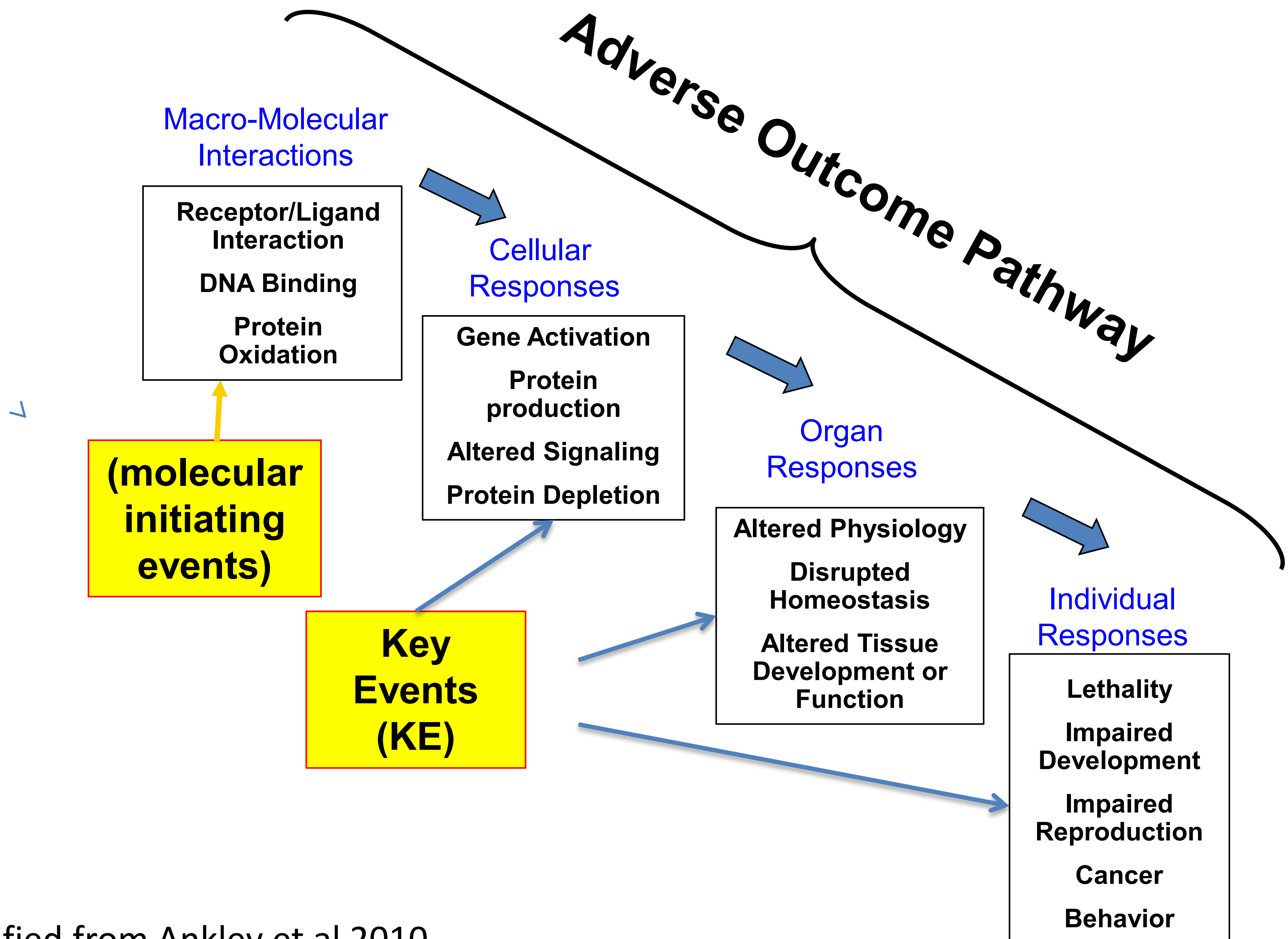


Red = standard medium;
Blue = standard medium with added organic material from algal cultures

