Numerical Methods in Mechanics and Environmental Flows

OCT 20, 2017

S.K. OOI

Outline for Environmental Flows

Oct 13
- Introduction
- Delft3D Introduction and Assignment 1: Spin-up?

Oct 20
- Box models and solution methods
- Delft3D Assignment 2 - Boundary conditions; initial conditions

Oct 27
- Solution methods / Transport processes
- Delft3D Assignment 3 – stratification (wind-driven flows)

Nov 3
- Transport processes in flows (1)
- Delft3d Project

Nov 10
- Transport processes in flows (2)
- Delft3d assignment 4 – model extend (estuarine stratification as an example)

Nov 17
- Presentation of term assignment (5 groups)

Last Week

We tried to understand if there were any differences to solving mechanic problems and environmental flow problems.

- BY first looking at what are Environmental flows?
- Then looking through box Models as a conceptual framework
- Introduction to numerical models and the use of the mass-spring system equivalent

Some relevant questions…

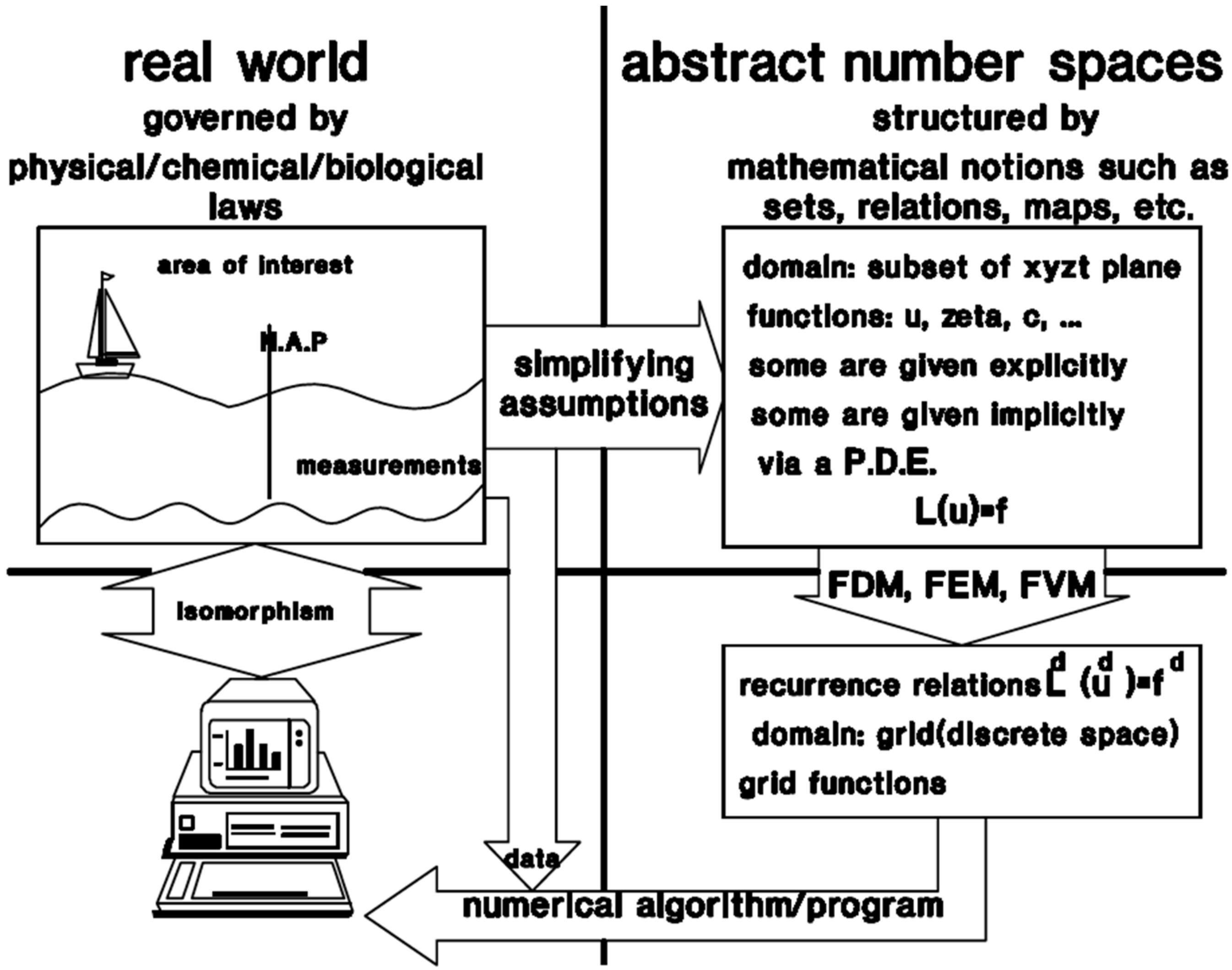
Given that we are only dealing with environmental surface flows and given what you have seen, what do you need to give a reasonably accurate value to a question e.g. what is ***the instantaneous and cumulative flux through the Singapore Straits over a year***

1.

2.

3.

Essentially:



A description of surface flows

Common description → conservation laws which are written as equations

What are three basic conservation laws or equations that can describe fluid flow?

A. [VERY BASIC]

B

C

Simplifying assumptions for surface flows?

What assumptions can we make for water to simplify our equations?

1.

2.

- Equation A

$$\frac{\partial(\rho)}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad \Rightarrow \quad \frac{\partial u_i}{\partial x_i} = 0$$

- Equation B

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} + b_i \quad \Rightarrow \quad \frac{du_i}{dt} = \frac{\mu}{\rho}\frac{\partial^2 u_i}{\partial x_j^2} - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{1}{\rho} b_i$$

Practical Approximations?

Density (Boussinesq approximation)

- Didn’t we remove it earlier? Yes but density can also be a function of salinity, temperature or sediment…

Turbulence (Time / Spatial Averaging)

- Averaging results in Equation B becoming:

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} + \frac{\partial \overline{(u_i' u_j')}}{\partial x_j} = \frac{\mu}{\rho_0} \frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{1}{\rho_0}\frac{\partial p}{\partial x_i} - f_i - \frac{\rho}{\rho_0} g \delta_{i=3}$$

- Assuming that one can approximate a so-called “eddy-viscosity” results in

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\nu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) - \frac{1}{\rho_0}\frac{\partial p}{\partial x_i} - f_i - \frac{\rho}{\rho_0} g \delta_{i=3}$$

$$\overline{u_i' u_j'} = -\nu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \frac{2}{3}\delta i_j k$$

A final approximation that is relevant to practical problems

Shallow Water Approximation:

- For this the flow is assumed to satisfy the following criteria:
  - Char. horizontal length >>> char. Vertical length
  - Char. Vertical velocity<< char. Horizontal velocity
- This results in the vertical (z) Equation B reducing to

$$\frac{\partial p}{\partial z} = -\frac{\rho}{\rho_0} g$$

  - Integrating the previous result: $p(x,y,z,t) = g\int_z^{\zeta} \rho \quad dz + p_a$
- The pressure terms in the remaining Equation B directions can then be written as:

$$-\frac{1}{\rho_0}\frac{\partial p}{\partial x_i} = -\frac{\rho g}{\rho_0}\frac{\partial \zeta}{\partial x_i} - \frac{g}{\rho_0}\int_z^{\zeta}\frac{\partial p}{\partial x_i}dz' - \frac{1}{\rho_0}\frac{\partial p_a}{\partial x_i}$$

**NOTE THIS APPROXIMATION IS USED FOR LOTS OF SURFACE FLOW CODES*

The issue is this…

Without simplifications the full Navier Stokes equations are 2nd order non-linear equations with 4 independent variables which means that they cannot be directly classified. But

- They do possess the properties inherent in the classification schemes and
- Some simplifications can be made for certain problems which allows us to classify these simplified flows

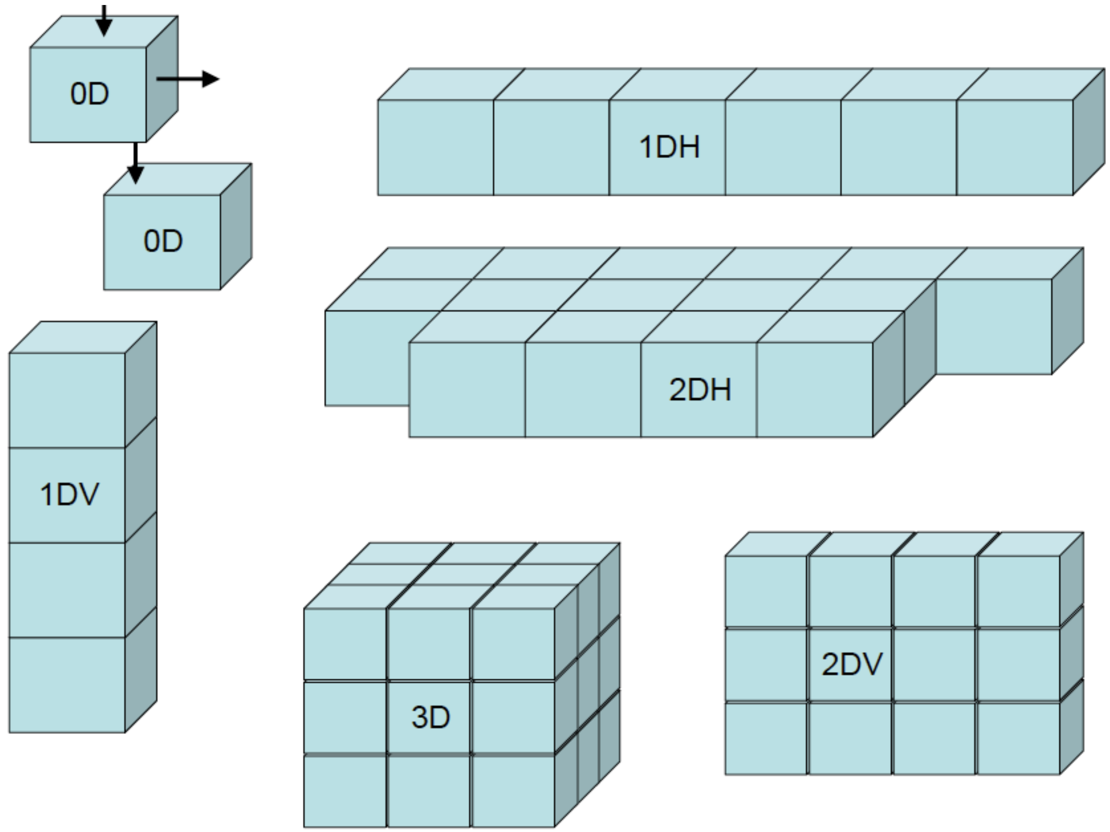
This leads to the fact that most flow problems cannot be solved analytically and an approximate numerical solution must be obtained.

How do we test and gauge if our solution is correct???

Types of Box Models

Remember the assumptions! They still apply.

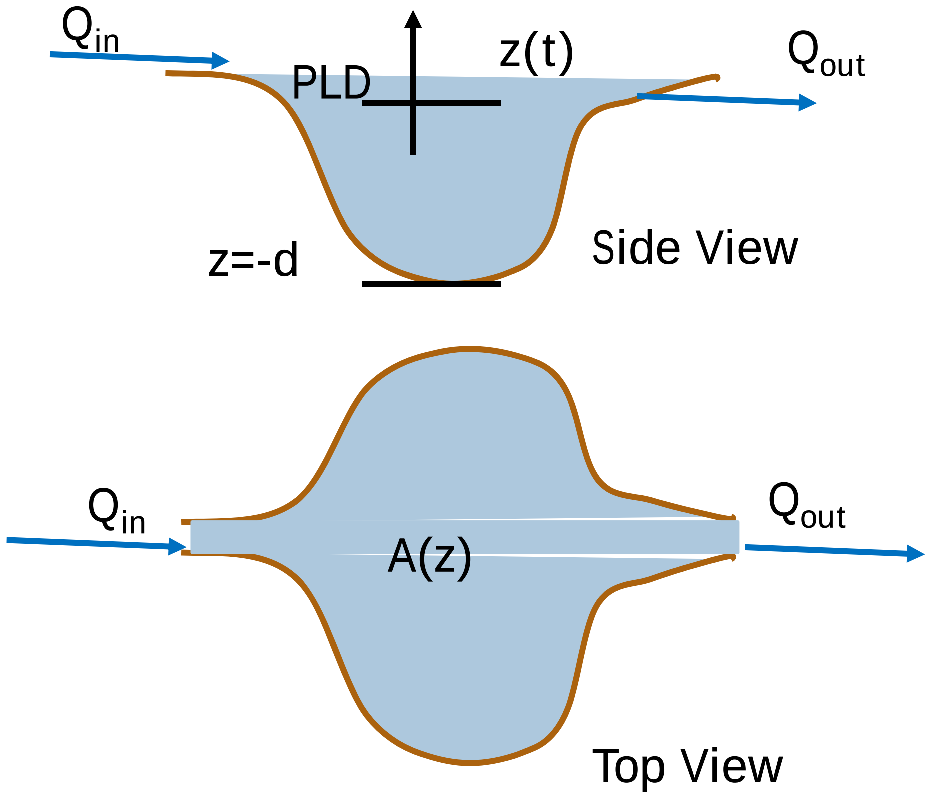
What would you use each system for?



Simple box model (2)

Reservoir / Lake:

What about this?



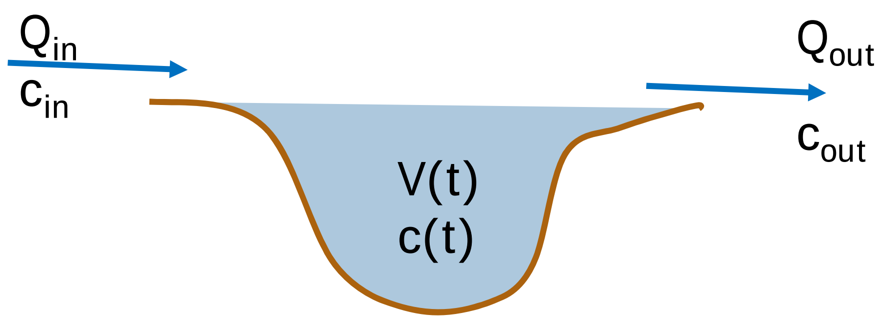
$$h(t) = d + z(t)$$

Solution method?

