Reliable Computation of Equilibrium States and Bifurcations in Nonlinear Dynamics

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Motivation

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

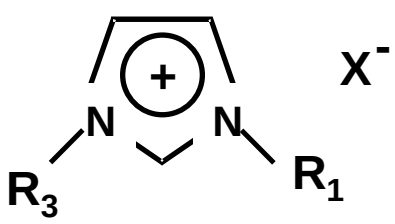
$$\dot{\boldsymbol{x}} = \frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{p}); \quad \boldsymbol{x} = \text{state variables}; \quad \boldsymbol{p} = \text{parameters}$$

- Common problems include computing
  - Equilibrium states $(\dot{\boldsymbol{x}} = \boldsymbol{0})$
  - Limit cycles
  - Bifurcations of equilibria
  - Bifurcations of cycles
- Of specific interest here are food chain/web models
  - Used to predict impact on ecosystems of introducing new materials (ionic liquids) into the environment

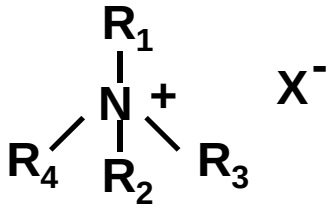
Motivation – Ionic Liquids

- Ionic liquids (ILs) are salts that are liquid at or near room temperature
- Many attractive properties
  - No measurable vapor pressure – ILs do not evaporate
  - Many potential applications, including replacement for volatile organic compounds (VOCs) currently used as solvents
  - Eliminates a major source of air pollution
- Could enter the environment via aqueous waste streams
  - Very little environmental toxicity information available
  - Single species toxicity information is not sufficient to predict ecosystem impacts
- Need for ecological risk assessment

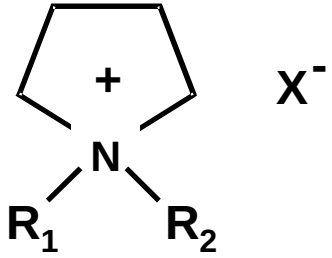
Example Ionic Liquids



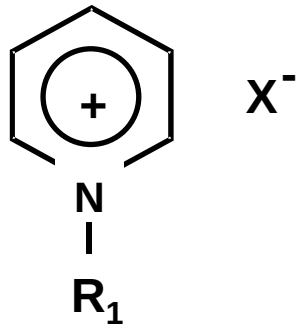
imidazolium



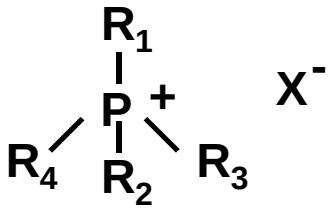
tetra alkylammonium



pyrrolidinium



pyridinium



tetra alkylphosphonium

X =		
	PF_6	Cl
	BF_4	NO_3
	CF_3SO_3	CH_3CO_2
	$(CF_3SO_2)_2N$	CF_3CO_2

Example:
1-n-butyl-3-methylimidazolium hexafluorophosphate
[bmim][PF_6]

