Computation of Equilibrium States and Bifurcations in Ecosystem Models Using Interval Analysis

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Motivation

- Nonlinear dynamic systems are of frequent interest in engineering and science

$$\dot{\mathbf{x}} = \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{p})$$

$$\mathbf{x} = \text{state variable vector}$$

$$\mathbf{p} = \text{parameter vector}$$

- Common problems include computing: equilibrium points, limit cycles, bifurcations of equilibria, bifurcations of cycles
- Need a method that is guaranteed to find all equilibrium points and bifurcations of equilibria
- Of specific interest here are food chain/web models
  - Used to predict impact on ecosystems of introducing new materials (ionic liquids) into the environment

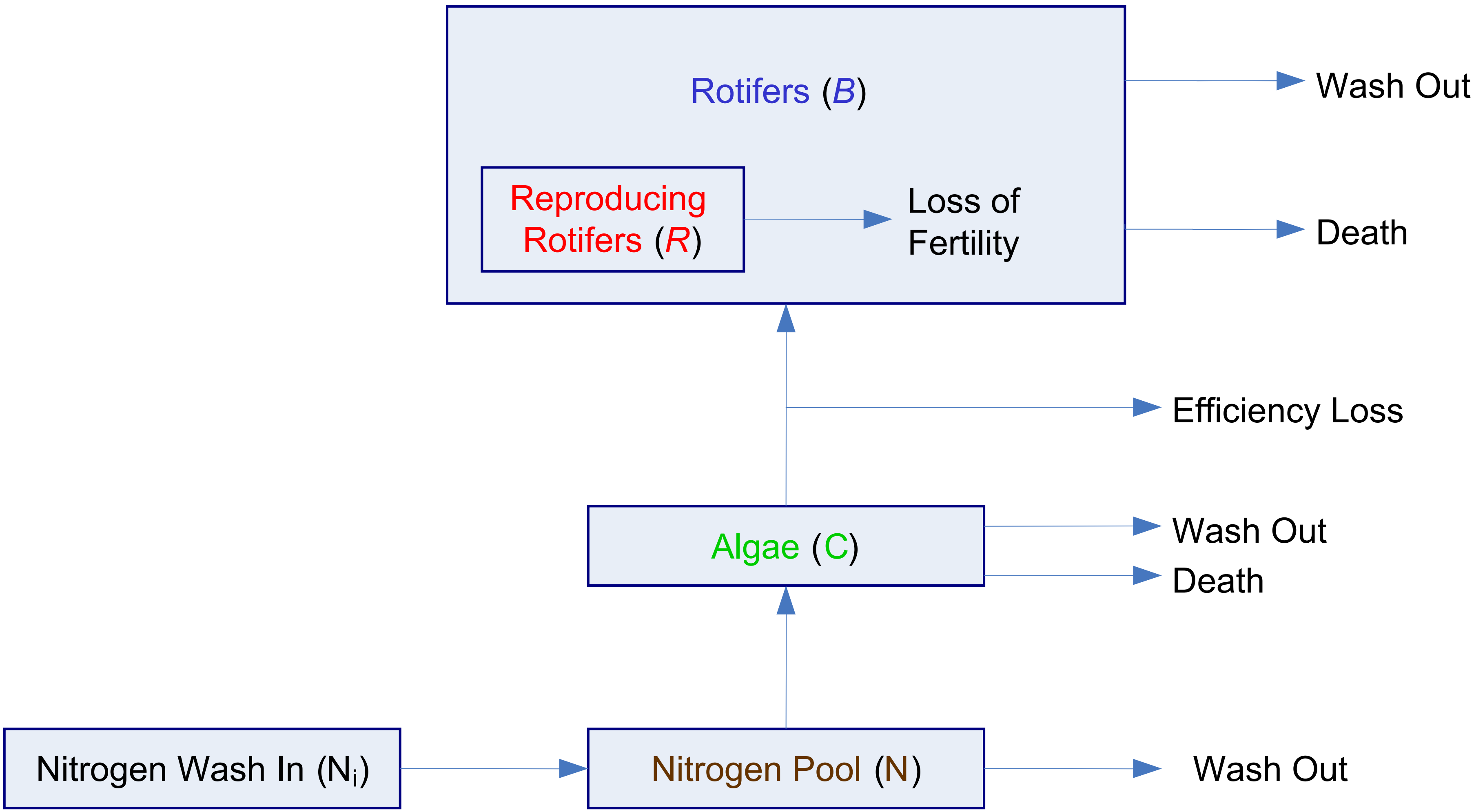
Motivation – Ionic Liquids

- Ionic liquids (ILs) are salts that are liquids at or near room temperature
- Many promising properties
  - Immeasurably low vapor pressure – Do not evaporate
  - Many potential applications, including replacement solvents for volatile organic compounds (VOCs) currently used as solvents
  - Eliminates a major source of air pollution
- Could enter the environment via aqueous waste streams
  - Relatively little environmental toxicity information available
  - Single species toxicity information alone is not sufficient to predict ecosystem impacts
- Need a tool that will predict ecosystem impacts from single species toxicity information