If you were given the following data, how would you obtain the solution by using a numerical model?

- $A = 1000\ m^2$
- $h(0) = 10\ m$
- $Q_{in} = 9\ m^3/s$
- $Q_{out} = 10\ m^3/s$ when $h > 0$; or 0 when $h \leq 0$

Extending (2) to pollutant transport - 1



What assumptions can or should you make ?

- 1.
- 2.

Numerical Solutions

ISSUES

Numerical Solution

What must we have to correctly solve the description (PDEs/ODEs) numerically if we have the data we need?

- A discretization method to approximate the PDEs with a system of algebraic equations
  - Typically applied so that the solution provides results at discrete locations in space and time.

- A solver to solve the system of algebraic equations
  - Direct solver
  - **Iterative solver**

How do we use iterative solution methods?

Choose a discretization method.

Built a matrix from the set of algebraic equations

Solve matrix from discretized equations

- Guess solution
- Improve by following a procedure until convergence criteria is satisfied.
- Typically split matrices into Lower, Upper, Diagonals

Some methods:

- Basic: Jacobi, Gauss-Seidel
- Over-relaxation: SOR, SLOR, Red-black point relaxation
- Other Methods: Stone’s, ADI, Multigrid

Errors in Numerical Solutions

Systematic Errors to be aware of

- Modeling Errors
  - Assumptions made in deriving equations
    - Incompressible, turbulence, shallow water etc.
  - Simplification of geometry; boundary conditions etc.
    - Unfortunately not known a priori, can only be known after comparing to data!
- Discretization Errors
    - Discussed earlier
    - Be AWARE for a particular grid, methods of the same order may produce differences in solution up to an order of magnitude
- Iteration Errors
  - Easiest to control, why?
  - Normall we when the difference between successive iterations are less than a pre-selected value (typically normalized)

Sometimes these errors can cancel each other

Components for Numerical Solution (1)

Mathematical Model (The Box Model)

- Incompressible? Inviscid? 1D? 2D? 2.5D? 3D?

Discretization method

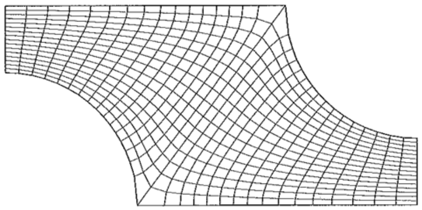
- Finite Element, Finite Volume, Finite Difference, etc.

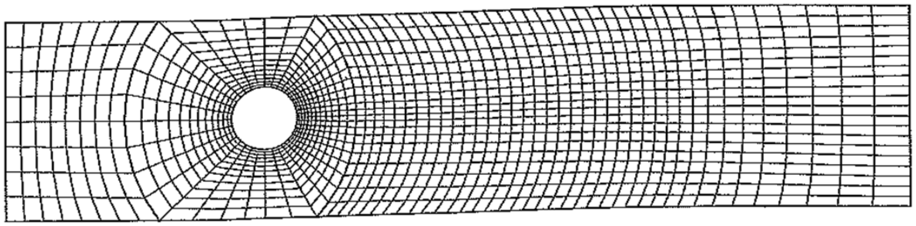
Coordinate systems

Components for Numerical Solution (2)

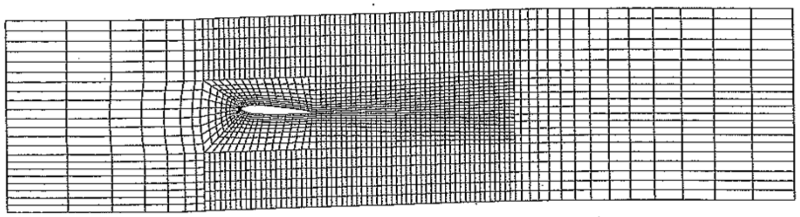
Types of numerical grid

- 1

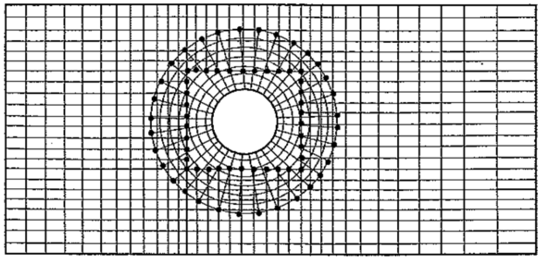




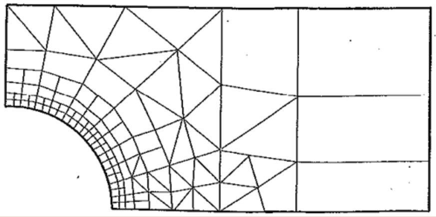
- 2



- 3



- 4



Components for Numerical Solution (3)

Finite approximations

- Approximations for derivatives
- Approximations for surface/vol. integrals
- Shape and weighting functions

Solution method (Solvers)

- Unsteady: time marching
- Steady: typically pseudo-time marching.
- Both typically use iterative techniques due to non-linearity

Convergence Criteria for Iterative method!

Important concepts that arise due to the use of Numerical Methods

Convergence

Consistency

Stability

Conservation

Boundedness

Realizability

Similar concept

Important concepts of Numerical Solution Methods (1)

Convergence

- Discretized solution $\longrightarrow$ exact solution of the differential equation as the grid spacing $\longrightarrow$ 0.
- Lax equivalence theorem is used for linear initial value problems
- However for real problems, we usually do a grid-independent study

Consistency

- Truncation error $\longrightarrow$ 0 as the time step / grid spacing $\longrightarrow$ 0
- Even if consistent, the solution may not become exact when step sizes are small. For this to occur the solution must be stable.

Stability

- The scheme is considered stable when errors from the solution process are not magnified in the solution process
- Mostly investigated with linear problems and constant coefficients without boundary conditions using von Neumann method
- Typically most schemes require some restrictions on time step or grid size (CFL criteria)

Important concepts of of Numerical Solution Methods (2)

Conservation

- Equations are conservation laws!
- Schemes should respect these laws.
- Becomes a constraint on the solution.
- Typically guaranteed for FV but not for other methods.

Boundedness

- Solutions should lie within proper bounds.

Realizability

- Not strictly a numerical issue
- Physical model we use should be physically realistic as well

Discretization Method

Various methods exist to discretize the equations

- Finite Difference
- Finite Volume
- Finite Element (similar to FV in many ways; typically use a triangular element in 2D
- And others:
  - Spectral methods
  - Boundary element
  - Vorticity-based
  - Lattice Boltzmann
  - And many more

Finite Element Method

More well known in structural analysis

- Developed for fluid flow solution in 1970s
- Similar in approach to Finite Volume but uses weights as multiplier to equations. Results in non-linear algebraic equations

Advantages

- Accurate for coarse grids
- Works well for viscous free surface problems

Disadvantages

- Slow for large problems
- Weak for solving turbulent flows

Finite Difference Overview

Oldest method

- Advantages: Easy to implement
- Disadvantages: Restricted to structured grids, doesn't conserve mass without special treatment

Methodology

- Requires a structured mesh (i,j,k)
- Discretize domain of interest into grid points
- Discretize equations –obtain derivatives from Taylor series expansions
- Each grid point has an algebraic equation that must be solved
- Solve resulting linear algebraic equations

Finite Volume Overview

Advantages

- Mass, momentum and energy are conserved in the formulation
- Well developed iterative solvers exist

Disadvantages

- False diffusion depending on numerical scheme

Methodology:

- Solve integral equations (not differential)
- Divide domain into Control Volumes, assign computational node to the centroid of the Control Volume
- Interpolate to obtain values at surfaces (f of node values)
- Approximate surface and volume integrals
- Each grid point has an algebraic equation but with neighboring values as well
- Solve a set of Linear Algebraic Equations

Finite Differences [FD] (1) - Space

Most FD schemes are based on Taylor series expansions

$$\phi(x) = \phi(x_i) + (x - x_i)\frac{d\phi}{dx}_i + \frac{(x-x_i)^2}{2!}\left(\frac{d^2\phi}{dx^2}\right)_i + \frac{(x-x_i)^3}{3!}\left(\frac{d^3\phi}{dx^3}\right)_i + \ldots$$

Methods to approximate the first derivative at point i from Taylor expansions

- Forward difference, $x=x_{i+1}$

$$\frac{d\phi}{dx}_i = \frac{\phi(x)-\phi(x_i)}{(x-x_i)} - \frac{(x-x_i)}{2!}\left(\frac{d^2\phi}{dx^2}\right)_i - \frac{(x-x_i)^2}{3!}\left(\frac{d^3\phi}{dx^3}\right)_i + h.o.t$$

- Backward difference, $x=x_{i-1}$

- Central difference (Homework?)

Finite Differences (2) - Space

Order of accuracy

- classified based on the leading error term
  - FDS?
  - BDS?
- What is it useful for?
- What doesn't it say?

Space differencing schemes for any order?

- Fit a polynomial and differentiate it
- Polynomial Fitting

Finite Differences - Temporal (1)

Unsteady flows can be considered initial value problems

- Illustration: $$\frac{d\phi(t)}{dt} = f(t,\phi(t)); \qquad \phi(t_0) = \phi_0$$
- How to find a solution for a short time after initial time?

$$\phi_i^{n+1} - \phi_{i-1}^{n} = \int_n^{n+1} f(t,\phi(t))dt$$

- Evaluate integral by numerical quadrature
  - Explicit $$\phi_i^{n+1} = \phi_{i-1}^{n} + f(t_n,\phi^n)\Delta t$$
  - Implicit $$\phi_i^{n+1} = \phi_{i-1}^{n} + f(t_{n+1},\phi^{n+1})\Delta t$$
  - Trapezoidal $$\phi_i^{n+1} = \phi_{i-1}^{n} + \frac{1}{2}\left[f(t_n,\phi^n) + f(t_{n+1},\phi^{n+1})\right]\Delta t$$
  - Mid-Point (Leap-frog) $$\phi_i^{n+1} = \phi_{i-1}^{n} + f(t_{n+\frac{1}{2}},\phi^{n+\frac{1}{2}})\Delta t$$

Finite Differences – Temporal (2)

Some general comments about unsteady schemes

- Order of accuracy
  - Euler schemes are 1st order; the other two schemes are 2nd order
- When time steps are increased
  - Explicit Euler is stable
  - Implicit Euler is stable
  - Trapezoid is unconditionally stable but oscillates; may be unstable for non-linear equations.
- Explicit methods are easy to program, use little memory and computation time.
- Implicit methods require iterative solution methods, use more memory and time per step, generally more stable than explicit schemes as time steps increase.

Finite Differences – Temporal (3)

Other methods to try and combine the best of both worlds

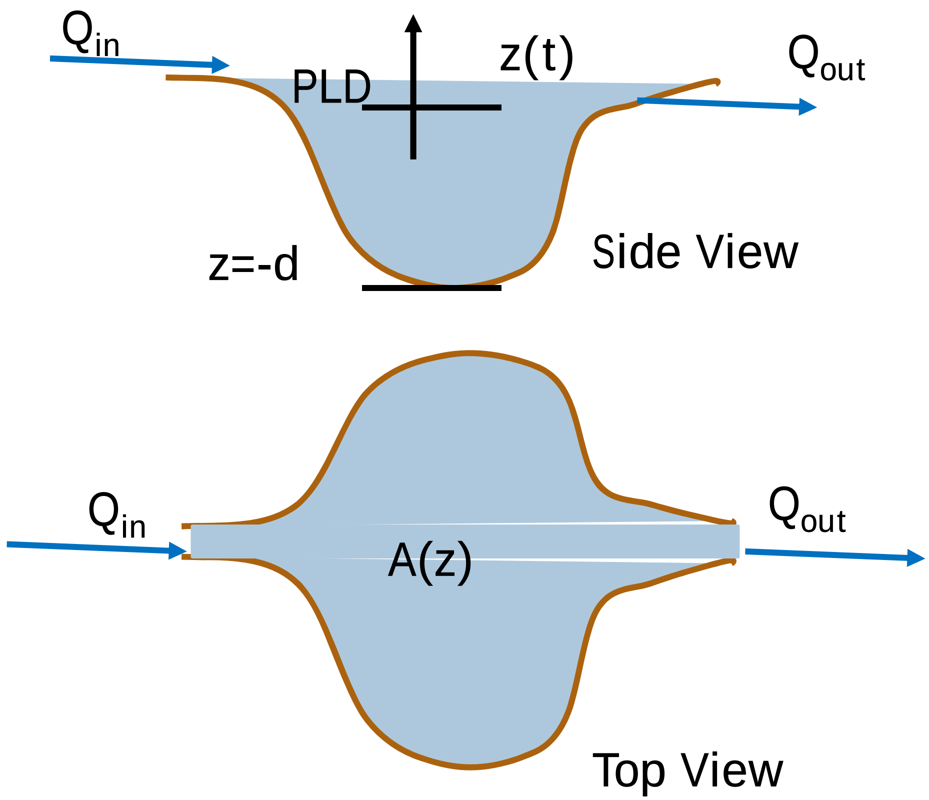
- 2^{nd} Order or Lower: Predictor-corrector
  - E.g. Predict using explicit Euler, correct with trapezoid
- > 2^{nd} Order
  - Multipoint: Adams Family
    - Adams-Bashforth, Adams-Moulton
  - Runge-Kutta

Can we solve the lake problem now?

Simple reservoir - Example 1

Reservoir / Lake:

What about this?



$h(t) = d + z(t)$

Solution method?