Suborganismal to Individual

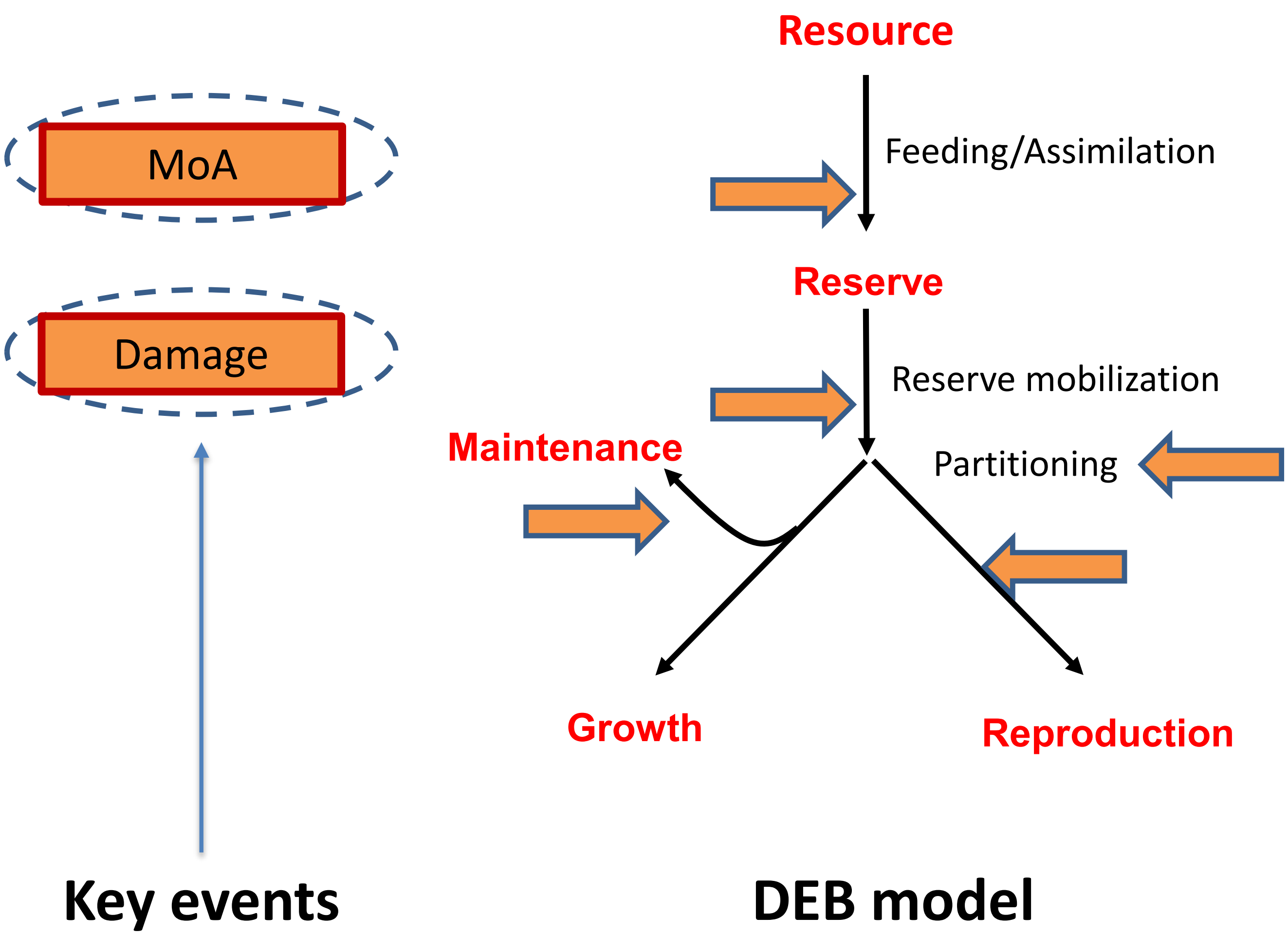
with AOPs

AOPs?



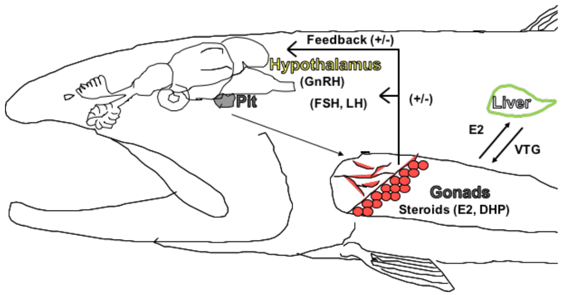
Modified from Ankley et al 2010

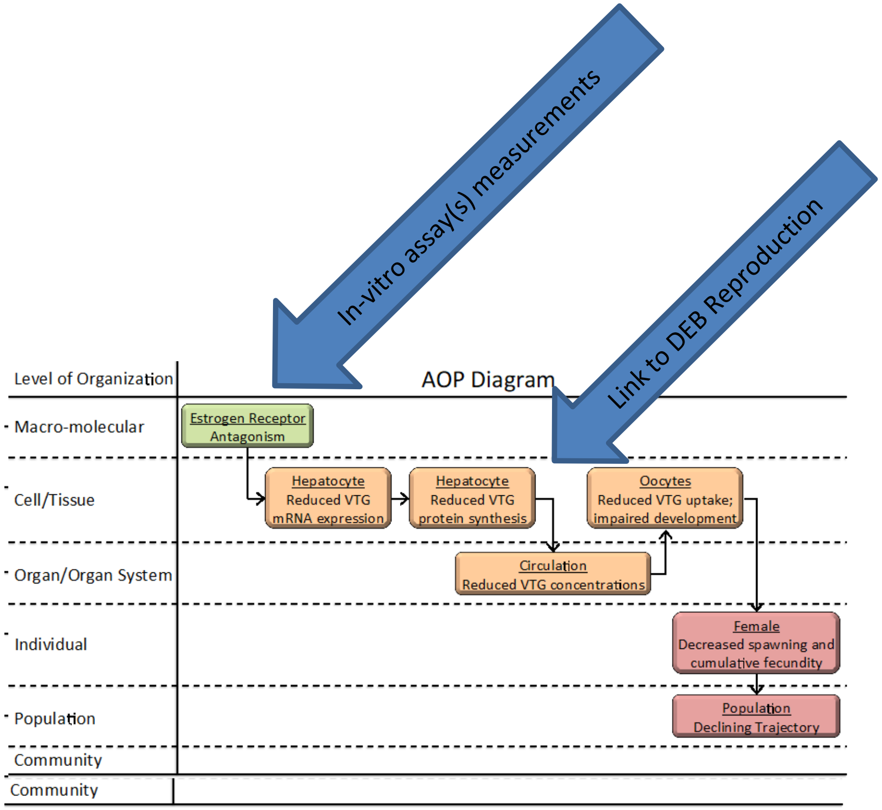
Conceptual model linking AOP and DEB approaches