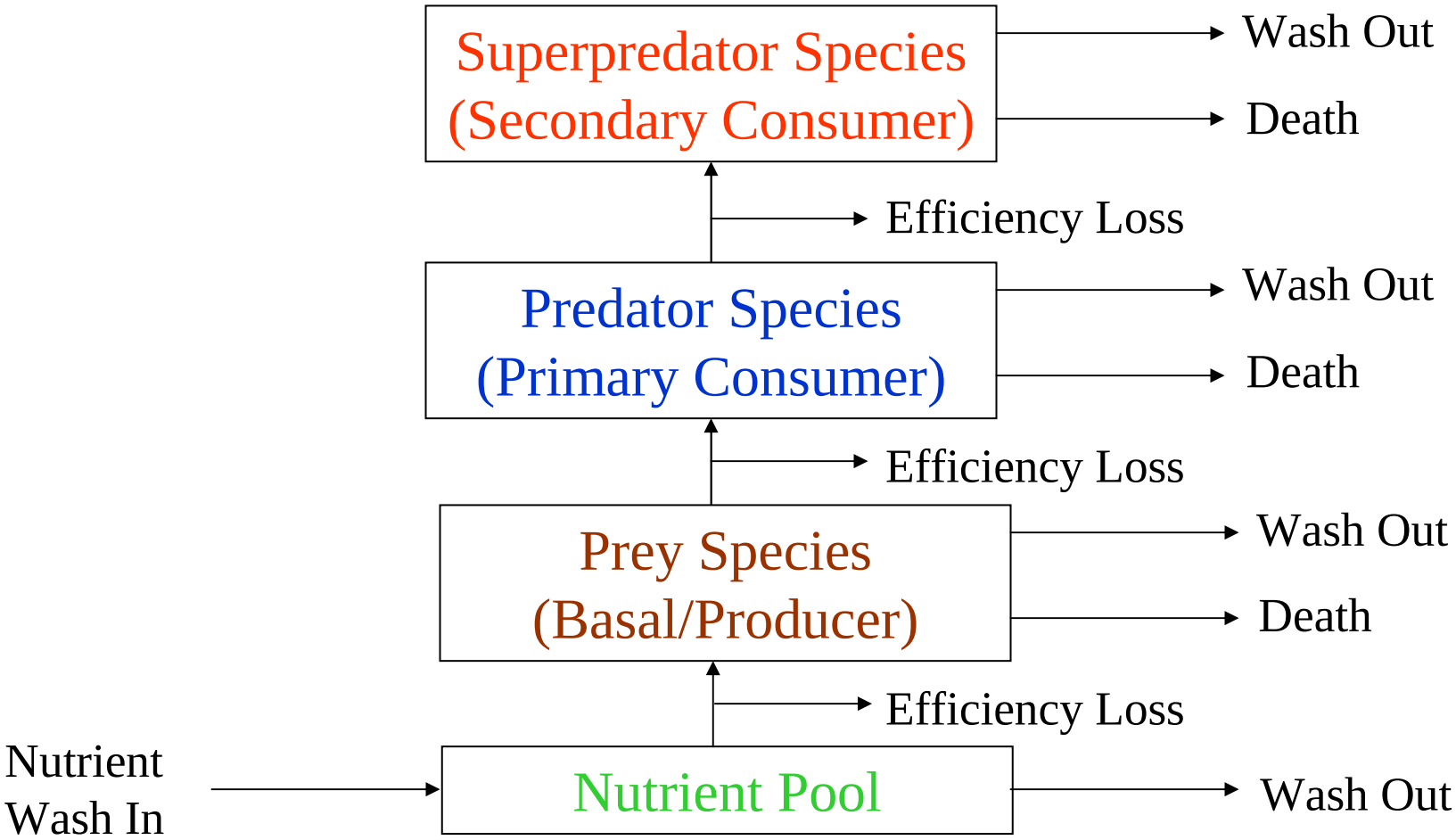
Ecological Risk Assessment

- Aim to predict a variety of different consequences, e.g.,
  - Bioaccumulation and biomagnification
  - Contaminant transport and fate
  - Ecosystem toxicity effects
- Use a variety of different strategies and tools, e.g.,
  - Toxicology
  - Microbiology
  - Hydrology
  - Ecological Modeling
- Currently, food chain/web models are used to link single species toxicity tests to ecosystem toxicity effects
  - Results indicate that modeling can provide a conservative estimate of allowable contaminate concentrations (e.g., Naito *et al.*, 2002)

Food Chain/Web Models

- Systems of ordinary differential equations that describe the rates of change in species biomass in an ecosystem
- 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 ecosystem models possible, depending on individual models of growth, predation, etc.
- Focus of this presentation is Canale's model: Tritrophic system in a chemostat with a hyperbolic predator and superpredator

Canale's Chemostat Model



Canale's Chemostat Model

$$\frac{dx_0}{dt} = D(x_n - x_0) - \frac{a_1 x_0 x_1}{b_1 + x_0}$$

$$\frac{dx_1}{dt} = x_1\left[e_1 \frac{a_1 x_0}{b_1 + x_0} - \frac{a_2 x_2}{b_2 + x_1} - d_1 - \varepsilon_1 D\right]$$

$$\frac{dx_2}{dt} = x_2\left[e_2 \frac{a_2 x_1}{b_2 + x_1} - \frac{a_3 x_3}{b_3 + x_2} - d_2 - \varepsilon_2 D\right]$$

$$\frac{dx_3}{dt} = x_3\left[e_3 \frac{a_3 x_2}{b_3 + x_2} - d_3 - \varepsilon_3 D\right]$$

x_0: nutrient
x_1: prey
x_2: predator
x_3: superpredator

x_n : inflow nutrient concentration
D : inflow rate

a_i : max predation rate; b_i : half saturation constant;
d_i : death rate; e_i : efficiency; $\varepsilon_i D$: washout rate

Model Computations

- Locate equilibrium points and bifurcations of equilibria in the food chain/web model
- 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 of equilibria are located by solving a nonlinear algebraic system consisting of the equilibrium conditions along with one or more augmenting (test) functions