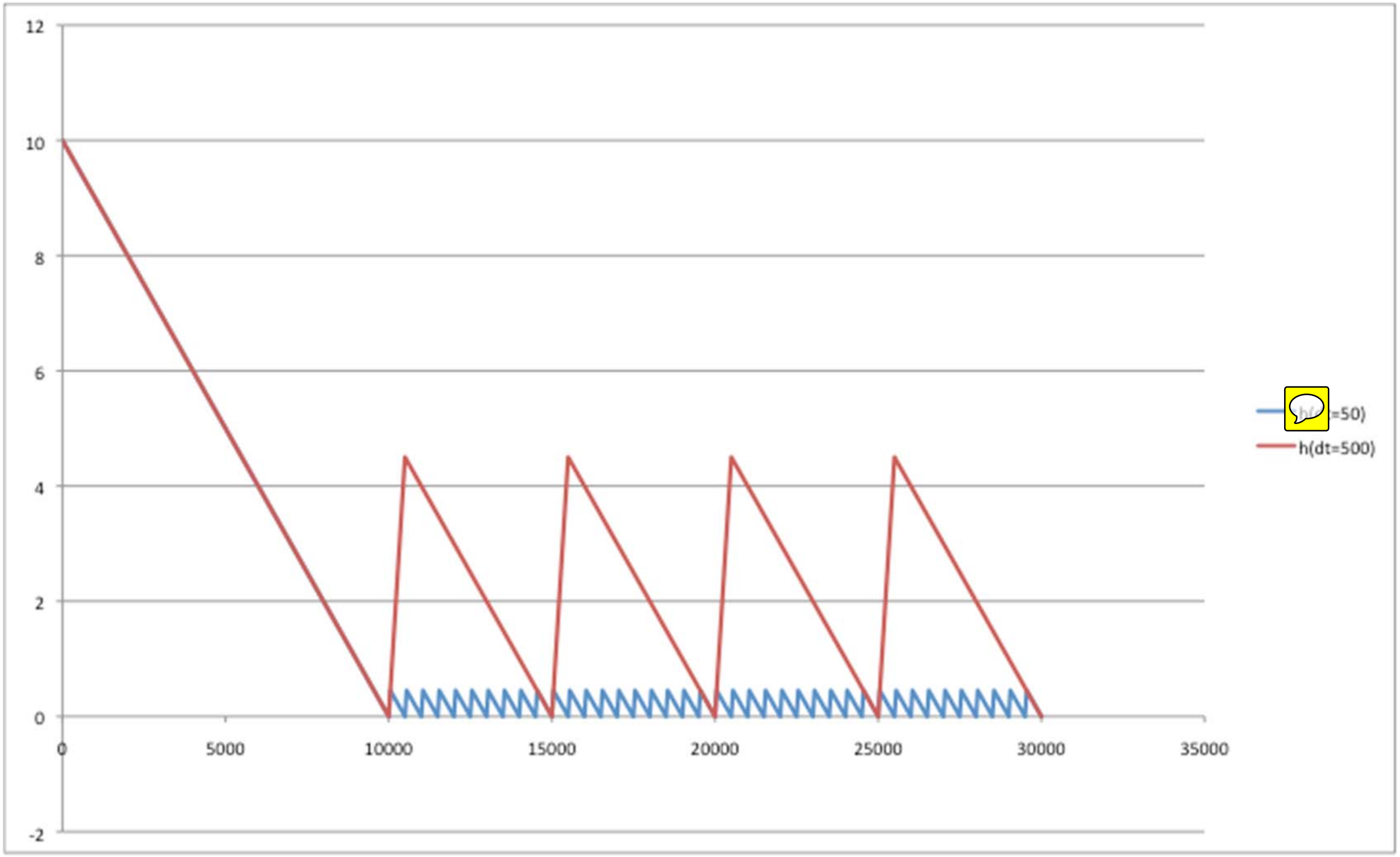
If you were given the following data, how would you obtain the solution by using a numerical model?

- $A = 1000\ m^2$
- $h(0) = 10\ m$
- $Q_{in} = 9\ m^3/s$
- $Q_{out} = 10\ m^3/s$ when $h > 0$; or 0 when $h \leq 0$

- What if you chose $h_{n+1} = h_n + \frac{\Delta t}{A}(Q_{in} - Q_{out})$

The result…

Is this a good solution?



Can we solve it differently?

With numerical tricks this can be disguised e.g.: “Patankar trick” :

$$A\frac{dh}{dt} = Q_{input} - Q_{output} \text{or } h_{n+1} = h_n + \Delta t\frac{Q_{input}}{A} - \Delta t\left(\frac{h_{n+1}}{h_n}\right)\frac{Q_{output}}{A}$$

$$\rightarrow h_{n+1} = \frac{Ah_n^2 + \Delta t h_n Q_{input}}{Ah_n + \Delta t Q_{output}}$$

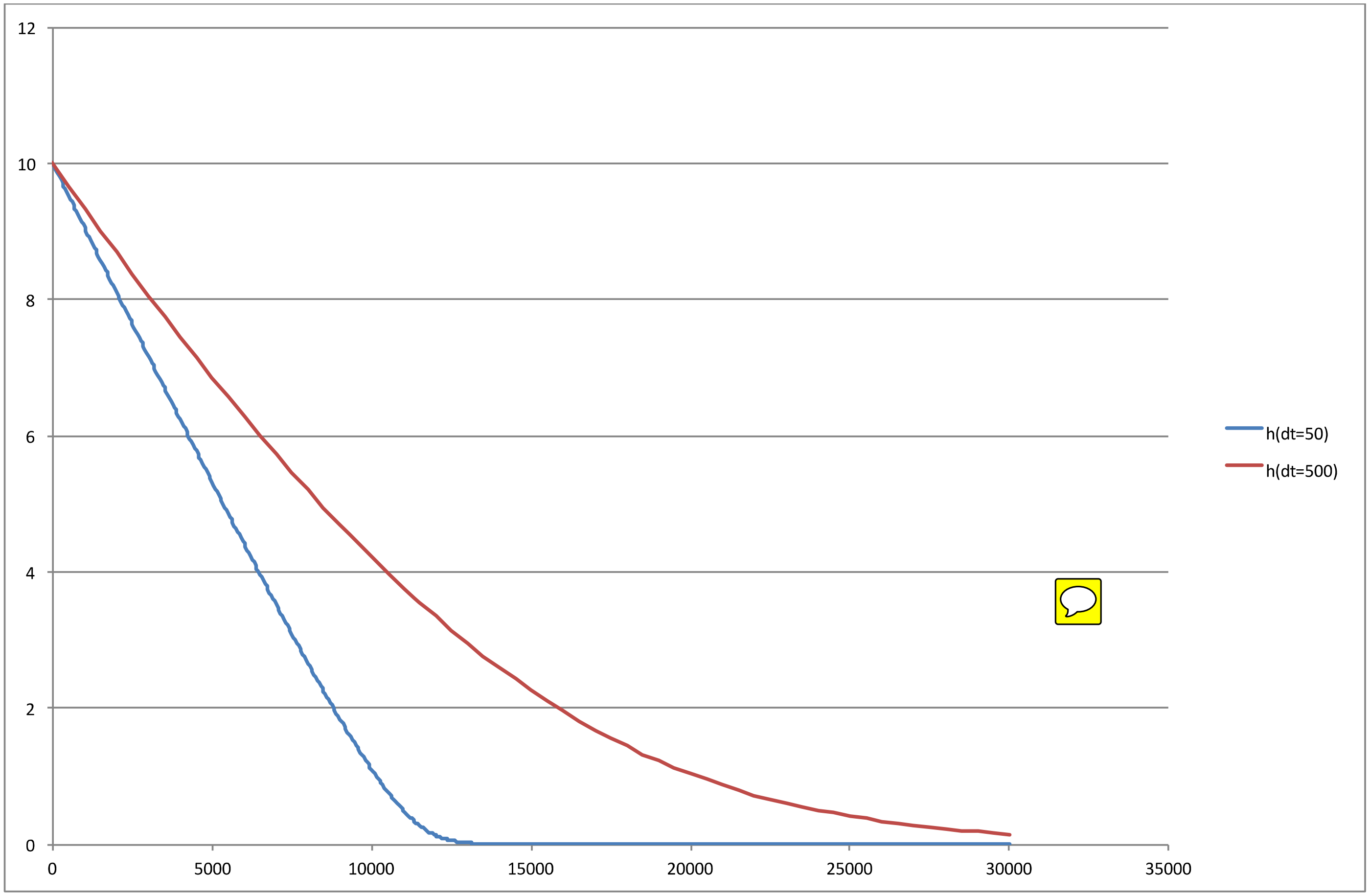
“Patankar trick 2” :

$$A\frac{dh}{dt} = Q_{input} - Q_{output} \text{or } h_{n+1} = h_k + \Delta t\left(\frac{h_{n+1}}{h_n}\right)\frac{Q_{input} - Q_{output}}{A}$$

$$\rightarrow h_{n+1} = \frac{Ah_n^2}{Ah_n - \Delta t\left(Q_{input} - Q_{output}\right)}$$

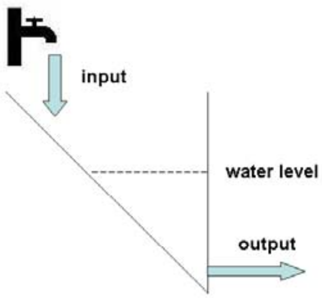
Result from a numerical trick…

Or do you prefer this?



Simple Reservoir – Example 2

Example



$$\frac{dV(h(t))}{dt} = Q_{input} - Q_{output}(h(t))$$

$$h(0)=0.5\ m$$

$$V(h) = 2\times\frac{1}{2}h^2,\ Q_{input} = 0.05,\ Q_{output}(h) = 0.01\sqrt{2g\max(0, h-1.0)},\ g = 9.81\ m^2/s$$

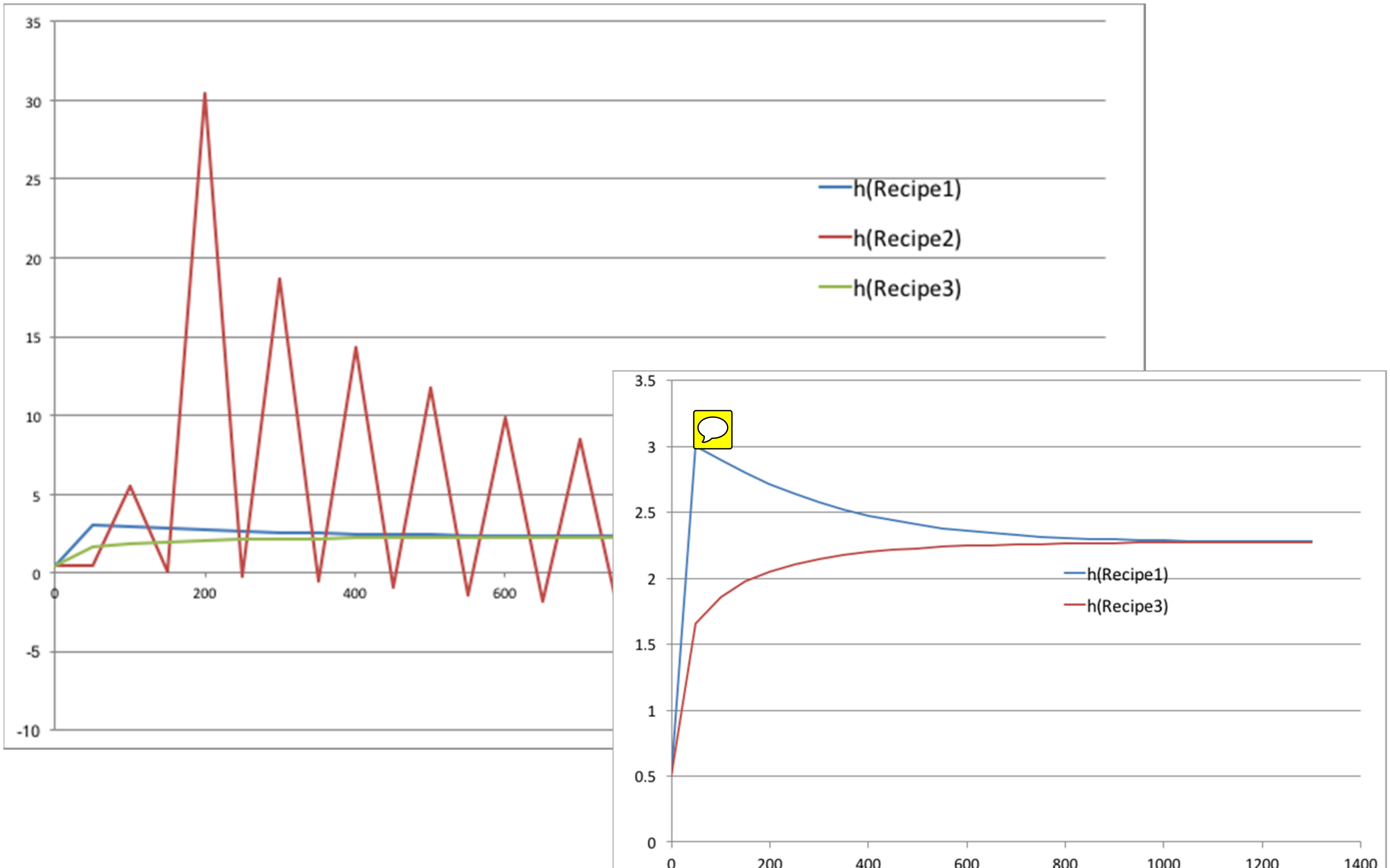
Recipe 1:
$$h_{n+1} = h_n + \Delta t\left(\frac{0.05 - 0.01\sqrt{2g\max(0, h_n - 1.0)}}{2h_n}\right)$$

:

Recipe 2:
$$h_{n+1} = h_{n-1} + 2\Delta t\left(\frac{0.05 - 0.01\sqrt{2g\max(0, h_n - 1.0)}}{2h_n}\right)$$

Recipe 3:
$$h_{n+1} = \sqrt{(h_n)^2 + \Delta t\left(0.05 - 0.01\sqrt{2g\max(0, h_n - 1.0)}\right)}$$

Solutions from the different recipes



Take home from this part

Two different examples with different reasons for the results you have seen

- Example 1: Actual reason for the fluctuations was due to the problem being ill-posed. But that can be solved through a numerical trick (known as the Patankar trick)

- Example 2: The fluctuations are due to the choice of the numerical schemes

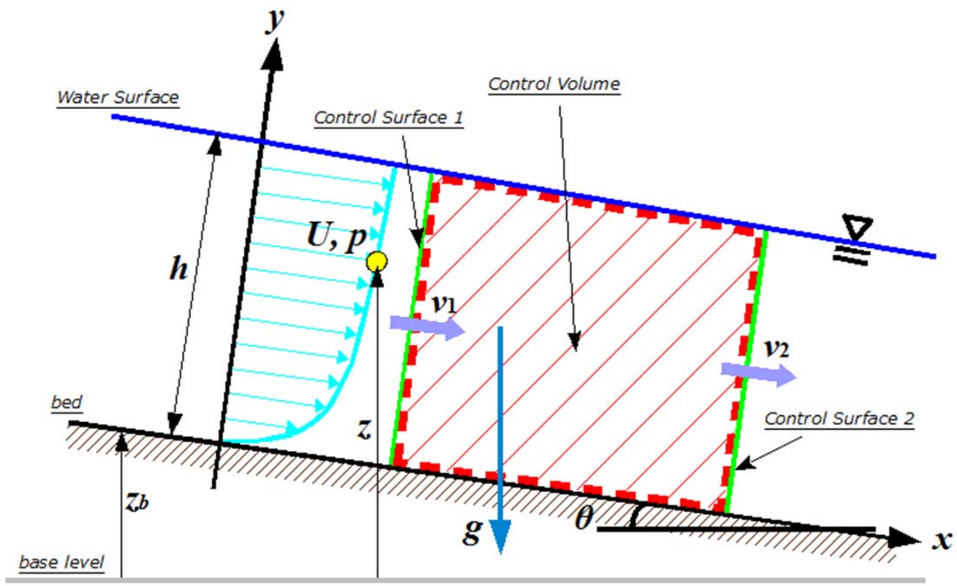
Assignment 2

REFRESHER ON OPEN CHANNEL FLOWS

What is an open-channel flow?