C. A. Murphy + NIMBioS group, *Integrated Environmental Assessment and Management*, 2018

Example: AOP for Estrogen Receptor Antagonism in trout





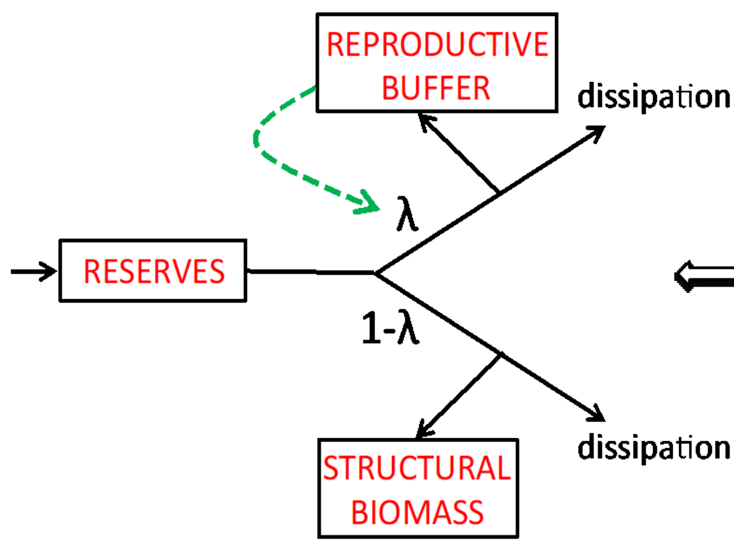
Slide from Karen Watanabe

Watanabe, K. H. and Schultz, I. R. (2015). Development of quantitative adverse outcome pathways for ecological risk assessment. In *SETAC North America 36th Annual Meeting Abstract Book*: p. 347.

How to relate to DEB?

Change <u>short term</u> energy allocation rules

Demand DEB is Standard DEB with feedback of reproductive buffer on reserve partitioning



⟺

Data from Gillies *et al*. (2016)
(10.1371/journal.pcbi.1004874)

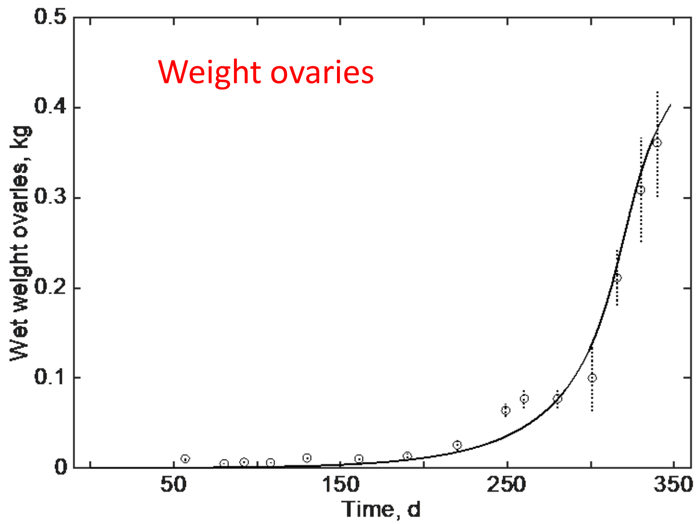
Weight ovaries (proportional to size reproductive buffer)

