
UNITED STATES
ENVIRONMENTAL PROTECTION AGENCY

Pesticides
Federal Insecticide, Fungicide & Rodenticide Act
(FIFRA)

≈2,000

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Chemicals under Federal Food, Drug, and Cosmetic Act
(FFDCA)

≈2,000

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Chemicals under Federal Food, Drug, and Cosmetic Act
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Industrial chemicals under Toxic Substances Control Act (TSCA)
≈84,000

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This is a lot of chemicals to evaluate

Traditional toxicity testing doesn't stand a chance

96hr Lethal Concentration at 50% mortality (LC50) takes 4 days to complete per chemical

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$$84000\ chemicals * 4 \frac{days}{chemical} \approx 920\ years$$

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Does anyone know approximately how many listed species there are in the US?

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There are currently around 1600 threatened or endangered species in the US

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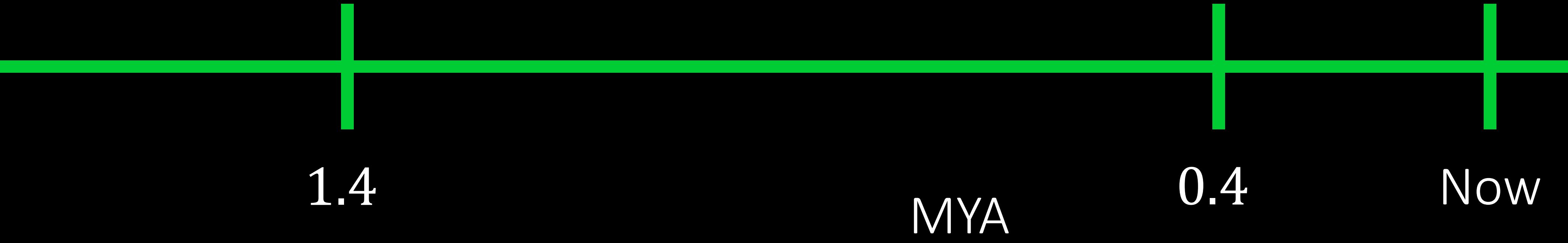
Evaluating chemicals for listed species in this way will take

1,472,000 years


1.4
MYA
0.4
Now

Homo erectus learned how to use fire

Homo sapiens

1.4

MYA

0.4

Now

Homo sapiens

1.4

MYA

0.4

Now

Traditional toxicity testing doesn't stand a chance

We need models

SIZE, AGE, SEX, AND/OR STAGE?

Developing structured population models for ecotoxicology

Nate Pollesch, PhD
USEPA
Office of Research and Development
Great Lakes Ecology and Toxicology Division
Duluth, MN

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Ecotoxicology is the study of how toxic chemicals affect populations, communities, and ecosystems

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Structured population models utilize traits of individuals to determine population dynamics

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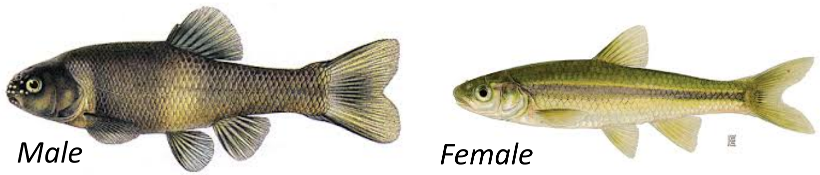
Fathead minnow
Pimephales promelas



Structured population models utilize traits of individuals to determine population dynamics

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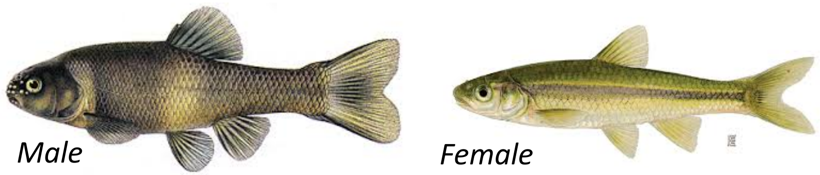
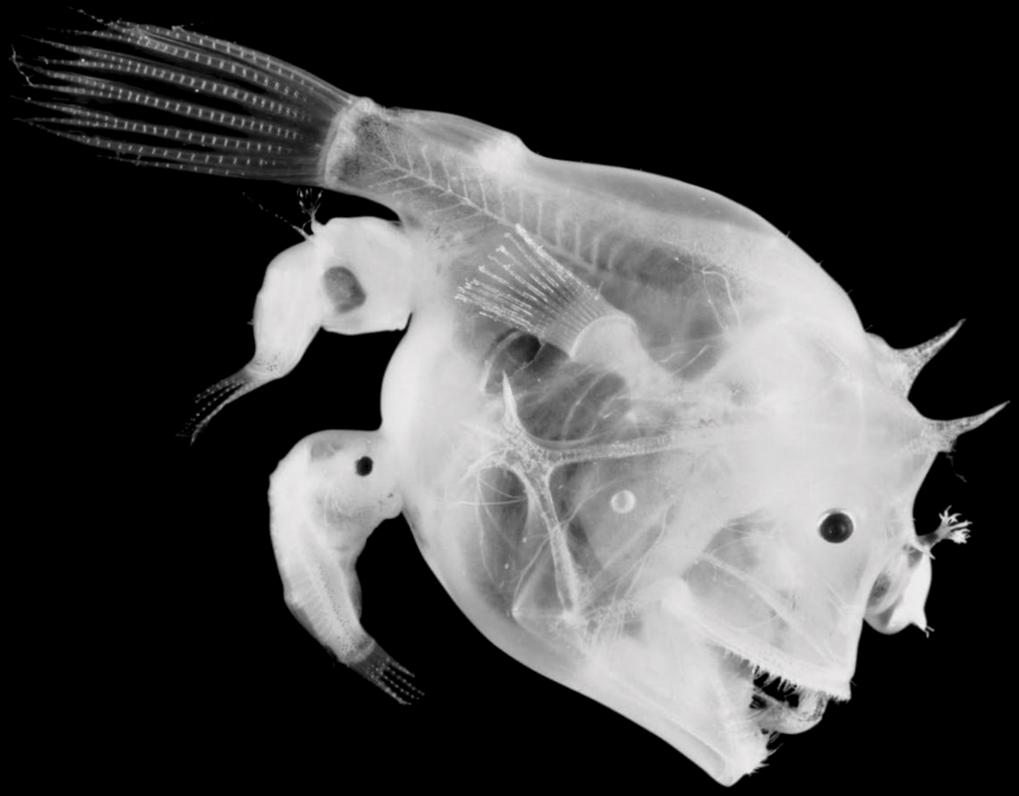


With Fatheads as our muse…

- What are some traits of fish?
- Are there traits that can be measured/observed in the lab, but not in the wild?
- What about the wild, but not the lab?

Examples of individual traits that may be important for population dynamics

- Age
- Size
- Developmental stage
- Disease status
- Toxic exposure/effect
- Sex
- Territory Possession
- Spatial Location



Examples of individual traits that may be important for population dynamics

- Age
  - Accumulation of time
- Size
  - Accumulation of length or mass
- Developmental stage
  - Juvenile vs adult
  - ‘breeder’ vs ‘non-breeder’
  - Seed, seedling, non-flowering plant, flowering plant
- Disease status
  - Susceptible, infected, recovered
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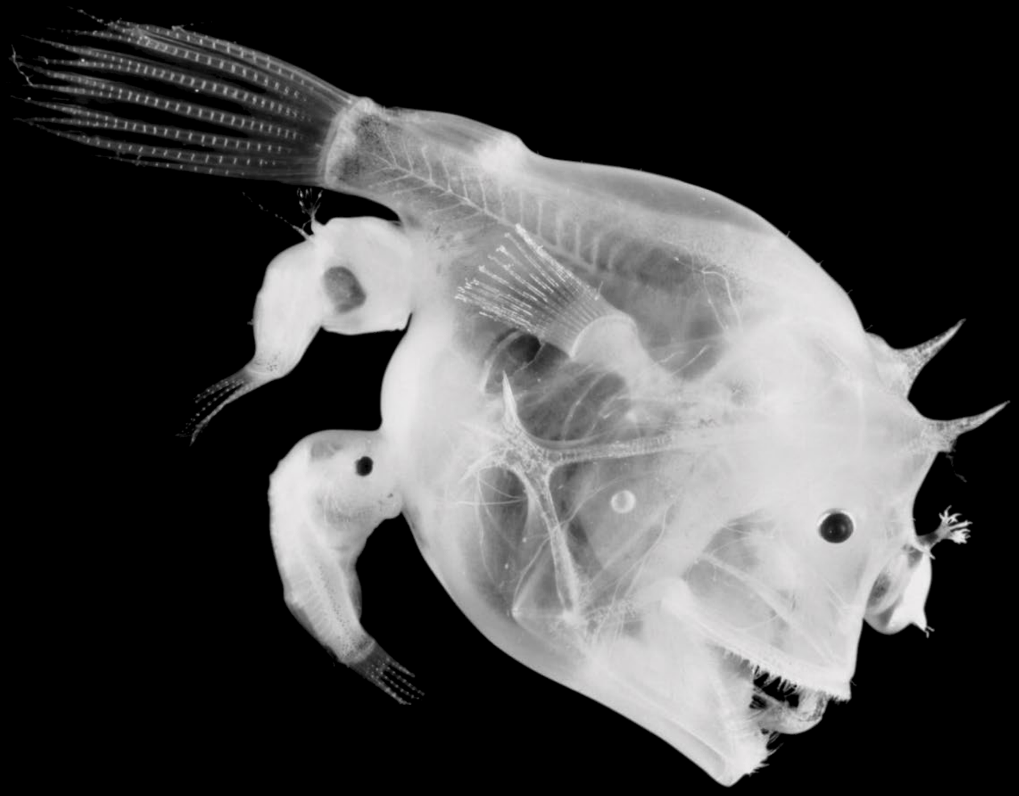

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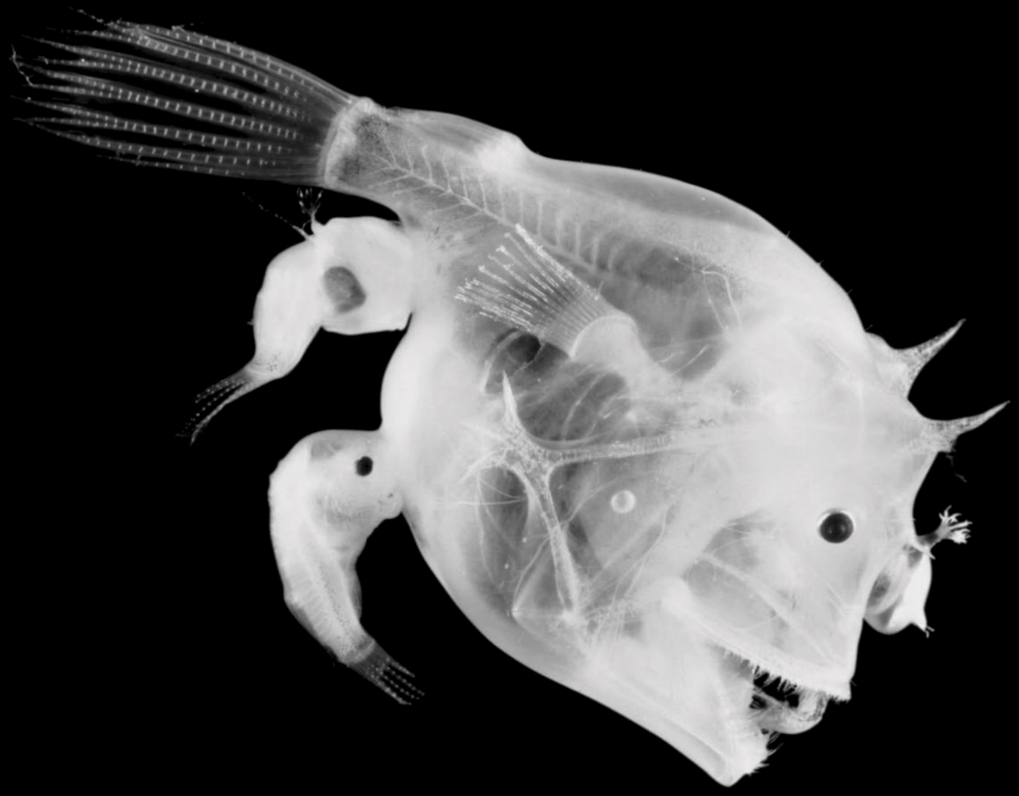
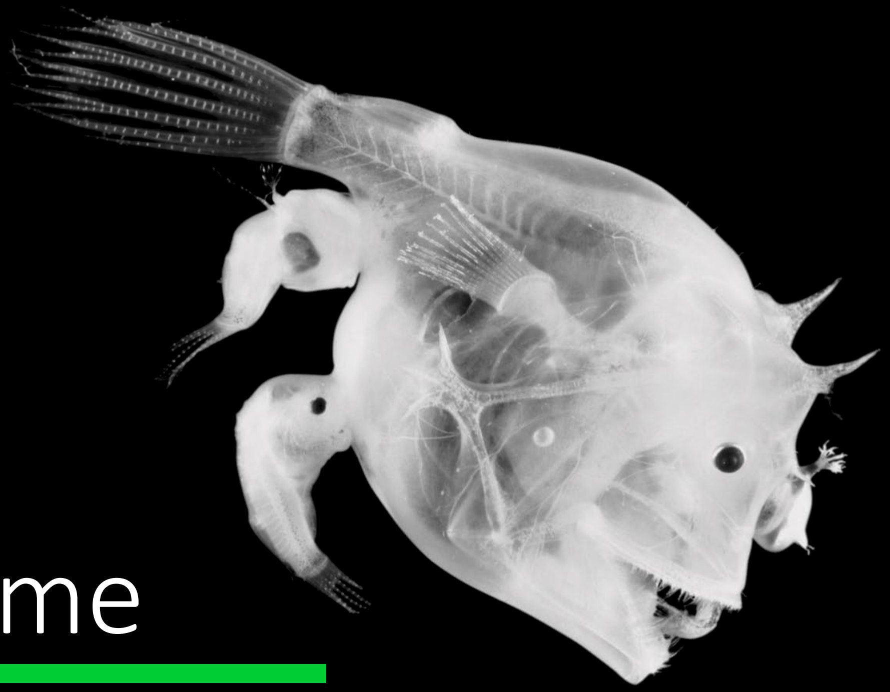
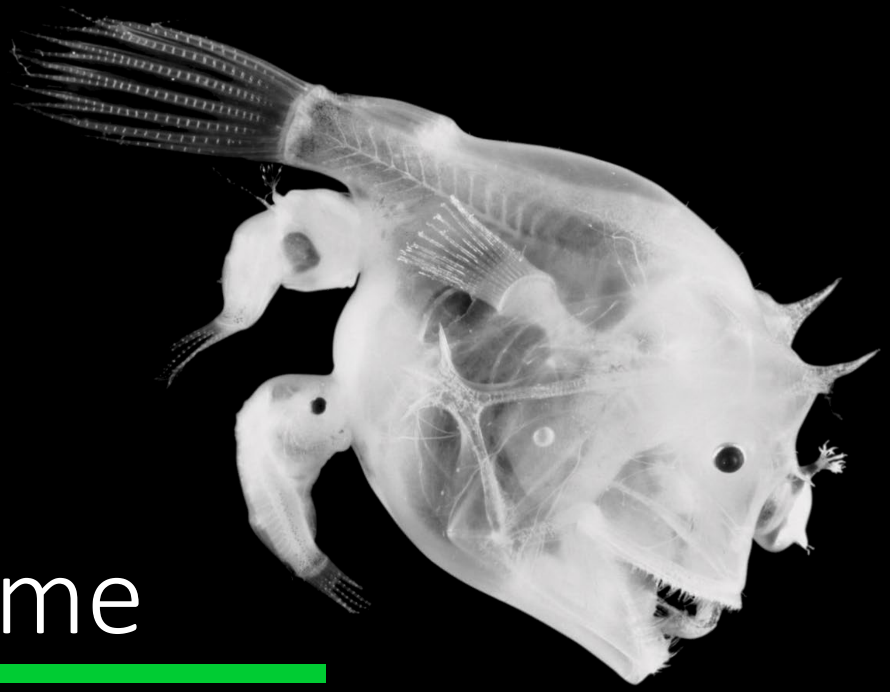