Characteristics?

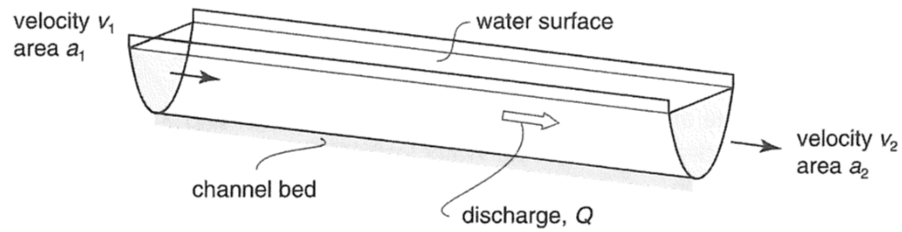
- Surface



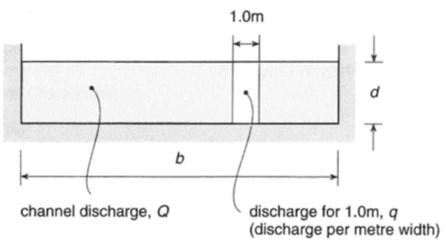
- Balance between?
- Typically water
- Typically turbulent (most practical examples)

Basic Tools Applied to Open Channel Flow

Continuity

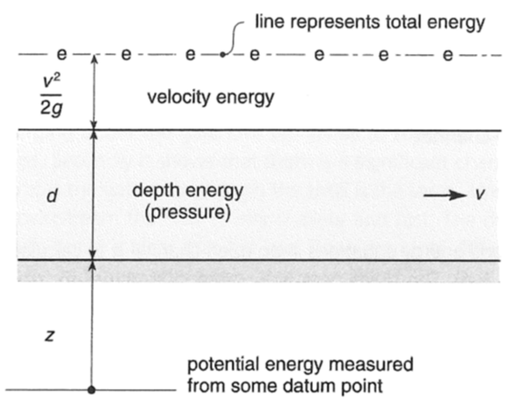


- Unit width discharge concept



Energy

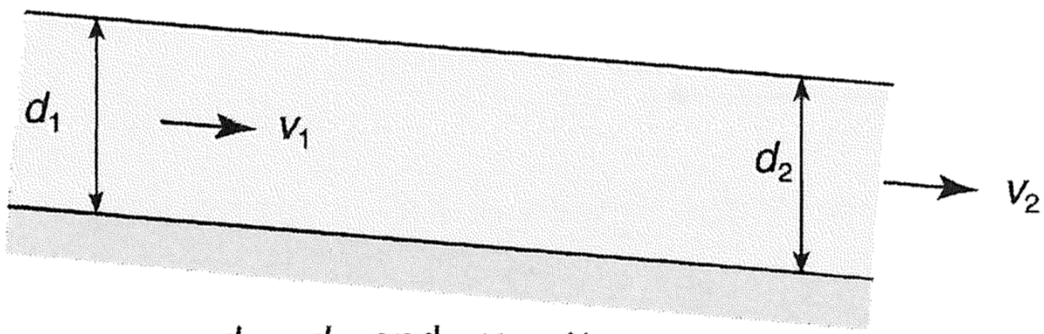
$$d + \frac{v^2}{2g} + z$$



The concept of uniform flow

Assumptions

- Long
- Gently Sloping
- Straight



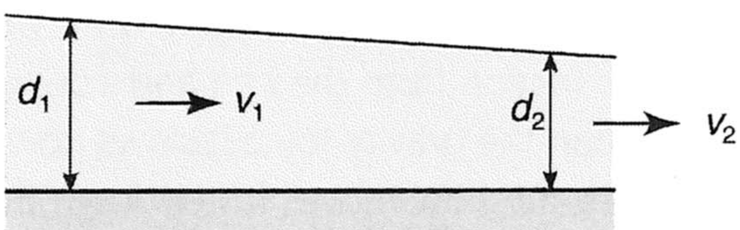
$d_1 = d_2$ and $v_1 = v_2$

Results in

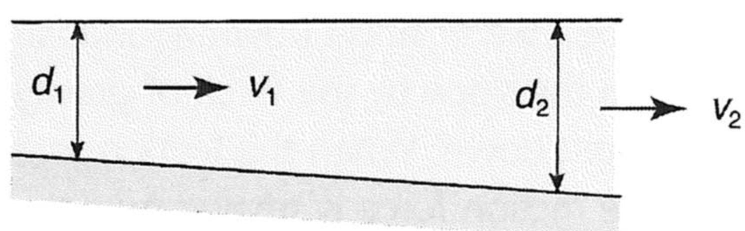
- Force balance
- Constant velocity

Does this happen in real life?

- Sometimes yes, Mostly no (real-life conditions are like below)



gravity force > friction force



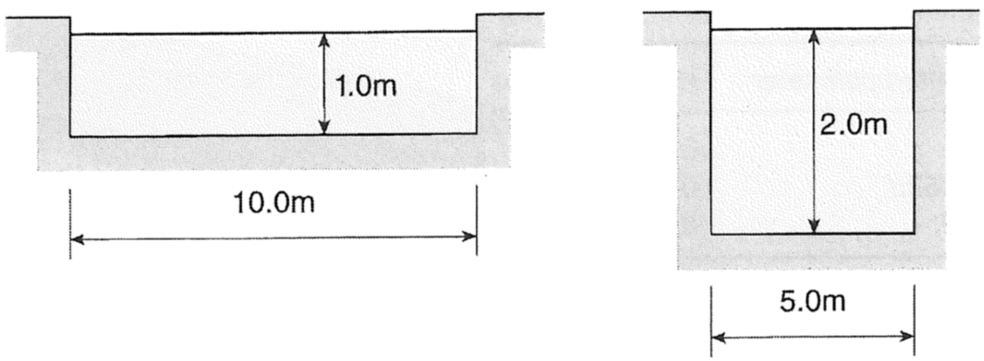
gravity force < friction force

$d_1 \neq d_2$ and $v_1 \neq v_2$

Considerations (1)

Unlike pipe flow – channel shape is important!

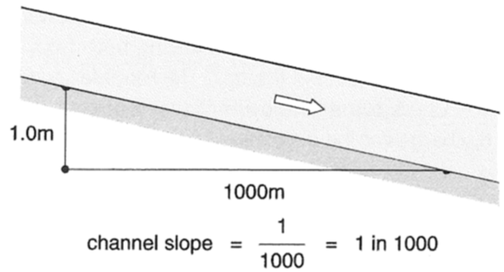
- Why?



- Area and wetted perimeter → Hydraulic radius

Considerations (2)

Slope



- (no other driving force other than gravity, so water flows downhill)

Roughness (i.e. Friction) accounted for in formulae

Typical Roughness values

Adapted from Chow (1959):

Material	*Manning's roughness coefficient, n* *Minimum*	*Average*	*Maximum*
Smooth brass	0.009	0.010	0.013
Welded steel	0.010	0.012	0.014
Riveted, spiral steel	0.013	0.016	0.017
Coated cast iron	0.010	0.013	0.014
Uncoated cast iron	0.011	0.014	0.016
Black wrought iron	0.012	0.014	0.015
Galvanized wrought iron	0.013	0.016	0.017
Glass	0.009	0.010	0.013
Concrete, finished	0.011	0.012	0.014
Concrete, unfinished smooth wood form	0.012	0.014	0.016
Clay, vitrified sewer	0.011	0.014	0.017
Sanitary sewers coated with biological slime	0.012	0.013	0.016

Roughness Coefficients (Manning's "N") for Sheet Flow

Surface Description	n^1
Smooth surfaces (concrete, asphalt, gravel, or bare soil)	0.011
Fallow (no residue)	0.05
Cultivated soils: Residue cover ≤ 20%	0.06
Cultivated soils: Residue cover > 20%	0.17
Grass: Short grass prairie	0.15
Grass: Dense grases[2]	0.24
Grass: Bermudagrass	0.41
Range (natural)	0.13
Woods[3]: Light underbrush	0.40
Woods[3]: Dense underbrush	0.80

Uniform flow design formula

Chezy:

- From Energy Equation the first assumption is $h_f = \frac{Lv^2}{C^2 R}$
- Using uniform flow approximations in the energy equation, one obtains

$$\frac{v^2}{C^2 R} = \frac{z_2 - z_1}{L} \rightarrow v = C\sqrt{RS}$$

Manning's: $v = \frac{1}{n} R^{2/3} \sqrt{S}$

What about non-uniform, steady flows?

Two types:

- Gradually varying
  - Essentially water surface follows a gradual curve
  - 12 types of curves typically thought of
  - Most curves are in the order of km
  - For treatment plants, typically length too short

- Rapidly varying
  - Occurs due to sudden change in channel’s
    - Shape
    - Size
  - Examples include:
    - Hydraulic structures
    - Weirs;
    - Change in width; depth
  - Transitions occur over metres

The issue of flow behavior

If Q same for 2 flows, but if b, d, v different; presence of obstruction is also different. Why?

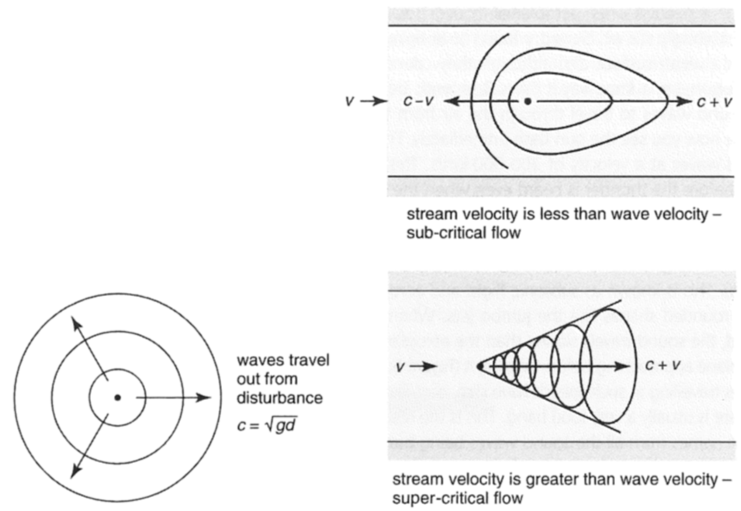
Criticality of flow

- 2 types: Sub and super
- With 1 transition point

How is it defined?

- Ratio of water velocity to wave celerity

→ Froude Number

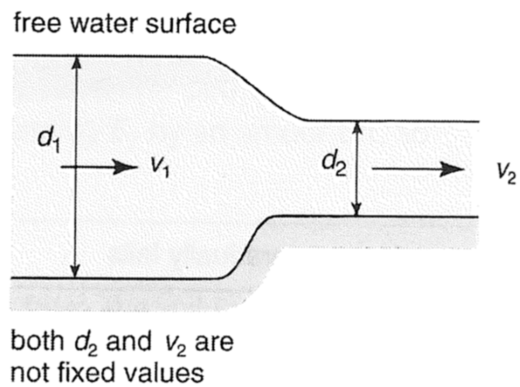


(a) Still pond

(b) Waves on a flowing stream

The concept of specific energy

Using energy and continuity will result in a cubic relationship; therefore another concept is needed.

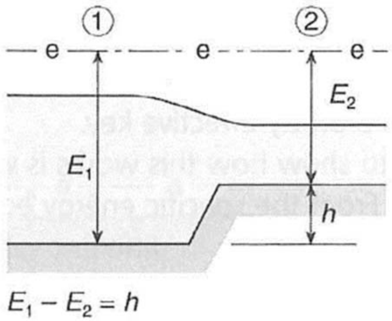


Specific Energy → $E = d + \frac{v^2}{2g} = d + \frac{q^2}{2gd^2}$

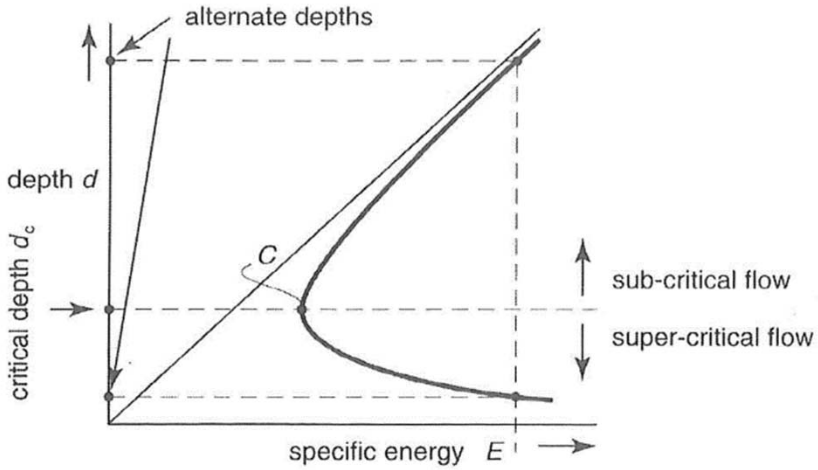
Energy as measured from the channel bed

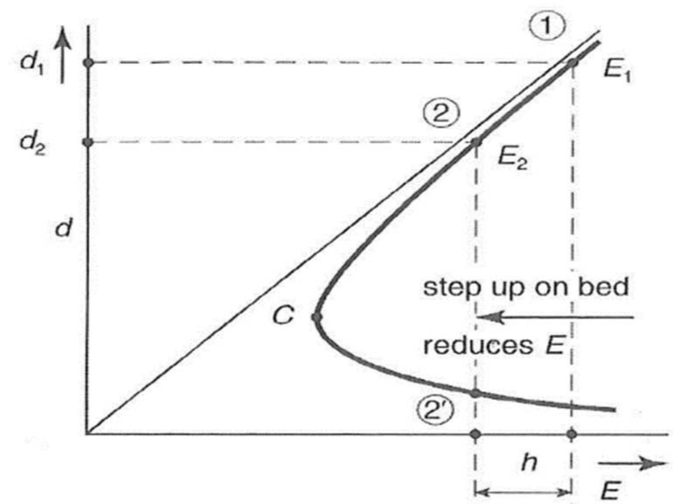
Quantifying the changes using the Specific Energy Diagram

Now if you want to know what happens here→



You can create a specific energy diagram





Critical Flow and Critical Depth

One can obtain the critical depth by differentiating the specific energy equation with respect to depth and setting the differential equation to 0, i.e.

