Problem 1

Stability Criteria. Let us derive the necessary and sufficient conditions for a 2×2 real matrix to have eigenvalues with negative real parts.

(a) Consider a 2×2 real matrix A with matrix elements a_{ij}. Show that the two conditions

$$\mathrm{tr}(A) = a_{11} + a_{22} < 0,$$
$$\det(A) = a_{11}a_{22} - a_{12}a_{21} > 0$$

are necessary and sufficient conditions for the two eigenvalues σ_i of A to both have negative real parts.

(b) Explain why these conditions are equivalent to the statement that all solutions $u(t)$ of the two-dimensional constant-coefficient linear dynamical system $d\mathbf{u}/dt = A\mathbf{u}$ decay to zero.

Problem 2

Linearized Brusselator Equations. Consider the "Brusselator" equations

$$\partial_t u_1 = a - (b+1)u_1 + u_1^2 u_2 + D_1 \partial_x^2 u_1,$$
$$\partial_t u_2 = b u_1 - u_1^2 u_2 + D_2 \partial_x^2 u_2.$$

(a) Derive the linearized equations for small perturbations about the stationary uniform solution.

(b) Determine the numerical value of the coherence length ξ_c for $a = 1.5$, $D_1 = 2.8$ and $D_2 = 22.4$ and compare that value with the critical wavelength $\lambda = 2\pi/q_c \approx 14.5$. Suggest a numerical experiment that can be used to verify this result for ξ_c?

(c) Determine where in the parameter space does the Type-III$_o$ instability take place. First find the critical value of b, as a function of the other parameters, $b_o = b_o(a, D_1, D_2)$. Next determine the condition a has to satisfy such that the mode $q = 0$ is marginal, while the mode $q = q_m$ is stable, for $b = b_o$ (otherwise, the type-III$_o$ instability can be pre-empted by the type-I$_s$ instability). Verify your result through numerical simulation (use $D_1 = 2.8$ and $D_2 = 22.4$).

Problem 3

The Oregonator. A more realistic, but still simplified, model of the Belousov-Zhabotinsky reaction is given by the following five reactions:

$$BrO_3^- + Br^- + 2H^+ \to HBrO_2 + HOBr,$$
$$HBrO_2 + Br^- + H^+ \to 2HOBr,$$
$$BrO_3^- + HBrO_2 + 3H^+ + 2Ce^{3+} \to 2HBrO_2 + 2Ce^{4+} + H_2O,$$
$$2HBrO_2 \to BrO_3^- + HOBr + H^+,$$
$$Z + Ce^{4+} + \alpha(h)H_2O \to hBr^- + Ce^{3+} + \beta(h)HCOOH + \gamma(h)CO_2 + \epsilon(h)H^+,$$

where h is some number (a stoichiometry factor) and the last reaction is a reaction of Ce^{4+} with a mixture of $CH_2(COOH)_2$ (malonic acid) and $CHBr(COOH)_2$ (bromomalonic acid) denoted as Z. Parameters α, β, γ, and ϵ denote numerical factors depending on h that are not necessary for this exercise.

(a) Use the law of mass action (the reaction rate with exponents equal to the stoichiometric coefficients of the reactants on the left side) to derive dynamical evolution equations for the three concentrations

$$u = [HBrO_2],$$
$$v = [Ce^{4+}],$$
$$w = [Br^-],$$

Assume that the concentrations $[H^+]$, $[Br0_3^-]$, $[CH_2(COOH)_2]$, $[CHBr(COOH)_2]$, $[Ce^{3+}]$, and $[H_20]$ are constant. The resulting three ODEs constitute the Oregonator model of the Belousov-Zhabotinsky reaction. The name comes from the University of Oregon, where a group of research chemists first proposed and analyzed this model.

(b) By an appropriate rescaling of time t and of the various concentrations, show that the rescaled equations can be written in the form

$$\eta \partial_t u = qw - uw + u - u^2, \tag{1}$$
$$\partial_t v = u - v, \tag{2}$$
$$\eta' \partial_t w = -qw - uw + bv, \tag{3}$$

The constants η, η', q, and b are related to the reaction rates and to the concentrations that are held constant.

(c) For some parameter values, the inequalities $\eta' \ll \eta \ll 1$ hold. Assuming in this case that the left side of equation (3) is approximately zero, show that the variable w can be eliminated so that the system (1-3) reduces to a two-variable model

$$\eta \partial_t u = u - u^2 - bv\frac{u-q}{u+q},$$
$$\partial_t v = u - v,$$

This illustrates how a non-polynomial reaction rate can arise from the elimination of a quickly changing variable.