Biology is awesome





Biology is awesome

Biology is messy

Synthetic Hormones in sewage are toxic to male fish over generations by K. Keteles

https://blog.epa.gov/blog/2014/06/synthetic-female-hormones-in-sewage-are-toxic-to-male-fish-over-generations/

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Sex structure
Spatial structure
Internal dose/exposure
Age structure
Parental effects

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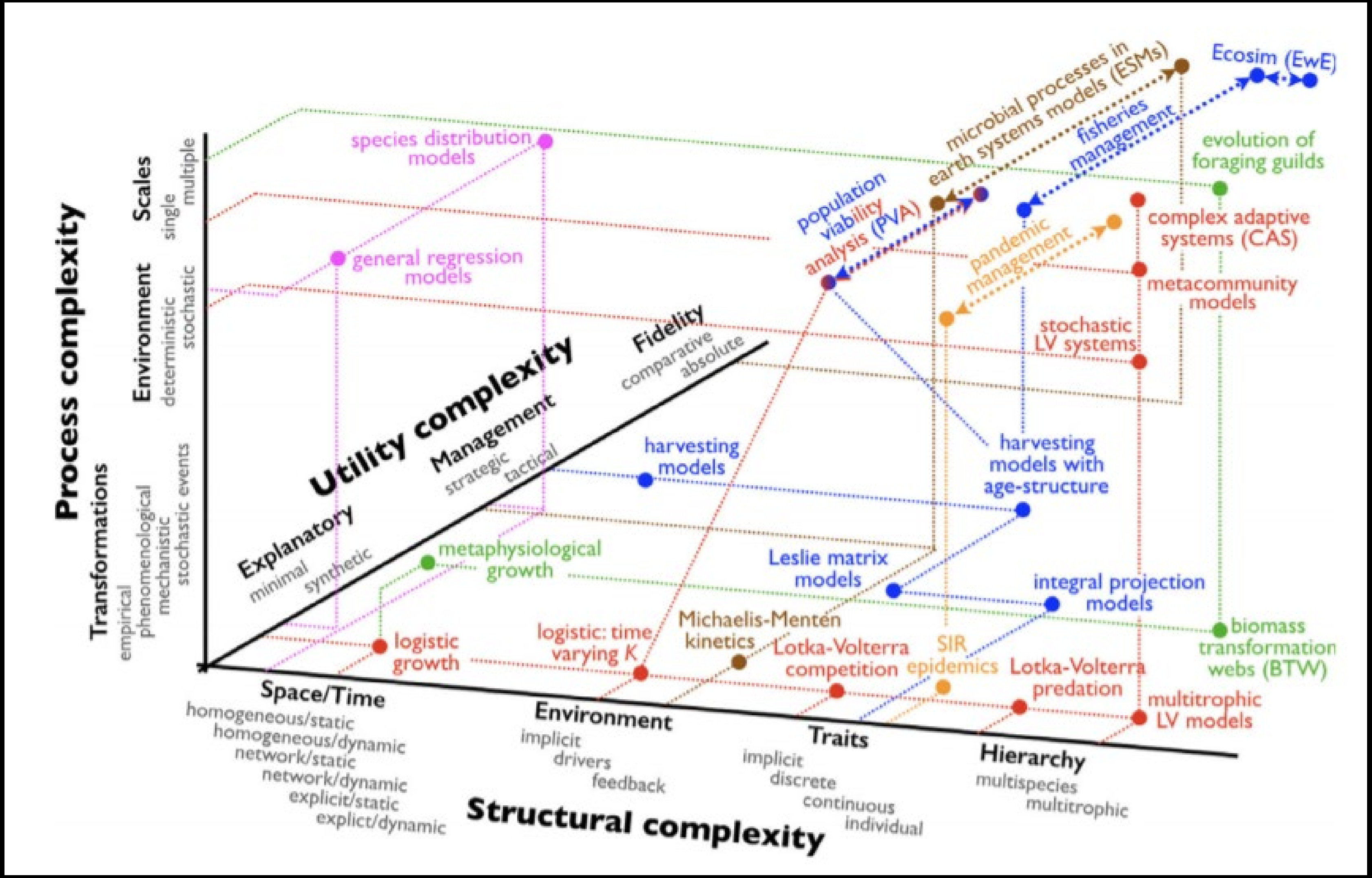

Model Typology from Getz et al., 2018 *Making ecological models adequate*

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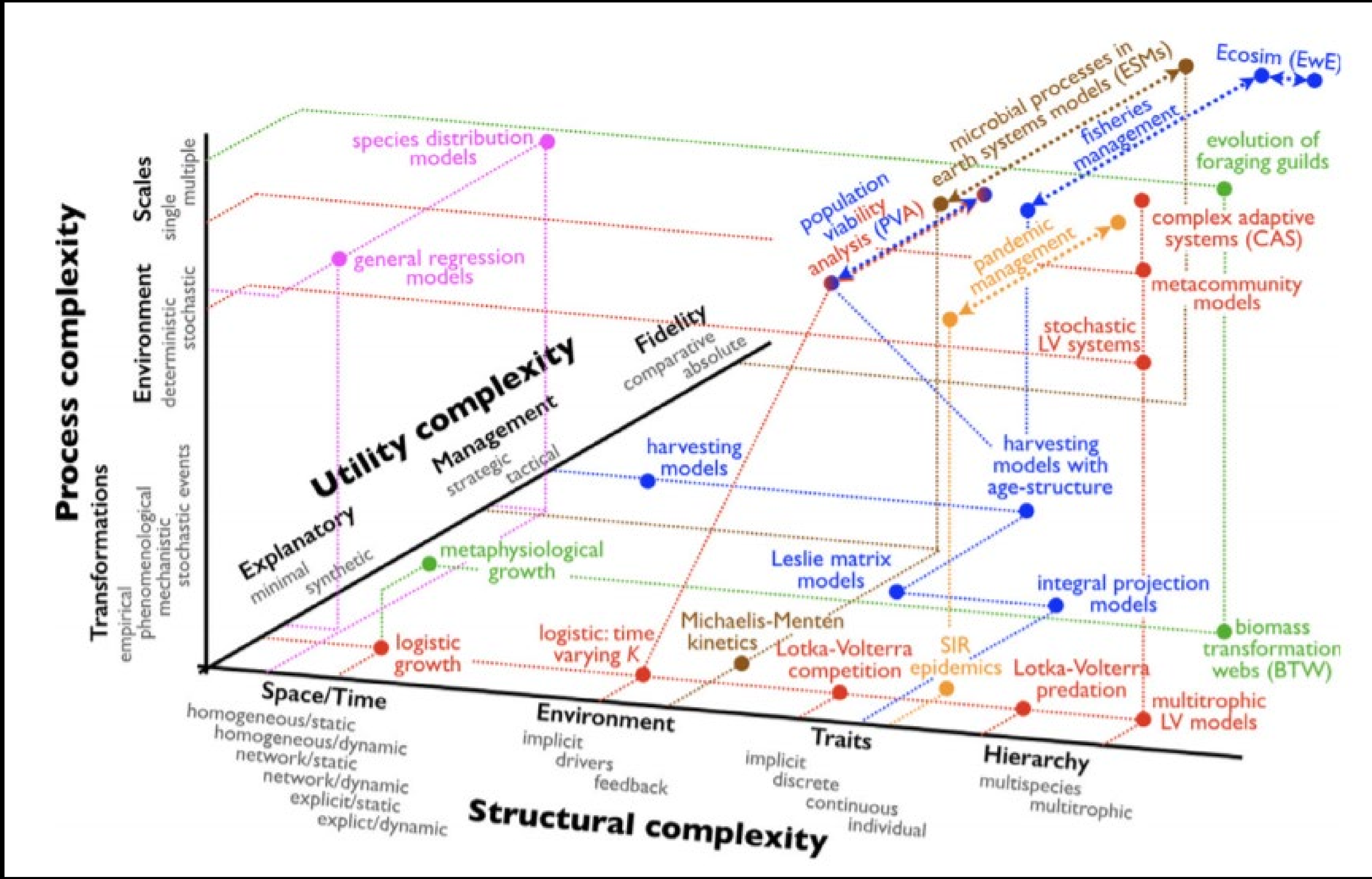

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Sex structure
Spatial structure
Internal dose/exposure
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Parental effects

Traits:

- Traits can be implicitly reflected in parameter values (e.g. Lotka–Volterra competition models)
- Or explicitly incorporated as discrete or continuous distributions (e.g. integral projection models – IPMs – are distributional generalisations of discrete matrix age or other trait structure models.
- The most comprehensive way to model multi-trait structure is to use an individual-based modelling (IBM) approach.

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What's a modeler to do?

What are you trying to study?

Are certain traits (relatively) more important to population dynamics than others?

What data do you have?

Can you measure and/or quantify the important traits?

Which traits are the MOST important?

Sex structure
Spatial structure
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What are you trying to study?

- Effect of synthetic hormones? Effect of living in wastewater effluent?

Are certain traits (relatively) more important to population dynamics than others?

- Sex reversal, acute toxicity, decrease reproductive fitness

What data do you have?

- What data, indeed*

Can you measure and/or quantify the important traits?

- "Males are indistinguishable"? Are there overt signs of reproductive fitness decreasing?

What's a modeler to do?

Which traits are the MOST important?

Sex structure
Spatial structure
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Sex structure
Spatial structure
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* Parental effects

What model should I use?

Sex structure
Spatial structure
Internal dose/exposure
Age structure
Parental effects

*

What model should I use?

Discrete time, discrete sex, discrete age matrix model

Sex and age structured matrix model applied to harvesting a white tailed deer population (Jensen, 2000)

$$\vec{N}_{t+1} = \vec{N}_t + D(N_t)(M - I)\vec{N}_t \qquad D(N_t) = \frac{(K - N_t)}{K}$$

$$* \quad \vec{N}_t = \begin{bmatrix} N_{t,0,\mathrm{m}} \\ N_{t,0,\mathrm{f}} \\ N_{t,1,\mathrm{m}} \\ N_{t,1,\mathrm{f}} \\ N_{t,2,\mathrm{m}} \\ N_{t,2,\mathrm{f}} \end{bmatrix} \qquad M = \begin{bmatrix} 0 & F_{\mathrm{m}0} & 0 & F_{\mathrm{m}1} & 0 & F_{\mathrm{m}2} \\ 0 & F_{\mathrm{f}0} & 0 & F_{\mathrm{f}1} & 0 & F_{\mathrm{f}2} \\ p_{\mathrm{m}0} & 0 & 0 & 0 & 0 & 0 \\ 0 & p_{\mathrm{f}0} & 0 & 0 & 0 & 0 \\ 0 & 0 & p_{\mathrm{m}1} & 0 & 0 & 0 \\ 0 & 0 & 0 & p_{\mathrm{f}1} & 0 & 0 \end{bmatrix}$$

Where N are individuals by age and sex, K is the carrying capacity, F are fecundities, and p are survival probabilities

What model should I use?

Continuous time, discrete sex, continuous age PDE model

Persistent Age Distributions for An Age-Structured Two-Sex Population Model (Inaba, 1999)

Sex structure
Spatial structure
Internal dose/exposure
Age structure
Parental effects

*

$$\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial a}\right)p_m(t,a) = -\mu_m(a)p_m(t,a) - \int_0^\infty \rho(t,a,\eta)d\eta + \int_0^a \int_0^\infty [\mu_f(\tau+\eta)+\delta(\tau;a-\tau,\eta)]s(t,\tau;a-\tau,\eta)d\eta d\tau,$$

$$\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial a}\right)p_f(t,a) = -\mu_f(a)p_f(t,a) - \int_0^\infty \rho(t,\zeta,a)d\zeta + \int_0^a \int_0^\infty [\mu_m(\tau+\zeta)+\delta(\tau;\zeta,a-\tau)]s(t,\tau;\zeta,a-\tau)d\zeta d\tau,$$

$$\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial \tau}\right)s(t,\tau;\zeta,\eta) = -[\mu_m(\tau+\zeta)+\mu_f(\tau+\eta)+\delta(\tau;\zeta,\eta)]s(t,\tau;\zeta,\eta),$$

$$p_m(t,0) = (1-\gamma)\int_0^\infty \int_0^\infty \int_0^\infty \beta(\tau;\zeta,\eta)s(t,\tau;\zeta,\eta)d\zeta d\eta d\tau$$

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$$s(t,0;\zeta,\eta) = \rho(t,\zeta,\eta) = \Psi(p_m(t,*),p_f(t,*))(\zeta,\eta).$$

Discrete vs continuous representation of traits matters

Sex structure
Spatial structure
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Models are awesome

*

Models are awesome

Models can be messy

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What data do you have?

- What data, indeed*

*For real though, what data do you have?

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Data availability is the largest constraint for ecotoxicological population modeling

- Expense
- Time
- Ecotoxicological data at the population level is supposed to be rare

*For real though, what data do you have?

