Implicit-Explicit Methods for Reaction-Diffusion Equations in Pattern Formation

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Outline

Explaining Pattern Formation in Biology

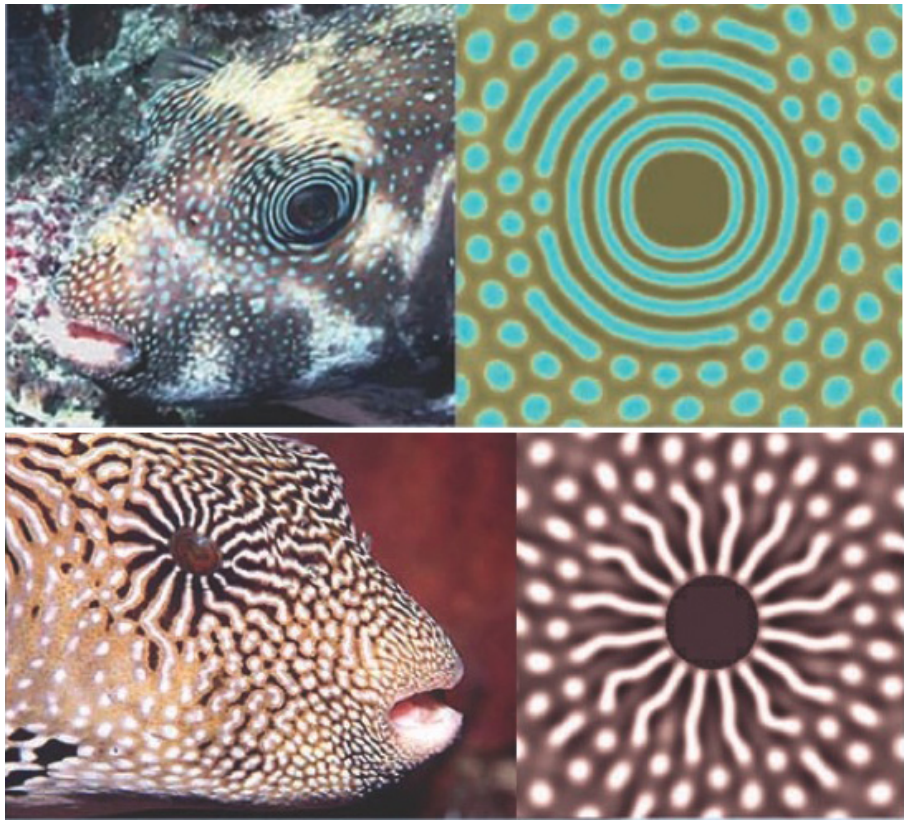


Figure: Juvenile and adult zebra-striped fish

What mathematical models can we use to explain the development of stripes, spots, or other patterns in nature?

Reaction-Diffusion model

$$w_t = F(w) + D\Delta w$$

- Alan Turing proposed a reaction-diffusion model for explaining pattern formation. Here w is a vector of chemical concentrations, F represents the reaction kinetics, D a diagonal matrix of diffusion rates.
- For simplicity, focus on two-chemical systems, $w = (u, v)$, in one spatial dimension. Turing showed that for certain reaction kinetics and diffusion constants, the system can evolve from a uniform steady state (u_*, v_*) into complex patterns.

Stability Analysis

- Linearize the equations about (u_*, v_*), and see what happens to perturbations.

$$\tilde{u}_t = f_u(u_*, v_*)\tilde{u} + f_v(u_*, v_*)\tilde{v} + D_u\tilde{u}_{xx}$$
$$\tilde{u}_t = g_u(u_*, v_*)\tilde{u} + g_v(u_*, v_*)\tilde{v} + D_u\tilde{v}_{xx}$$

  where $(u, v) = (u_* + \tilde{u}, v_* + \tilde{v})$ is the solution to the PDE.
- Apply changes of variables to rescale the equations:

$$\tilde{u}_t = k_1\tilde{u} - \tilde{v} + \tilde{u}_{xx}$$
$$\tilde{u}_t = \tilde{u} + k_4\tilde{v} + \nu\tilde{v}_{xx}$$

  where $\nu = \frac{D_v}{D_u}$ is the ratio of the diffusion rates.