Predator/Prey Models

- Systems of ordinary differential equations that describe the rates of change in species biomass
- Model parameters have real-life, physical meaning
- Though often simple in form, these models can exhibit rich mathematical behavior including varying numbers and stability of equilibria
- Many different models are possible, depending on the models for growth, predation, etc.
- We would like to use single species IL toxicity data in conjunction with these predator/prey models to predict the impact of IL contamination

Experimentally Verified Algae-Rotifer Model



Experimentally Verified Algae-Rotifer Model

$$\frac{dN}{dt} = \delta\left(N_i - N\right) - \frac{b_C NC}{K_C + N}$$

$$\frac{dC}{dt} = \frac{b_C NC}{K_C + N} - \frac{1}{\varepsilon}\frac{b_B CB}{K_B + C} - \delta C$$

$$\frac{dR}{dt} = \frac{b_B CR}{K_B + C} - \left(\delta + m + \lambda\right)R$$

$$\frac{dB}{dt} = \frac{b_B CR}{K_B + C} - \left(\delta + m\right)B$$

N : Nitrogen (μmol/L)
C : *C. vulgaris* (μmol/L)
R : Reproducing *B. calyciflorus* (μmol/L)
B : Total *B. calyciflorus* (μmol/L)

N_i : Nitrogen concentration of the inflow medium (μmol/L)
δ : Dilution rate (/day)

m : Mortality rate (/day)
ε : Assimilation efficiency
λ : Fecundity decay rate (/day)
b_C : Max birth rate of *C. vulgaris* (/day)
b_B : Max birth rate of *B. calyciflorus* (/day)
K_C : Half-saturation constant for *C. vulgaris* (μmol/L)
K_B : Half-saturation constant for *B. calyciflorus* (μmol/L)

Bifurcations of Equilibria

- Goal – locate equilibrium points and bifurcations in predator/prey models
- A bifurcation is a change in the topological type of the phase portrait as one or more system parameters are varied
  - Codimension-one: One parameter (α) can be varied
  - Codimension-two: Two parameters (α, β) can be varied
- Bifurcations are located by solving a nonlinear algebraic system consisting of the equilibrium conditions along with one or more augmenting (test) functions

Bifurcations and Test Functions

- Codim 1: Fold and transcritical bifurcations
  - As α is varied, two equilibria collide
  - Convenient test function (avoiding calculation of eigenvalues):

$$\boxed{\det\left(\mathrm{J}(\boldsymbol{x},\alpha)\right) = 0}$$

- Codim 1: Hopf bifurcation
  - As α is varied, $\mathrm{J}(\boldsymbol{x},\alpha)$ has a pair of imaginary complex conjugate eigenvalues that cross the imaginary axis: possible stability change
  - Convenient test function based on bialternate product:

$$\boxed{\det\left(2\mathrm{J}(\boldsymbol{x},\alpha) \otimes \mathrm{I}\right) = 0}$$

- Codim 2: Fold-Fold and Fold-Hopf
  - Located by using both augmenting functions:

$$\boxed{\det\left(\mathrm{J}(\boldsymbol{x},\alpha,\beta)\right) = 0 \;\&\; \det\left(2\mathrm{J}(\boldsymbol{x},\alpha,\beta) \otimes \mathrm{I}\right) = 0}$$

Locating Equilibrium States and Bifurcations

- Equilibrium states: Set the equilibrium conditions (model equations) equal to zero and solve for $\boldsymbol{x}$
- Bifurcations of equilibria: Solve equilibrium conditions and augmenting function(s) for $\boldsymbol{x}$ and α (and β)
- These equation systems may have multiple solutions
- Typically these systems are solved using a continuation-based strategy
  - Initialization dependent
  - No guarantee of locating all branches
- Interval mathematics provides a method that is:
  - Initialization independent
  - Capable of locating all solution branches with certainty (see also Gehrke & Marquardt, 1997)

Interval-Newton/Generalized Bisection Method (IN/GB)

- Given a system of equations, an initial interval (bounds on all variables), and a solution tolerance:
  - IN/GB can find (enclose), with mathematical and computational certainty, all solutions to the equation system, or it can determine that no solutions exist
  - The equation system must have a finite number of real roots in the initial interval
  - No strong assumptions or simplifications to the equation system are needed

IN/GB Method

Problem: Solve $\boldsymbol{f}(\boldsymbol{x}) = \mathbf{0}$ for all roots in the interval $\mathbf{X}^{(0)}$