Data availability is the largest constraint for ecotoxicological population modeling

- Expense
- Time
- Ecotoxicological data at the population level is supposed to be rare
  - We are asking questions that we don't ever want actual answers for

Toxicity Translation

- Leveraging data from standard toxicity tests to infer population level effects of chemical exposure

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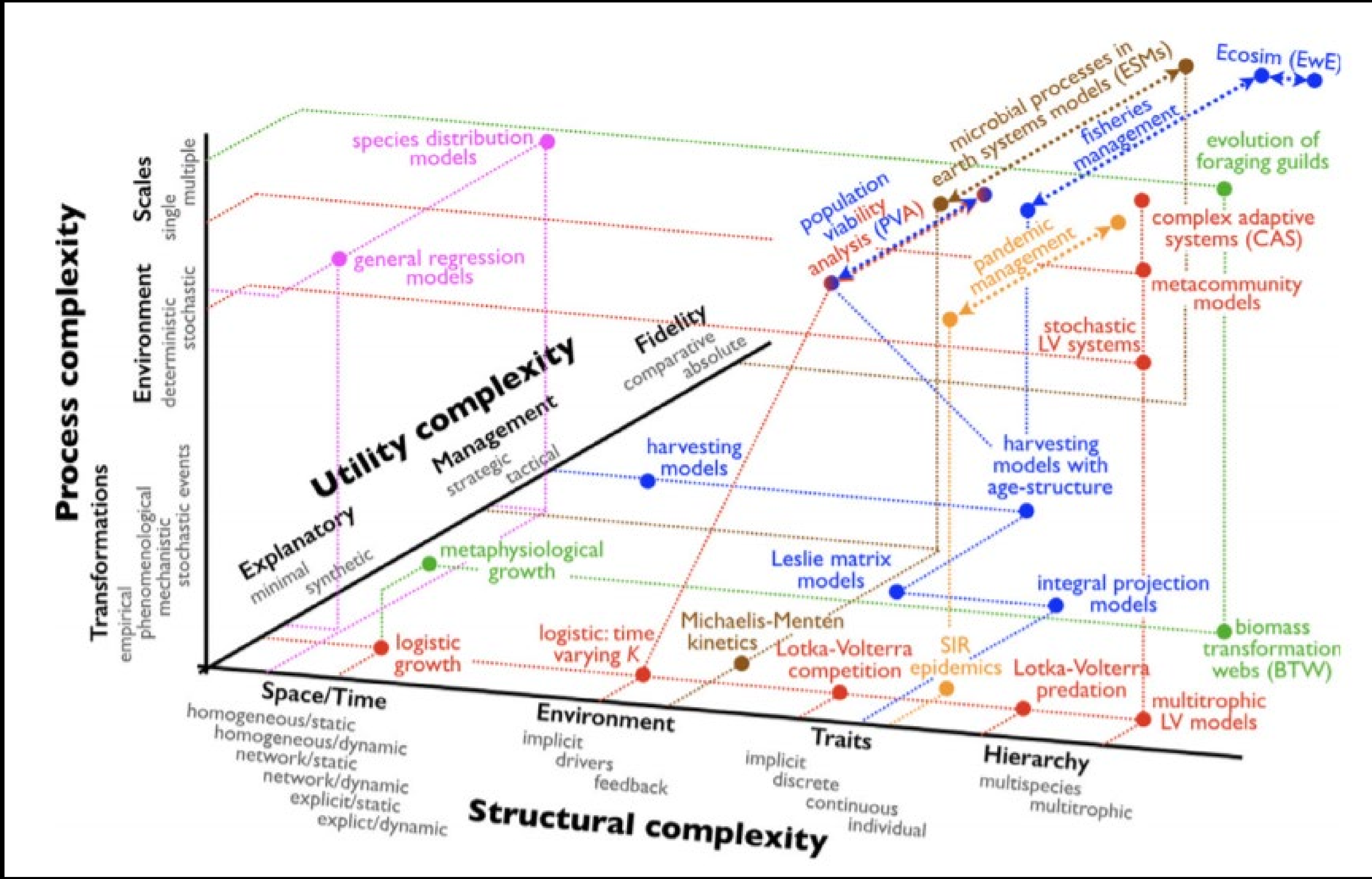
Growth

Survival

Reproduction

Integral Projection Models

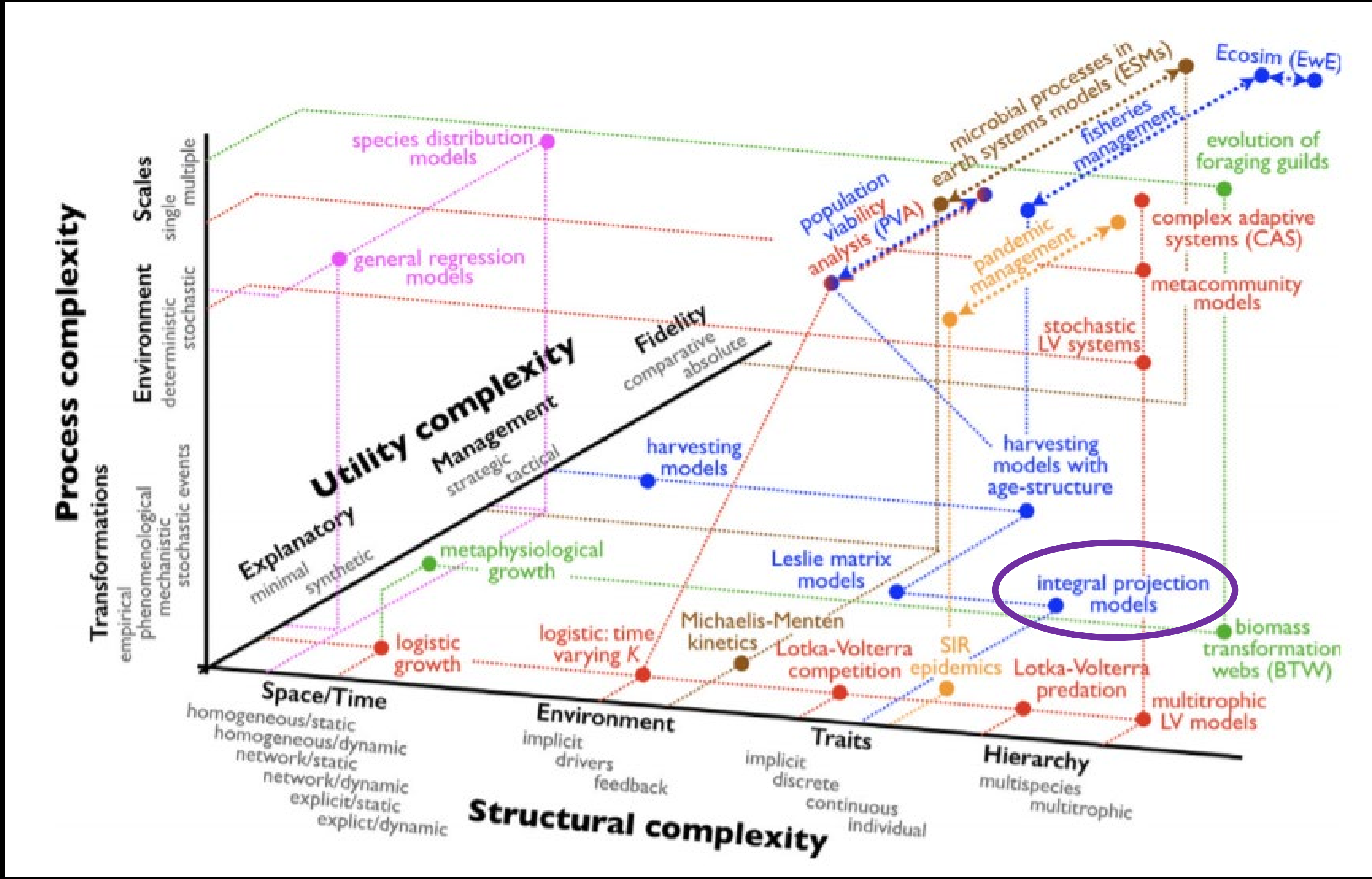
Integral Projection Models



Discrete time
Continuous Trait

Model Typology from Getz et al., 2018 *Making ecological models adequate*

Integral Projection Models



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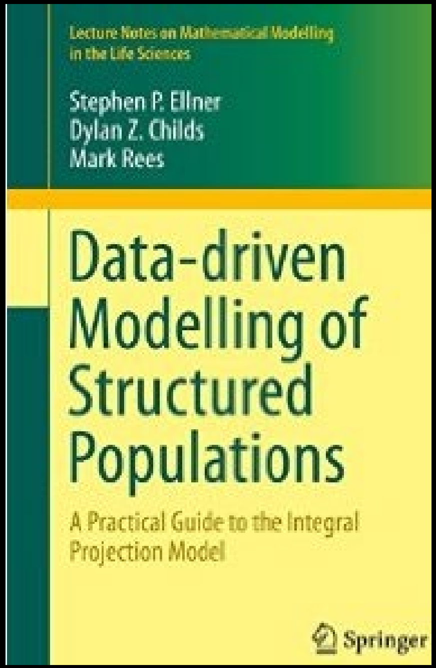
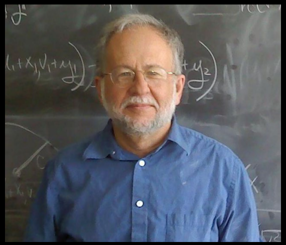
Discrete time

Continuous ~~Trait~~

Size



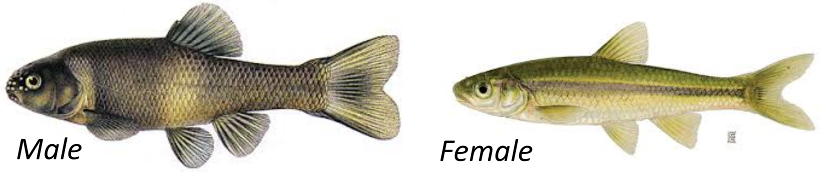
Ellner et al., 2016



Steve Ellner, Cornell

Fathead minnow

Pimephales promelas



For fish, why is size an important trait for growth, reproduction, and survival?

Fish Toxicity Translator Integral Projection Model

Fish Toxicity Translator Integral Projection Model

Size-structured model

Bringing size into the equation

- For fish, size is important toxicologically and ecologically
- IPMs link size to dynamics
- Our approach uses ***realistic exposure profiles (PWC)*** interpreted by different effect models (***TK-TD, threshold)*** to predict ***population-level impacts*** of exposures and stressors
- Most size measures are non-destructive in the laboratory

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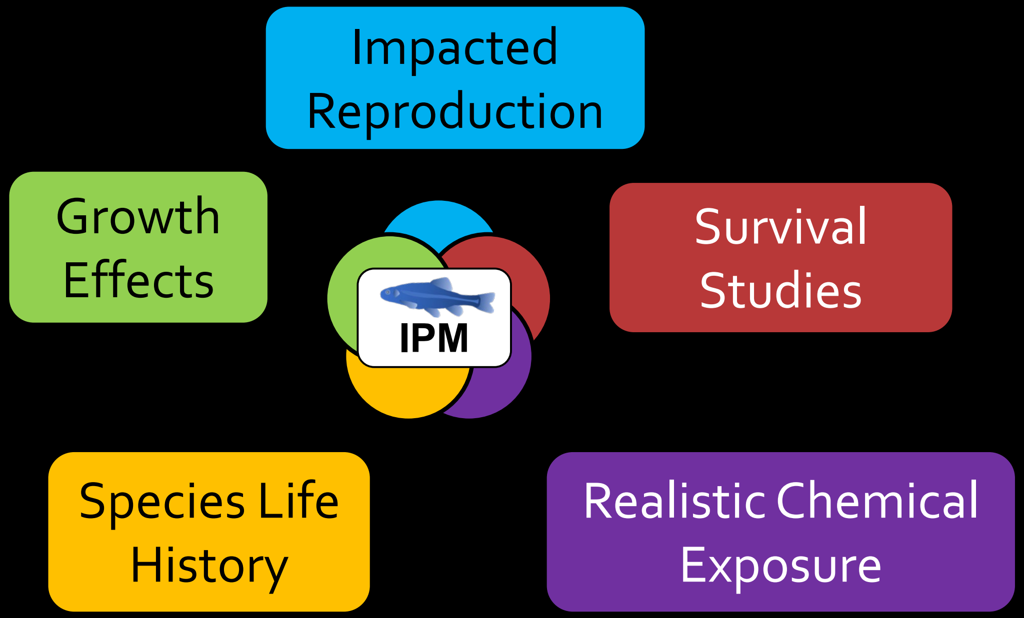
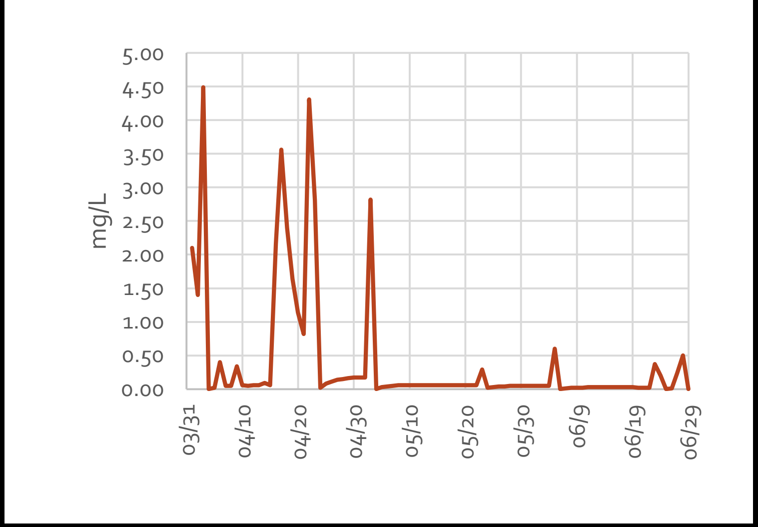


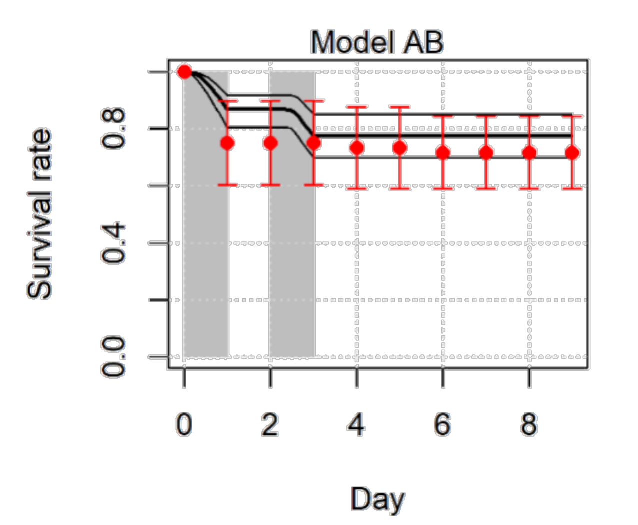
Pulsed exposure survival modeling

Realistic Chemical Exposure



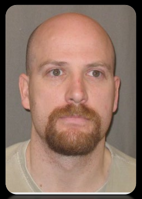
Predicted environmental concentrations can vary based on timing of use, precipitation, etc.

Survival Studies



Grey bars: Exposure periods
Black lines: Model-predicted survival
Red dots: Laboratory-observed survival


F. Whiteman


K. Flynn

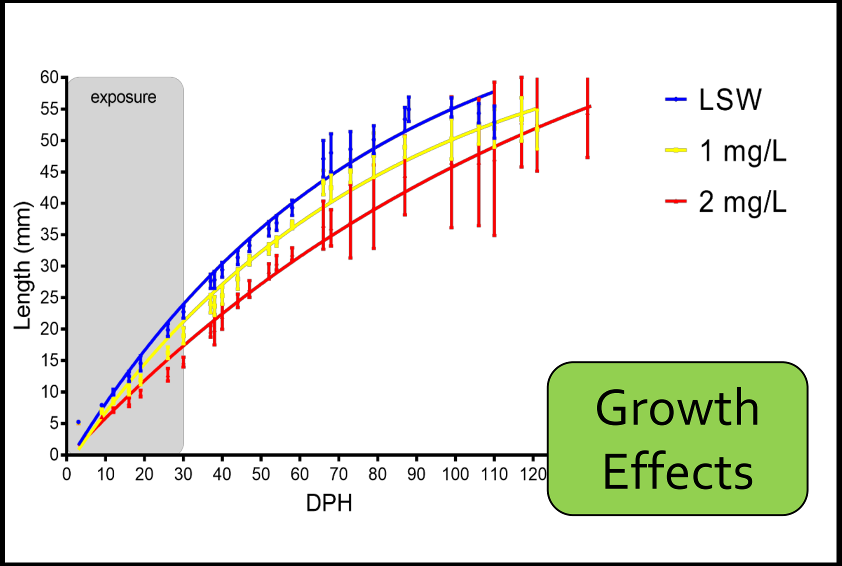

V.Kurker


S. Kadlec

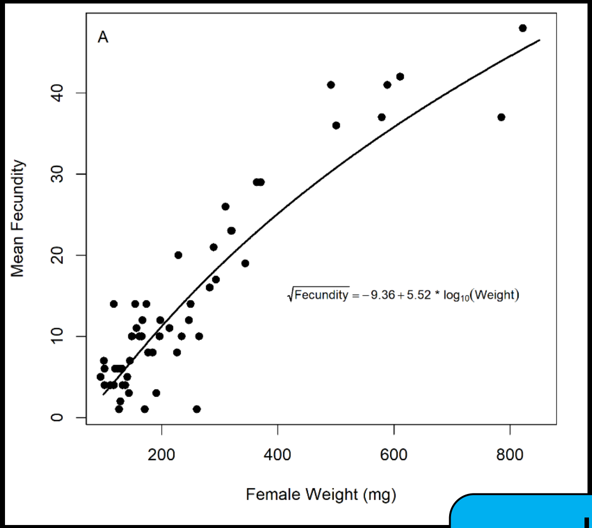
Toxicokinetic-toxicodynamic (TK-TD) models