Stability Analysis

- To see which patterns can develop, apply Fourier transform to the spatial variable to get:

$$\frac{d}{dt}\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} k_1 - \omega^2 & -1 \\ 1 & k_4 - \nu\omega^2 \end{pmatrix}\begin{pmatrix} U \\ V \end{pmatrix}$$

  where U, V are the Fourier transforms of $\tilde{u}, \tilde{v}$.
- Thus a perturbation of wavenumber ω will decay or grow depending on the eigenvalue $\lambda(\omega)$ with the largest real part. For a fixed diffusion ratio ν, we can thus find the areas in the $k_1 - k_4$ parameter space where patterns may form.
- Special case: a stable equilibrium in the absence of diffusion may become unstable when diffusion is added. (Turing instability)

Pattern forming regions

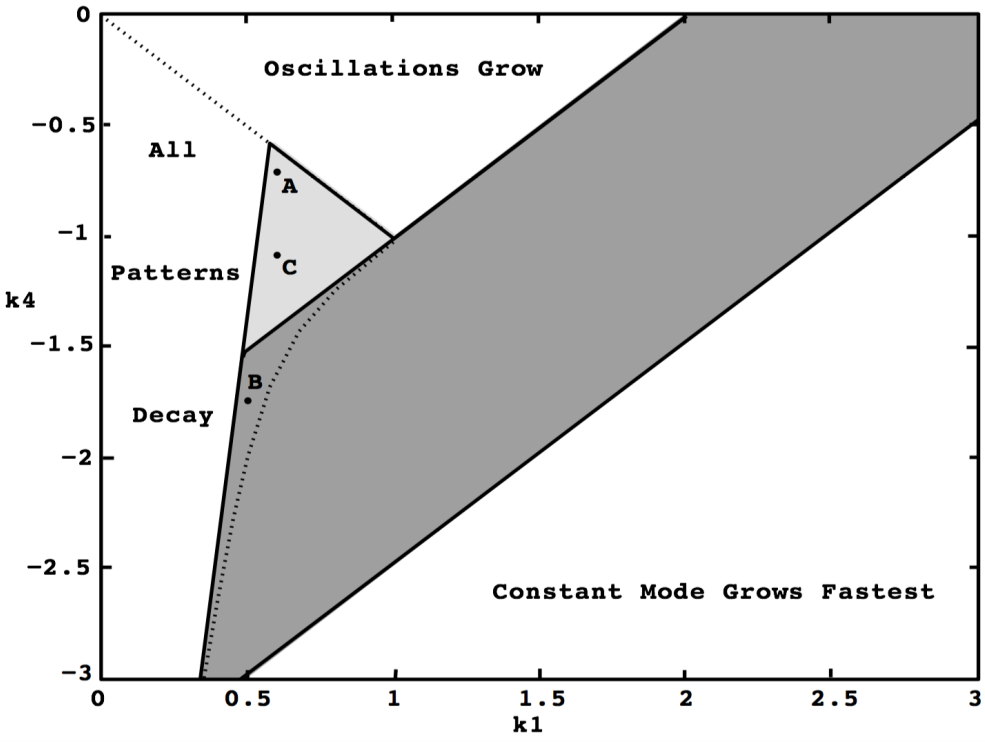


Figure: Pattern-forming region, $\nu = 10$

- All patterns decay if $\forall\omega, Re(\lambda(\omega)) < 0$
- Oscillations grow if λ is not purely real and $Re(\lambda) > 0$.
- The constant mode grows most quickly if $Re(\lambda(0)) > Re(\lambda(\omega))$
- Gray areas indicate regions where pattern formation may occur.

- Note: There may be competing patterns in certain parameter regimes.
- The dominant wavenumber is the wavenumber ω such that $Re(\lambda(\omega))$ is maximized. Patterns of these wavenumbers will grow the fastest and dominate the solution over time.
- When assessing finite difference schemes, we will thus want to see how accurately the pattern forming region and the dominant wavenumber can be estimated.

IMEX schemes

- One way to find numerical solutions to reaction-diffusion equations is to use implicit-explicit schemes.
- Use an implicit scheme for diffusion to avoid needing very small time steps.
- On the other hand, the reaction term is more suited to an explicit treatment.
- eg: The first-order, semi-implicit backward differentiation (1-SBDF) scheme is given by

$$\frac{w^{n+1} - w^n}{\Delta t} = F(w^n) + DL_h w^{n+1}$$

IMEX schemes

- Similar to the previous analysis, we apply the Fourier transform and get a matrix equation:

$$\begin{pmatrix} U^{n+1} \\ V^{n+1} \end{pmatrix} = M(k_1, k_4, \omega) \begin{pmatrix} U^{n} \\ V^{n} \end{pmatrix}$$