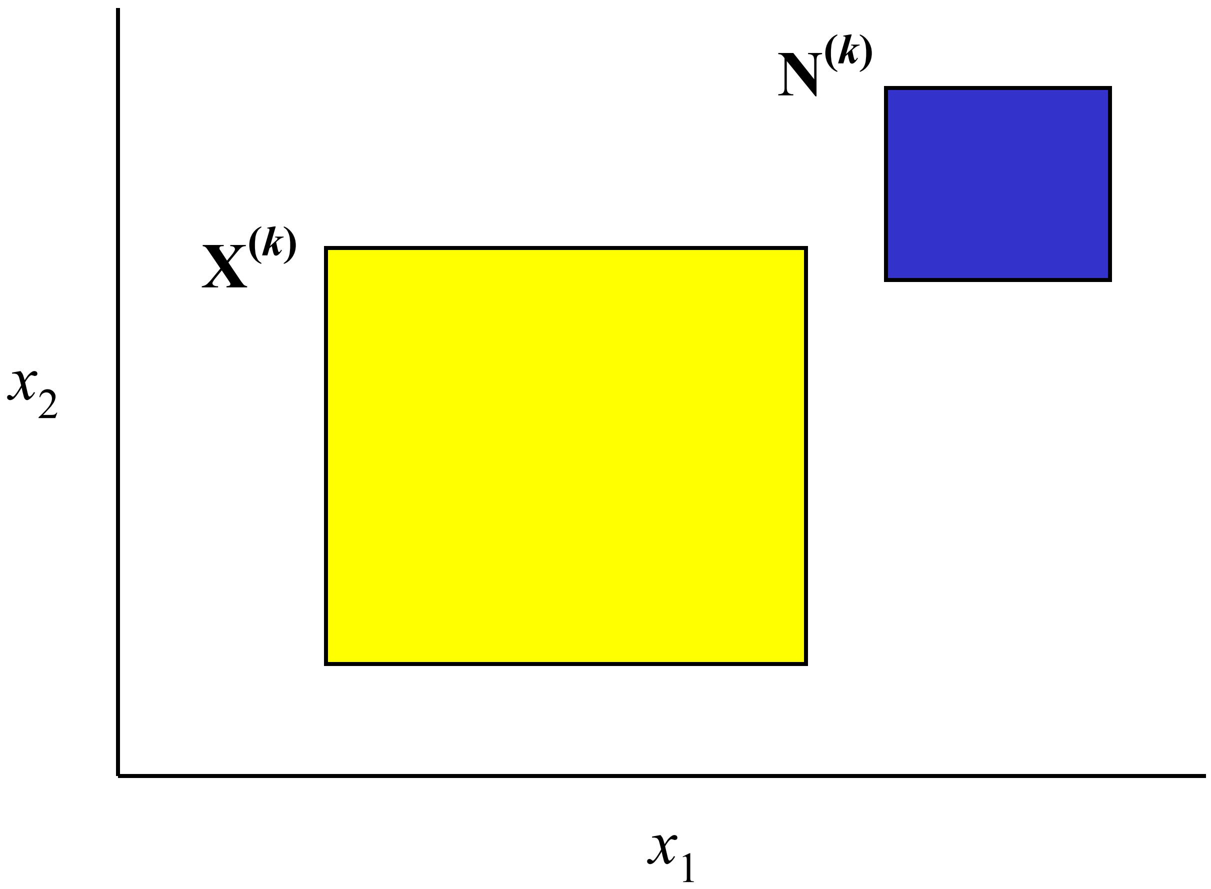
Basic iteration scheme: For a particular subinterval (box), $\mathbf{X}^{(k)}$, perform root inclusion test:

- Range test: Compute an interval extension (bounds on range) for each function in the system: $\mathbf{F}(\mathbf{X}^{(\boldsymbol{k})})$
  - If $\mathbf{0}$ is not a member of $\mathbf{F}(\mathbf{X}^{(\boldsymbol{k})})$, delete the box
- Interval Newton test: Compute the image, $\mathbf{N}^{(\boldsymbol{k})}$, of the box by solving the linear interval equation system

$$F'(\mathbf{X}^{(\boldsymbol{k})})(\mathbf{N}^{(\boldsymbol{k})} - \boldsymbol{x}^{(\boldsymbol{k})}) = -\boldsymbol{f}(\boldsymbol{x}^{(\boldsymbol{k})})$$