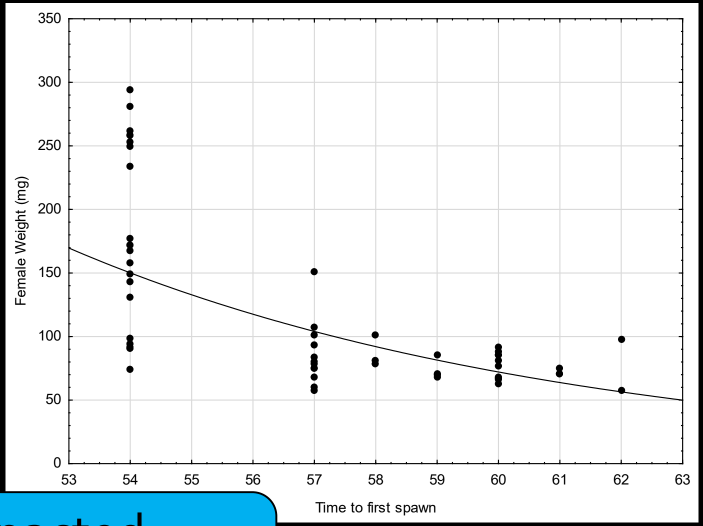
- Are effects of time-variable exposures different than constant exposures of the same average concentration?
- Simplified TK-TD models
  - Are calibrated with standard toxicity test data (constant exposure concentrations)
  - Can predict effects of simple and complex time-variable exposure scenarios

Growth and Reproductive Effects of Exposure

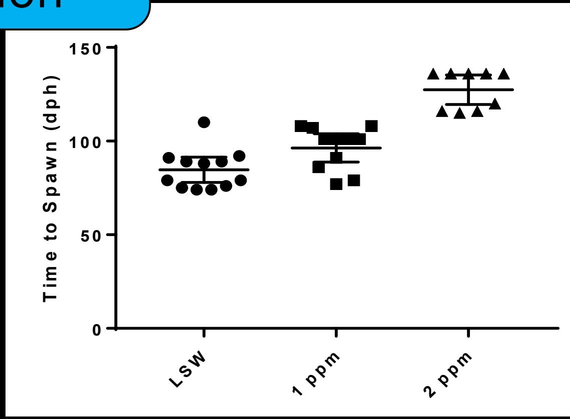


Growth Effects





Impacted Reproduction

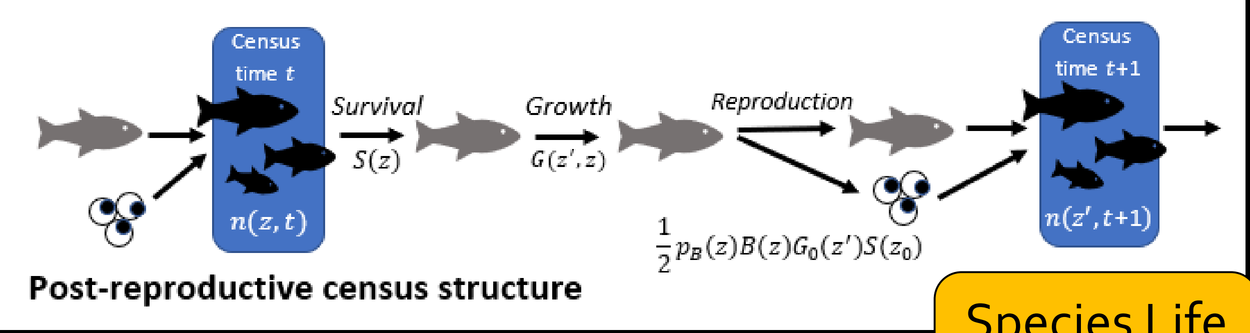


Exposure reduces growth

- Effects are persistent even after exposure ends
- Effects can be direct or indirect (food availability)
- Size is related to survival (ex., predation, over-winter)
- Size is related to fecundity, time to 1st spawn (i.e., spawning season)

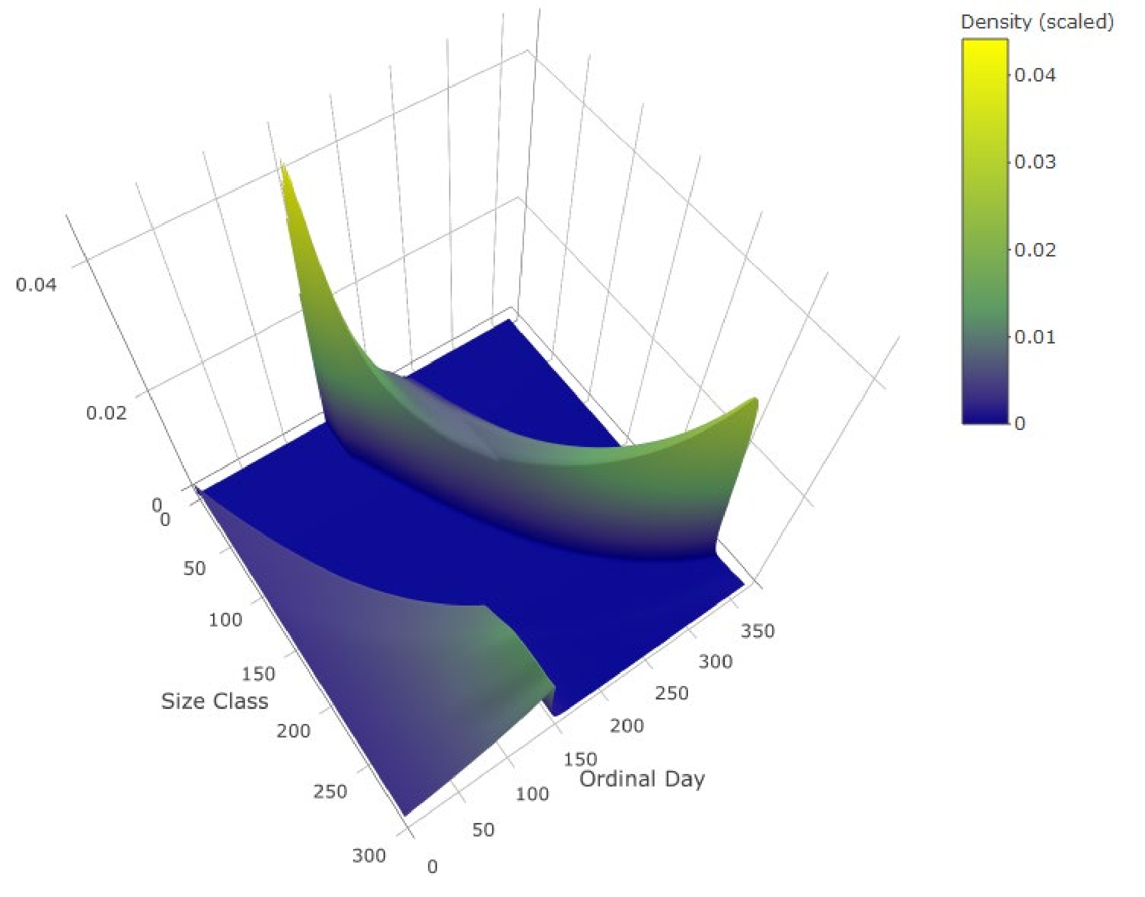
Scenario Building

- Parameterizable growth, reproduction, and survival functions for different species
- Different reproductive strategies
- Non-chemical stressors
  - Over-winter survival
- Chemical stressors
  - Type, magnitude, and timing of exposure
  - Multiple approaches for modeling chemical effects (eg TKTD or Threshold)

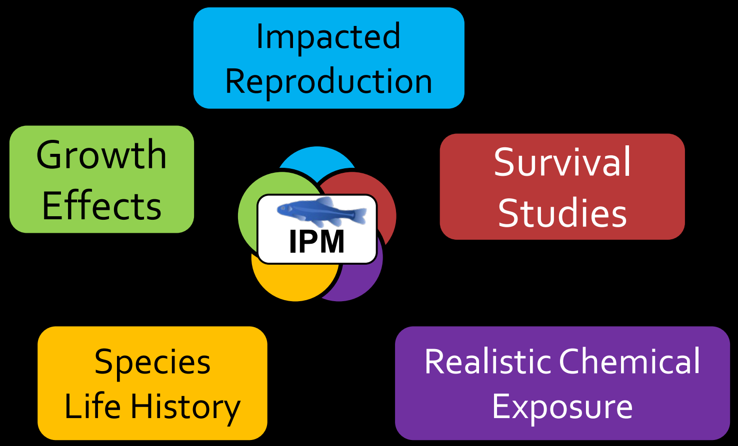


Species Life History

Example IPM Output:
Baseline daily size distributions for fathead minnow



IPM: 101



$K(z', z)$ The transition Kernel

$$n(z', t+1) = \int_L^U \left(\overbrace{G(z', z)S(z) + \frac{1}{2} p_B(z) B(z) G_0(z') s(z_0)} \right) n(z, t) dz$$

New population size-distribution

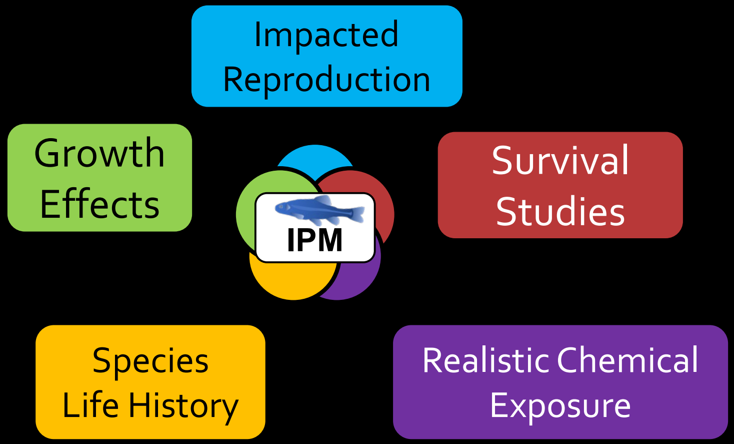
Growth and Survival Kernel

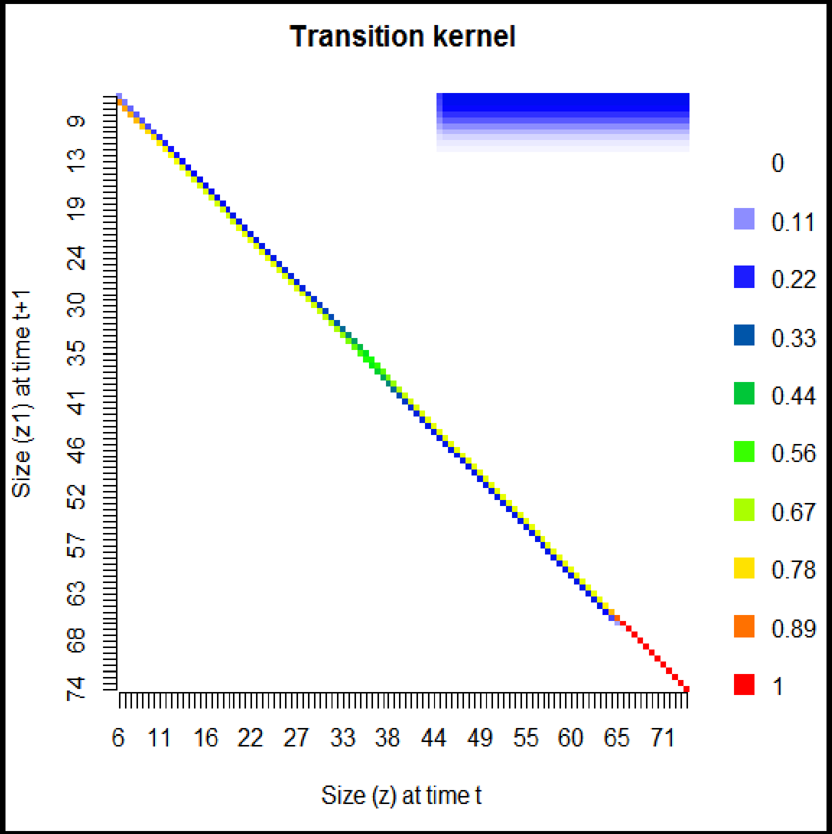
Reproduction Kernel

Population size-distribution

Where z and z' are size, t is time
U and L are the upper and lower limits of size.

IPM: 101





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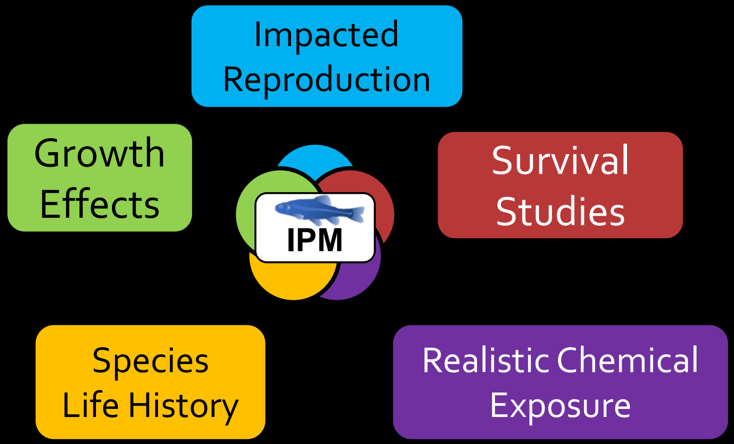

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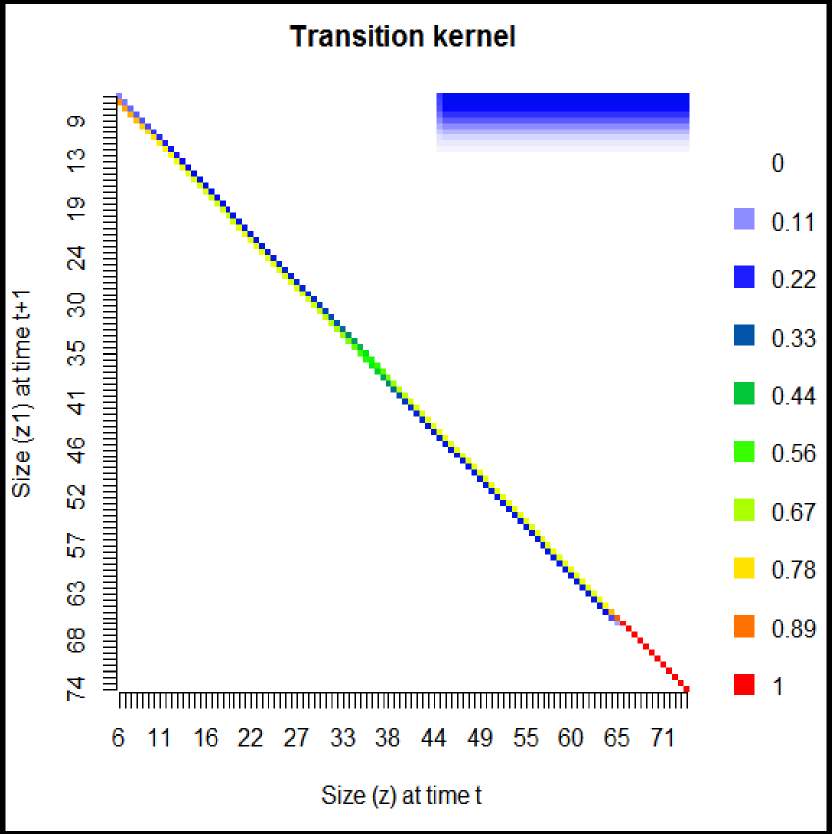


$$\begin{bmatrix} f_0 & f_1 & f_2 & \cdots & f_{\omega-2} & f_{\omega-1} \\ s_0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & s_1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & s_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & s_{\omega-2} & 0 \end{bmatrix}$$