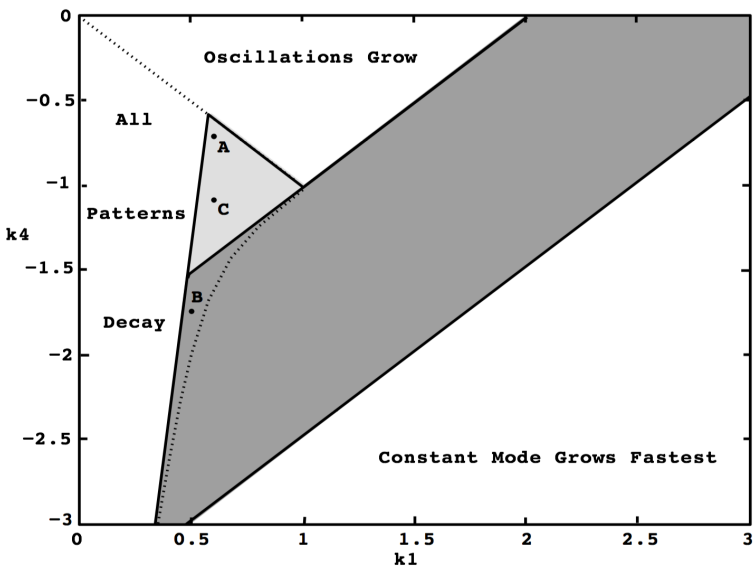
- Approximate the pattern-forming region by calculating the spectral radius of M, $\rho(k_1, k_4, \omega)$.
- Approximate the dominant wavenumber by analyzing the eigenvalues of $M(k_1, k_4, \omega)$.

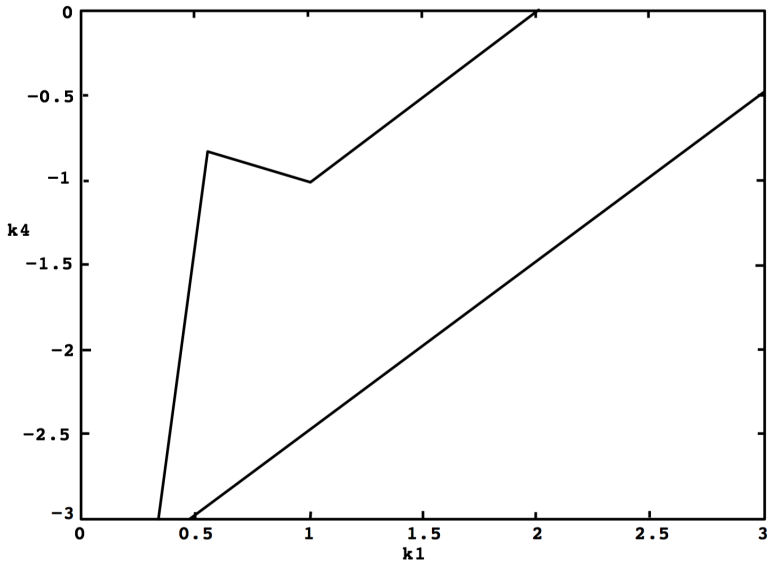
Estimating the pattern forming region and dominant wavenumber

1. If $\rho(k_1, k_4, \omega) < 1$ for all ω, then all modes decay. This approximates the left boundary of the region.
2. If $\rho(k_1, k_4, 0) \geq \rho(k_1, k_4, \omega)$ for all ω, then the constant mode grows the fastest. This approximates the lower boundary of the region.
3. If there exists $\omega \geq 0$ for which $M(k_1, k_4, \omega)$ has a non-real eigenvalue with real part greater than one, than oscillations will grow. This approximates the upper boundary.
4. One can estimate the dominant wavenumber ω_0 if $\rho(k_1, k_4, \omega_0) > \rho(k_1, k_4, \omega)$ for all $\omega \geq 0$.