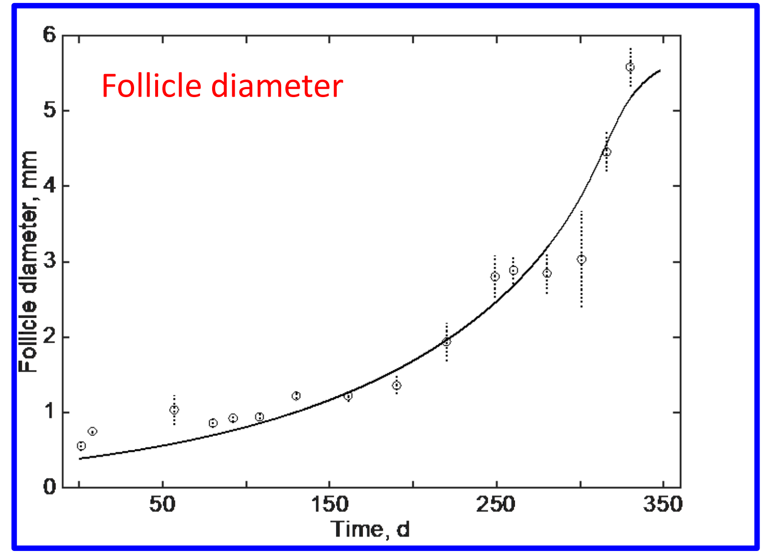
- Weight (wet)
- Follicle diameter
- Plasma estradiol
- Plasma vitellogenin

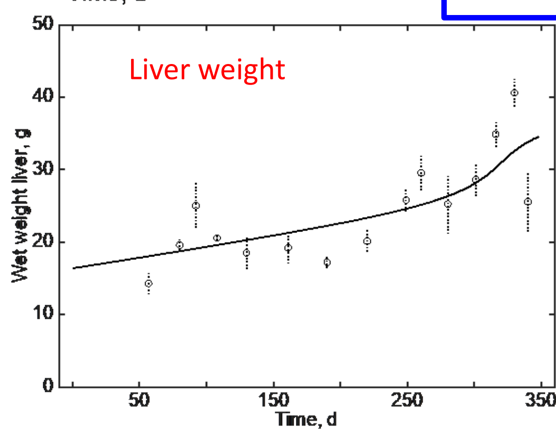
Weight liver (consists of reserves, structure and reproductive matter

Muller, Lika, Nisbet, Schutz, Casas, Gergs, Murphy, Nacci, Watanabe. Regulation of reproductive processes with dynamic energy budgets , *Functional Ecology,019*

Rainbow Trout, third year –*DemandDEB* fits

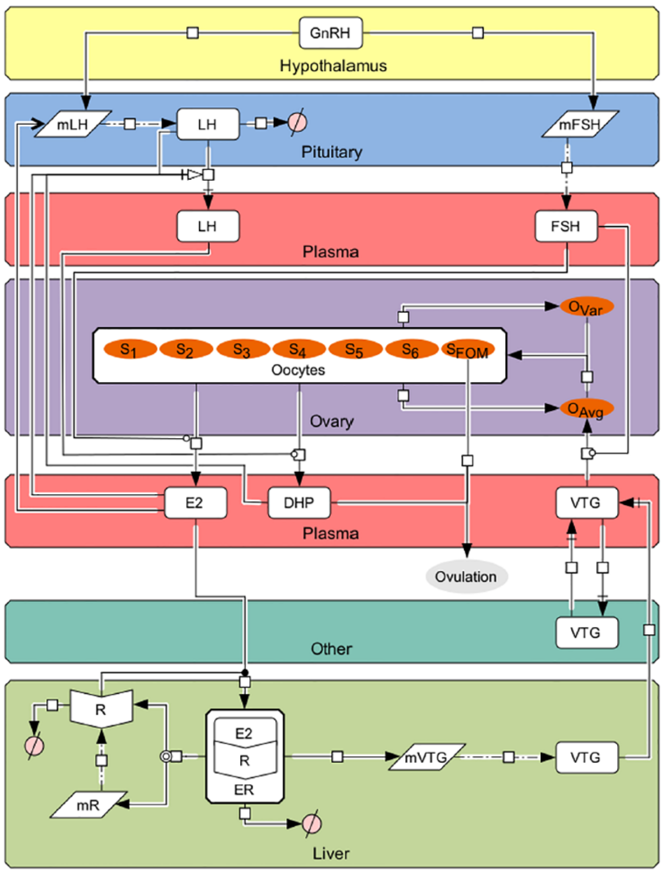




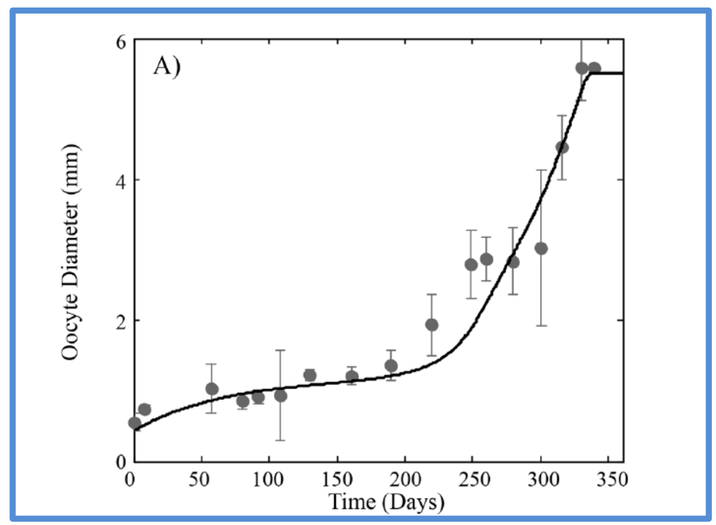


Data from Gillies *et al* (2016)
10.1371/journal.pcbi.1004874

"Bottom-up" model of same system



- Many feedbacks – positive and negative
- Model predicts rate of oocyte growth (primarily driven by Vitellogenin ("VTG" in diagram) supply.



