Reaction-Diffusion with Alternate-Direction Implicit

High Performance Computing for Science and Engineering

CSElab
Computational Science & Engineering Laboratory
http://www.cse-lab.ethz.ch

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Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

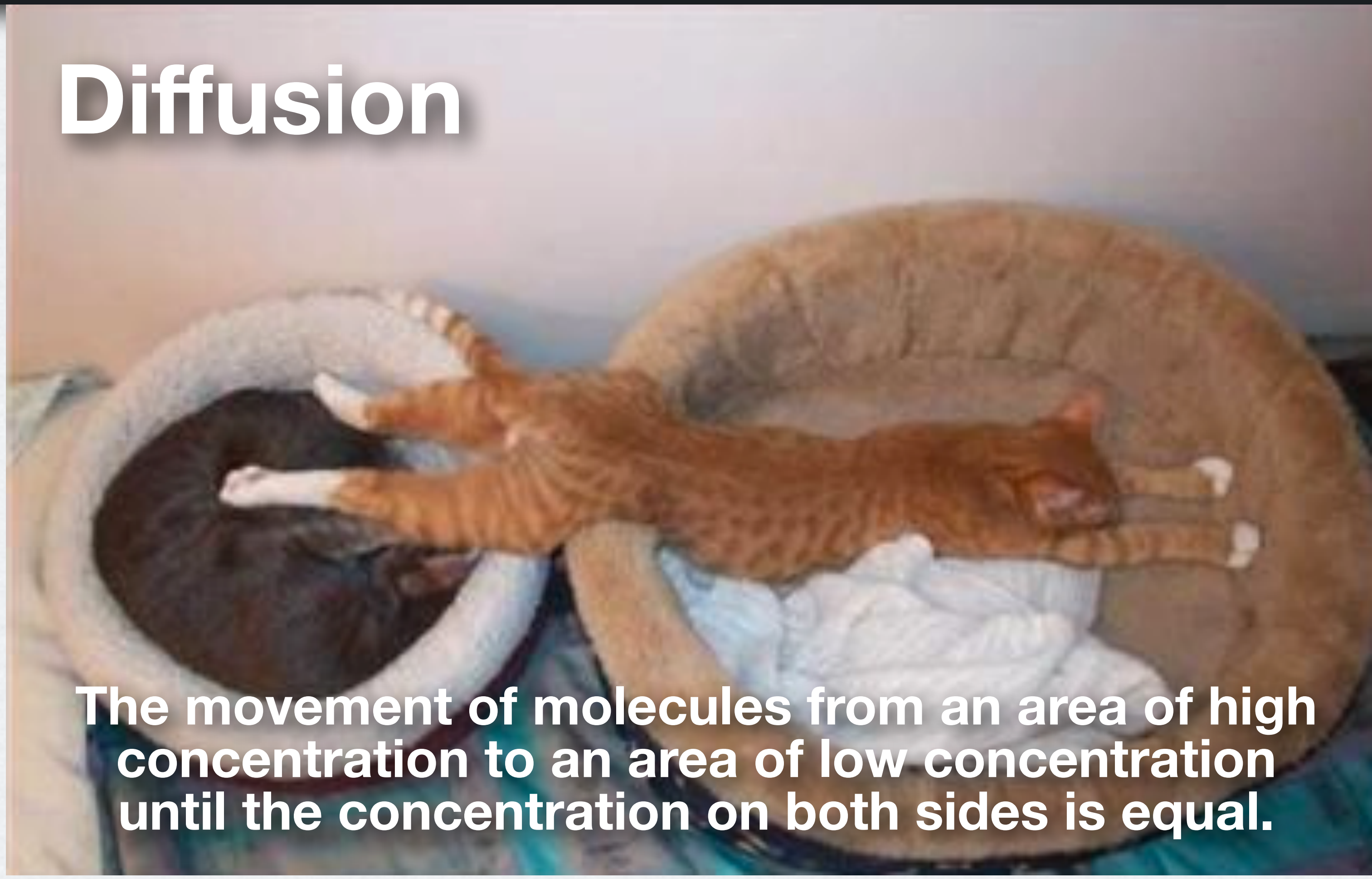
Diffusion

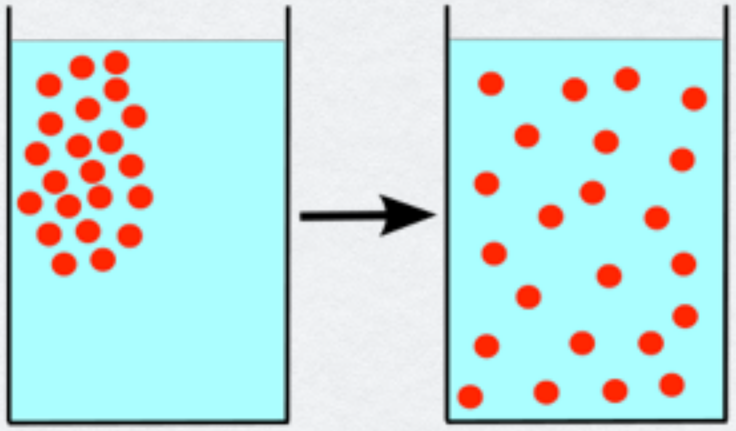
Diffusion

▸ describes spread of the quantity driven by its concentration gradient towards regions with lower density