IPM: 101

$K(z', z)$ The transition Kernel

$$n(z', t+1) = \int_L^U \left(G(z', z)S(z) + \frac{1}{2} p_B(z)B(z)G_0(z')s(z_0) \right) n(z, t)dz$$

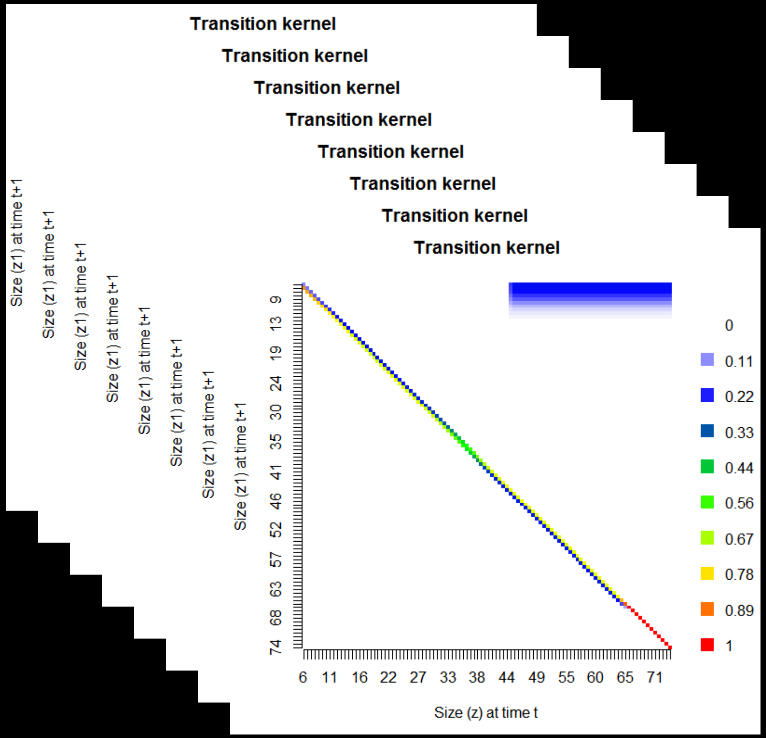
New population size-distribution

Growth and Survival Kernel

Reproduction Kernel

Population size-distribution

In Practice…

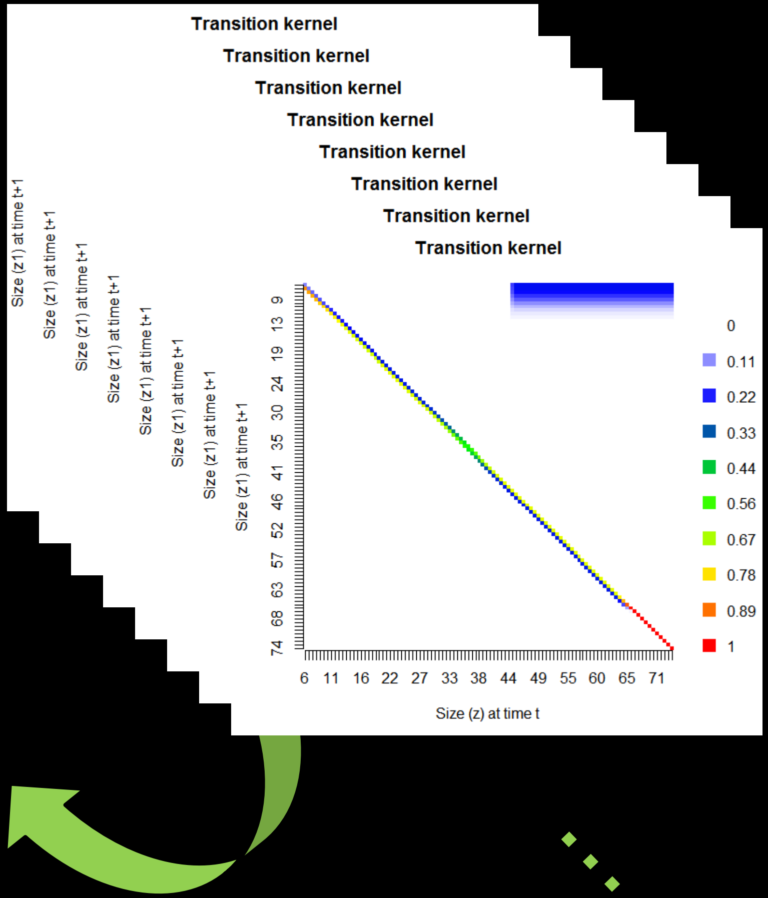


IPM: 101

$K(z', z)$ The transition Kernel

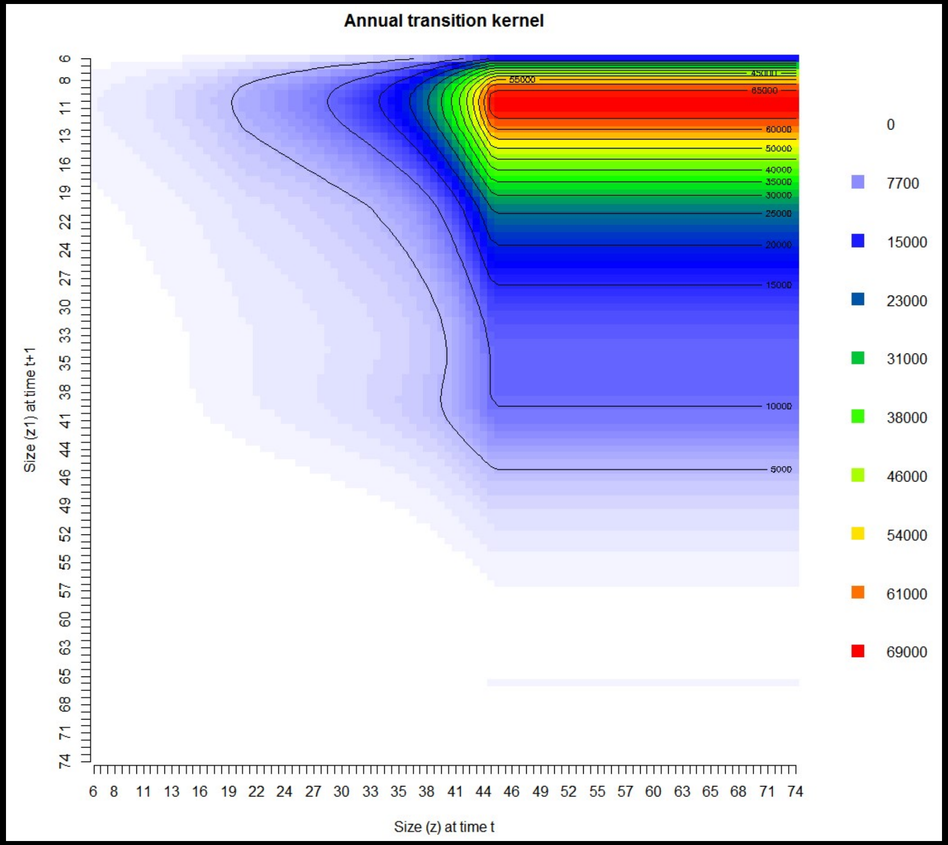
$$n(z', t+1) = \int_L^U \left(\overbrace{G(z', z)S(z) + \frac{1}{2} p_B(z) B(z) G_0(z') s(z_0)}^{K(z',z)} \right) n(z,t)dz$$

In Practice…



Which can be analyzed for:

- Asymptotic growth rate (λ)
- Stable size distribution
- Annual class size-transitions

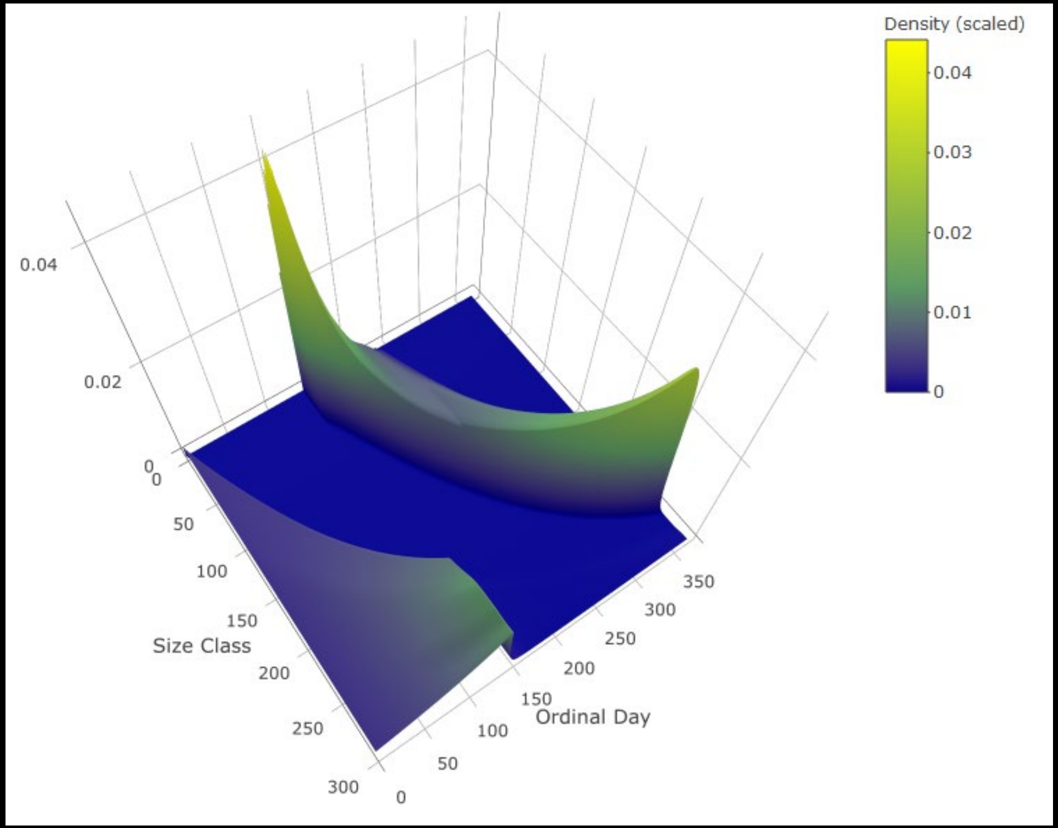


IPM: 101

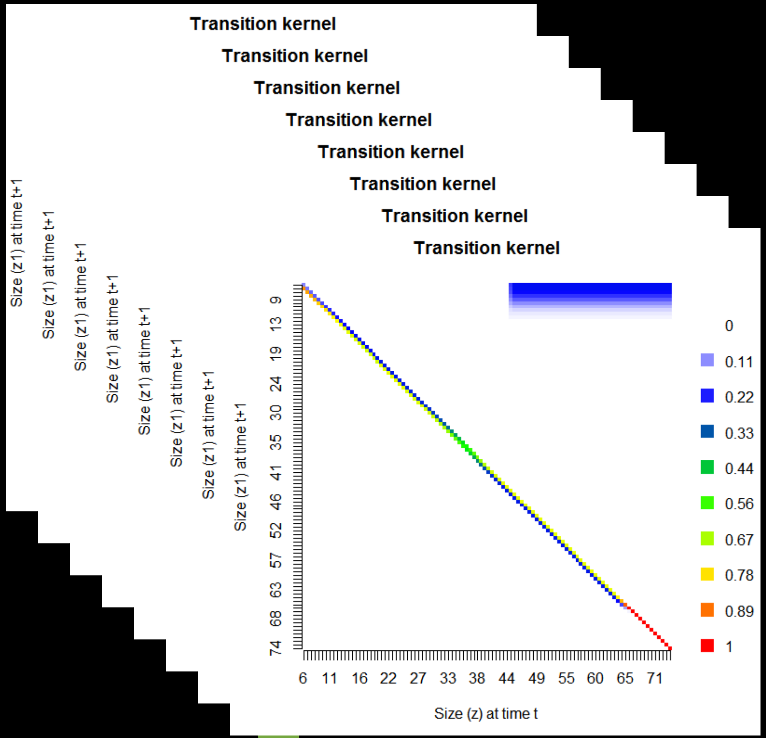
$$n(z',t+1) = \int_L^U \overbrace{\left(G(z',z)S(z) + \frac{1}{2}p_B(z)B(z)G_0(z')s(z_0)\right)}^{K(z',z)\text{ The transition Kernel}} n(z,t)dz$$

Which can be analyzed for:

- Number of individuals
- Daily size-distributions



In Practice…



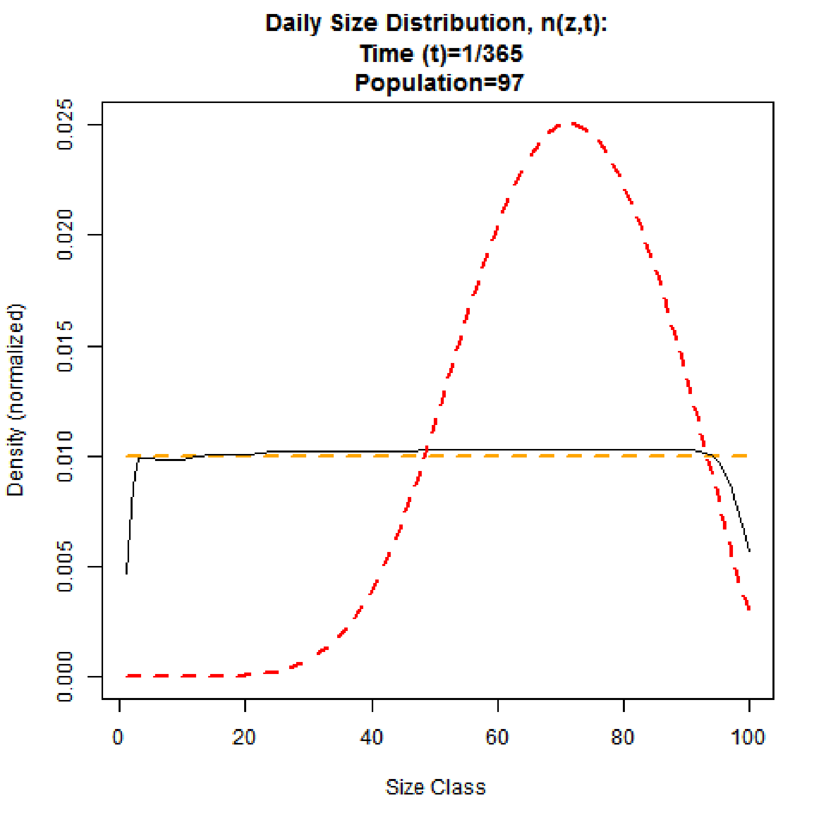
+ ⋱

Initial dist.