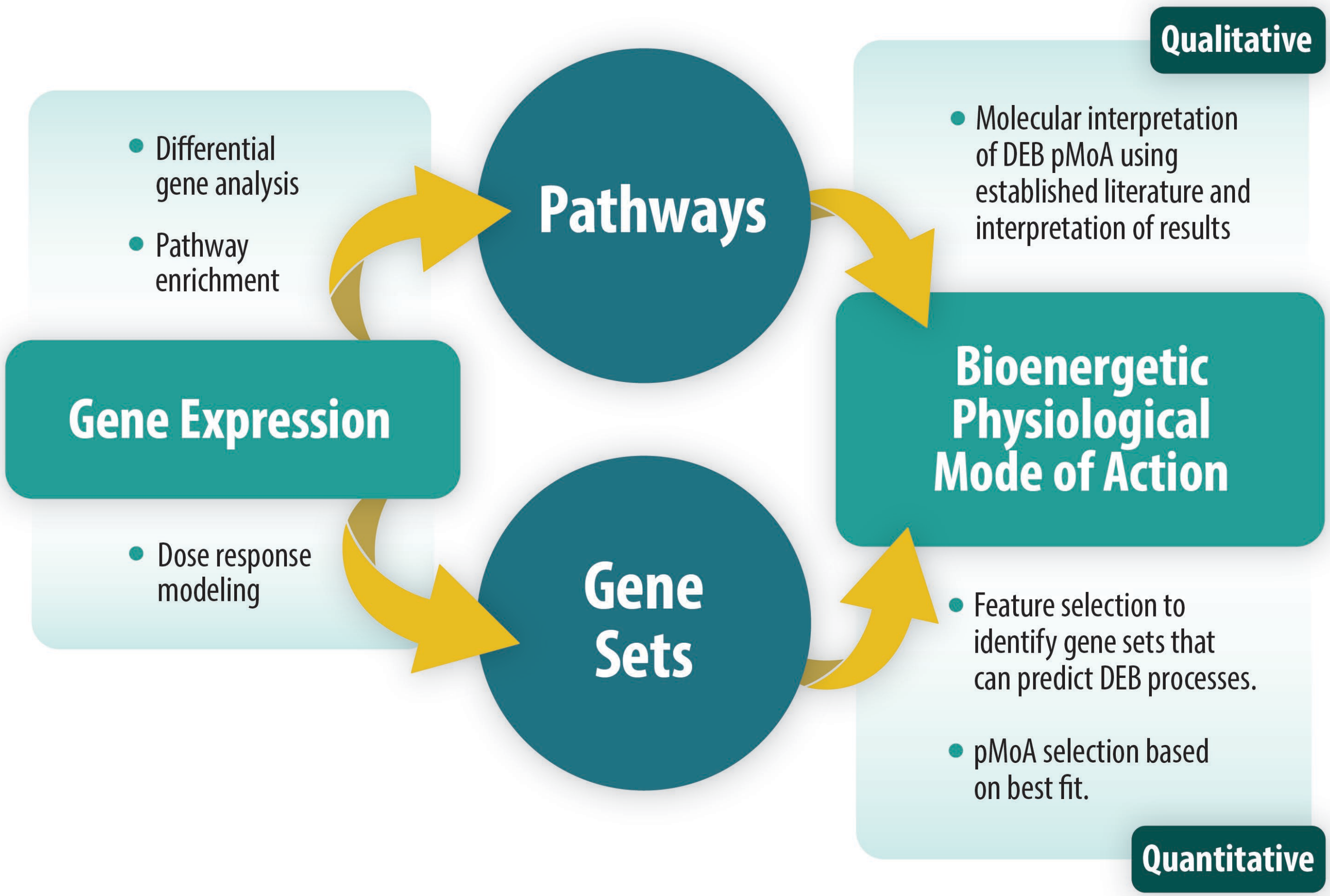
Gillies K, Krone SM, Nagler JJ, **Schultz IR** (2016). PLoS Comput Biol 12(4): e1004874. doi:10.1371/journal.pcbi.1004874