1-SBDF

$$\frac{w^{n+1} - w^n}{\Delta t} = F(w^n) + DL_h w^{n+1}$$

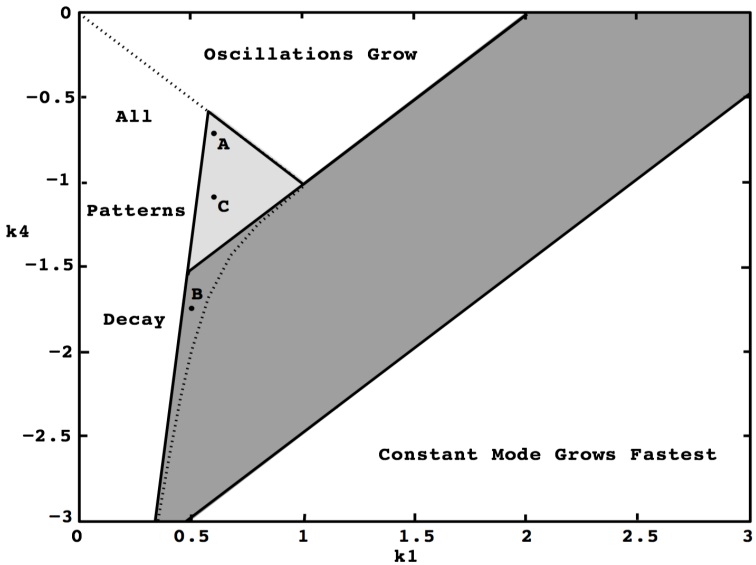


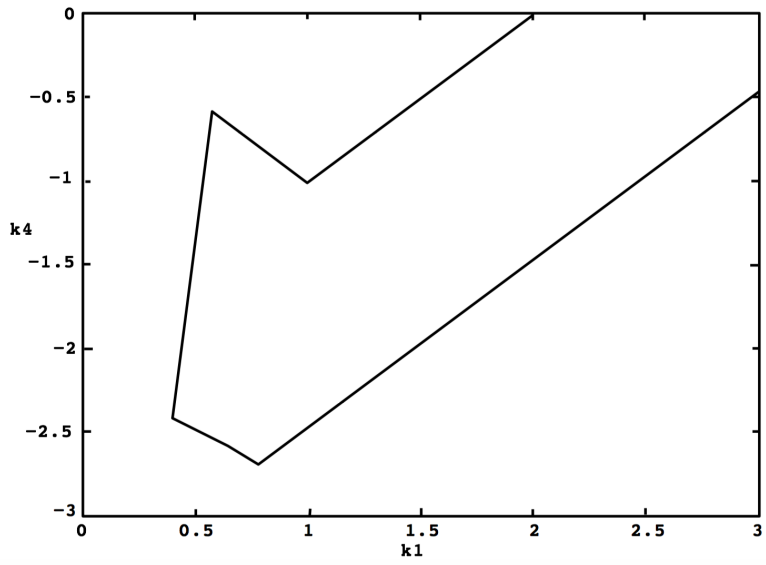


- Pattern-forming region is well-approximated, except for the boundary $k_1 + k_4 = 0$.
- Requires small time steps to get good approximation for the dominant wavenumber, because it is first order.
- Wrong dominant wavenumber can lead to qualitatively incorrect patterns.

MCNAB (Modified Crank-Nicolson Adams-Bashforth)

$$\frac{w^{n+1}-w^n}{\Delta t} = \frac{3F(w^n)}{2} - \frac{F(w^{n-1})}{2} + DL_h\left(\frac{9w^{n+1}}{16} + \frac{3w^n}{8} + \frac{w^{n-1}}{16}\right)$$

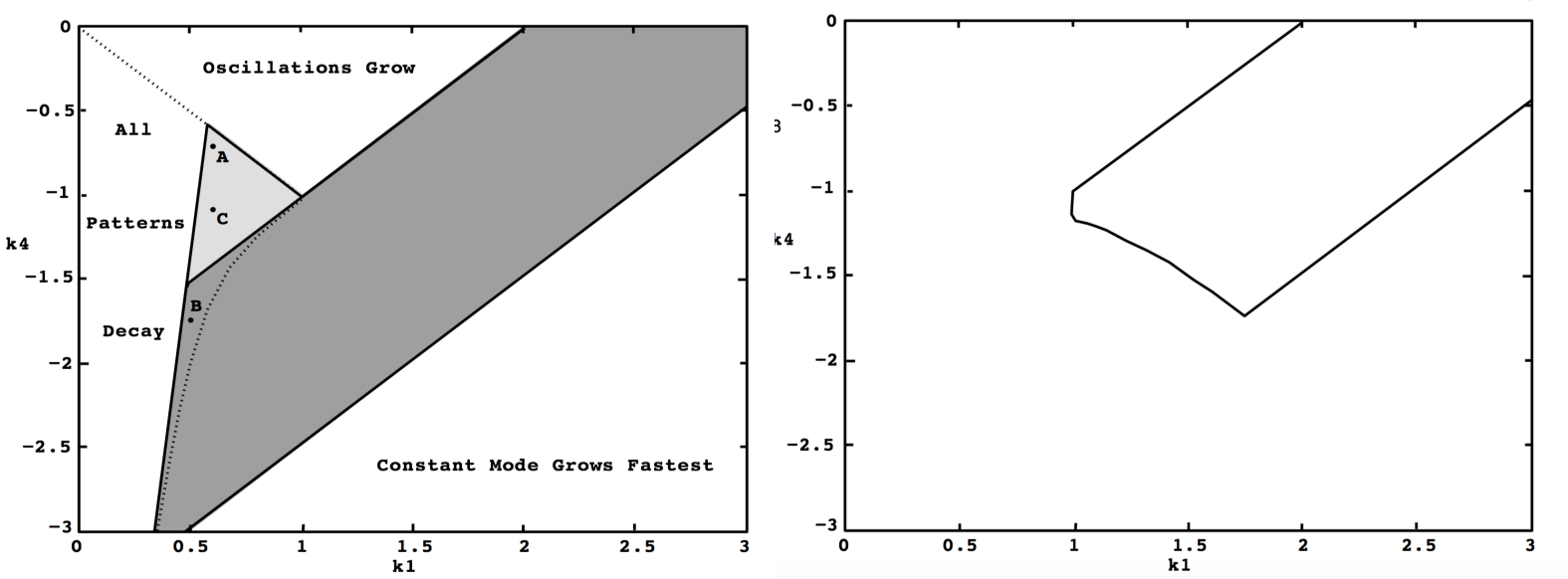




- Pattern-forming region require small time steps (eg $\Delta t < 0.2$) for a good approximation.
- Has small truncation error and gives a good approximation to the dominant wavenumber.