Examples:

- distribution of heat in given region
- drop of ink in the glass of water
- teabag diffusion





Diffusion Equation

- Diffusion of quantity **ρ** (e.g. heat flow) can be described by diffusion equation of the form:

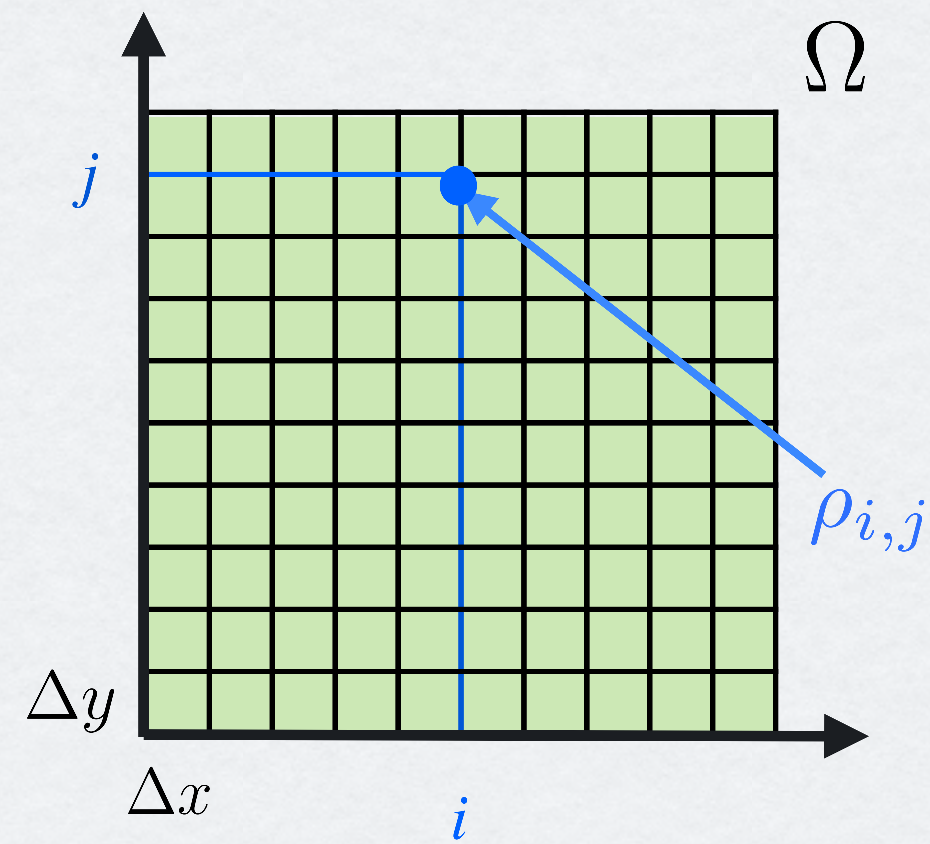
$$\frac{\partial \rho(\boldsymbol{r},t)}{\partial t} = D\nabla^2 \rho(\boldsymbol{r},t) \quad \text{in} \quad \Omega \qquad (1)$$

ρ(r,t) - measure for the amount of heat at position $r=(x,y)$ and time t

D - diffusion coefficient (constant here)

- Discretizing eq. (1) using forward Euler in time and central differences in space yields:

$$\frac{\rho_{i,j}^{(n+1)} - \rho_{i,j}^{(n)}}{\Delta t} = D\left(\frac{\rho_{i+1,j}^{(n)} - 2\rho_{i,j}^{(n)} + \rho_{i-1,j}^{(n)}}{\Delta x^2} + \frac{\rho_{i,j+1}^{(n)} - 2\rho_{i,j}^{(n)} + \rho_{i,j-1}^{(n)}}{\Delta y^2}\right)$$



- where *n* is the index of time step: $t_n = n \cdot \Delta t$
- i, j are indices of spatial discretization: $x_i = i \cdot \Delta x$, $y_j = j \cdot \Delta y$
- and $\rho_{i,j}^{n} = \rho(x_i, y_j, t_n)$