Codim-1 Bifurcations and Test Functions

- Fold and transcritical bifurcations
  - As α is varied, two equilibria collide, resulting in annihilation (fold) or exchange of stability (transcritical)
  - The Jacobian, $J(\boldsymbol{x},\alpha)$, of the model has a single zero eigenvalue
  - Product of all eigenvalues must be zero: $\lambda_1\lambda_2\lambda_3\lambda_4 = 0$
  - Convenient test function (avoiding calculation of eigenvalues):

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

Codim-1 Bifurcations and Test Functions

- Hopf bifurcation
  - J($\boldsymbol{x}, \alpha$) has a pair of complex conjugate eigenvalues that cross the imaginary axis as α is varied: possible change in stability
  - Product of all possible pair sums must be zero:

$$(\lambda_1+\lambda_2)(\lambda_1+\lambda_3)(\lambda_1+\lambda_4)(\lambda_2+\lambda_3)(\lambda_2+\lambda_4)(\lambda_3+\lambda_4) = 0$$

  - Convenient test function based on bialternate product

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

  - Can produce false-positives
  - Must screen solutions by checking if eigenvalues are imaginary conjugates

Codim-2 Bifurcations and Test Functions

- Fold-Fold: Two eigenvalues are zero
- Fold-Hopf: One eigenvalue is zero and a pair of pure imaginary complex conjugate eigenvalues
- Located by using both augmenting functions

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

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

Locating Equilibrium States and Bifurcations

- Equilibrium states: Solve equilibrium conditions for $\boldsymbol{x}$.
- Bifurcations of equilibria: Solve augmented equilibrium conditions for $\boldsymbol{x}$ and α (and β)
- These equation systems may have multiple solutions
- Typically these systems are solved using a continuation-based strategy (e.g., Kuznetsov, 1991; AUTO software)
  - Initialization dependent
  - No guarantee of locating all solution branches
- Interval mathematics provides a method that is:
  - Initialization independent
  - Capable of locating all solution branches with certainty

Methodology

Core methodology is interval-Newton: Solve $\boldsymbol{f}(\boldsymbol{x}) = \mathbf{0}$ for all roots in the interval $\mathbf{X}^{(0)}$

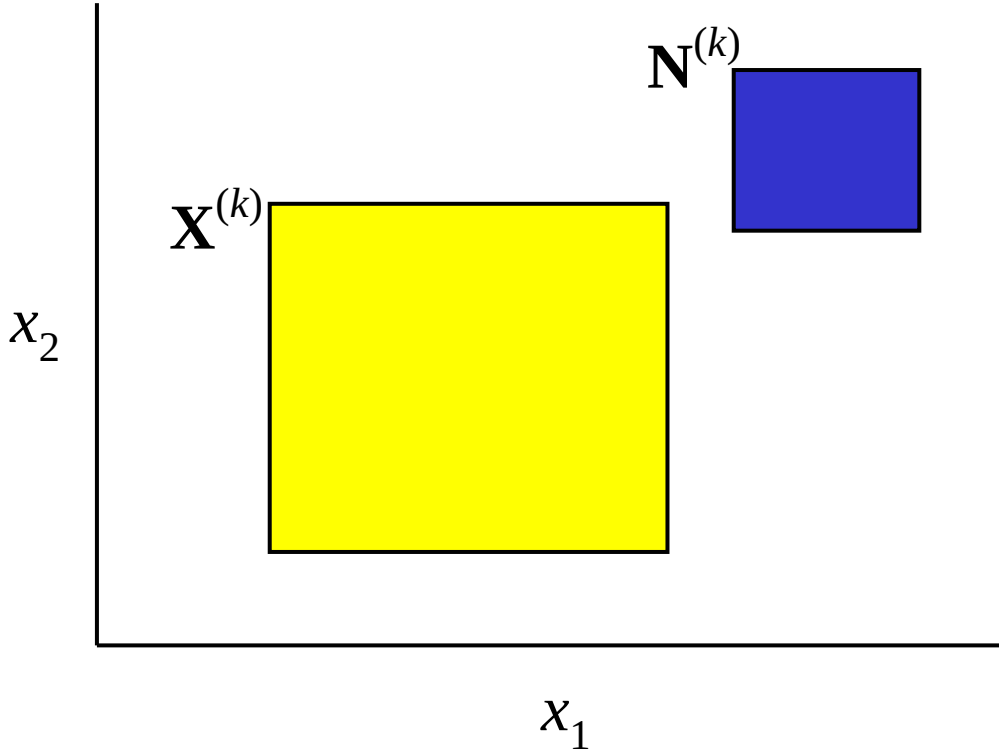
Basic iteration scheme: For a particular subinterval (box), $\mathbf{X}^{(k)}$, perform root inclusion test:

- Range test: Compute an interval extension (bounds on range) $\mathbf{F}(\mathbf{X}^{(k)})$
  - If $\mathbf{0} \notin \mathbf{F}(\mathbf{X}^{(k)})$, delete the box
- Interval Newton test: Compute the image, $\mathbf{N}^{(k)}$, of the box by solving the linear interval equation system

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

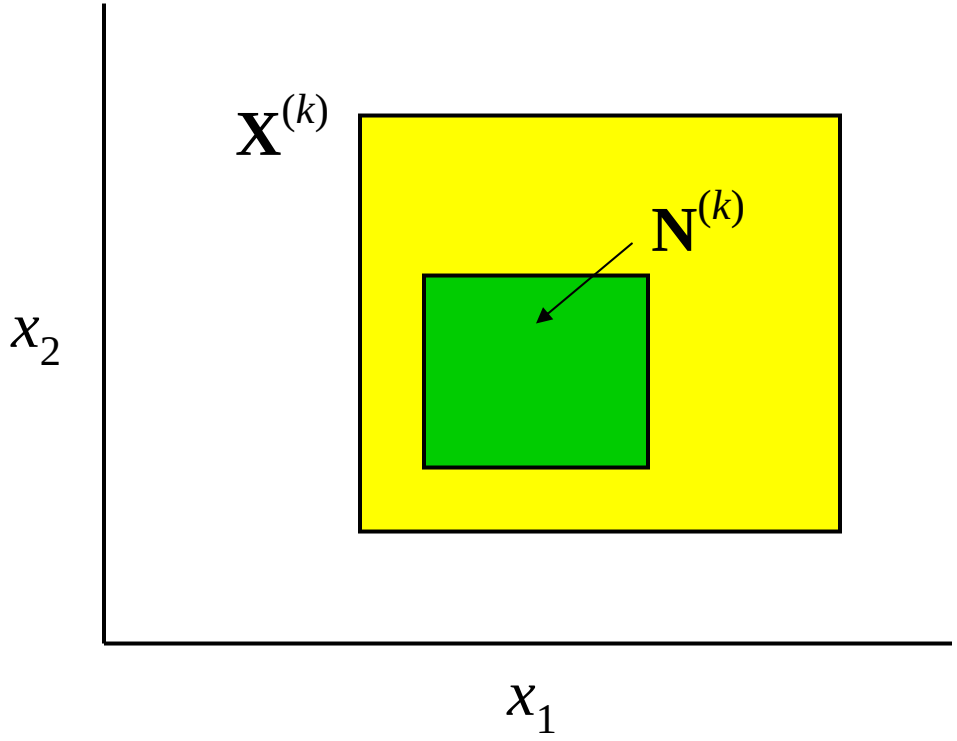
  - $\boldsymbol{x}^{(k)}$ is a point in $\mathbf{X}^{(k)}$
  - $\mathrm{F}'(\mathbf{X}^{(k)})$ is the interval extension of the Jacobian matrix of $\boldsymbol{f}(\boldsymbol{x})$ over the interval $\mathbf{X}^{(k)}$

Interval-Newton Test



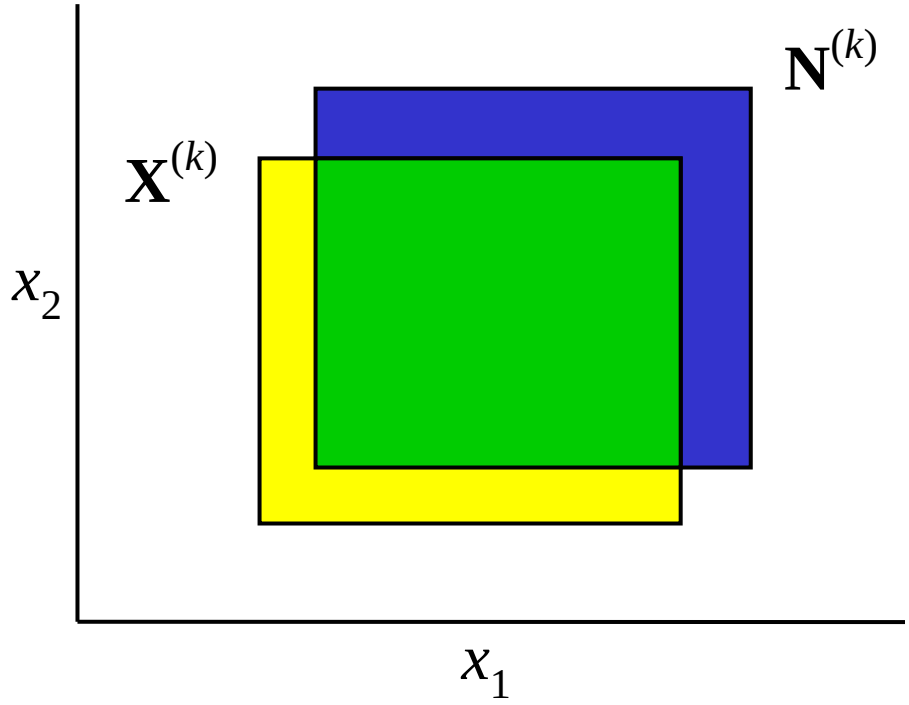
- There is no solution in $\mathbf{X}^{(k)}$