CNLF (Crank-Nicolson Leapfrog)

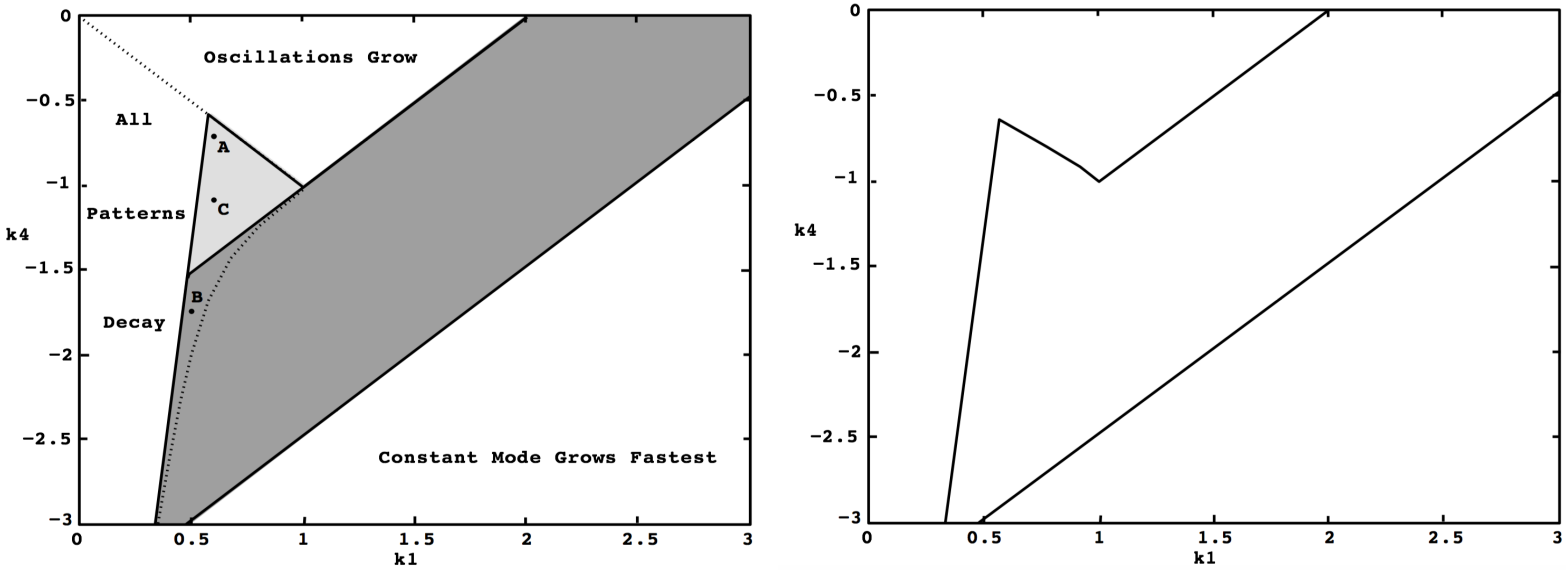
$$\frac{w^{n+1} - w^{n-1}}{2\Delta t} = F(w^n) + DL_h\left(\frac{w^{n+1} + w^{n-1}}{2}\right)$$



- Pattern-forming region is not reproduced even for small time steps. Never use this scheme for this setting!
- This is because leapfrog is unstable for diffusion equation.

2-SBDF (Second-order Backward Differentiation)

$$\frac{3w^{n+1} - 4w^n + w^{n-1}}{2\Delta t} = 2F(w^n) - F(w^{n-1}) + DL_h w^{n+1}$$



- Very good approximation for pattern-forming region even for large time steps ($\Delta t = 0.5$).
- Also estimates the dominant wavenumber well, although less accurately than MCNAB.