Reaction-Diffusion

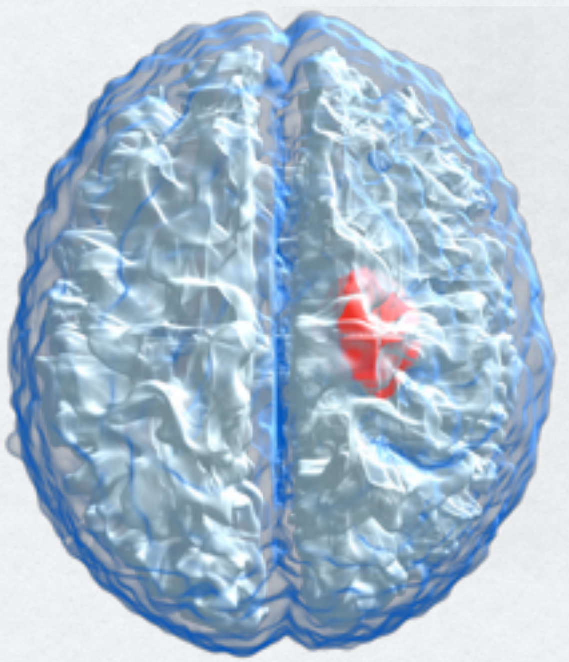
Reaction-Diffusion Processes

describe evolution of concentration of one or more substances whose

- state is modified by ***reactions***
- movement is governed by ***diffusion***

- **reaction = "cell proliferation"**

  e.g. brain cancer



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  e.g pattern formation

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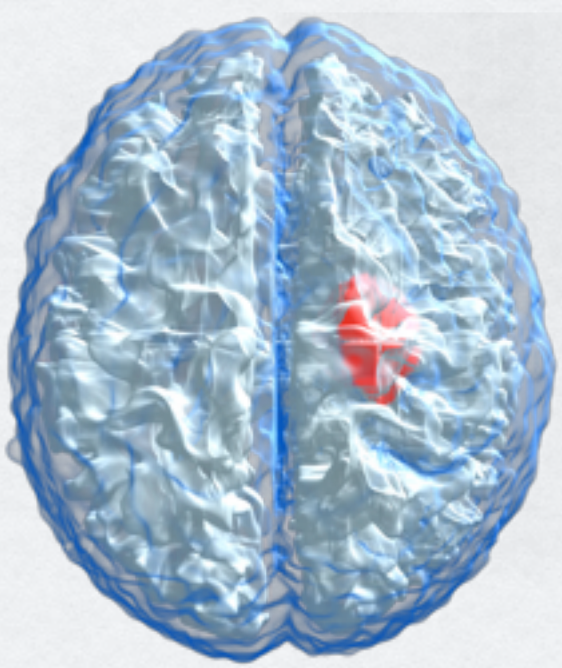

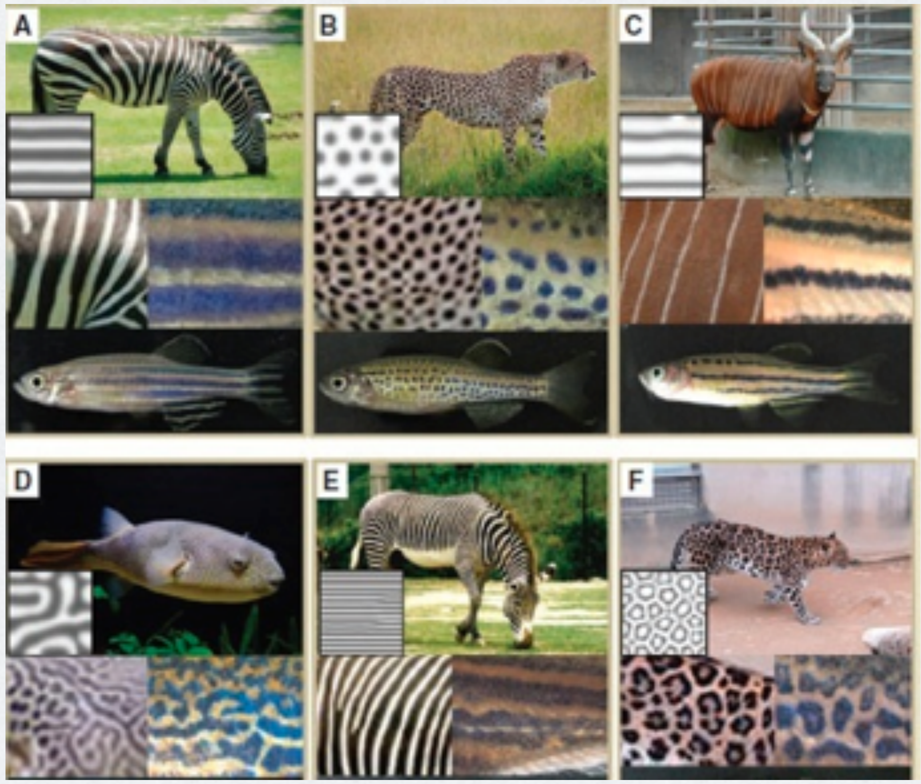

Figure: Watanabe M, Kondo S.
Pigment Cell Melanoma Res. 2012 Feb 7. doi: 10.1111/j.1755-148X.2012.00984.x.