$\frac{dE}{dd} = 0$, results in two useful relationships:

$$d_c = \sqrt[3]{\frac{q^2}{g}} \quad \text{and} \quad E_c = 1.5 d_c$$

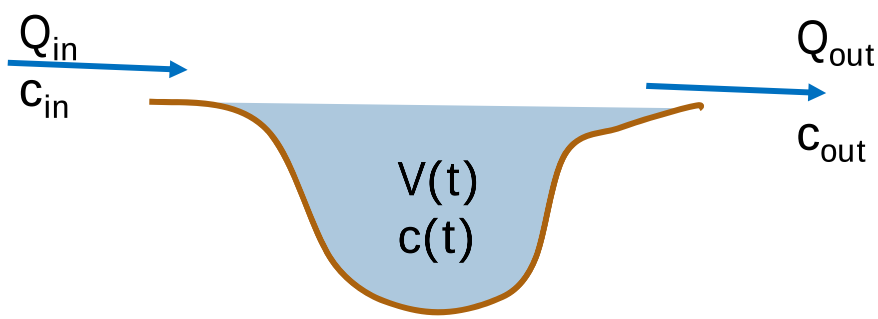
Points about critical flow:

- For plant design, make sure flows in channels are not

Lake with pollutant

A DETAILED LOOK AT NUMERICAL SOLUTION ISSUES

Pollutants in a reservoir…



Using the assumptions discussed earlier, we are able to start with

$$\frac{d(Vc)}{dt} = Q_{in}c_{in} - Q_{out}c$$

And proceed to solving this equation

$$V\frac{dc}{dt} = Q_{in}(c_{in} - c)$$

Some numerical integration methods

Some numerical integration methods for: $\dfrac{dc}{dt} = f(c)$, example: $f(c) = \lambda c$

Euler's explicit rule: $\dfrac{c_{n+1} - c_n}{\Delta t} = f_n \quad \left(E_{n+1} = \dfrac{\Delta t}{2} c^{(2)}(t_n) + O(\Delta t^2) \right)$

Euler's implicit rule: $\dfrac{c_{n+1} - c_n}{\Delta t} = f_{n+1} \quad \left(E_{n+1} = -\dfrac{\Delta t}{2} c^{(2)}(t_n) + O(\Delta t^2) \right)$

Trapezoidal rule: $\dfrac{c_{n+1} - c_n}{\Delta t} = \dfrac{1}{2} f_n + \dfrac{1}{2} f_{n+1} \quad \left(E_{n+1} = -\dfrac{\Delta t^2}{12} c^{(3)}(t_n) + O(\Delta t^3) \right)$

Midpoint rule: $\dfrac{c_{n+1} - c_{n-1}}{2\Delta t} = f_{n+1} \quad \left(E_{n+1} = \dfrac{\Delta t^2}{6} c^{(3)}(t_n) + O(\Delta t^3) \right)$

2nd order BDF: $\dfrac{3c_{n+2} - 4c_{n+1} + c_n}{2\Delta t} = f_{n+2}$

θ method: $\dfrac{c_{n+1} - c_n}{\Delta t} = \theta f_{n+1} + (1-\theta) f_n$

2nd order Adams Bashforth: $\dfrac{c_{n+1} - c_n}{\Delta t} = 1.5 f_n - 0.5 f_{n-1}$

Convergence: $\lim\limits_{\Delta t\to 0}\left|c(t_n)-c_n\right|=0, \forall n, t_n=n\Delta t, n=1,\ldots,\frac{T}{\Delta t}$

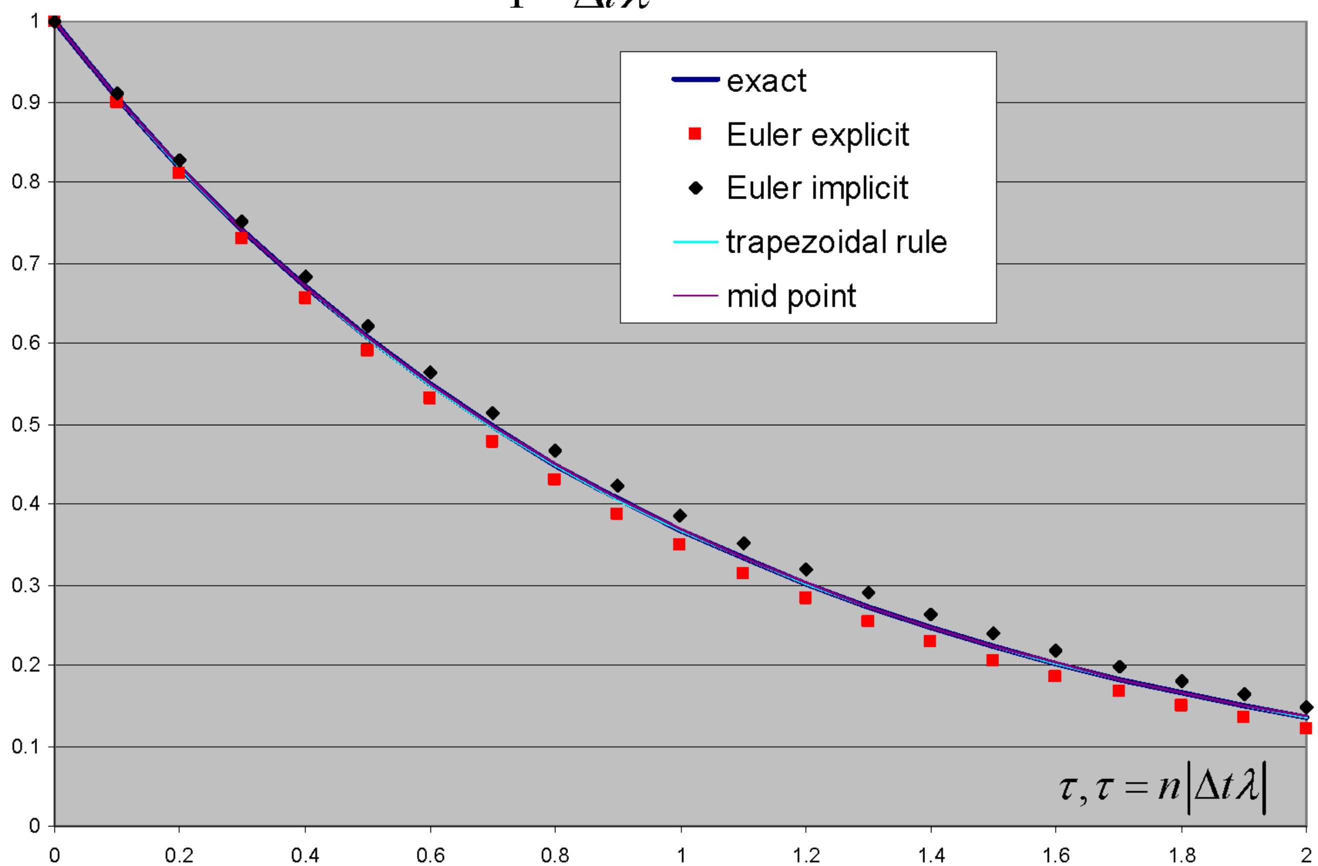
examples for the test equation:

Euler's explicit rule: $c_{n+1}=\left(1+\Delta t\lambda\right)c_n$

Trapezoidal rule: $c_{n+1}=\dfrac{1+\frac{1}{2}\Delta t\lambda}{1-\frac{1}{2}\Delta t\lambda}c_n$