Summary of schemes

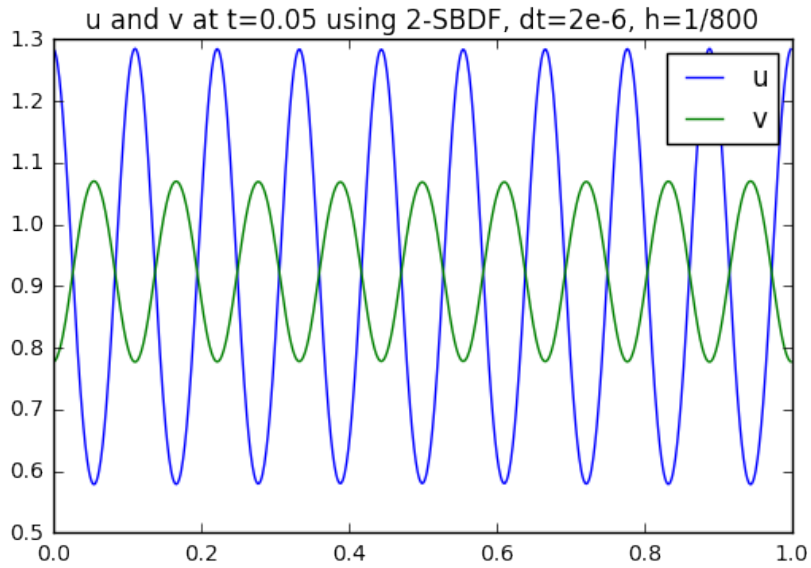
- Instability of a scheme can lead to errors in estimating the pattern-forming region.
- 2-SBDF is a good choice for most problems in this setting.
- MCNAB may be preferred when more accuracy is preferred, or near the boundary $k_1 + k_4 = 0$.

Schnakenberg model

$$u_t = \gamma(a - u + u^2 v) + \Delta u$$
$$v_t = \gamma(b - u^2 v) + \nu \Delta v$$

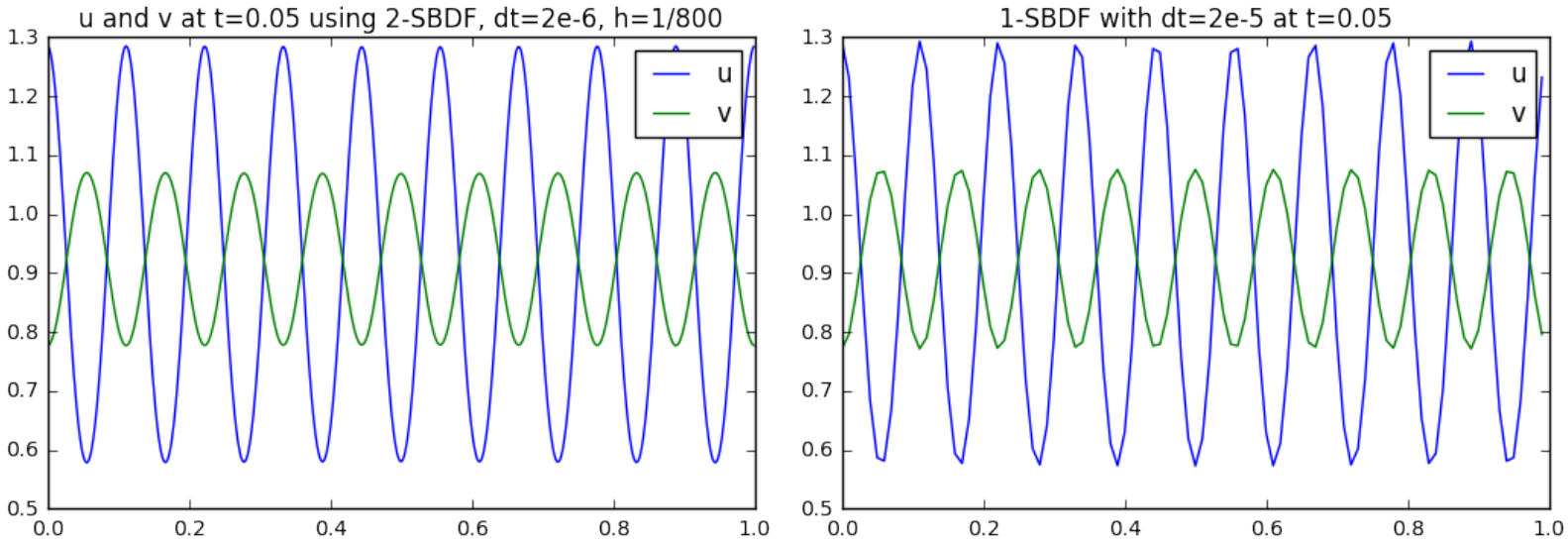
- Simple model for describing glycolysis.
- Reaction kinetics exhibit limit cycle oscillations.
- Consider the above model in 1 spatial dimension on $(0, 1)$ subject to periodic boundary conditions.