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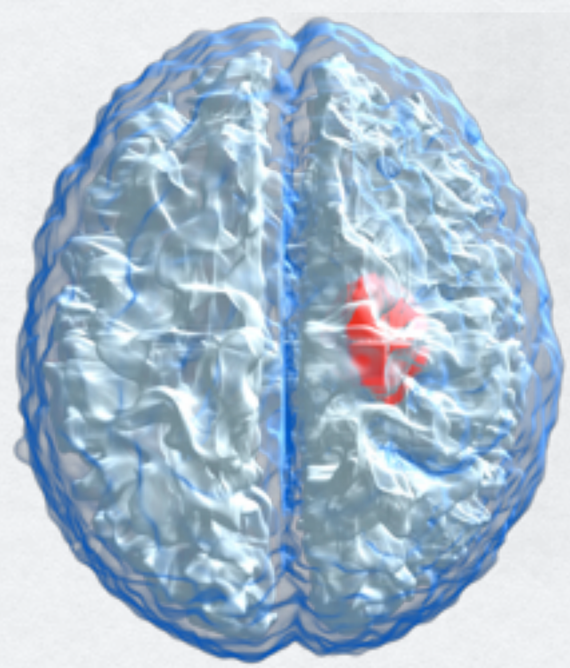
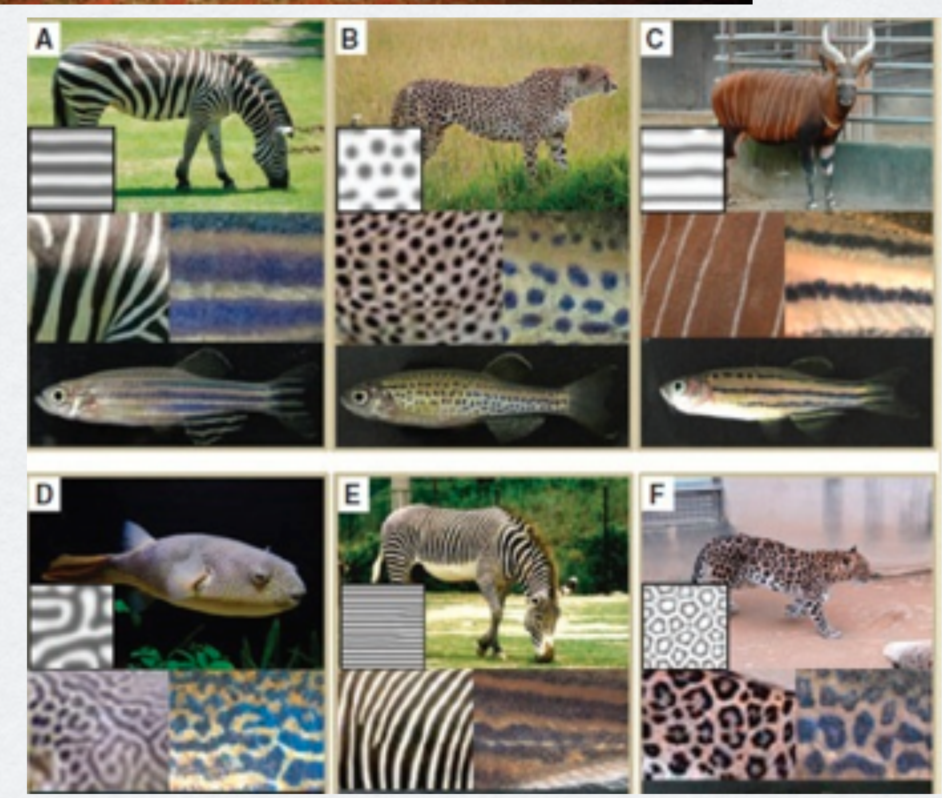
Examples

- **reaction = “chemical reaction”**
  e.g pattern formation
- **reaction = “interaction”**
  e.g. predator-prey model
- **reaction = “cell proliferation”**
  e.g. brain cancer





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Reaction-Diffusion Equation

Reaction-diffusion equation for M different species with respective

- concentrations u_i and
- diffusion terms D_i

$$\boxed{\frac{\partial u_i}{\partial t} = D_i \Delta u_i + f_i(\mathbf{u}),\ \forall i = 1 \cdots M.}$$

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Gray-Scott system

two species U & V reacting according:

$$\begin{aligned} U + 2V &\to 3V \\ V &\to P \end{aligned}$$

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corresponding dimensionless RD equations:

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_u \Delta u - uv^2 + F(1-u) \\ \frac{\partial v}{\partial t} &= D_v \Delta v + uv^2 - (F+k)v \end{aligned}$$