Suborganismal to Individual

with Transcriptomics

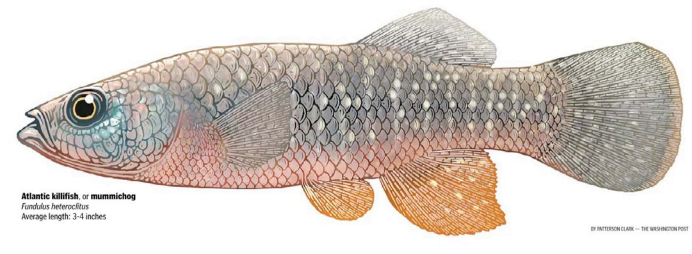
Linking gene expression to DEB

Gene expression quantified using RNAseq

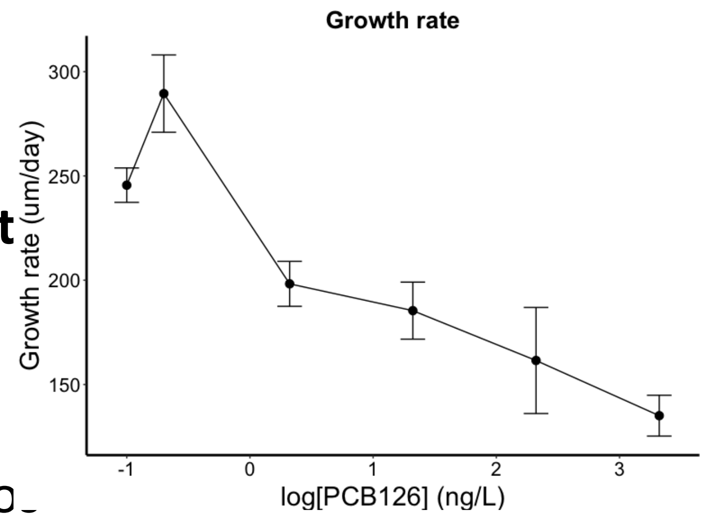


Example study: ‘omics to DEB

<u>Case Study:</u> *Fundulus* and dioxin-like chemicals (DLCs)



- *Fundulus heteroclitus*
- Established AOP for DLC – AHR pathway activation
  - Precise mode of action unknown
- DLCs in *Fundulus*
  - Embryo-larval exposures result in **lethality at ng/L concentrations**
  - AHR binding evident (CYP1A -> EROD) at **sublethal concentrations**
  - **Sublethal effect on larval growth** for embryos surviving exposures (unpublished data)



Stevenson, Clark, Muller, Nacci, Whitehead, Nisbet (in press) *Environmental Toxicology and Chemistry*

Transcriptomic response to sublethal DLC exposure

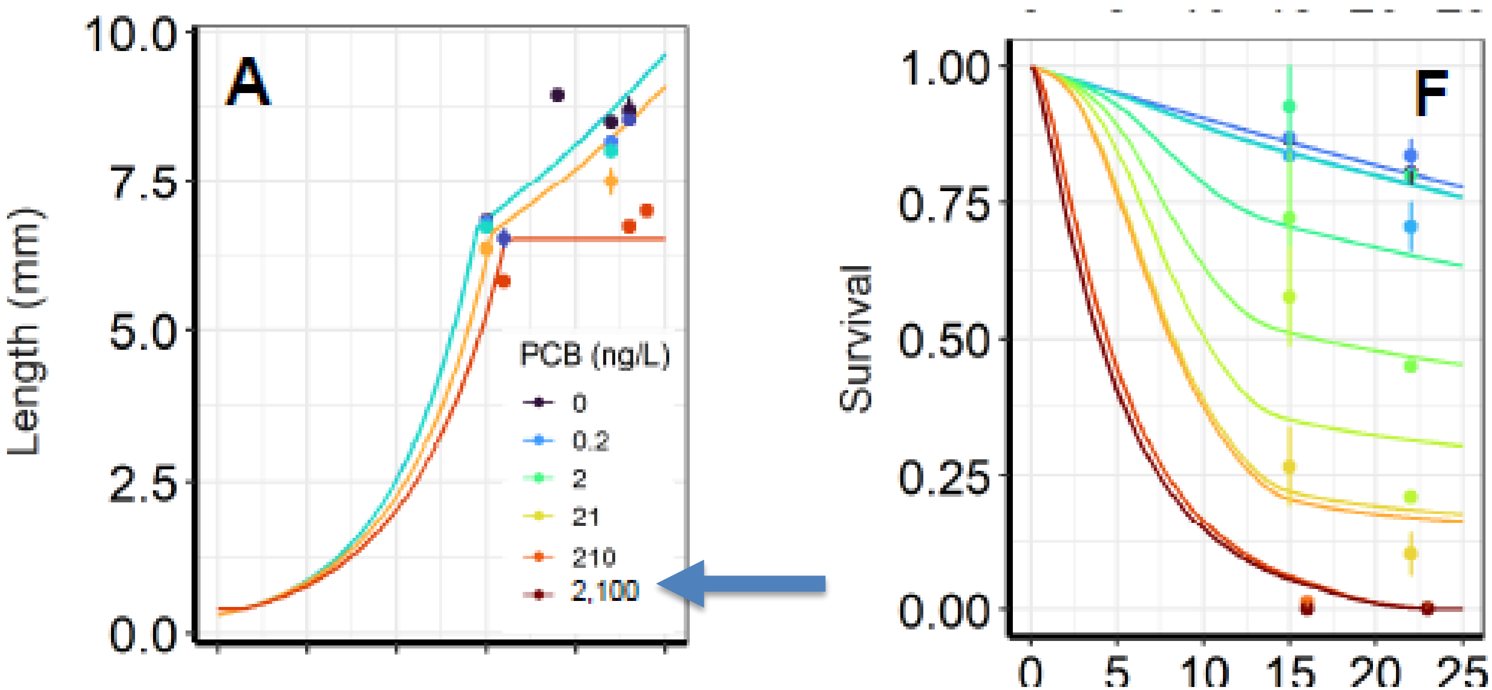
- Clusters common among concentrations:
  - Up regulated
    - Oxidoreductase (stress response)
    - Signaling (neurotransmission, muscle contraction, proper heart function)
    - Cytochrome P450
    - Xenobiotic metabolism
  - Down regulated
    - Muscles (muscle proteins, tropomyosin, and actin filaments), specifically muscle contraction
    - Glycolysis