Example



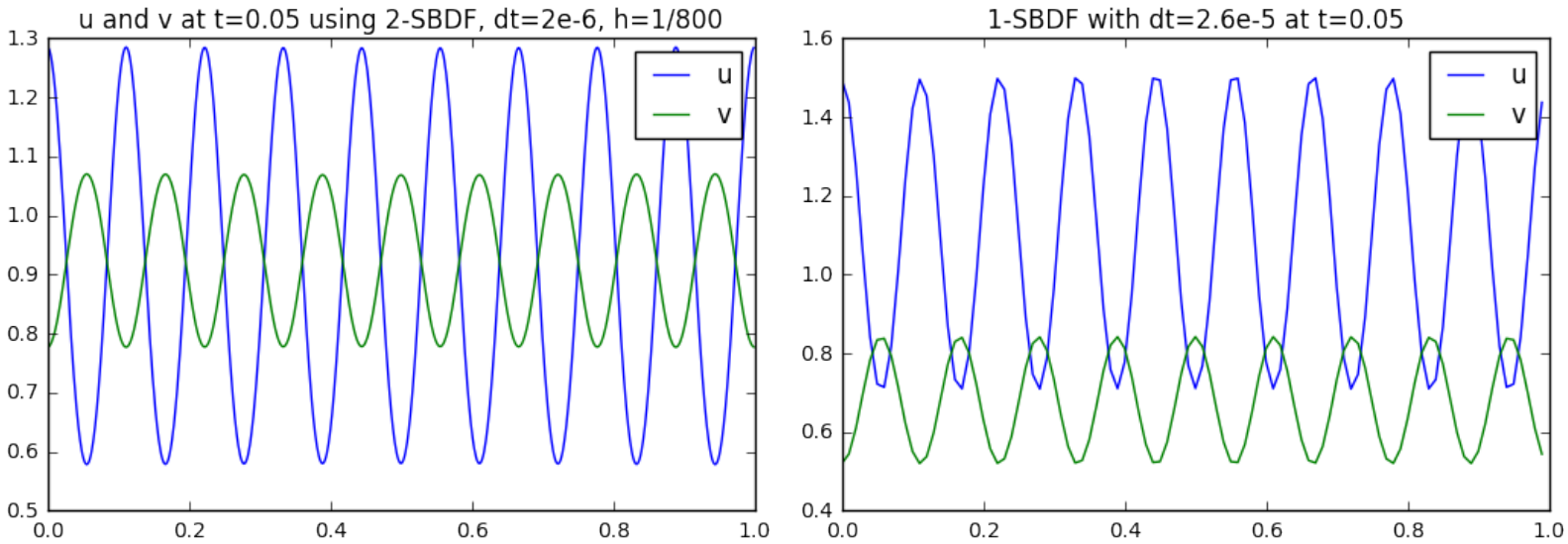
- Set $a = 0.126779, b = 0.792366, \gamma = 10^4$. This corresponds to $(k_1, k_4) = (0.6, -0.7)$
- Set initial conditions $u(x, 0), v(x, 0)$ as small perturbations away from the unique homogeneous fixed point.
- From theoretical analysis, we expect this parameter regime to exhibit damped oscillatory solutions.
- We know 2-SBDF is accurate so use a solution using 2-SBDF with $\Delta t = 2 \times 10^{-6}$, $h = 1/800$ as the "exact solution".

Example



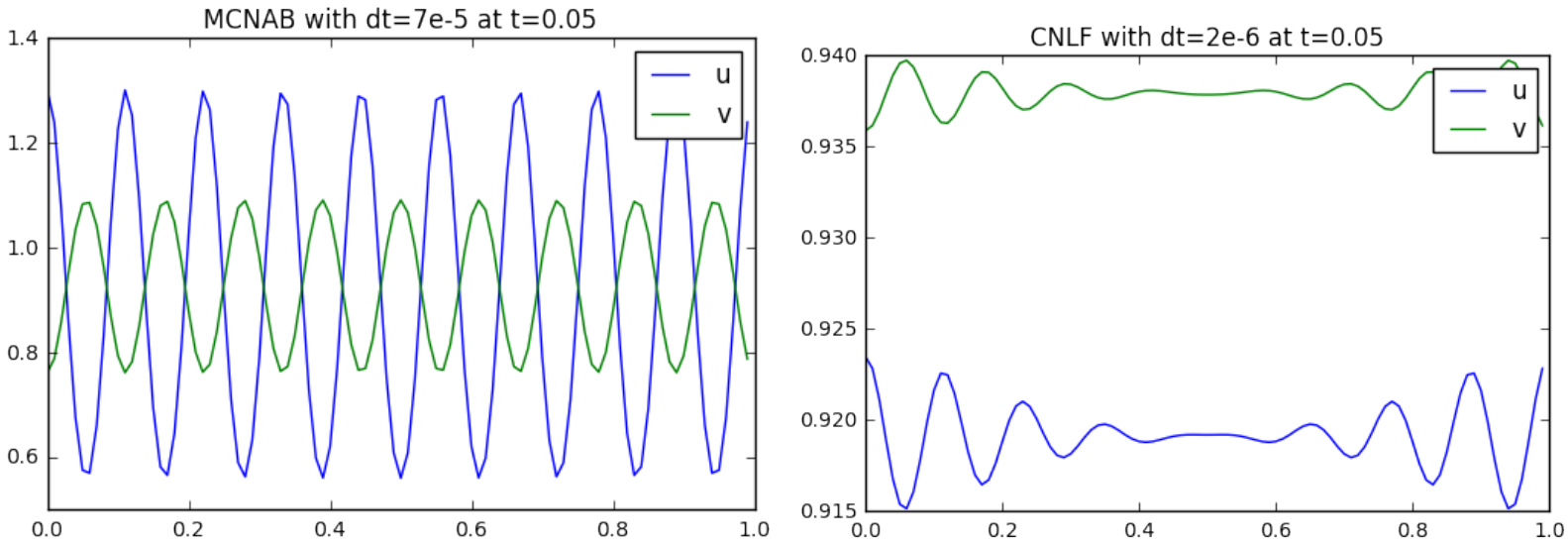
- Now solve using 1-SBDF with $h = 0.01$, $\Delta t = 2 \times 10^{-5}$. Even after increasing the time step by an order of magnitude, the solution looks accurate.