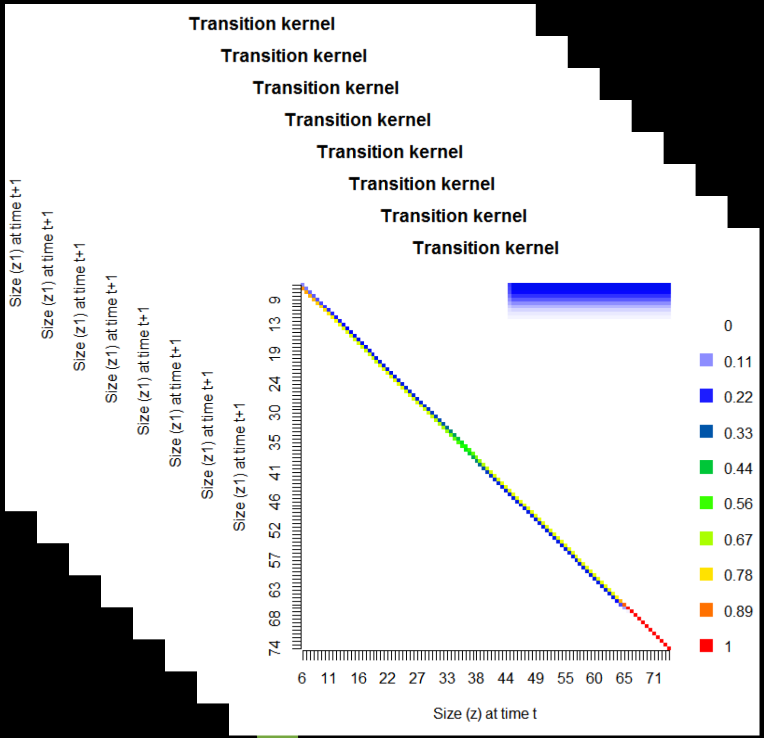
IPM: 101

$$n(z',t+1) = \int_L^U \Big(\overbrace{G(z',z)S(z) + \frac{1}{2}p_B(z)B(z)G_0(z')s(z_0)}^{K(z',z)\ \text{The transition Kernel}}\Big)\, n(z,t)dz$$

These can be combined for daily and asymptotic behavior.



In Practice…



+ ⋱

Initial dist.

ANNUAL DISCRETIZED TRANSITION KERNEL SUMMARY

COLOR KEY: % BASELINE

(+)100%-80%	80%- 60%	60% - 40%	40% -20%	20% - 0%

	BASELINE	WINTER		CHEMICAL EXPOSURE			
		Calendar Year Start Jan1-Dec31	*Reproductive Season Start May22-May21*	*GUTS-Uniform*	*GUTS- Step*	*TCEM-Uniform*	*TCEM-Step*
Simulated Population Size – N *Units: # of individuals*	23130	18131	16341	12479	17347	2889	9582
$N/N_{Baseline}$	-	78.39%	70.65%	53.95%	75.00%	12.49%	41.43%
Dominant Eigenvalue – λ *Unitless*	248.41	248.40	248.40	134.03	186.30	31.03	102.91
$\lambda/\lambda_{Baseline}$	-	100.00%	100.00%	53.95%	75.00%	12.49%	41.43%
Mean Stable Size - $\bar{\zeta}$ *Units: mm*	60.14	58.83	65.30	60.14	60.14	60.14	60.15
$\bar{\zeta}/\bar{\zeta}_{Baseline}$	-	97.82%	108.59%	100.00%	100.00%	100.00%	100.02%
Maximum Annual Growth Potential – α *Unitless*	248.41	248.41	248.40	134.03	186.30	31.03	102.91
$\alpha/\alpha_{Baseline}$	-	100.00%	100.00%	53.95%	75.00%	12.49%	41.43%
Minimum Annual Growth Potential – ω *Unitless*	181.35	0	1.20	97.85	136.01	22.66	75.13
$\omega/\omega_{Baseline}$	-	0.[illegible]%	0.66%	53.95%	75.00%	12.49%	41.43%

Traditional toxicity testing doesn't stand a chance

We need models

*

Traditional toxicity testing doesn't stand a chance

We need models

Biology is awesome

Biology is messy

*

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Biology is messy

Models are awesome

Models can be messy

*

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Models can be messy

*For real though, what data do you have?

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*For real though, what data do you have?

THERE IS A LOT OF WORK TO BE DONE

1.4

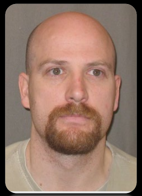
MYA

0.4

Now

FISH TOXICITY TRANSLATOR
Integral Projection Model Team

J. Swintek



K. Flynn

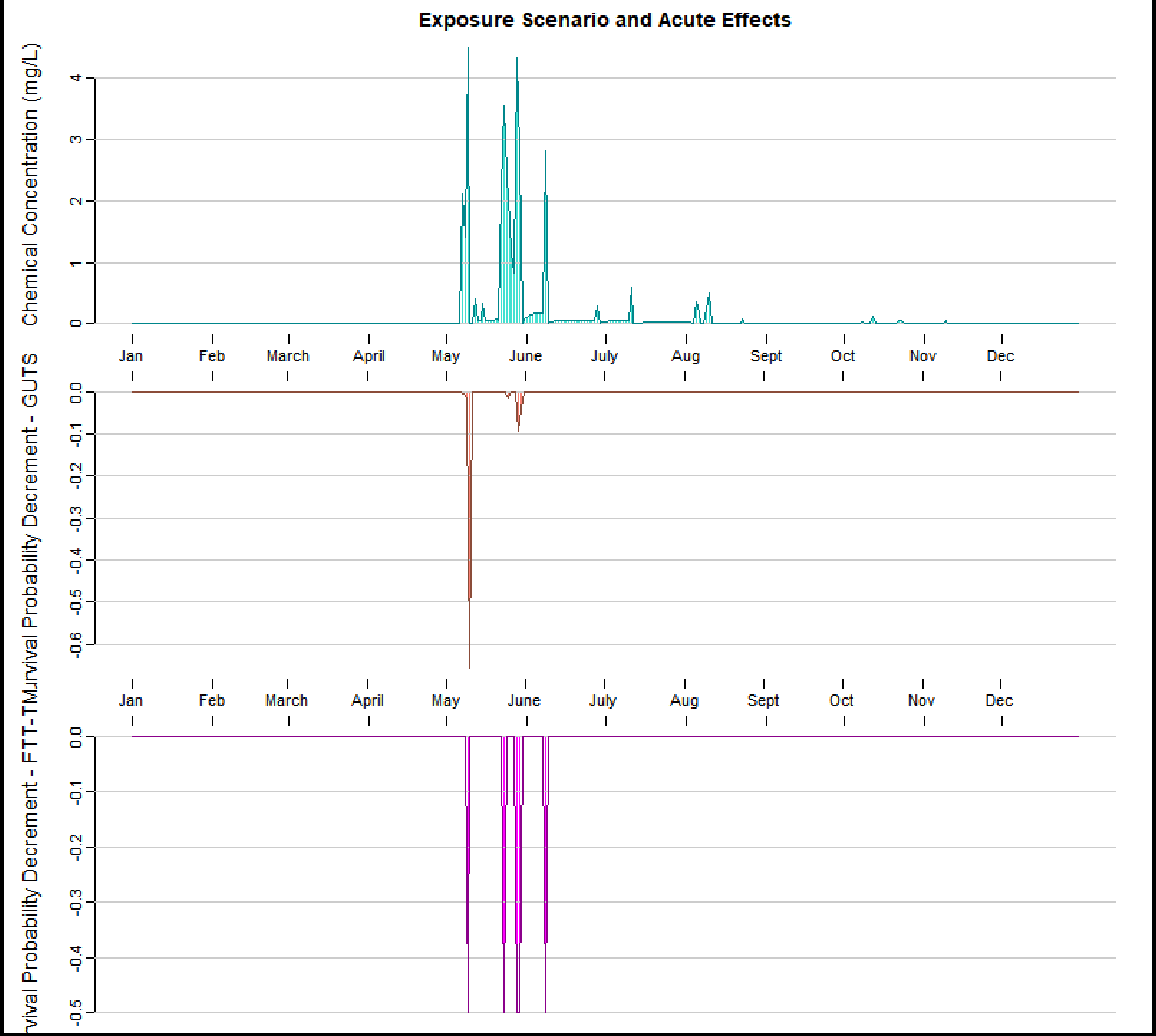
F. Whiteman

S. Kadlec

M. Etterson

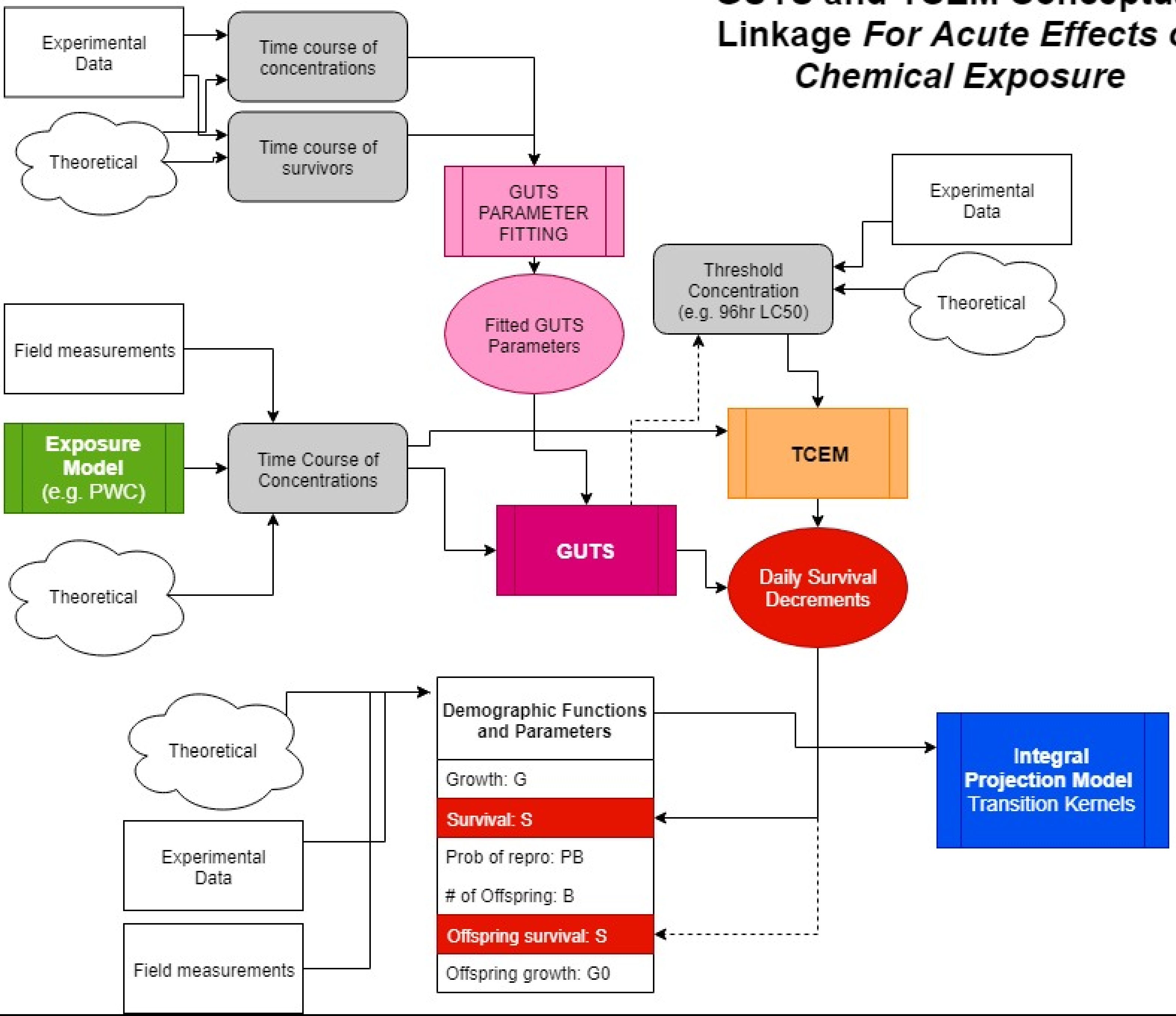
V.Kurker

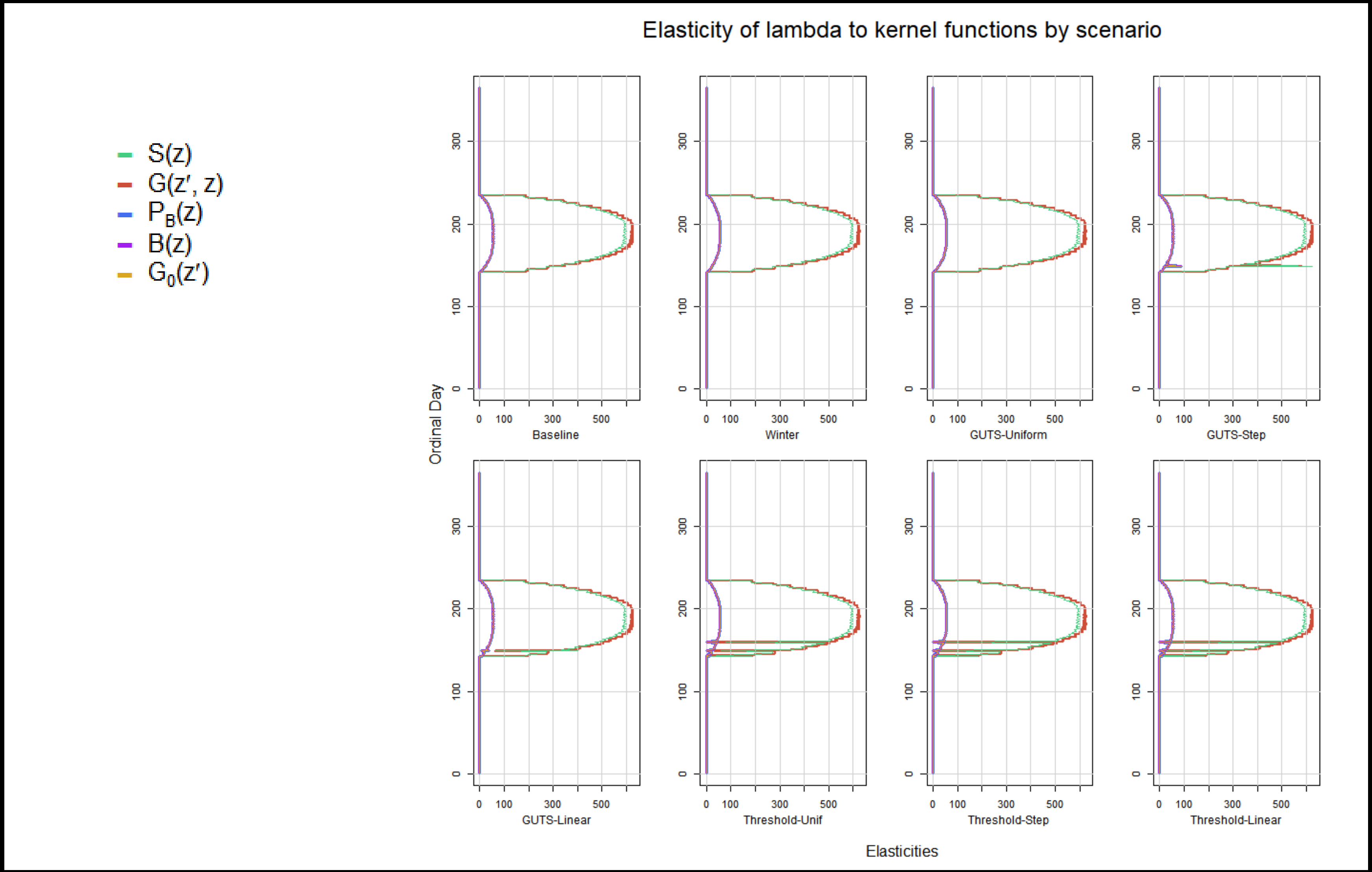
BONUS MATERIAL



Exposure Scenario and Acute Effects
Chemical Concentration (mg/L)
0
1
2
3
4
Jan
Feb
March
April
May
June
July
Aug
Sept
Oct
Nov
Dec
Survival Probability Decrement - GUTS
0.0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
Survival Probability Decrement - FTT-TM
0.0
-0.1
-0.2
-0.3
-0.4
-0.5