<u>OVERALL:</u>

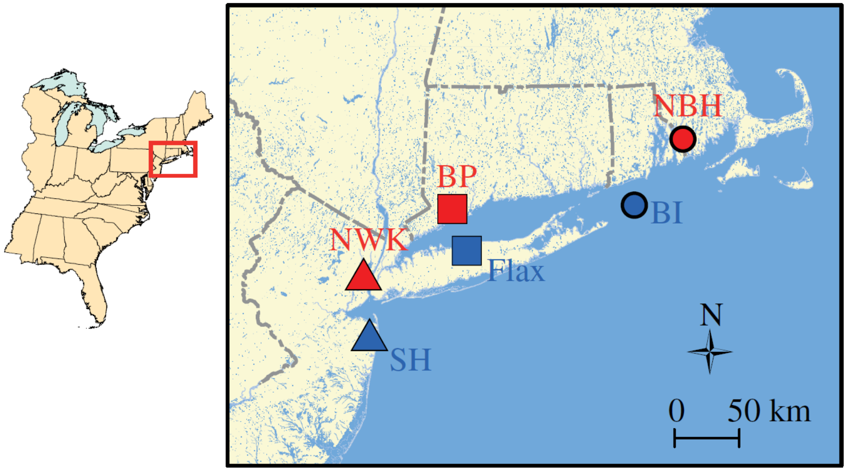
- Increase in detoxification response
- Signs of AhR pathway activation (e.g. CYPs)
- Cardiac impairment (PCBs teratogenic by messing with heart development)

→ Hypothesis: **maintenance costs increasing with DLC exposure**

Model Fits – sensitive fish



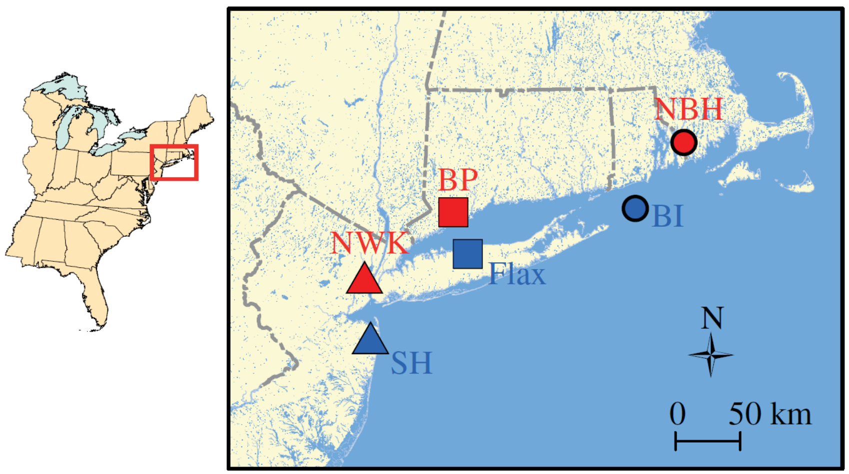
"Postdiction"/model verification of resistant populations



- Matched sensitive (blue) and tolerant (red) populations of *Fundulus heteroclitus*
- Model fit to sensitive fish, can it predict impact of DLCs on resistant fish?