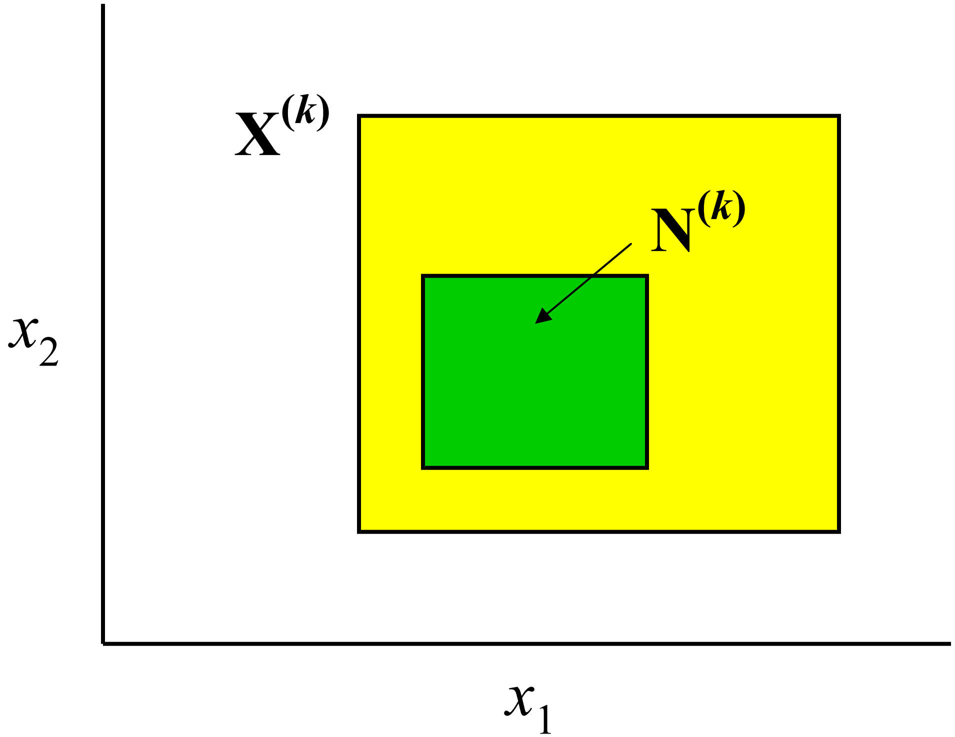
  - $\boldsymbol{x}^{(\boldsymbol{k})}$ is a point in $\mathbf{X}^{(\boldsymbol{k})}$
  - $F'(\mathbf{X}^{(\boldsymbol{k})})$ is the interval extension of the Jacobian matrix of $\boldsymbol{f}(\boldsymbol{x})$ over the interval $\mathbf{X}^{(\boldsymbol{k})}$

IN/GB Method: Interval Newton Test



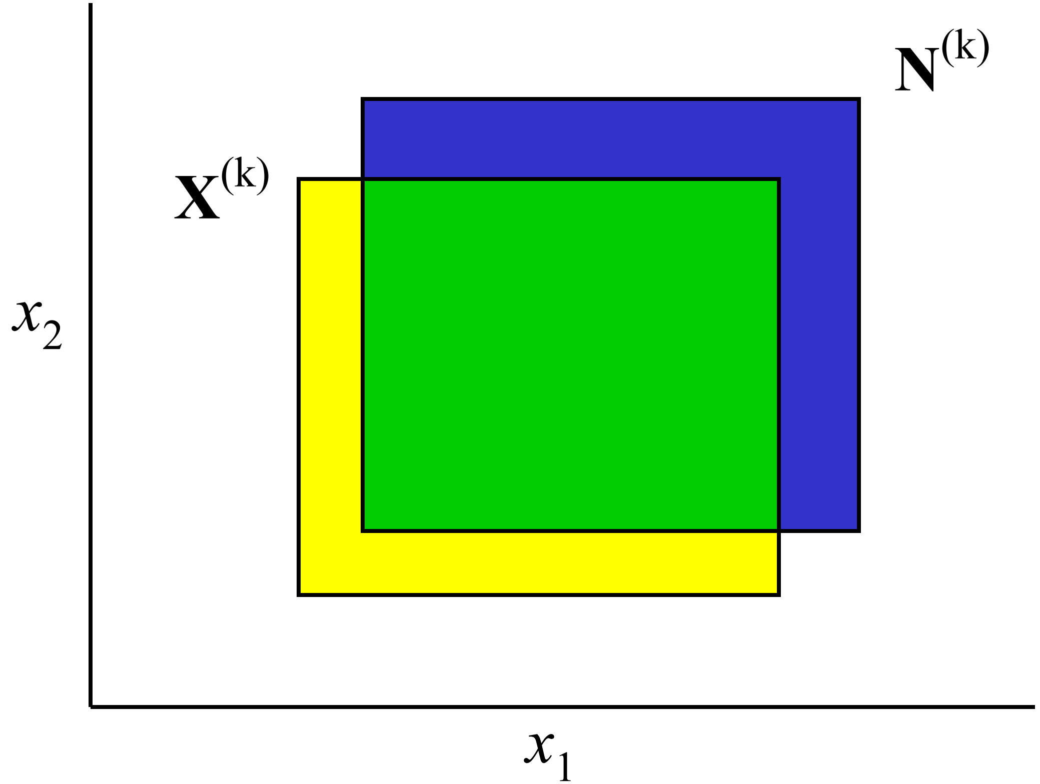
- There is no solution in $\mathbf{X}^{(k)}$