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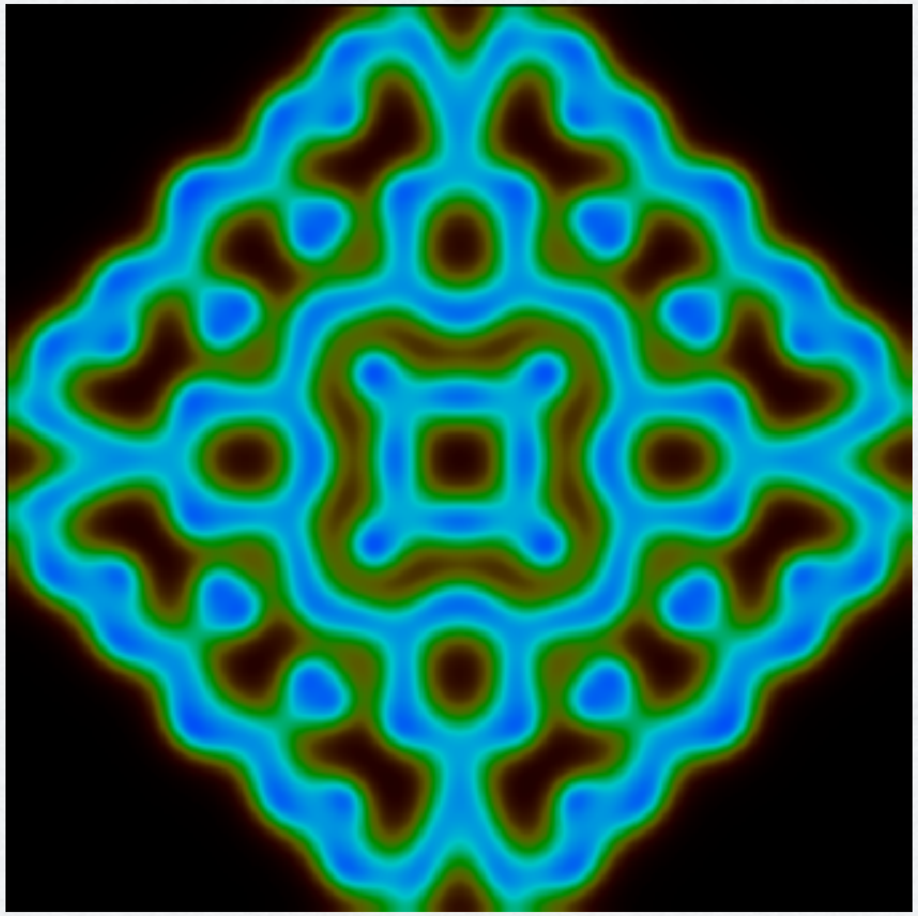

Gray-Scott
F=0.04, k = 0.06

Gray-Scott Pattern Formation

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Gray-Scott model result in pattern formation including:

- spots
- stripes
- mixed spot-stripes
- traveling waves
- labyrinth stripes
- chaos