Interval-Newton Test



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

Interval-Newton Test



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

Methodology

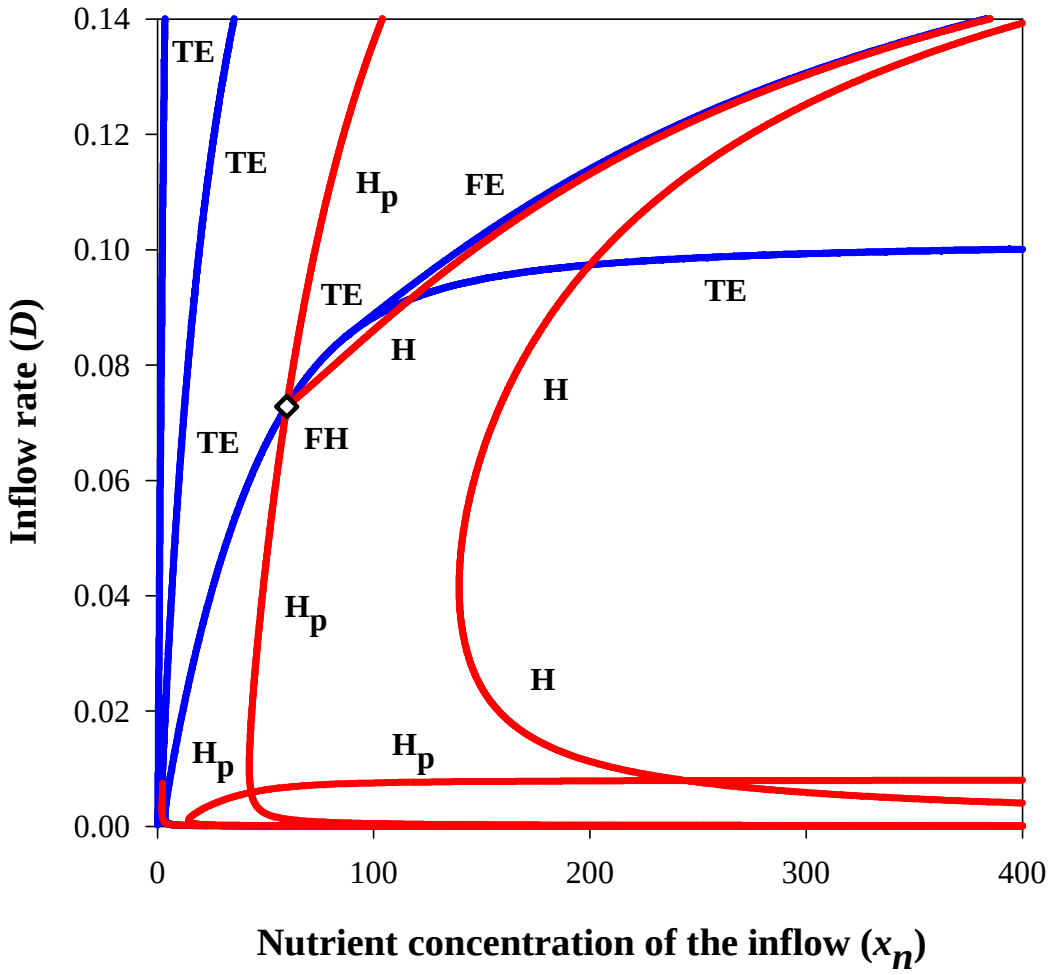
Available enhancements to basic methodology:

- LP-based strategy for computing image $\mathbf{N}^{(k)}$ in interval-Newton test (Lin and Stadtherr, 2003, 2004)
  - Exact bounds on $\mathbf{N}^{(k)}$ (within roundout)
- Constraint propagation (problem specific)
- Tighten interval extensions using known function properties (problem specific)

Generating Solution Diagrams

- Solution branch diagrams (say $\boldsymbol{x}$ vs. x_n)
  - Set x_n , use interval-Newton to solve equilibrium conditions for $\boldsymbol{x}$
  - Make small increment in x_n and repeat
- Bifurcation diagrams (say x_n vs. D)
  - Set D, solve for values of x_n and $\boldsymbol{x}$ at which bifurcations occur
  - Make small increment in D and repeat
  - Set x_n, solve for values of D and $\boldsymbol{x}$ at which bifurcations occur
  - Make small increment in x_n and repeat

Canale's Chemostat Model
x_n vs. D Bifurcation Diagram

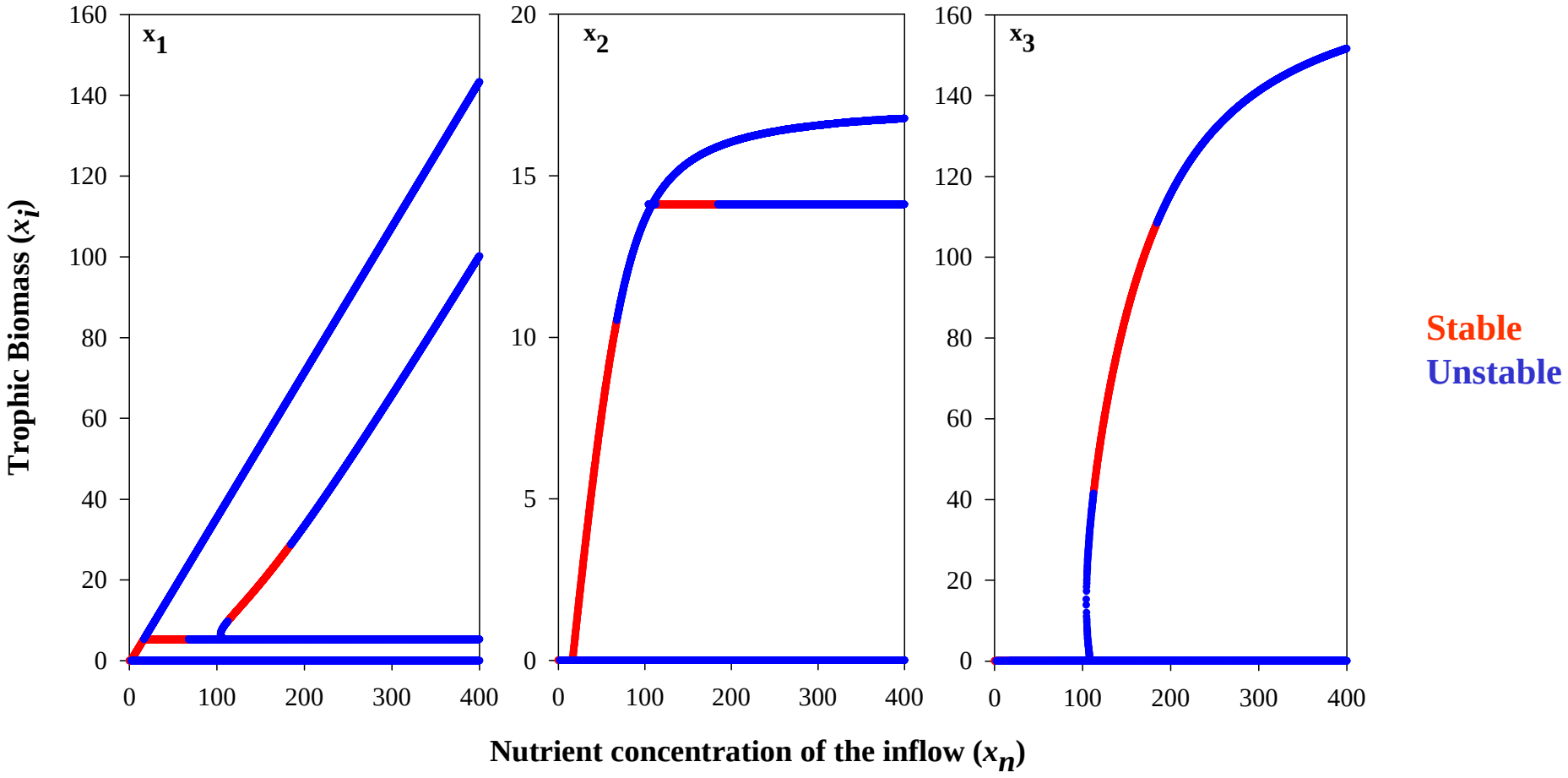


TE: Transcritical of Equilibria
FE: Fold of Equilibria

H: Hopf
H_p: Planar Hopf

FH: Fold-Hopf Codimension 2

Canale's Chemostat Model
x vs. x_n Solution Branch Diagram (D = 0.09)