IN/GB Method: Interval Newton Test



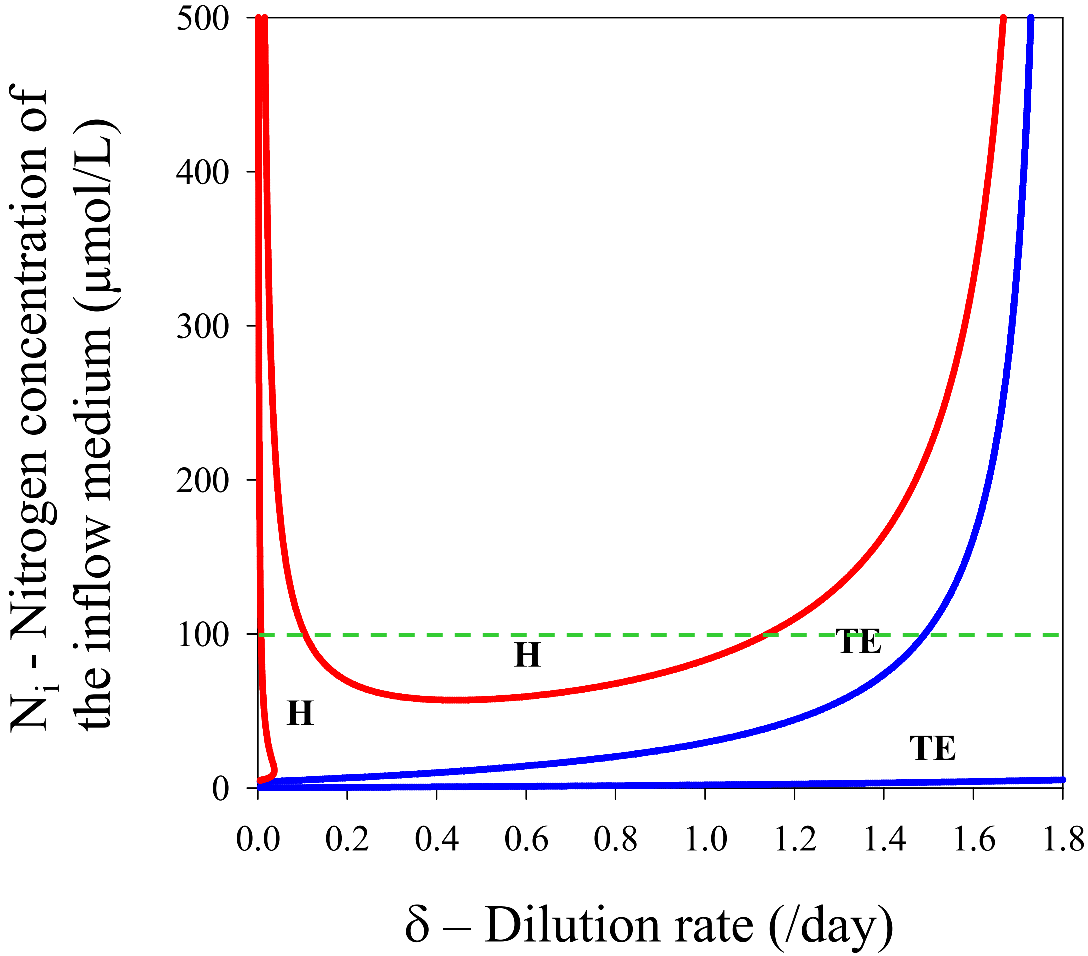
- There is a unique solution in $\mathbf{X}^{(k)}$ that is also in $\mathbf{N}^{(k)}$
- Additional interval-Newton steps will tightly enclose the solution with quadratic convergence

IN/GB Method: Interval Newton Test



- Any solutions in $\mathbf{X}^{(k)}$ are in $\mathbf{X}^{(k)} \cap \mathbf{N}^{(k)}$
- If the intersection is sufficiently small, repeat the root inclusion test
- Otherwise, bisect the intersection and apply the root inclusion test to each resulting subinterval