Accuracy



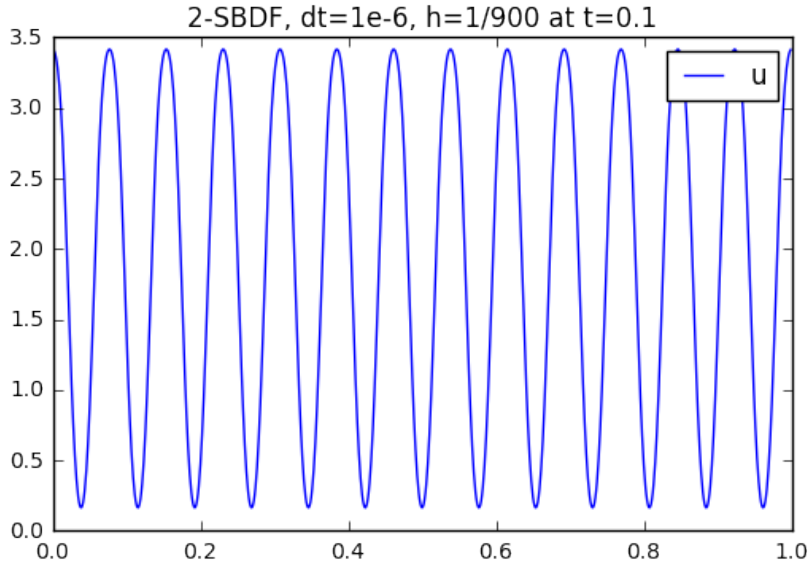
- However, if we just increase the time step to $\Delta t = 2.6 \times 10^{-5}$, the solution becomes very inaccurate.

Other schemes



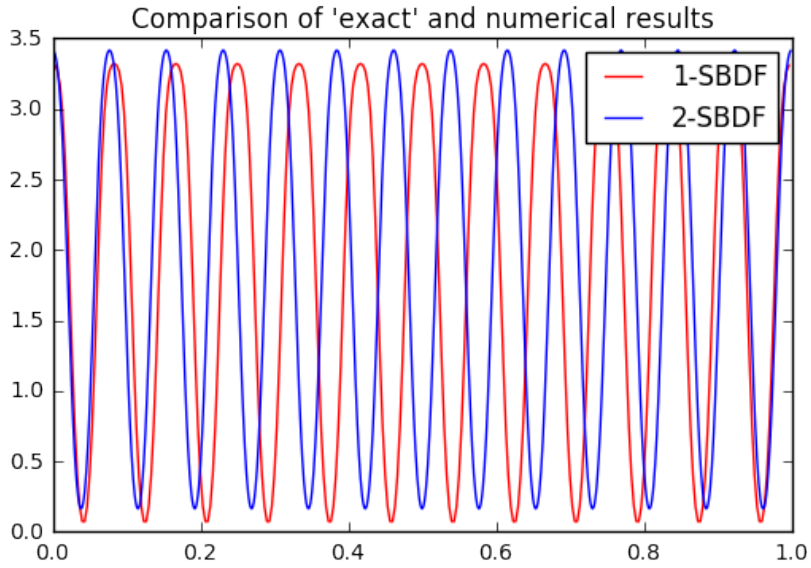
- MCNAB estimates the solution well for larger time steps than 1-SBDF.
- CNLF fails to approximate the result even for small time steps

Another example



- Previous example showed that 1-SBDF required smaller time steps than MCNAB and 2-SBDF.
- Now consider the 1-D Schnakenberg with constants $a = -0.887757, b = 2.774242$ instead.
- "Exact" solution calculated with 2-SBDF with $h = 1/900, \Delta t = 10^{-6}$.

Pitfalls of 1-SBDF



- A numerical solution with 1-SBDF produces patterns that look plausible, but have a different wave number than the exact solution.
- Decreasing the time step and mesh width produces similar results, which could lead one to believe that further refinement is not necessary.