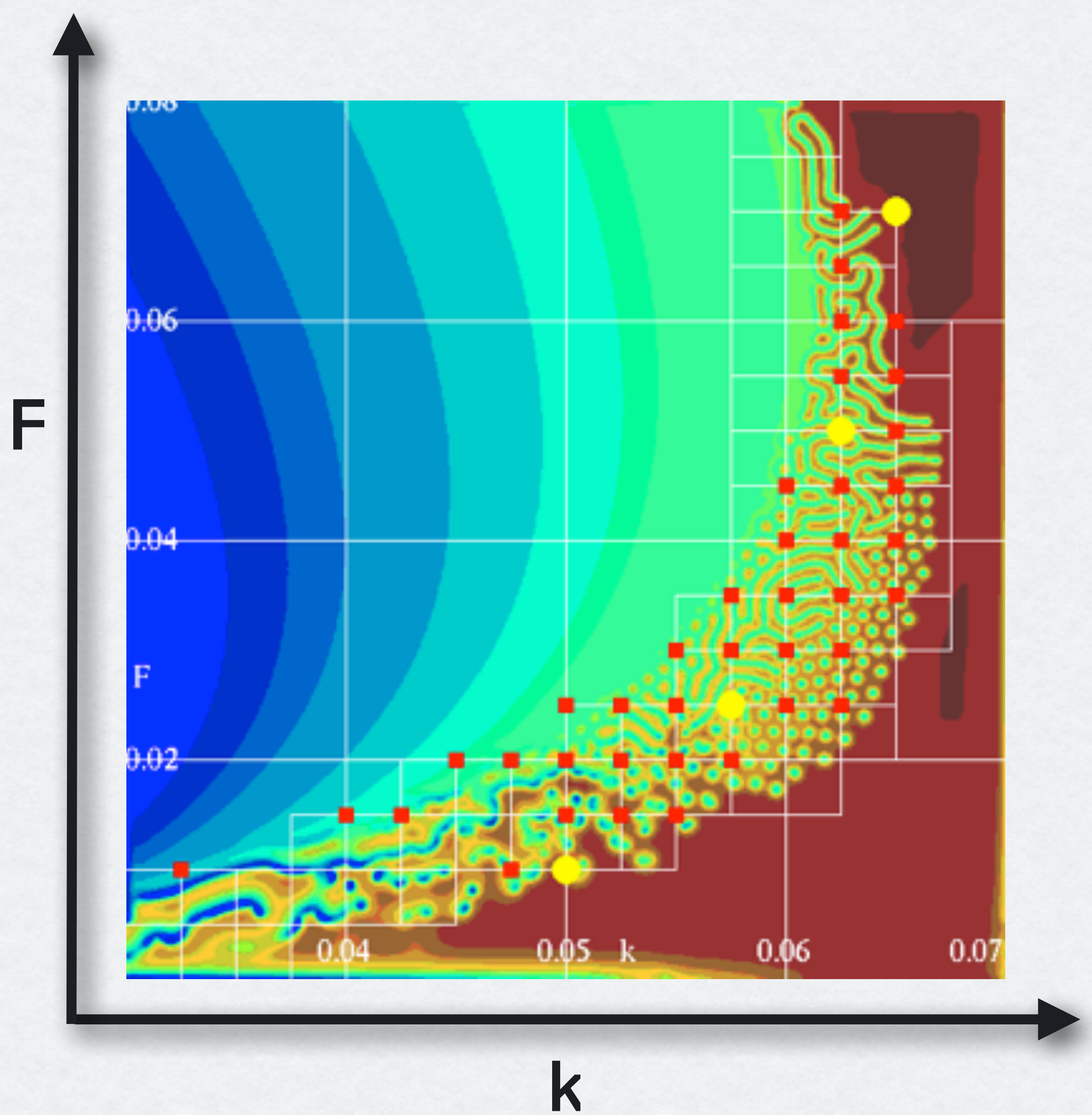
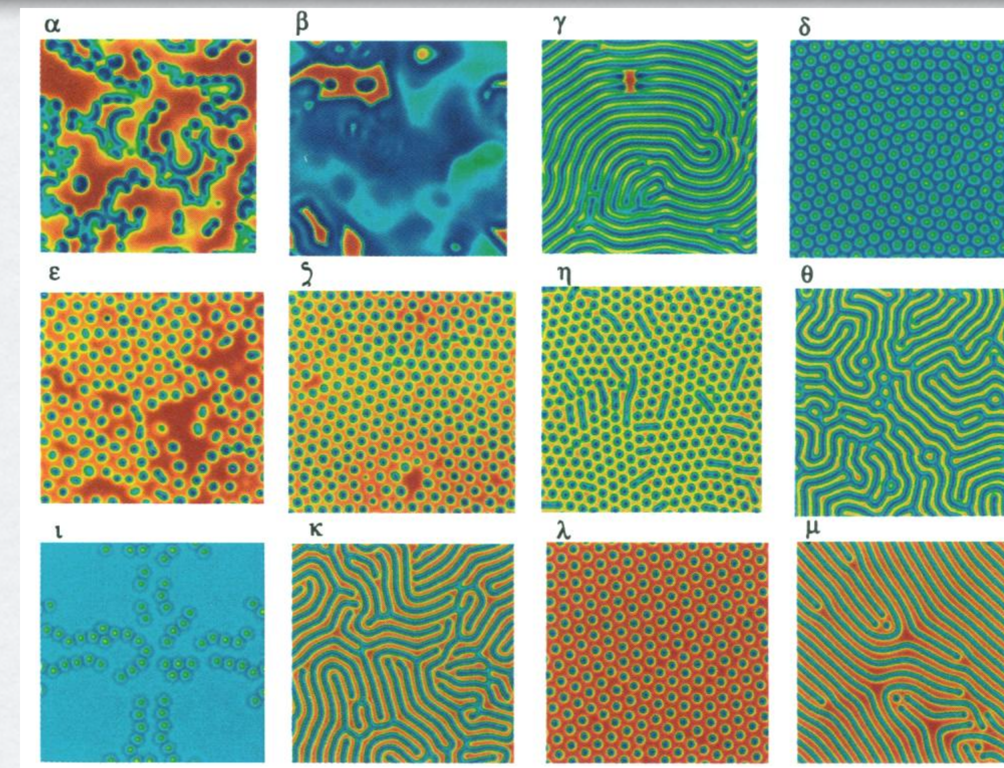
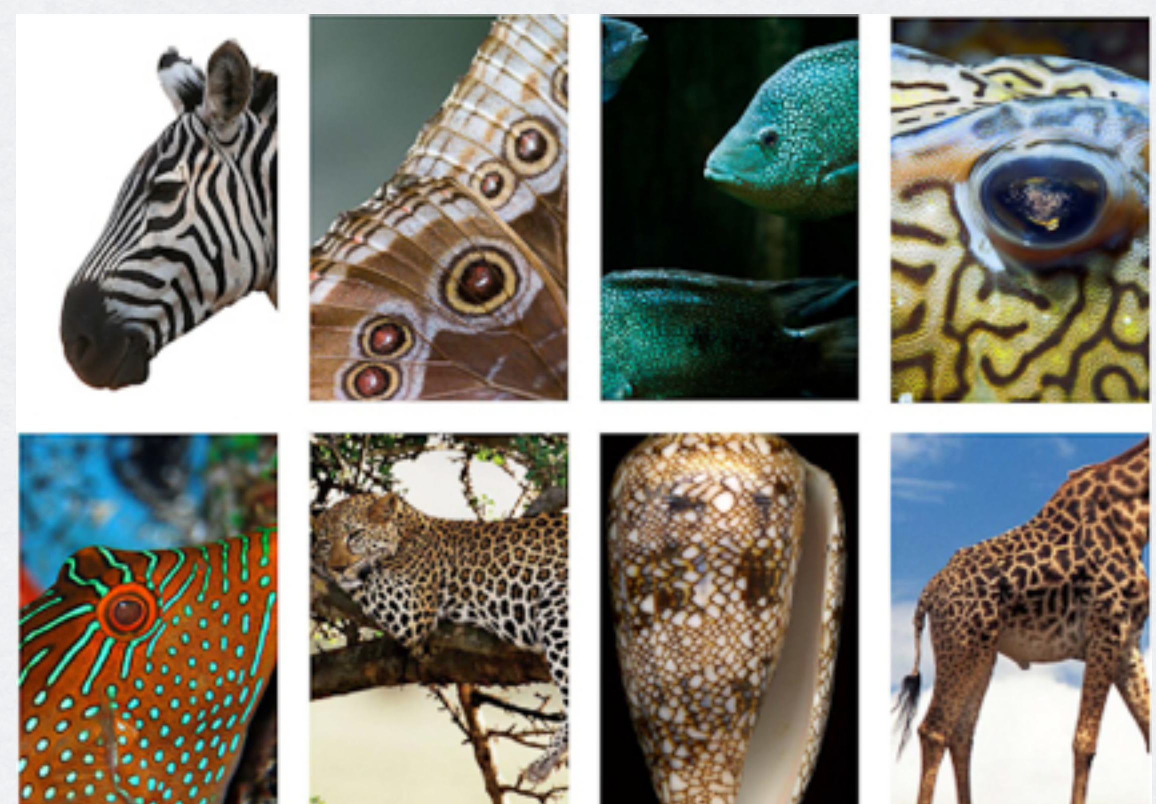