Canale's Model with Contaminant

- Can link the death rate parameter in each trophic level with a hypothetical contaminate concentration (Gwaltney and Stadtherr, 2004)

$$d_i = d_i^o + \frac{1}{2C_i^{LC50}} C$$

d_i^0 : base-line death rate

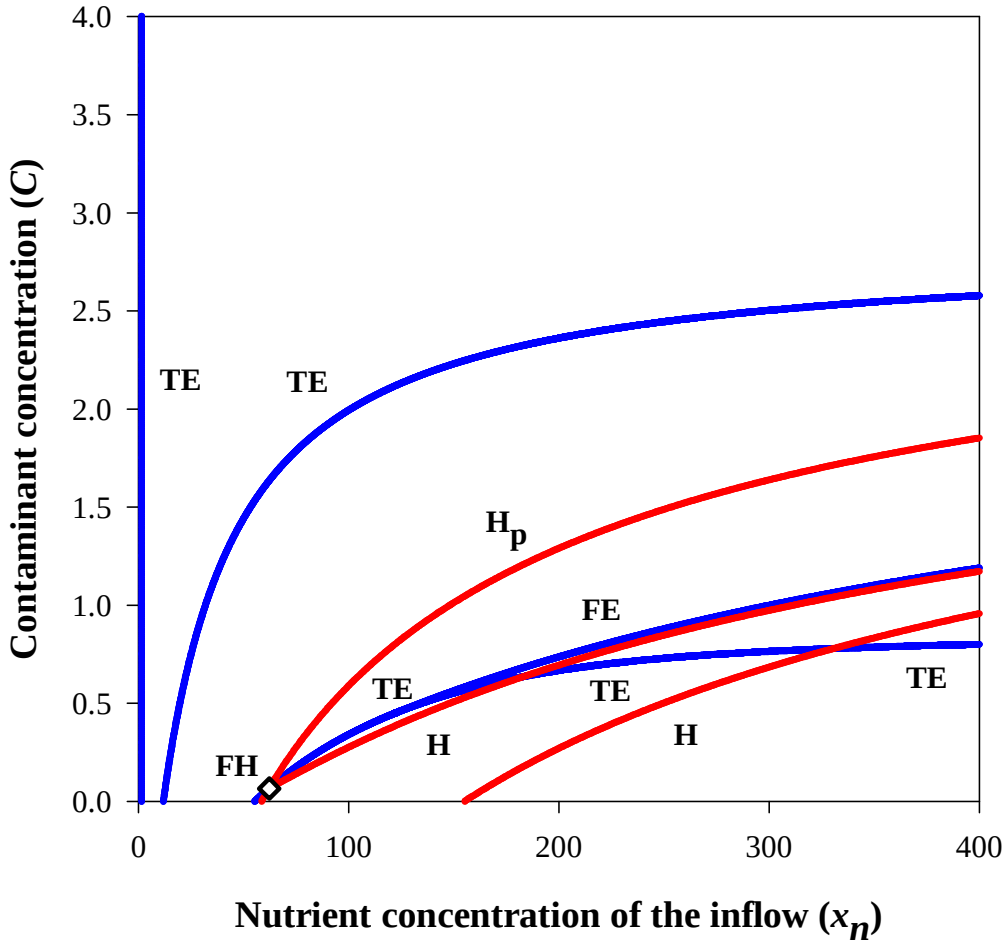
d_i : death rate

C_i^{LC50} : LC50 value

C: Contaminate Concentration

- LC50 value is concentration of contaminant that is lethal to 50% of a population of test animals in a given period of time (measured experimentally)