Algae-Rotifer Model



TE: Transcritical of Equilibria

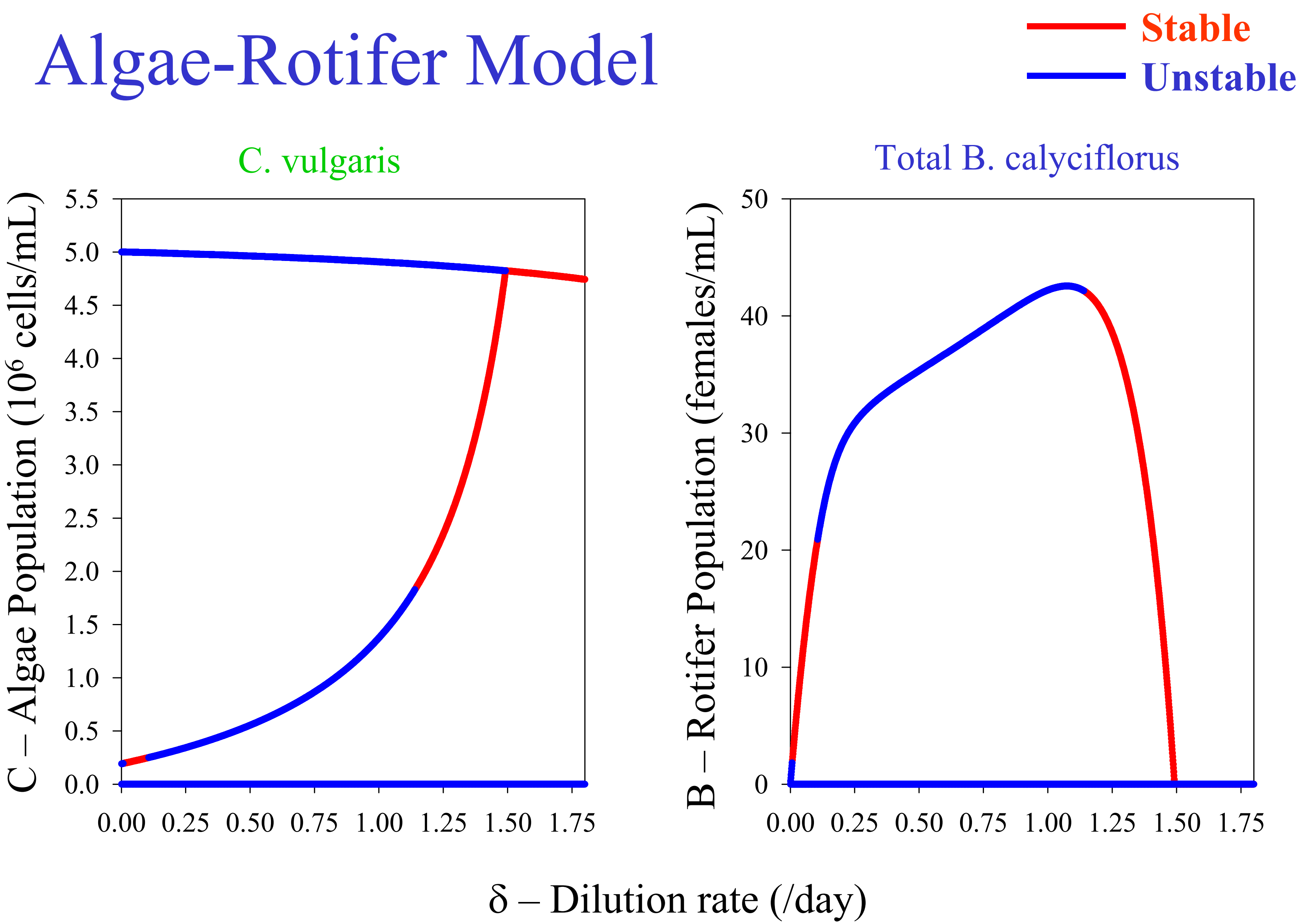
H: Hopf

Diagram generated using IN/GB

Consistent with Fussmann, et al., 2000

δ vs. N_i Bifurcation Diagram

Algae-Rotifer Model



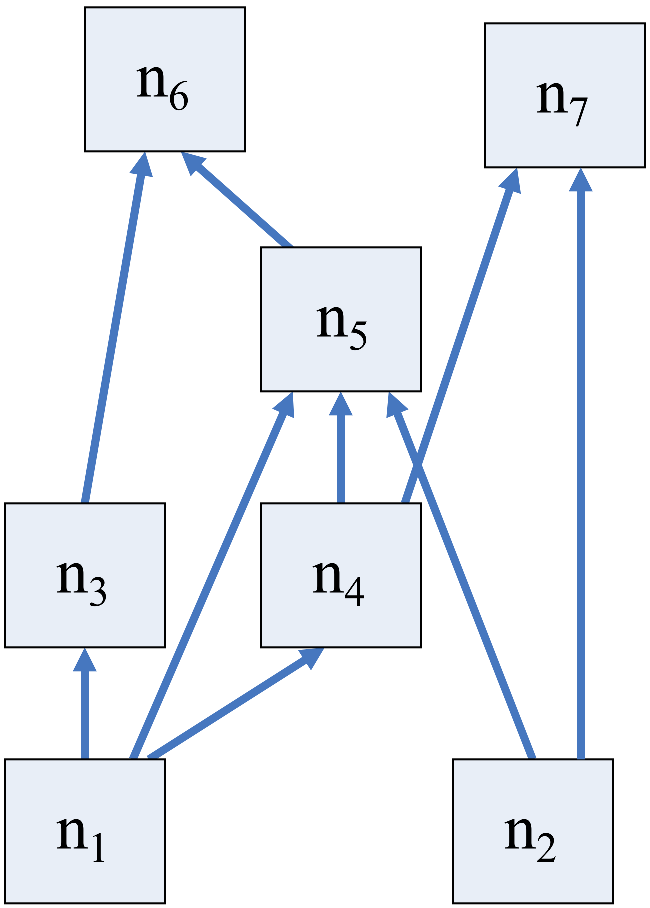
Solution Branch Diagram ($N_i = 100$)