Figure source: http://www.aliensaint.com/uo/java/rd/



J.E. Pearson "Complex patterns in a simple system" arXiv preprint patt-sol/9304003



http://n-e-r-v-o-u-s.com/education/simulation/ethworkshop.php

Alternate Direction Implicit

Explicit Euler

- Forward Euler is very easy to implement, requires few computations and often has acceptable accuracy.

- The main drawback of FE is *instability* – thought the local errors are small, the divergence of the numerical solution from the exact one will exponentially grow over time.

- The condition on time-step size for *stability* is very strong:

$$\Delta t < \frac{\Delta x^2 \Delta y^2}{D\left(\Delta x^2 + \Delta y^2\right)}$$

- This means that for $\Delta x \simeq h, \Delta y \simeq h$ we get $\Delta t = \Theta(h^2)$

Implicit Euler

- To overcome the issue of instability implicit Euler can be used:

Note the difference compared to Explicit Euler

$$\frac{\rho_{i,j}^{(n+1)} - \rho_{i,j}^{(n)}}{\Delta t} = D\left(\frac{\rho_{i-1,j}^{(n+1)} - 2\rho_{i,j}^{(n+1)} + \rho_{i+1,j}^{(n+1)}}{\Delta x^2} + \frac{\rho_{i,j-1}^{(n+1)} - 2\rho_{i,j}^{(n+1)} + \rho_{i,j+1}^{(n+1)}}{\Delta y^2}\right)$$

- It is always stable
- The difficulty now is to evaluate one iteration.
- You have to solve a system of linear equations with sparse but not regular matrix (note that in 1D case the matrix is just tridiagonal)

Alternating Direction Implicit

- The idea of ADI is to split one iteration into two steps in order to separate the “implicitness” of X and Y dimensions

- Smart splitting gives you not only a stable and easy to evaluate method, but also the second order of accuracy in time

- The method is read like this:

$$\frac{\rho_{i,j}^{(n+1/2)} - \rho_{i,j}^{(n)}}{\Delta t/2} = D\left(\frac{\rho_{i-1,j}^{(n+1/2)} - 2\rho_{i,j}^{(n+1/2)} + \rho_{i+1,j}^{(n+1/2)}}{\Delta x^2} + \frac{\rho_{i,j-1}^{(n)} - 2\rho_{i,j}^{(n)} + \rho_{i,j+1}^{(n)}}{\Delta y^2}\right)$$

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Note the different time indices