Canale's Model with Contaminant
x_n vs. C Bifurcation Diagram



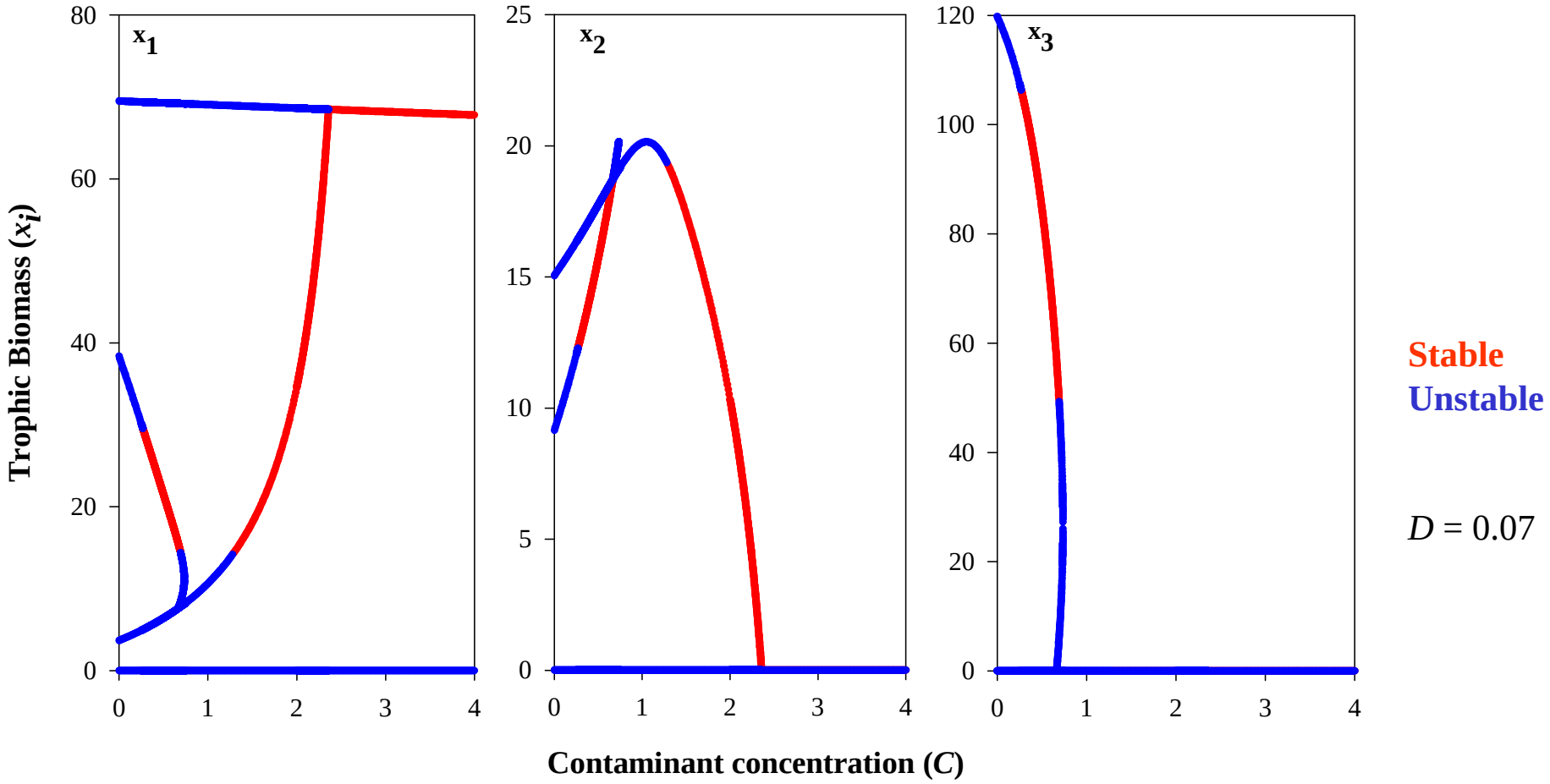
***D* = 0.07**

TE: Transcritical of Equilibria
FE: Fold of Equilibria

H: Hopf
H_p: Planar Hopf

FH: Fold-Hopf Codimension 2

Canale's Model with Contaminant
x vs. *C* Solution Branch Diagram (x_n = 200)



Concluding Remarks

- Computation times (1.7GHz Xeon/Linux) are reasonable
  - Average 0.06 s to solve for equilibrium states
  - Average 15 s to solve for fold/transcritical bifurcations
  - Average 100 s to solve for Hopf bifurcations
- Using interval methodology, can generate solution branch and bifurcation diagrams with confidence, without need for initialization or *a priori* insights
- Diagrams can be generated automatically without user intervention to deal with initialization issues
- Applicable to a wide variety of problems in nonlinear dynamics

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