Euler's implicit rule: $c_{n+1}=\dfrac{1}{1-\Delta t\lambda}c_n$

Midpoint rule: $c_{n+1}=c_{n-1}+2\Delta t\lambda c_n$

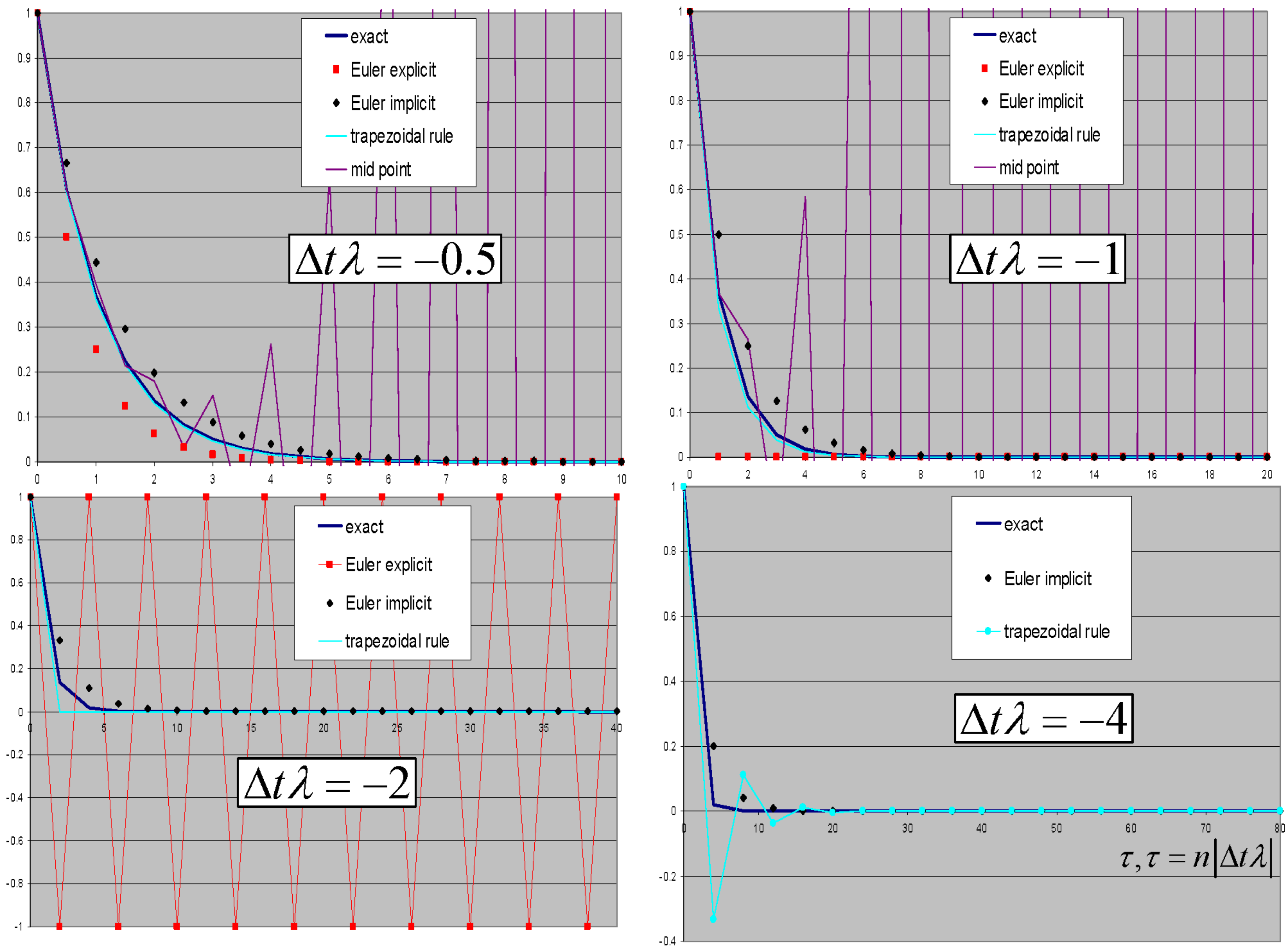


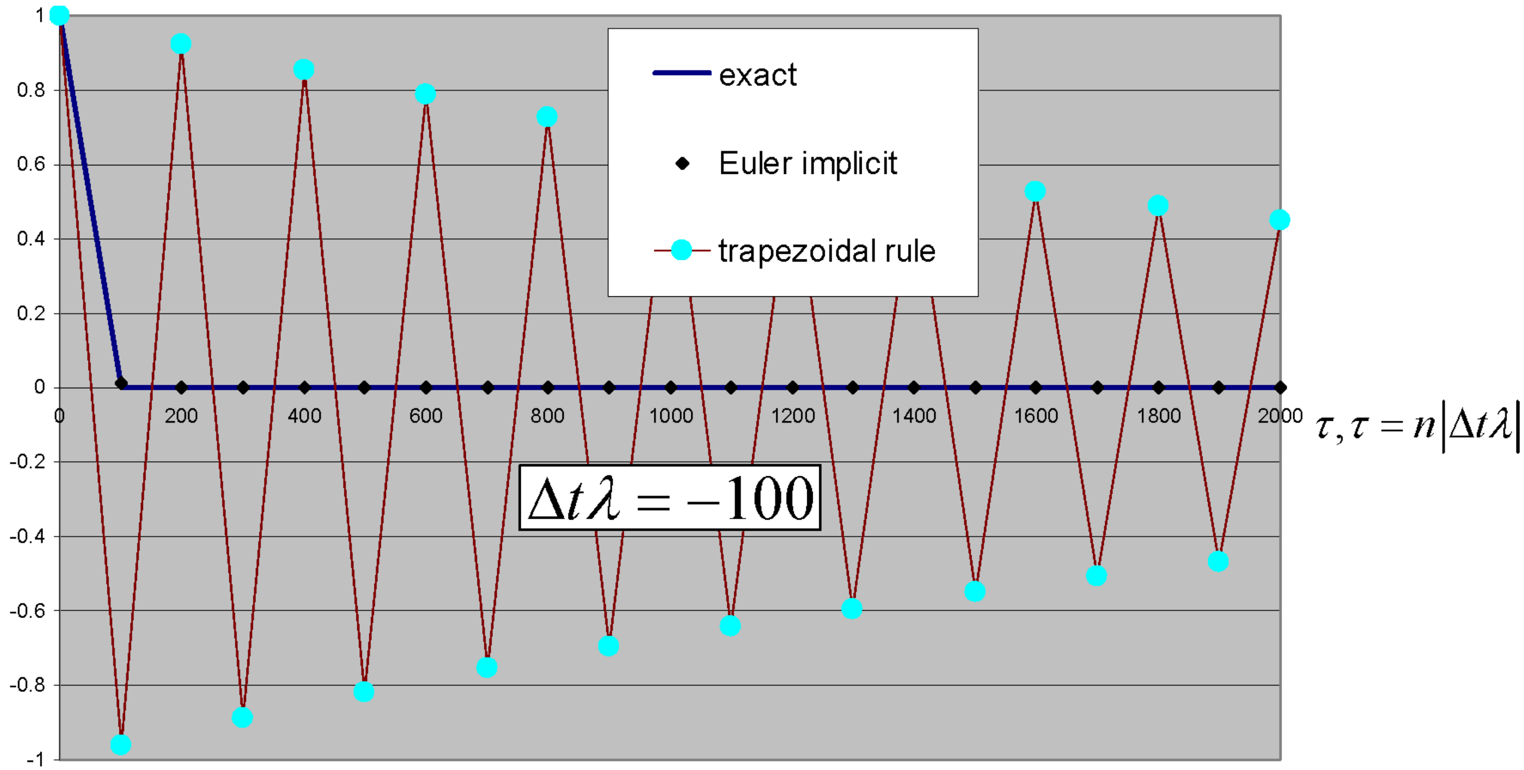
$$\Delta t\lambda=-0.1$$

$$c(t_n)=e^{\lambda t_n}$$

$$=e^{n\Delta t\lambda}=$$

$$=e^{-0.1n}$$


exact
Euler explicit
Euler implicit
trapezoidal rule
mid point
$\Delta t\lambda = -0.5$
$\Delta t\lambda = -1$
$\Delta t\lambda = -2$
$\Delta t\lambda = -4$
$\tau, \tau = n|\Delta t\lambda|$



Euler's implicit rule: $c_{n+1} = \dfrac{1}{1-\Delta t\lambda} c_n, \ \lim\limits_{\Delta t\lambda \to -\infty} c_{n+1} = 0 \longrightarrow$ Stiffly stable! (and positive and monotonic)

Trapezoidal rule: $c_{n+1} = \dfrac{1+\frac{1}{2}\Delta t\lambda}{1-\frac{1}{2}\Delta t\lambda} c_n, \ \lim\limits_{\Delta t\lambda \to -\infty} c_{n+1} = (-1)^{n+1} c_0$

Stability analysis for test equation: $\dfrac{dc}{dt} = \lambda c$

Suppose $c_n = r^n c_0$ this is stable if: $\boxed{\|r\| \le 1}$

Euler's explicit rule:

$$\frac{c_{n+1} - c_n}{\Delta t} = \lambda c_n \rightarrow c_{n+1} = (1+\Delta t\lambda)c_n \rightarrow c_1 = (1+\Delta t\lambda)c_0, c_2 = (1+\Delta t\lambda)c_1$$

$$\rightarrow c_2 = (1+\Delta t\lambda)^2 c_0 \rightarrow c_{n+1} = (1+\Delta t\lambda)^{n+1} c_0 \rightarrow r = 1+\Delta t\lambda \rightarrow \boxed{-2 \le \Delta t\lambda < 0}$$

Euler's implicit rule:

$$\frac{c_{n+1} - c_n}{\Delta t} = \lambda c_{n+1} \rightarrow c_{n+1} = \frac{1}{1-\Delta t\lambda} c_n \rightarrow r = \frac{1}{1-\Delta t\lambda} \longrightarrow \boxed{\text{Unconditional stable!}}$$

Stability analysis of midpoint rule for test equation: $\dfrac{dc}{dt} = \lambda c$

midpoint rule: $\dfrac{c_{n+2} - c_n}{2\Delta t} = \lambda c_{n+1} \rightarrow c_{n+2} = c_n + 2\Delta t \lambda c_{n+1}$

Suppose $c_n = r^n c_0$ this is stable if: $\boxed{\|r\| \le 1}$

Substutution of $c_n = r^n c_0$ into $c_{n+2} = c_n + 2\Delta t \lambda c_{n+1}$ yields:

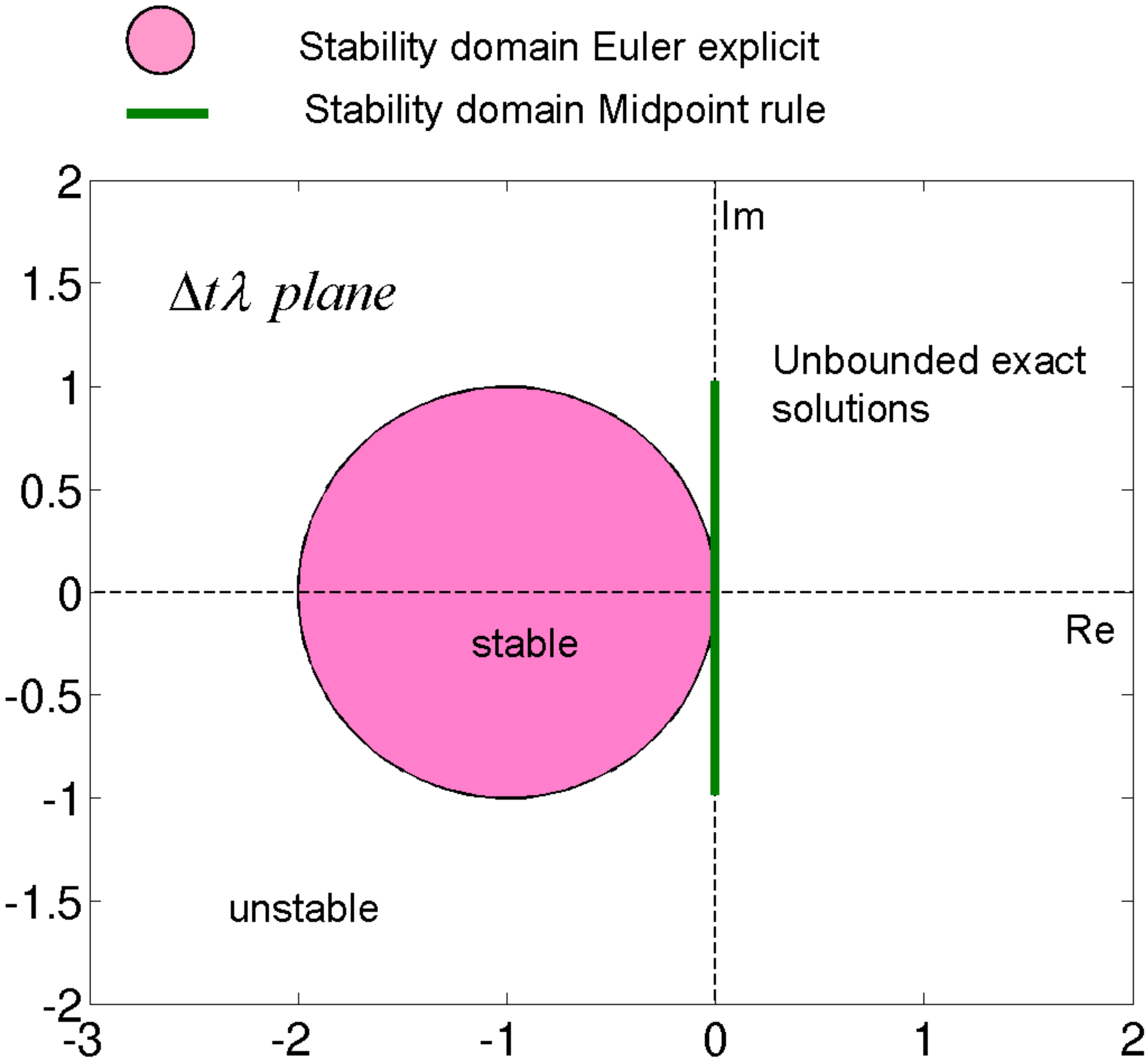
$$r^{n+2} c_0 = r^n c_0 + 2\Delta t \lambda r^{n+1} c_0 \rightarrow \frac{r^{n+2} c_0}{r^n c_0} = \frac{r^n c_0 + 2\Delta t \lambda r^{n+1} c_0}{r^n c_0} \rightarrow$$

$$\rightarrow \boxed{r^2 - 2\Delta t \lambda r - 1 = 0} \longleftarrow$$ Characteristic equation! $$\boxed{c_n = d_1 r_1^n + d_2 r_2^n}$$

Principal root: $r_1 = \Delta t \lambda + \sqrt{(\Delta t \lambda)^2 + 1} \rightarrow r_1^n \approx e^{n \Delta t \lambda}$

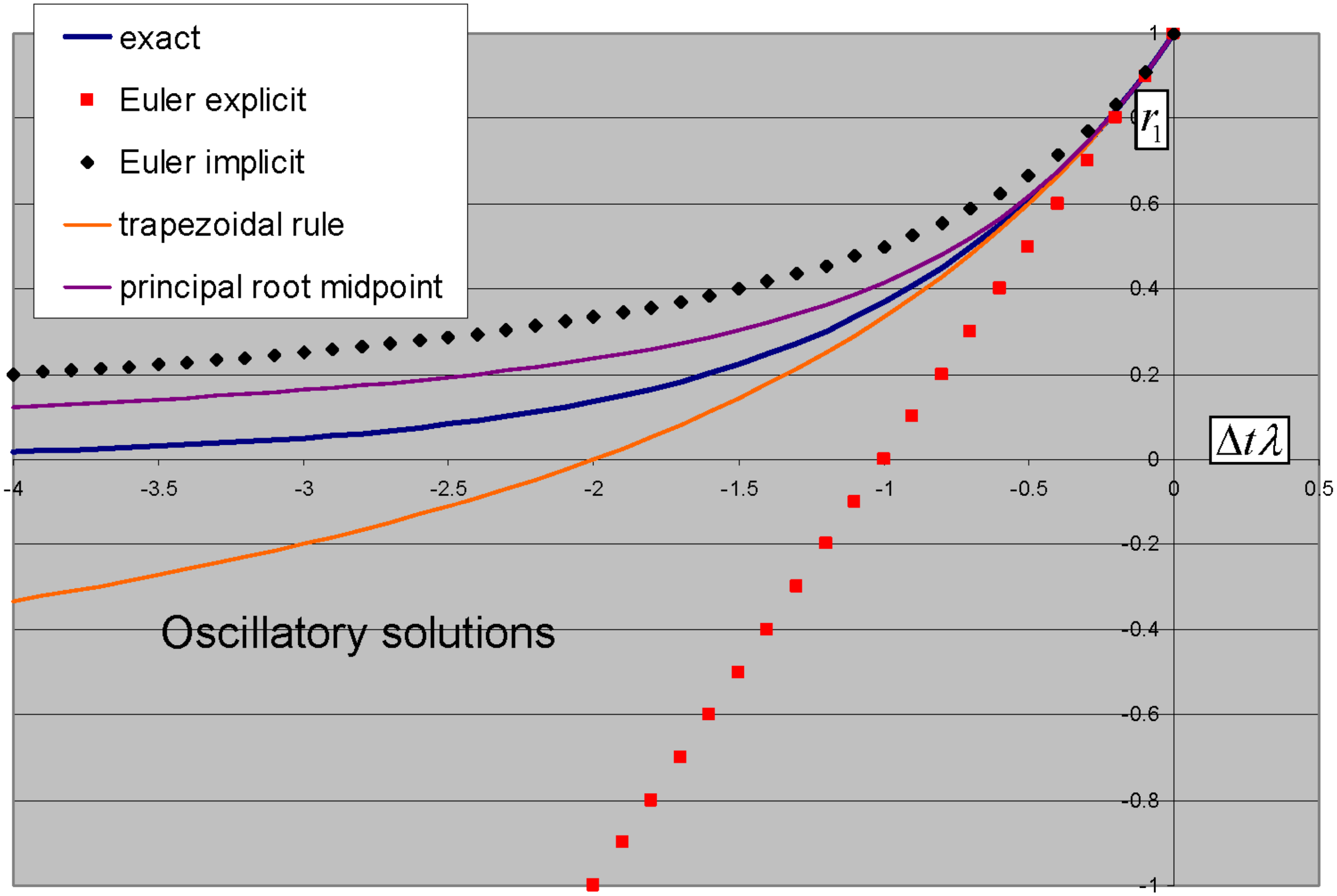
Spurious root: $r_2 = \Delta t \lambda - \sqrt{(\Delta t \lambda)^2 + 1} \rightarrow |r_2| > 1 \forall \Delta t \lambda < 0$

> Midpoint rule always unstable for real values of $\Delta t \lambda$ even if $d_2 = 0$
>
> Only stable for imaginary values iff: $-i \le \Delta t \lambda \le i$


Stability domain Euler explicit
Stability domain Midpoint rule
$\Delta t\lambda$ plane
Im
Unbounded exact solutions
stable
Re
unstable
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-3
-2
-1
0
1
2

Comparison of $\dfrac{c_{n+1}}{c_n}, \dfrac{c(t_{n+1})}{c(t_n)}$

$$c(n\Delta t) = \left(e^{\Delta t\lambda}\right)^n \to \frac{c(t_n + \Delta t)}{c(t_n)} = e^{\Delta t\lambda}, c_n = \left(r_1(\Delta t\lambda)\right)^n \to \frac{c_{n+1}}{c_n} = r_1(\Delta t\lambda)$$