GUTS and TCEM Conceptual Linkage *For Acute Effects of Chemical Exposure*





Elasticity of lambda to kernel functions by scenario
S(z)
G(z′, z)
P_B(z)
B(z)
G_0(z′)
Ordinal Day
Elasticities
Baseline
Winter
GUTS-Uniform
GUTS-Step
GUTS-Linear
Threshold-Unif
Threshold-Step
Threshold-Linear

IPM 101: The Kernel Functions

$$n(z',t+1) = \int_L^U \left(G(z',z)S(z) + P_B(z)B(z)g(z')s(z) \right) n(z,t)dz$$

growth, reproduction, and survival

IPM 101: The Kernel Functions

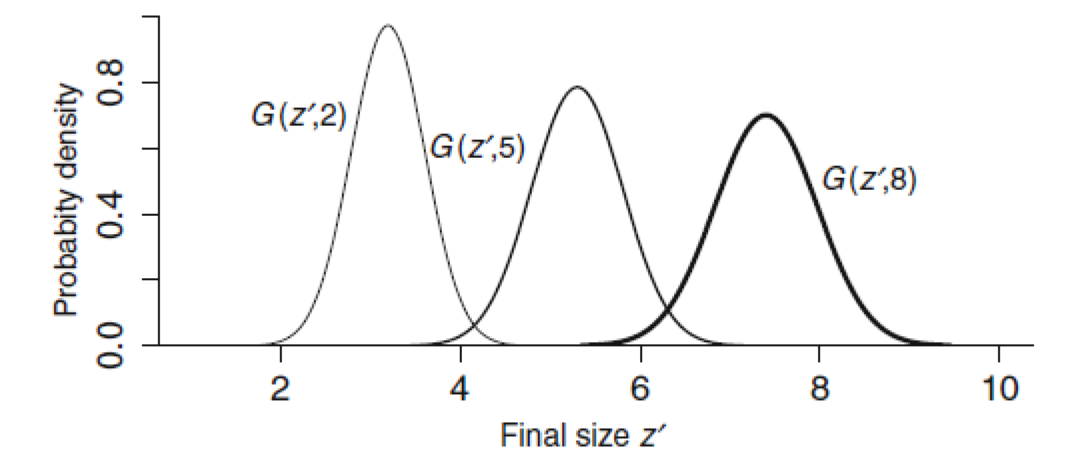
$$n(z',t+1) = \int_L^U \left(G(z',z)S(z) + P_B(z)B(z)g(z')s(z)\right)n(z,t)dz$$

Growth transitions

$$G(z',z) : Normal\left(\mu = vB(z,\Delta t), \sigma = .1vB(z,\Delta t)\right)$$

Normal distribution with mean as size-dependent vonBertalanffy growth and SD proportional to mean

$$vB(z,\Delta t) = L_\infty - (L_\infty - z)e^{-k\Delta t}$$



Karl Ludwig
von Bertalanffy

IPM 101: The Kernel Functions

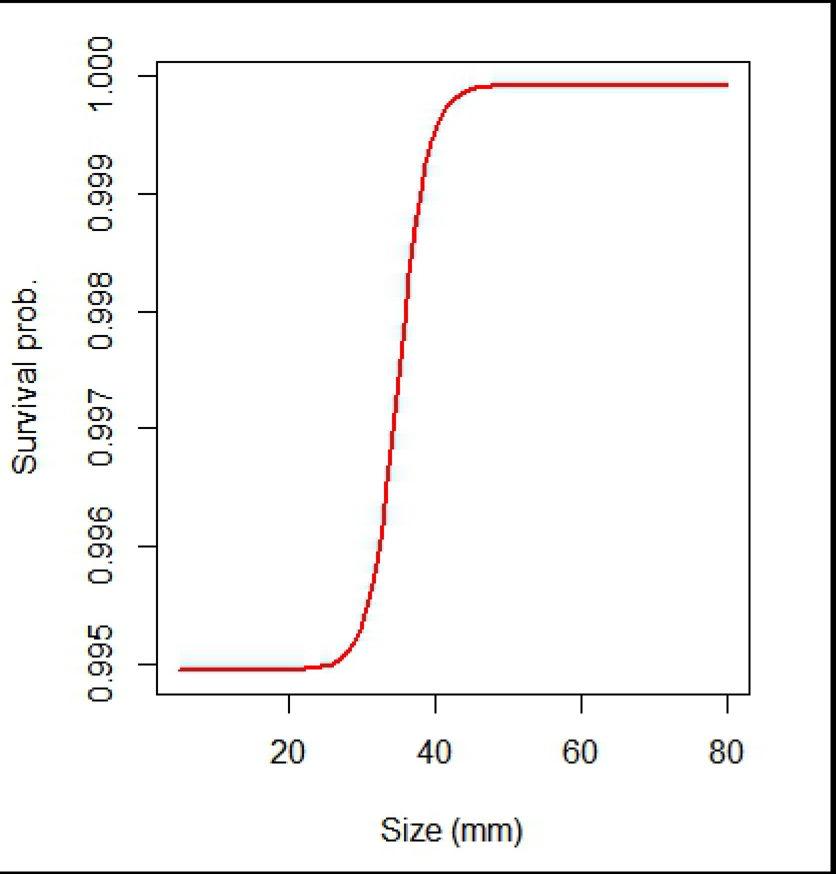
$$(z', t+1) = \int_L^U \left(G(z',z)S(z) + P_B(z)B(z)g(z')s(z)\right)n(z,t)dz$$

Survival Function

$S(z)$: Logistic size−dependent survival

$$S(z) = S_{min} + \frac{(S_{max} - S_{min})}{1 + e^{(S_b(S_a - z))}}$$

via *Erickson et al., 2017*



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Fecundity

Step functions, minimum size needed to reproduce.

$$P_B(z) = \begin{cases} 0 & z < z_{repro} \\ p_{spawn} & z \geq z_{repro} \end{cases}.$$

Hatchlings per spawn, $B(z)$ is, also a step-function,

$$B(z) = \begin{cases} 0 & z < z_{repro} \\ B_{spawn} & z \geq z_{repro} \end{cases},$$

IPM 101: The Kernel Functions

$$n(z',t+1) = \int_L^U \Big(G(z',z)S(z) + P_B(z)B(z)g(z')s(z)\Big)n(z,t)dz$$

Reproductive strategies vary

- There are multiple life histories for fish that lead to different ways to parameterize daily spawning probability.
- Batch spawning is used by Fathead minnow *(Pimephales promelas)*
- Semelparity (one and done) is the approach of Delta smelt *(hypomesus transpacificus)*

IPM 101: The Kernel Functions

$$n(z', t+1) = \int_L^U \left(G(z', z)S(z) + P_B(z)B(z)g(z')s(z)\right)n(z,t)dz$$

Batch spawning algorithm developed accounting for:

- # of spawns per season
- # of hatchlings per spawn
- Distribution of spawn timings
- Inter-spawn interval

Semelparous spawning kernel derived

- Modified survival based on spawning probability
  - i.e. after you spawn, you die

Reproductive strategies vary

- There are multiple life histories for fish that lead to different ways to parameterize daily spawning probability.
- Batch spawning is used by Fathead minnow *(Pimephales promelas)*
- Semelparity (one and done) is the approach of Delta smelt *(hypomesus transpacificus)*

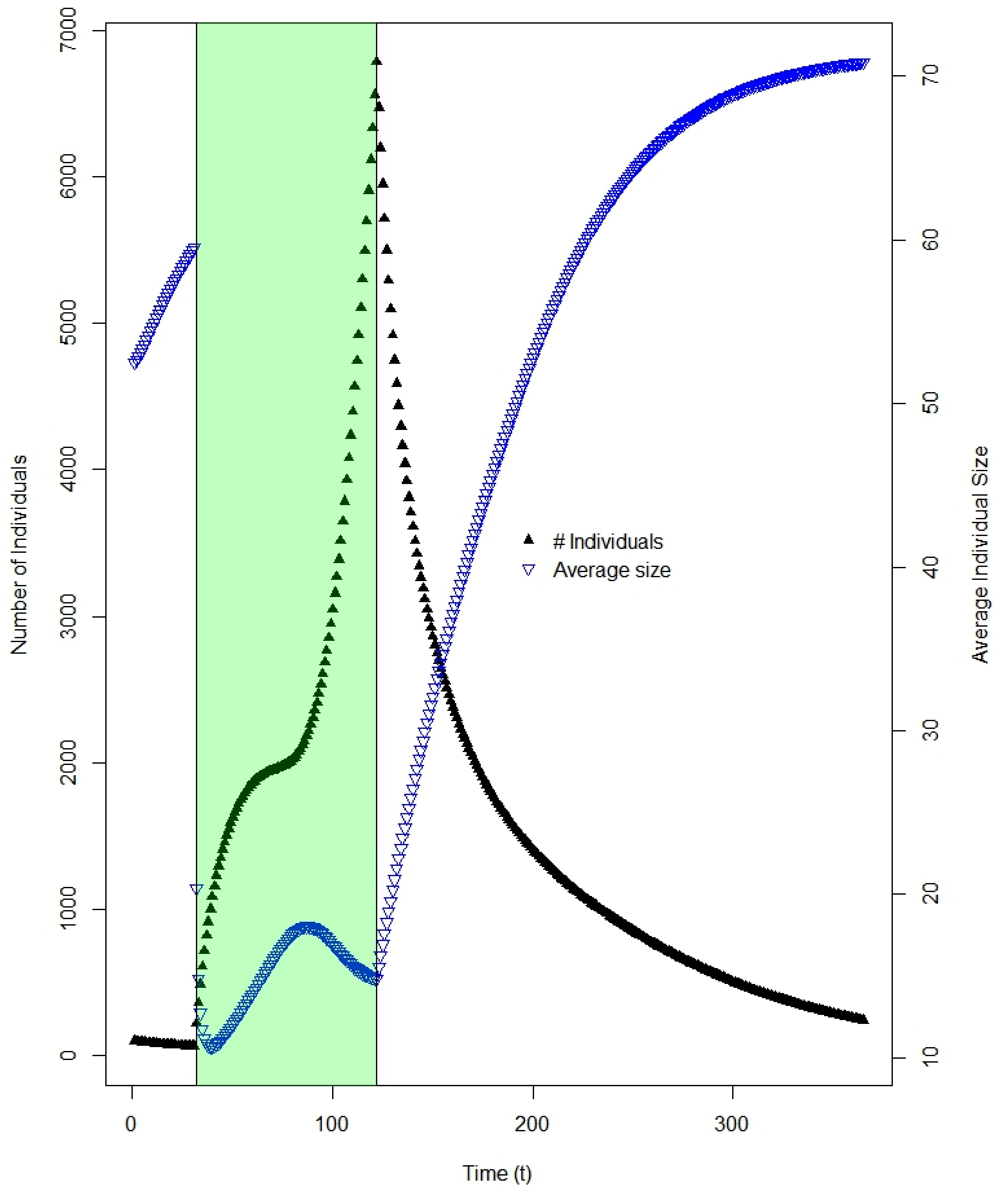
Preliminary Results for Delta smelt

100 individuals, uniformly distributed by size, annual simulation beginning Jan 1st

Intrinsically stable population growth (without explicit inclusion of stressors)
100 -> 237 $(\lambda = 3.39)$

vonBertalanffy Growth model matched well to time/stage transitions

$$l_\infty = 100mm, \kappa = 0.0059$$



Reclamation Photograph by René Reyes

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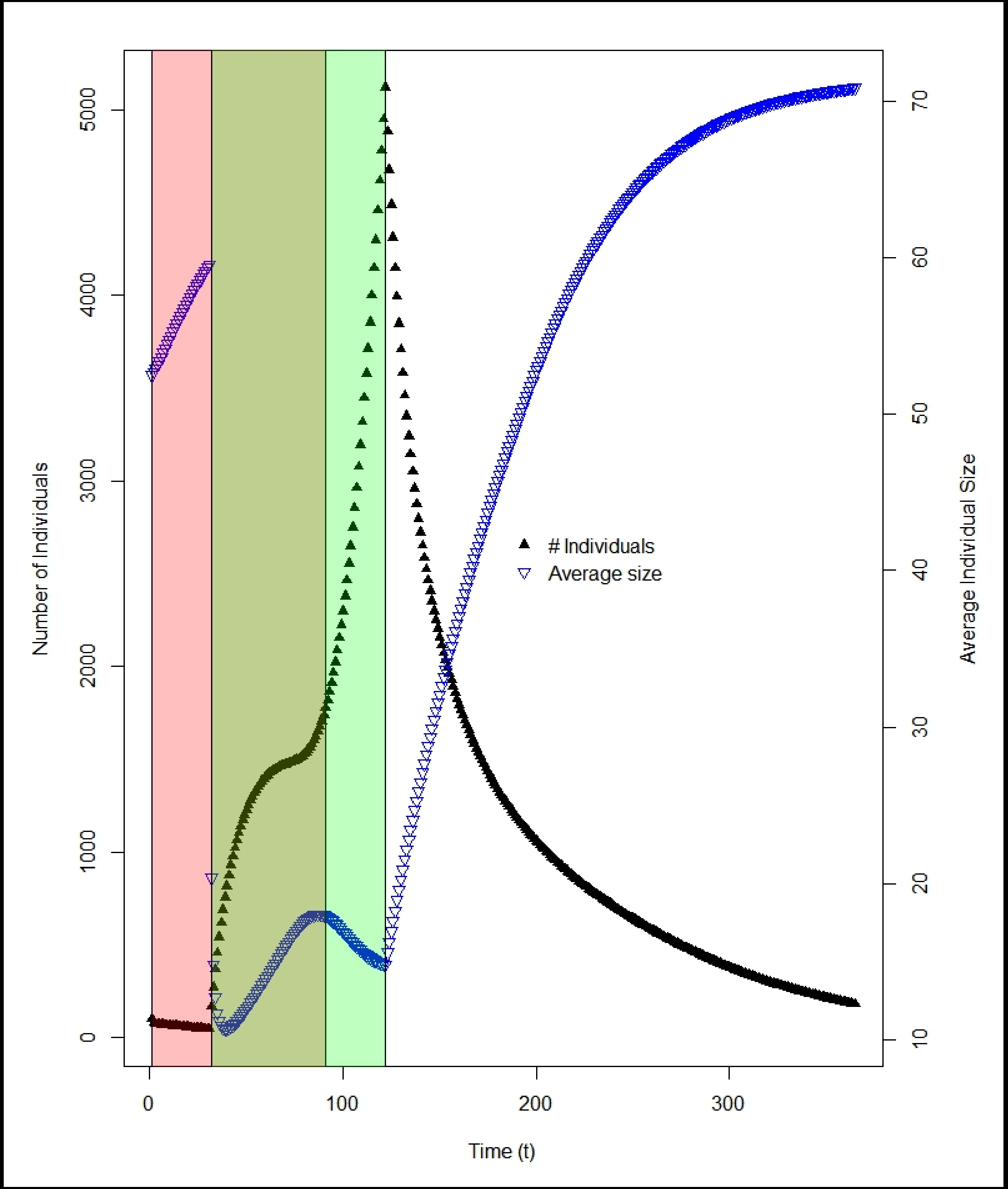