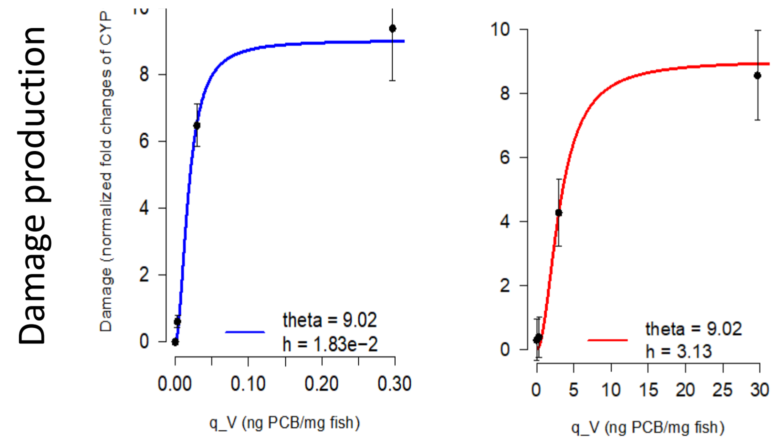
Whitehead et al. Proc. R. Soc. B (2012) 279, 427–433

“Postdiction”/model verification of resistant populations



Sensitive populations
h = 1.83e-2

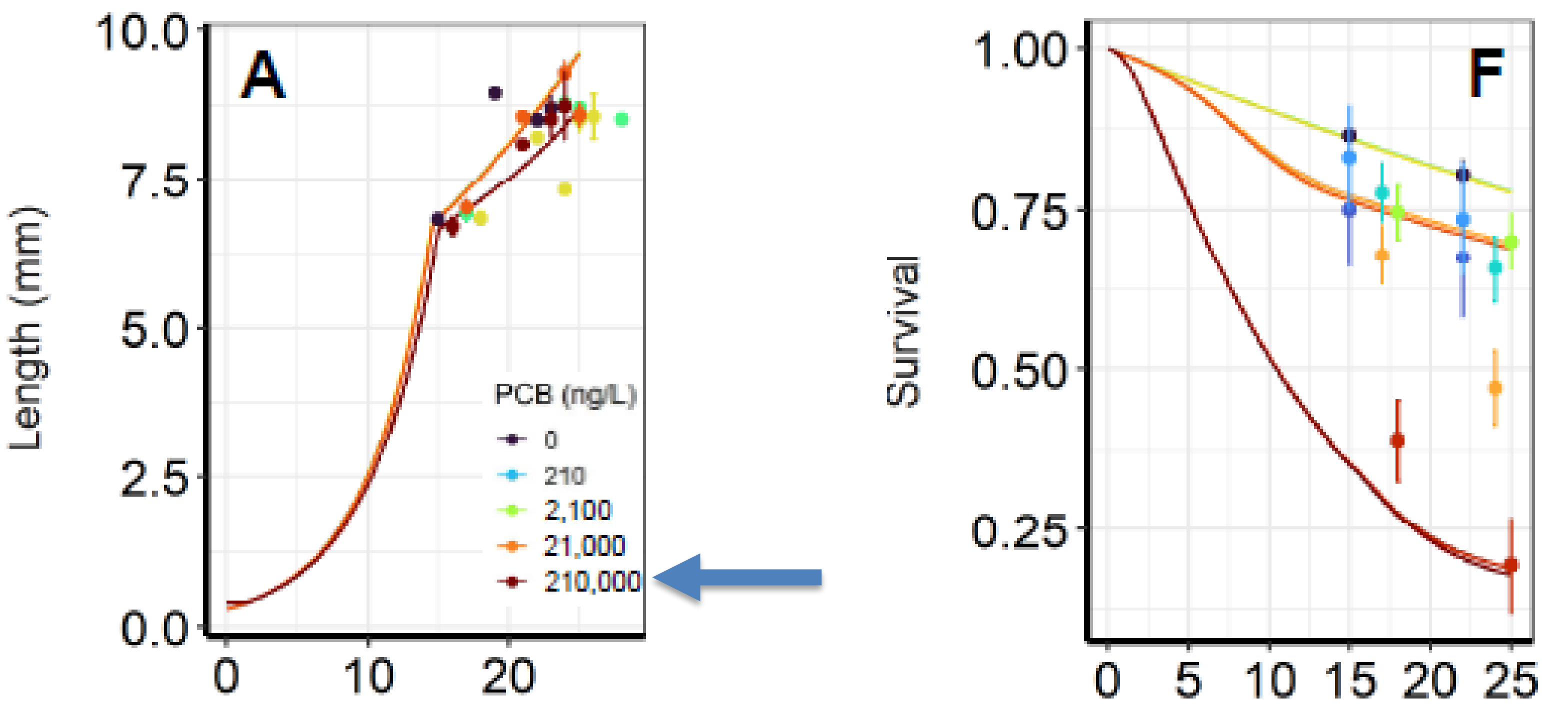
Resistant populations
h = 3.13



Internal concentration of PCB-126 (ng PCB/mg fish)

Changed **one parameter** between sensitive and tolerant populations (*h* describing damage production) → how well does model “postdict” resistant data?

Model Fits – tolerant fish



Take home message