Discussion – Algae-Rotifer Model

- Computation times are good (3.0 GHz Xeon/Linux)
  - Average 0.06 s to solve for equilibrium states
  - Average 7 s to solve for fold/transcritical bifurcations
  - Average 27 s to solve for Hopf bifurcations
- Increasing the dilution rate has two effects
  - Washing in more nutrient
  - Washing out more species biomass
- Initially, increasing the nutrient wash in to the system has the predominate effect of increasing the biomass of b. calyciflorus
  - After a point, further enriching the system becomes counter productive and the state becomes unstable
- Further increasing the dilution rate will eventually stabilize the system, and then cause a decrease in the b. calyciflorus population due to washout

Food Web Model

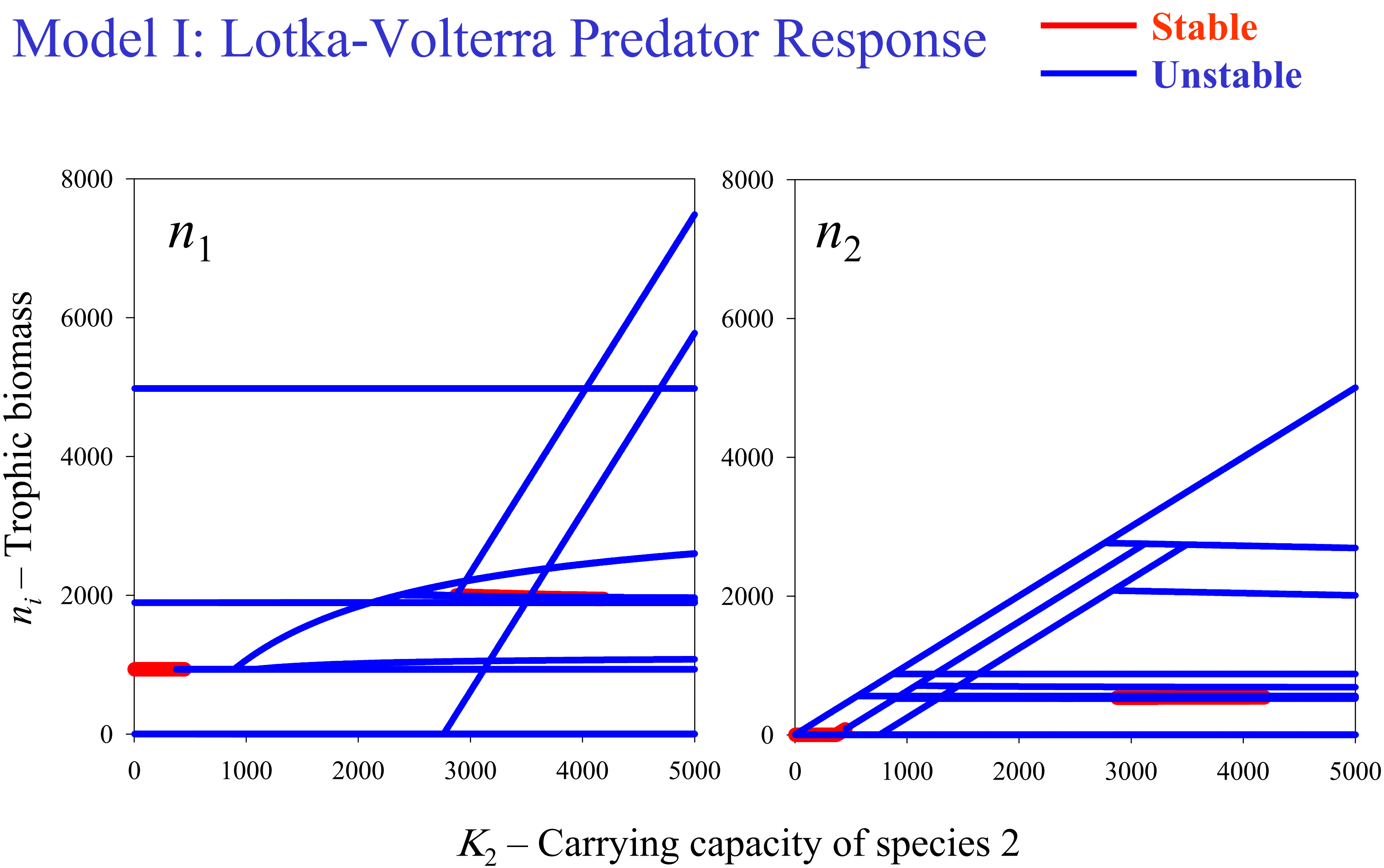
- Hypothetical food web model
  - 7 species
  - 2 producers that compete for resources
  - 5 predators
- Predator response functions:
  - Linear (Lotka-Volterra)
  - Hyperbolic (Holling II)
  - Combination of above



Food Web Model

- Simultaneous approach
  - Solve nonlinear equations (7 x 7) for all steady-states simultaneously
- Sequential approach
  - Solve sequence of subproblems corresponding to feasible zero-nonzero states
  - In this case, $2^7 = 128$ zero-nonzero states are possible; analysis shows that 55 are feasible
  - Subproblems may be linear or nonlinear depending on the model
- Here we apply IN/GB to the simultaneous approach