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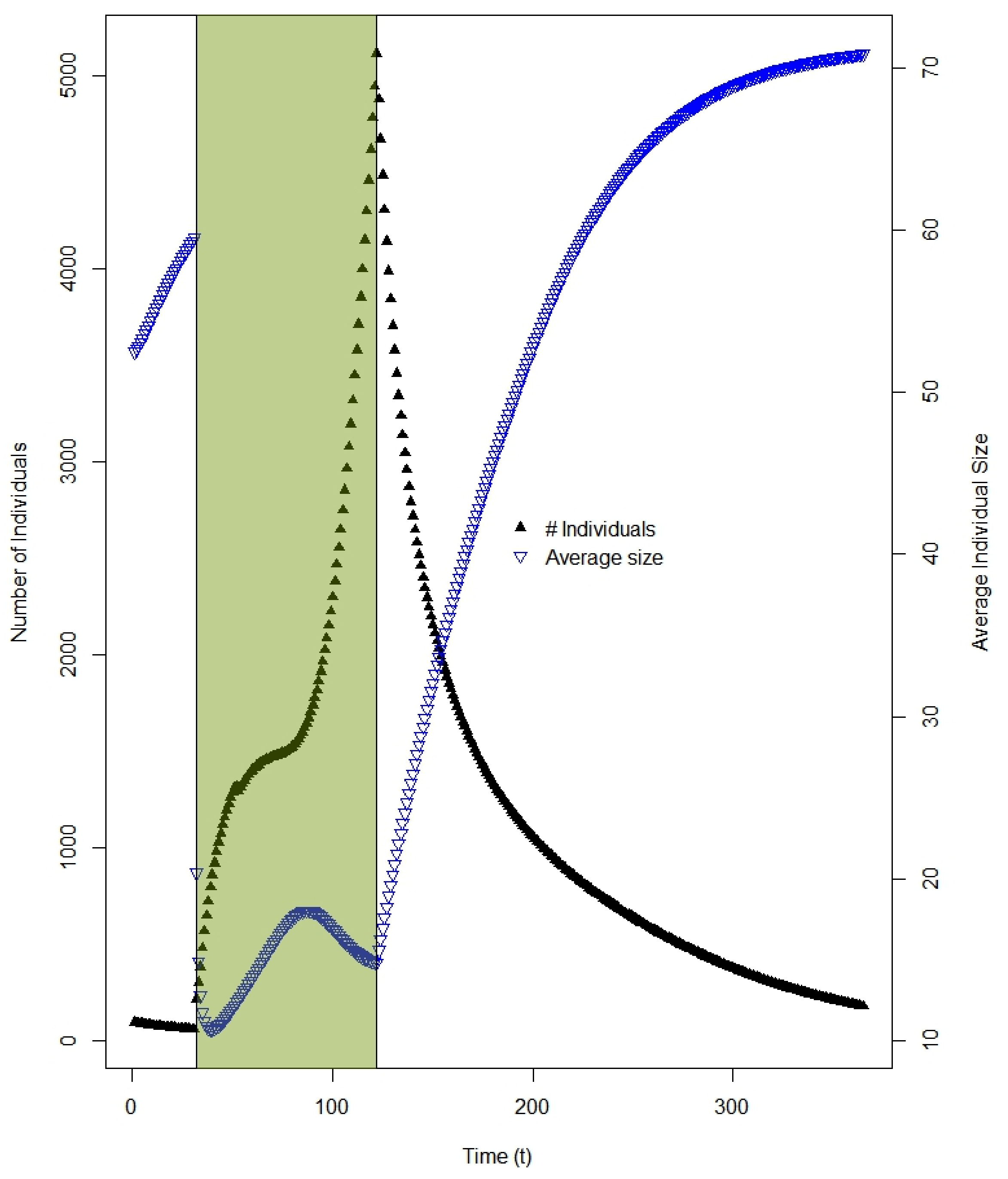

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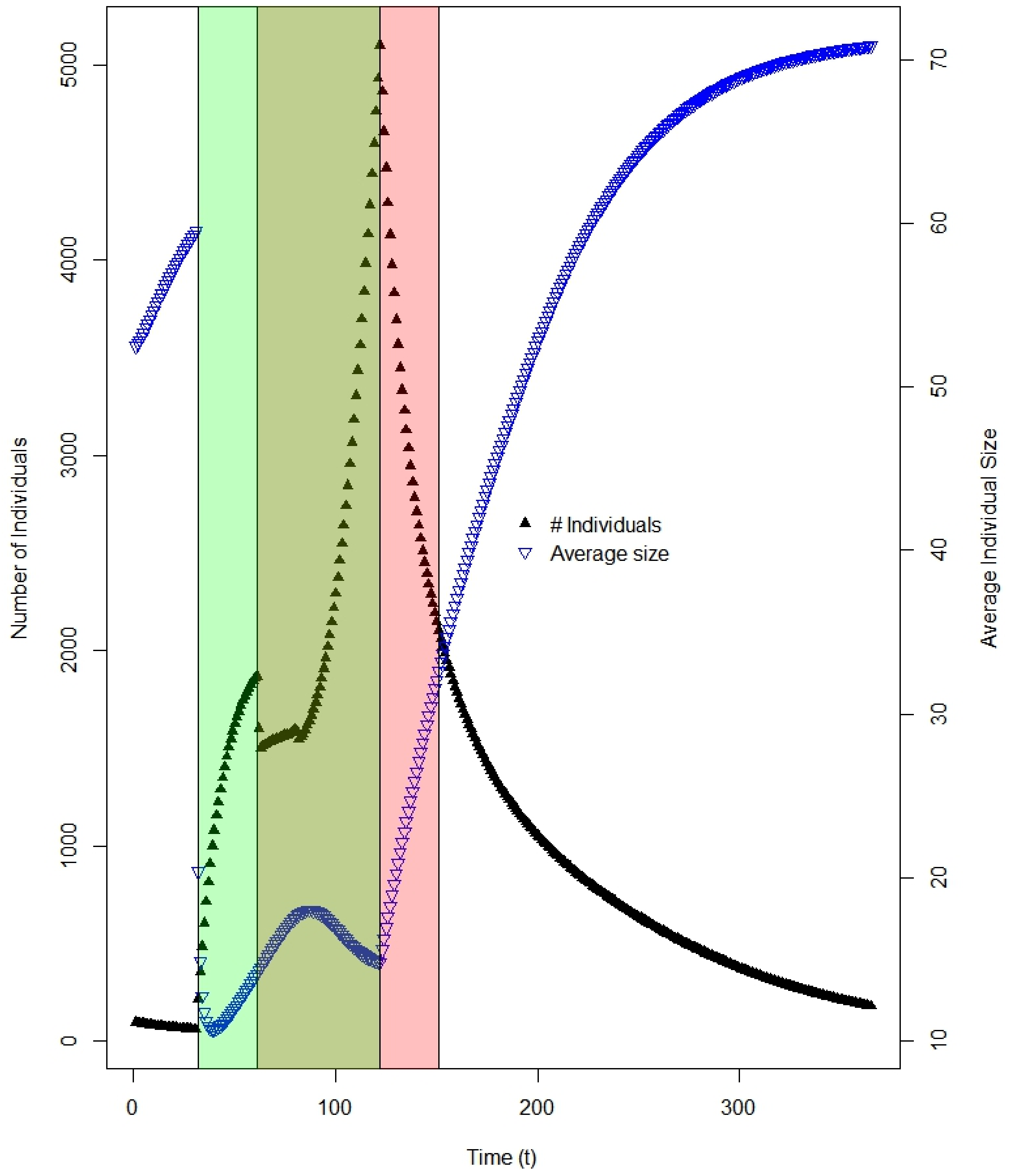

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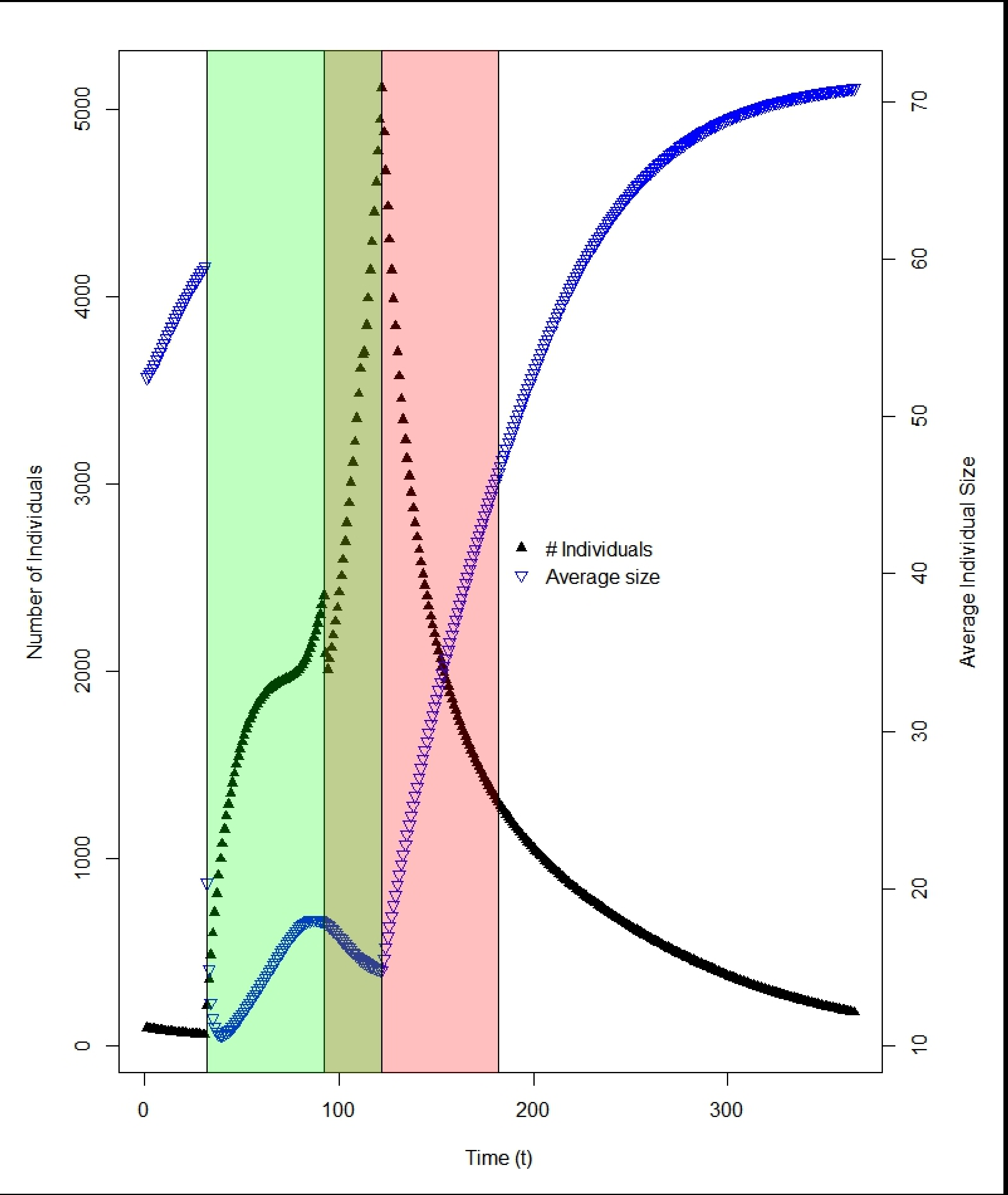

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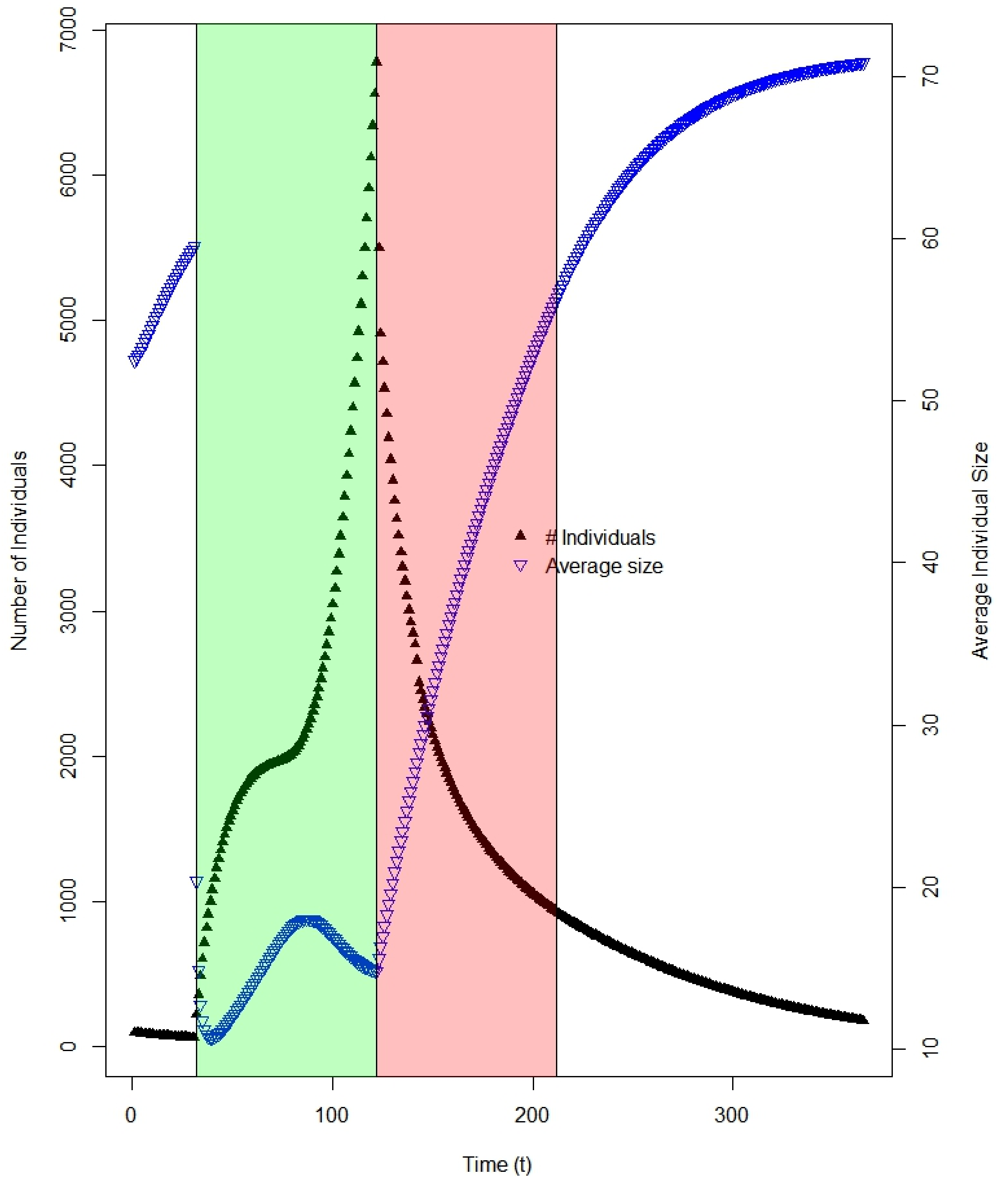

"But to be driven by impelling odor headlong upon a mate so gigantic, in such immense and forbidding darkness, and willfully eat a hole in her soft side, to feel the gradually increasing transfusion of her blood through one's veins, to lose everything that marked one as other than a worm, to become a brainless, senseless thing that was a fish—this is sheer fiction, beyond all belief unless we have seen the proof of it."