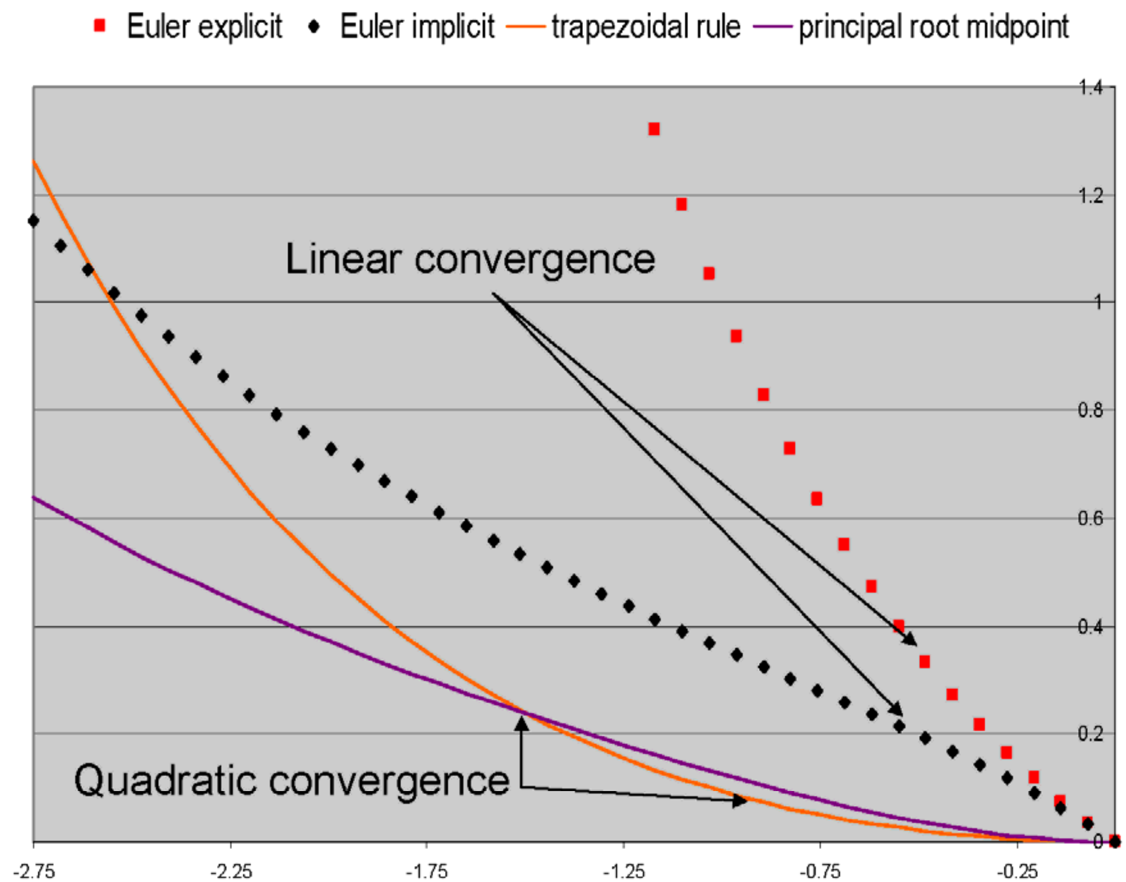


Comparison of relative local errors,
i.e. assuming that no previous
errors are made, i.e.:

$$c_n = c(t_n) =$$

$$= c_0 e^{n\Delta t\lambda} \rightarrow$$

$$c_{n+1} = r c_0 e^{n\Delta t\lambda}$$



$$\varepsilon = \left| \frac{\dfrac{c(n\Delta t + \Delta t) - c(n\Delta t)}{\Delta t} - \dfrac{c_{n+1} - c_n}{\Delta t}}{\dfrac{dc(n\Delta t + \Delta t)}{dt}} \right| = \left| \frac{c(n\Delta t + \Delta t) - c_{n+1}}{\Delta t \dfrac{dc(n\Delta t + \Delta t)}{dt}} \right| = \left| \frac{e^{\lambda\Delta t} - r}{\lambda \Delta t e^{\lambda\Delta t}} \right|$$

Error per time step, local truncation error, consistency

An ODE given by:
$$\frac{dc}{dt} = f(c,t), \quad c(t_0) = C_0$$

Approximated with Euler explicit:
$$\frac{c_{n+1} - c_n}{\Delta t} = f_n \rightarrow c_{n+1} = c_n + \Delta t f_n$$

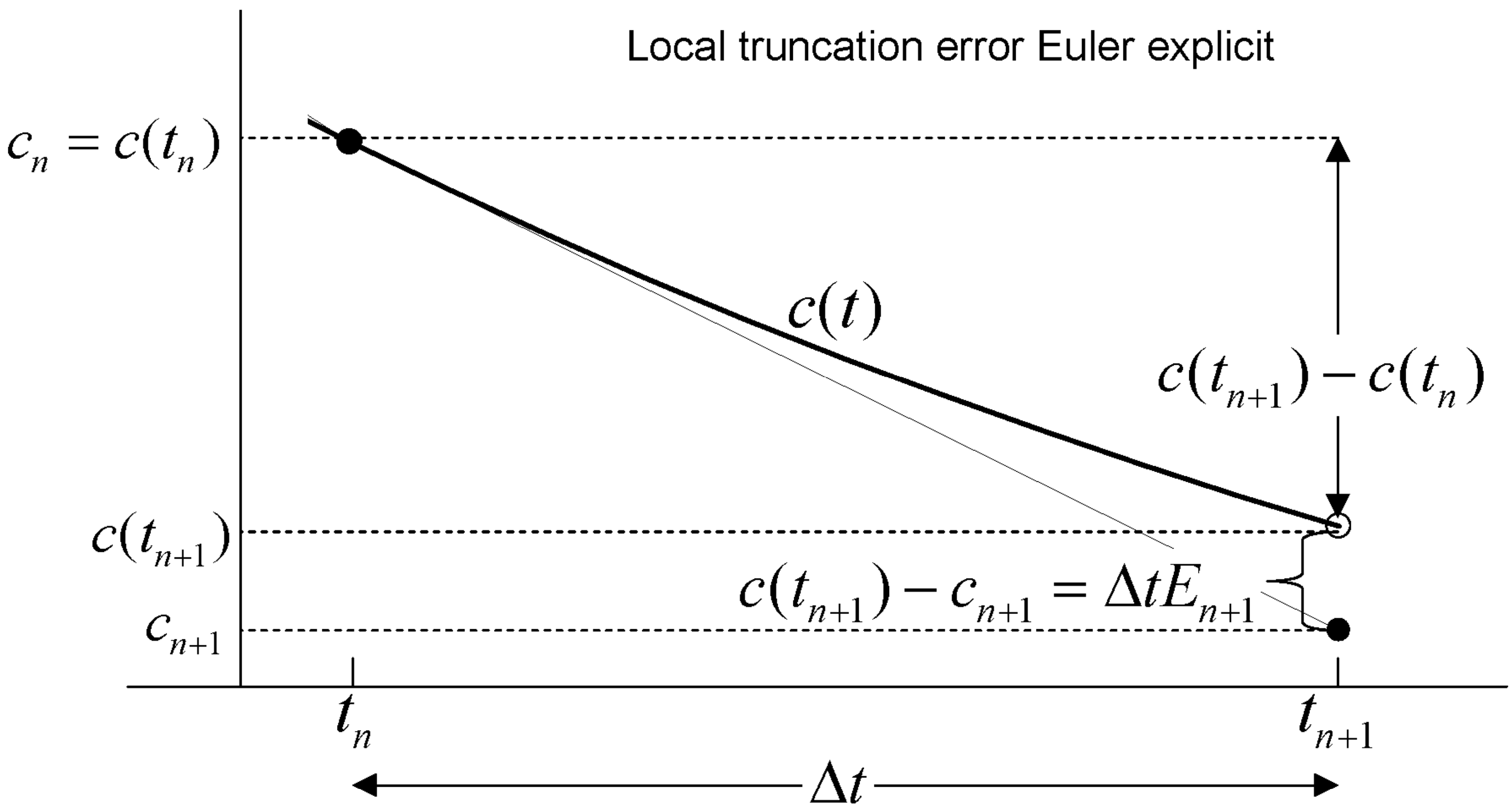
Assume no previous errors:
$$c_{n+1} = c(t_n) + \Delta t f\left(c(t_n), t_n\right)$$

The local truncation error E_{n+1} is now defined by:

$$E_{n+1} = \frac{c(t_n + \Delta t) - c_{n+1}}{\Delta t} = \frac{c(t_n + \Delta t) - c(t_n)}{\Delta t} - f\left(c(t_n), t_n\right) = D_{\Delta t} c(t_n)$$

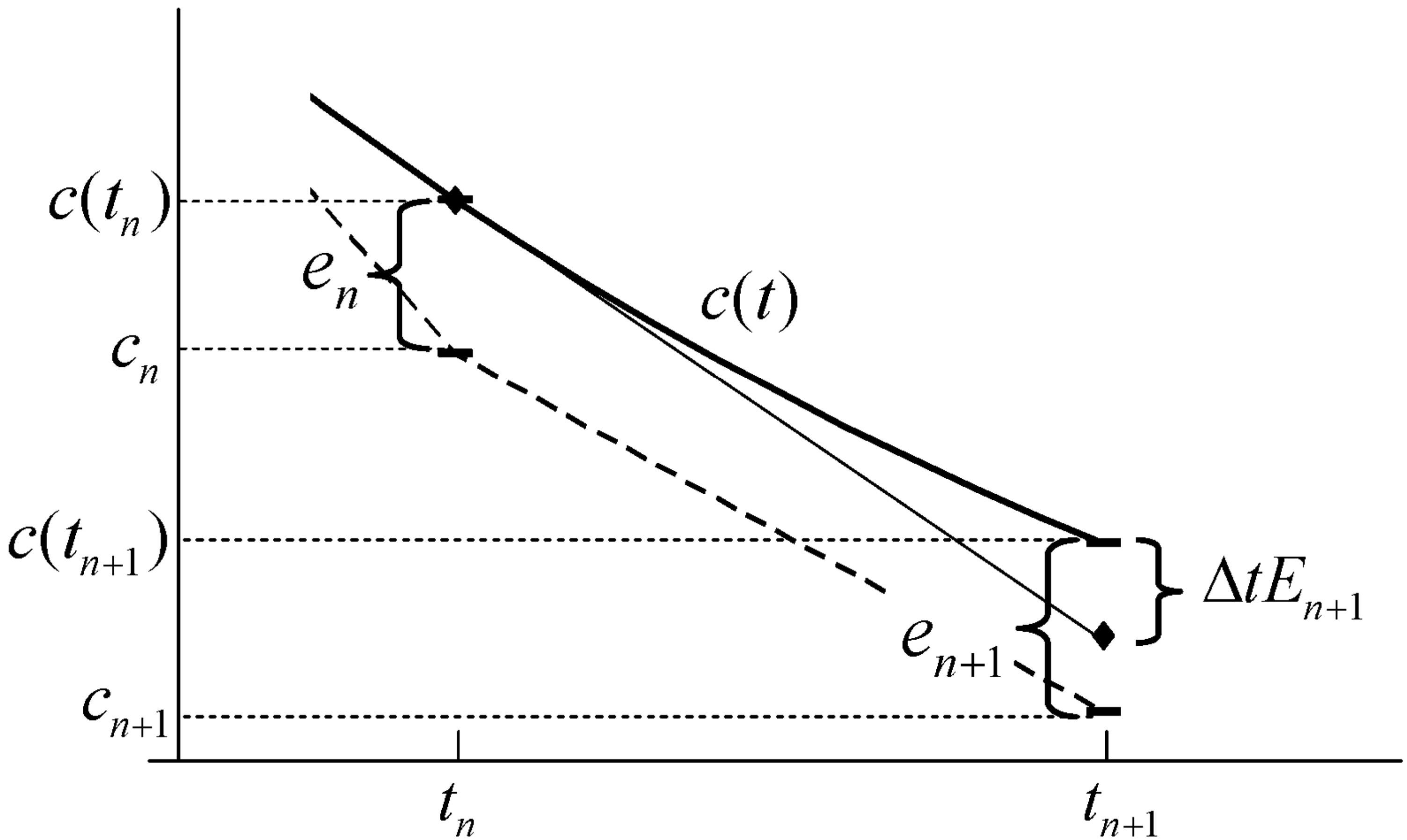
Consistency means:
$$\lim_{\Delta t \to 0} D_{\Delta t}[c(t_n)] = 0$$

Note that by definition:
$$\lim_{\Delta t \to 0} \frac{c(t + \Delta t) - c(t)}{\Delta t} - f[c(t), t] = 0$$



$$E_{n+1} = \frac{c(t_n + \Delta t) - c_{n+1}}{\Delta t} = \frac{c(t_n + \Delta t) - c(t_n)}{\Delta t} - \frac{c_{n+1} - c(t_n)}{\Delta t} \rightarrow$$

$$\boxed{E_{n+1} = \frac{c(t_n + \Delta t) - c(t_n)}{\Delta t} - f\left(c(t_n), t_n\right)} \qquad \left(c_{n+1} = c(t_n) + \Delta t f\left(c(t_n), t_n\right)\right)$$



$$e_n = c(t_n) - c_n, e_{n+1} = c(t_{n+1}) - c_{n+1}, E_{n+1} \approx \frac{e_{n+1} - e_n}{\Delta t}$$

Local truncation error is roughly the rate of change of the error

Summary

An ODE is given by:

$$\frac{dc}{dt} = f(c,t), \quad c(t_0) = C_0$$

An approximation by a linear multistep method is given by:

$$\sum_{j=0}^{k} \alpha_j \frac{c_{n+j}}{\Delta t} - \sum_{j=0}^{k} \beta_j f_{n+j} = 0$$

The difference operator is defined by:

$$D_{\Delta t}[c(t)] = \sum_{j=0}^{k} \left\{ \frac{\alpha_j c(t + j\Delta t)}{\Delta t} - \beta_j f[c(t + j\Delta t), t + j\Delta t] \right\}$$

Consistency means:

$$\lim_{\Delta t \to 0} D_{\Delta t}[c(t)] = 0$$

The local truncation error is :

$$E_{n+k} = \sum_{j=0}^{k} \left\{ \frac{\alpha_j c(t_{n+j})}{\Delta t} - \beta_j f[c(t_{n+j}), t_{n+j}] \right\}$$

The necessary and sufficient conditions for a linear multistep method to be convergent are that it be consistent and zero-stable.