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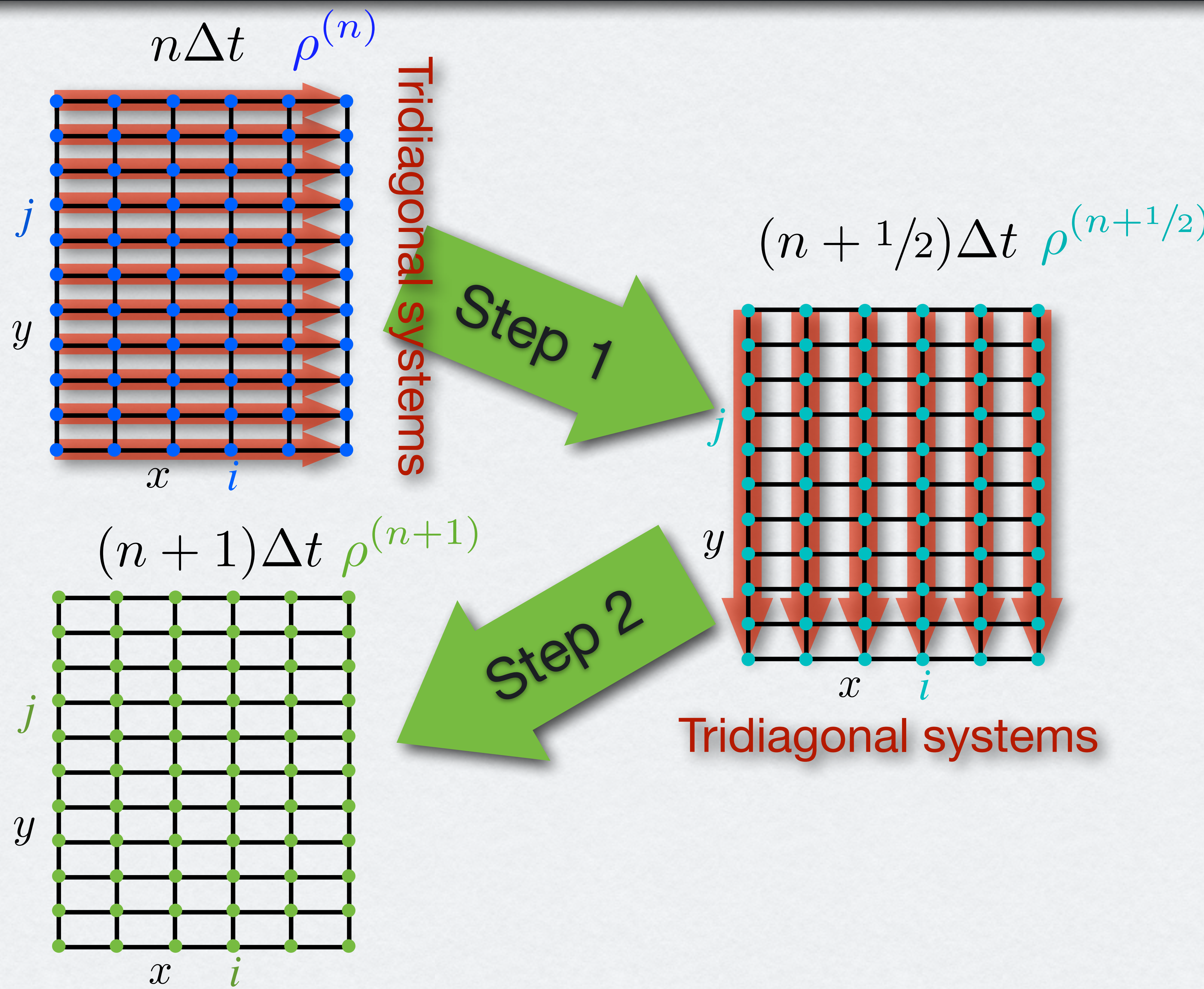
Tridiagonal systems

Alternating Direction Implicit



Tridiagonal system and Thomas algorithm

We look now into solving a linear system $A\mathbf{x} = \mathbf{v}$ with a tridiagonal matrix:

$$A = \begin{pmatrix} b_0 & c_0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ a_1 & b_1 & c_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & a_2 & b_2 & c_2 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & a_{n-2} & b_{n-2} & c_{n-2} \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_{n-1} & b_{n-1} \end{pmatrix}$$

We first eliminate the sub-diagonal elements a_i and obtain a system $A'\mathbf{x} = \mathbf{v}'$

$$A' = \begin{pmatrix} b'_0 & c_0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & b'_1 & c_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & b'_2 & c_2 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & b'_{n-2} & c_{n-2} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & b'_{n-1} \end{pmatrix}, v' = \begin{pmatrix} v'_0 \\ v'_1 \\ v'_2 \\ \vdots \\ v'_{n-2} \\ v'_{n-1} \end{pmatrix},$$

$$\boxed{\begin{aligned} b'_i &= b_i - c_{i-1}\frac{a_i}{b'_{i-1}}\,,\ i = 1..n-1 \\ v'_i &= v_i - v_{i-1}\frac{a_i}{b'_{i-1}}\,,\ i = 1..n-1 \end{aligned}}$$

Now we can easily solve the new system:

$$\boxed{\begin{aligned} x_{n-1} &= \frac{v'_{n-1}}{b'_{n-1}} \\ x_i &= \frac{1}{b'_i}\left(v'_i - c_i x_{i+1}\right),\ i = (n-2)\,..\,0 \end{aligned}}$$