Model I: Lotka-Volterra Predator Response

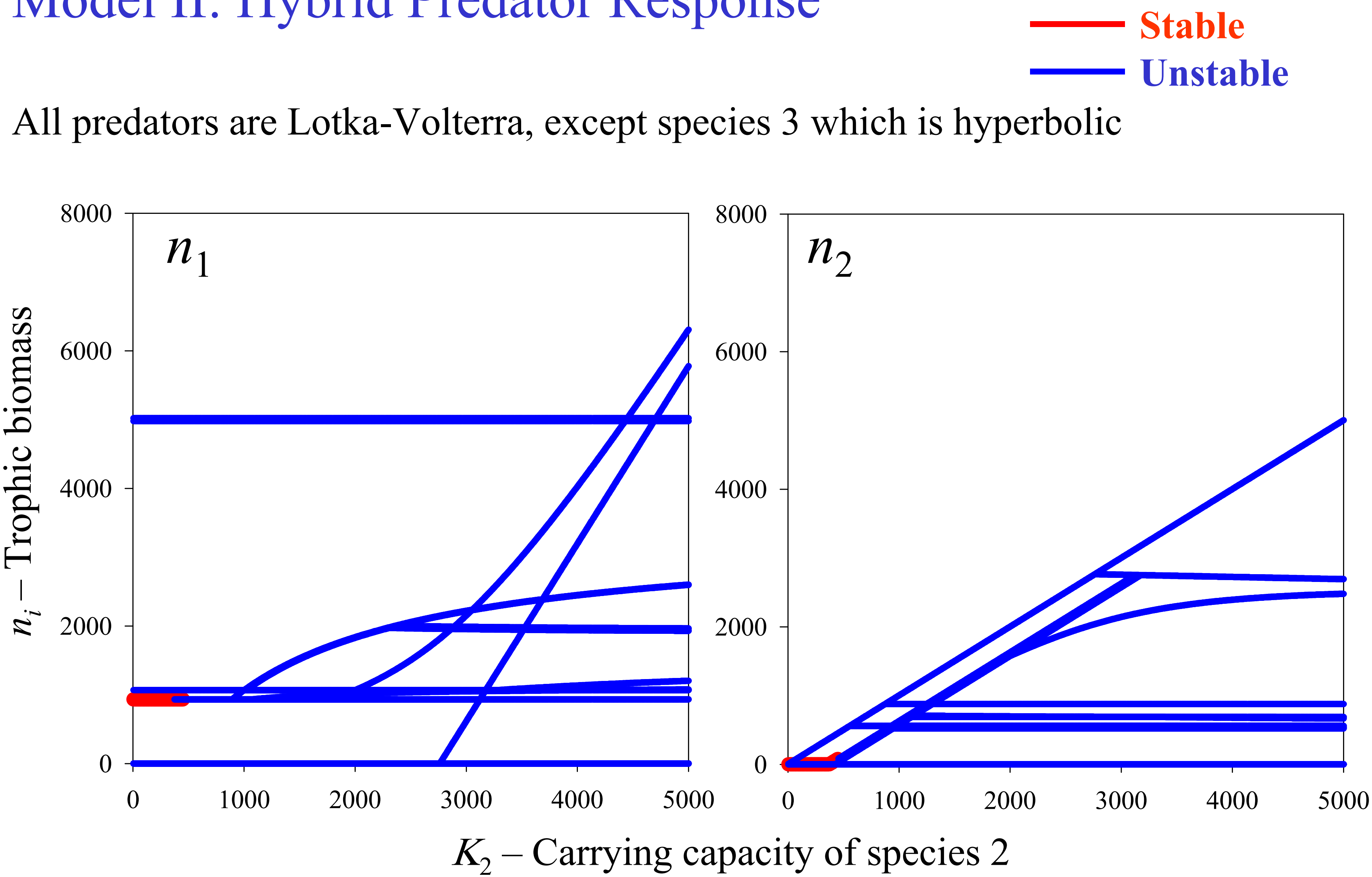


Solution Branch Diagram

Average 5.1 s per parameter set

Model II: Hybrid Predator Response

All predators are Lotka-Volterra, except species 3 which is hyperbolic



Solution Branch Diagram

Average 60 s per parameter set

Discussion – Food Web Model

- System behavior between the two models is identical when comparing states with zero biomass levels for species 3
- Changing species 3 to a hyperbolic predator destabilizes what was previously a stable, coexisting steady-state
- In both cases, a minimum carrying capacity is necessary for species 2 to coexist in a stable steady-state with the competitor species 1

Concluding Remarks

- Demonstrated the utility of an interval-Newton method combined with generalized bisection for the computationally rigorous and reliable location of
  - Fold, transcritical, and Hopf codimension-1 bifurcations
  - Fold-fold or Fold-Hopf codimension-2 bifurcations
  - Equilibrium states
- The utility of this method may be quite useful in dealing with systems with large numbers of solutions
  - The number of solutions is often unknown *a priori* and may not be a trivial problem to discern

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