Verify consistency with Taylor's series expansion given by:

$$c(t+\Delta t) = c(t) + \Delta t c^{(1)}(t) + \frac{\Delta t^2}{2!}c^{(2)} + \frac{\Delta t^3}{3!}c^{(3)} + \ldots, c^{(q)}(t) = \frac{d^q c}{dc^q}, q = 1,2,\ldots$$

$$D_{\Delta t}[c(t)] = \frac{b_0}{\Delta t}c(t) + b_1 c^{(1)}(t) + b_2 \Delta t c^{(2)}(t) + \ldots + b_q \Delta t^{q-1} c^{(q)}(t) + \ldots$$

Consistency implies at least b_0=0 and b_1=0.

Example: Trapezoidal rule

$$D_{\Delta t}[c(t)] = \frac{c(t+\Delta t) - c(t)}{\Delta t} - \frac{1}{2}c^{(1)}(t+\Delta t) - \frac{1}{2}c^{(1)}(t) =$$

$$= \frac{c(t) + \Delta t c^{(1)}(t) + \frac{\Delta t^2}{2!}c^{(2)}(t) + \frac{\Delta t^3}{3!}c^{(3)}(t) + \cdots - c(t)}{\Delta t}$$

$$-\frac{1}{2}\left(c^{(1)}(t) + \Delta t c^{(2)}(t) + \frac{\Delta t^2}{2!}c^{(3)}(t) + \cdots\right) - \frac{1}{2}c^{(1)}(t) = \left(\frac{\Delta t^2}{3!} - \frac{1}{2}\frac{\Delta t^2}{2!}\right)c^{(3)}(t) + H.O.T$$

Here b_0=0, b_1=0 and b_2=0. $\longrightarrow$

$\longrightarrow$ *Local truncation error of second order* : $E_{n+1} = -\frac{\Delta t^2}{12}c^{(3)}(t_n) + H.O.T$

The problem of stiffness

$$\frac{dc}{dt}=\frac{Q}{V}(c_{inp}-c),c_{inp}=\hat{C}(\sin(\omega t)+1),c(0)=?$$

$$c'=\frac{c}{\hat{C}},t'=\omega t,\Omega=\frac{\omega V}{Q}\rightarrow\frac{dc'}{dt'}=\frac{1}{\Omega}\left(\sin t'+1-c'\right),c'(0)=?$$

$$\rightarrow c'(t')=\frac{1}{1+\Omega^2}\left(\sin(t')-\Omega\cos(t')\right)+1 \quad + \quad a.e^{-\frac{t'}{\Omega}}$$

$$c'(t')=\frac{1}{\sqrt{1+\Omega^2}}\sin(t'-\Phi)+1$$

$$\Phi=\tan^{-1}\Omega$$

particular solution

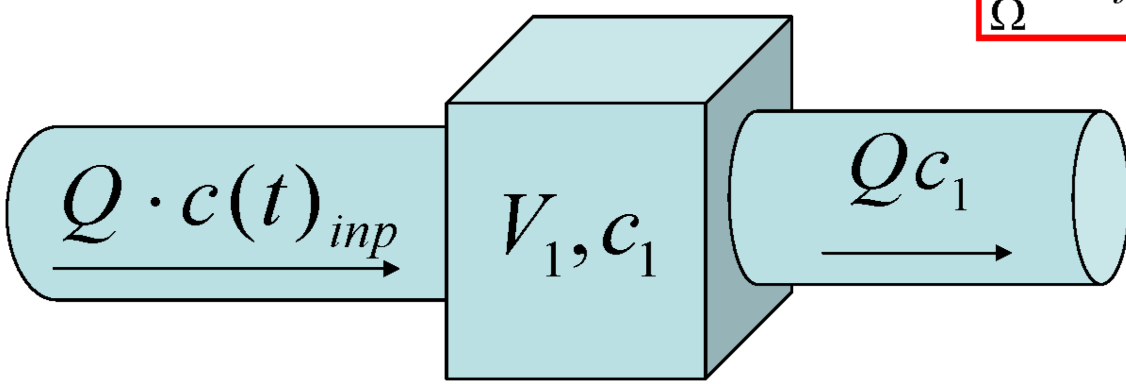
$+$

$$a.e^{-\frac{t'}{\Omega}}$$

homogeneous solution

$$a=c(0)-1+\frac{\Omega}{1+\Omega^2}, if\ c(0)=1-\frac{\Omega}{1+\Omega^2}\rightarrow a=0$$

$$\boxed{\frac{1}{\Omega}=stiffness\ ratio}$$



Numerical schemes:

$$c'_{n+1} = \left(1 - \frac{\Delta t'}{\Omega}\right) c'_n + \frac{\Delta t'}{\Omega}\left(\sin\left(t'_n\right) + 1\right)$$

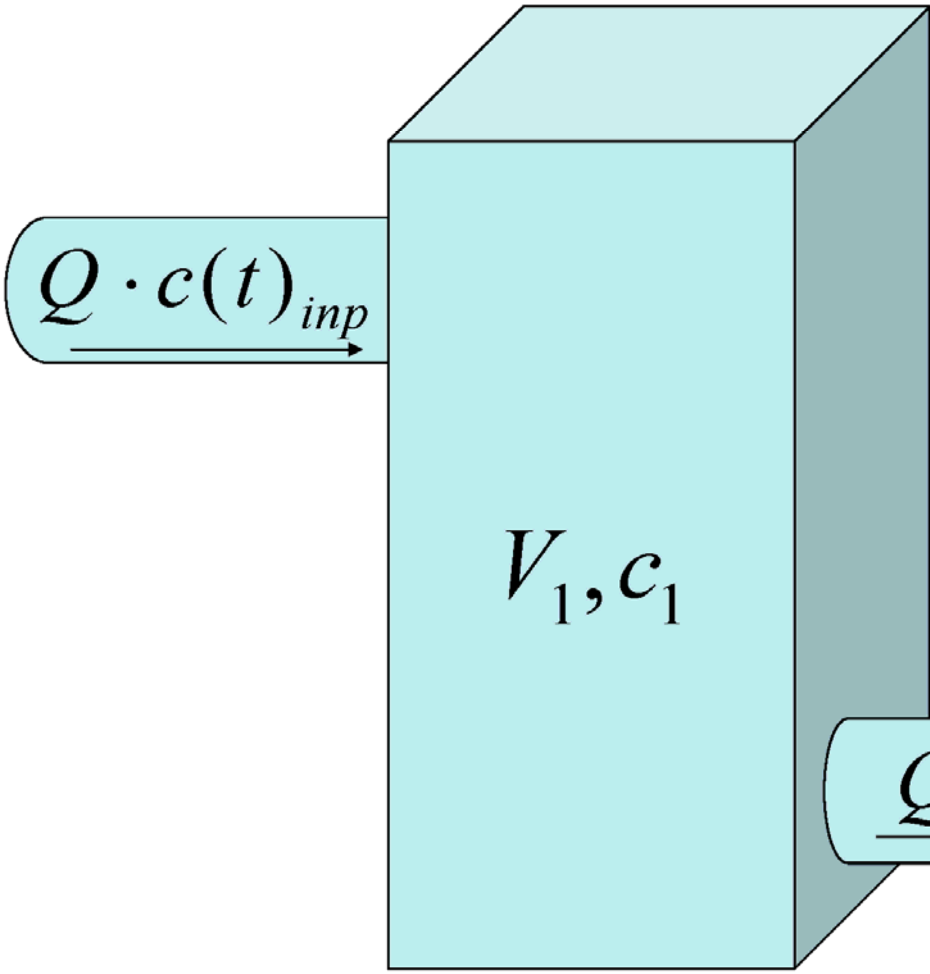
$$c'_{n+1} = \frac{\left(1 - \frac{1}{2}\frac{\Delta t'}{\Omega}\right) c'_n + \frac{1}{2}\frac{\Delta t'}{\Omega}\left(\sin\left(t'_n\right) + \sin\left(t'_{n+1}\right) + 1\right)}{1 + \frac{1}{2}\frac{\Delta t'}{\Omega}}$$

$$c'_{n+1} = \frac{c'_n + \frac{\Delta t'}{\Omega}\left(\sin\left(t'_n\right) + 1\right)}{1 + \frac{\Delta t'}{\Omega}}$$

SYSTEM OF EQUATIONS

NUMERICAL SOLUTIONS AND ISSUES

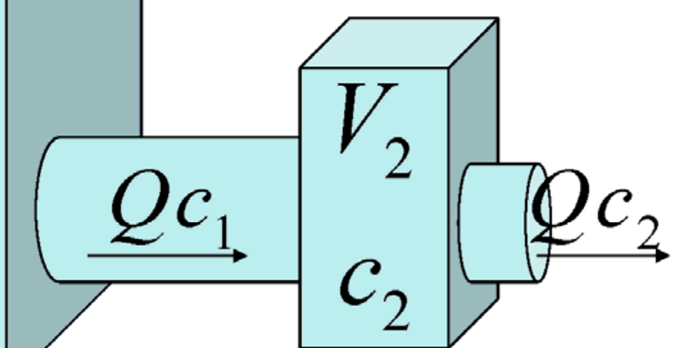
Systems of ODE's, non linear aspects



$$\frac{dc_1}{dt} = \frac{Q}{V_1}(c_{inp} - c_1)$$

$$\frac{dc_2}{dt} = \frac{Q}{V_2}(c_1 - c_2)$$

$$V_2 \ll V_1$$

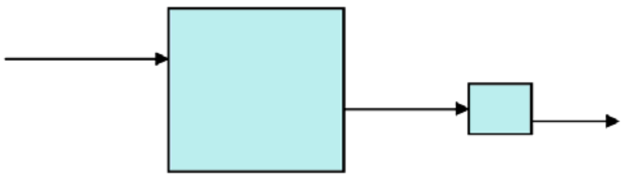


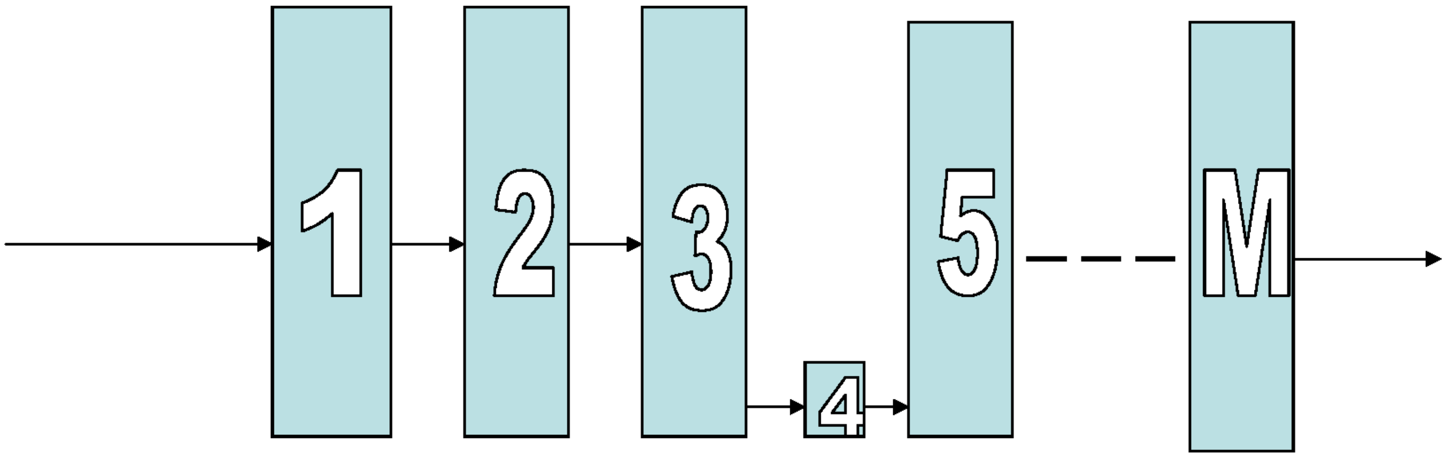
How do you build systems?

$$\frac{dc_1}{dt} = \frac{Q}{V_1}(c_{inp} - c_1) \qquad \frac{dc_2}{dt} = \frac{Q}{V_2}(c_1 - c_2) \leftrightarrow \begin{bmatrix} \frac{dc_1}{dt} \\ \frac{dc_2}{dt} \end{bmatrix} + \begin{bmatrix} \frac{Q}{V_1} & 0 \\ -\frac{Q}{V_2} & \frac{Q}{V_2} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \frac{Q}{V_1} c_{inp} \\ 0 \end{bmatrix}$$

$$\frac{d\vec{c}}{dt} = \vec{f}(\vec{c}, t), \quad \vec{c}(t_0) = \vec{C}^0$$

$$\sum_{j=0}^{k} \frac{\alpha_j}{\Delta t} c^{n+j} = \sum_{j=0}^{k} \beta_j f^{n+j} \qquad \vec{c} = \begin{bmatrix} c_1 \\ \vdots \\ c_m \end{bmatrix}, \ \vec{f} = \begin{bmatrix} f_1 \\ \vdots \\ f_m \end{bmatrix}, \ \vec{C}^0 = \begin{bmatrix} C_1^0 \\ \vdots \\ C_m^0 \end{bmatrix}$$





$$\frac{dc_1}{dt} = \frac{Q}{V_1}(c_{inp} - c_1)$$

$$\frac{dc_2}{dt} = \frac{Q}{V_2}(c_1 - c_2)$$

$$\vdots$$

$$\frac{dc_M}{dt} = \frac{Q}{V_2}(c_{M-1} - c_M)$$

$$\leftrightarrow \begin{bmatrix} \frac{dc_1}{dt} \\ \frac{dc_2}{dt} \\ \vdots \\ \frac{dc_M}{dt} \end{bmatrix} + \begin{bmatrix} \frac{Q}{V_1} & & \bigcirc & \\ -\frac{Q}{V_2} & \frac{Q}{V_2} & & \\ & \ddots & \ddots & \\ \bigcirc & & -\frac{Q}{V_M} & \frac{Q}{V_M} \end{bmatrix} \times \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_M \end{bmatrix} = \begin{bmatrix} \frac{Q}{V_1} c_{inp} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$