Hydraulic groundwater modeling

- Week 5

- Temporal discretization and stability concerns

Discretization of time

- Similar to space, continuous time needs to be discretized
- Discretization of time is based on finite differences

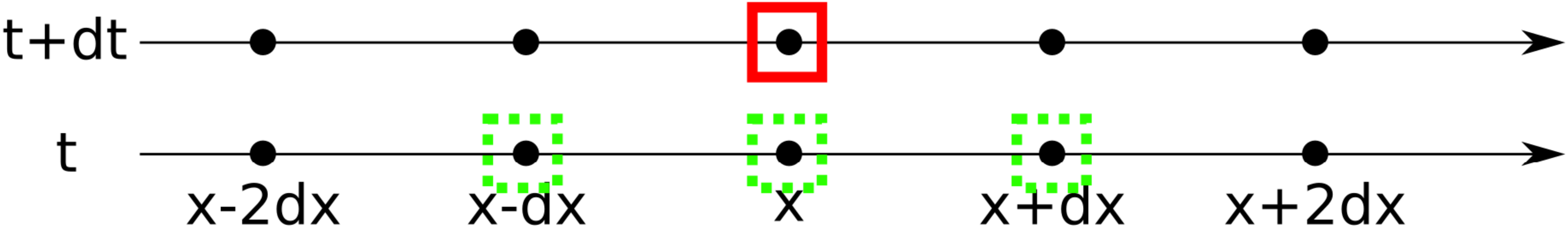
$$\frac{\partial f(x,t)}{\partial t} = \frac{f(x,t+dt) - f(x,t)}{dt}$$

Time step

- Time step dt = difference between discrete points in time
- Value of dt depends on
  - Time scale of the process
  - Spatial discretization
  - Stability of the numerical method
  - Desired accuracy
  - Discretization method/scheme

Explicit time discretization

- One time step after another in a sequence
- conditionally stable



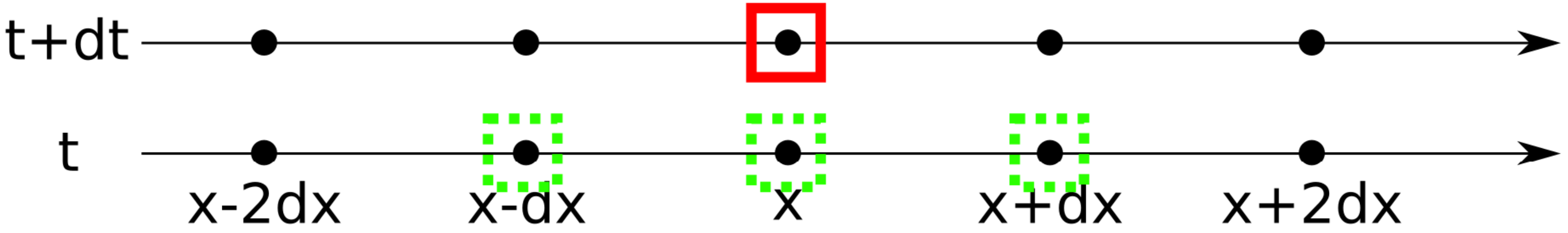
Example for explicit time discretization

- 1d GW flow: $S\frac{\partial h(x,t)}{\partial t} = T\frac{\partial^2 h(x,t)}{\partial x^2}$

- Finite difference discretization in time and space

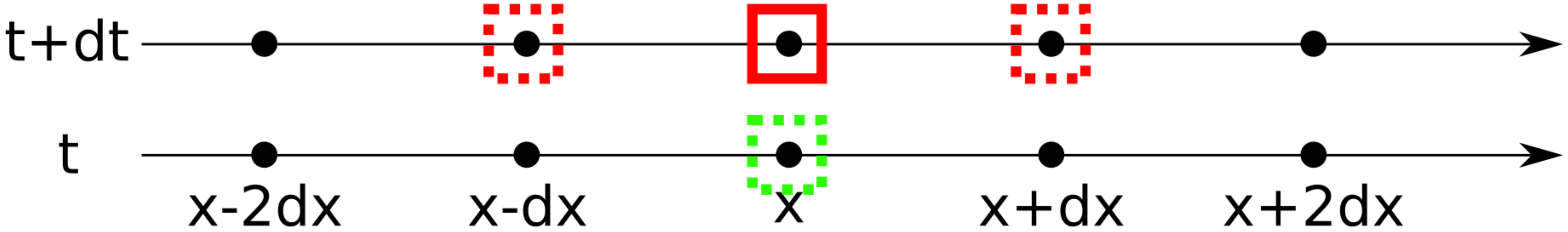
$$S\,\frac{h(x,t+dt)-h(x,t)}{dt} = T\,\frac{h(x+dx,t)\,-2\,h(x,t)+h(x-dx,t)}{dx^2}$$

$$h(x,t+dt)\;=h(x,t)+\frac{Tdt}{Sdx^2}\left(h(x+dx,t)\;-2\,h(x,t)+h(x-dx,t)\right)$$



Implicit time discretization

- A set of equations solved by linear algebra or iterative procedures
- unconditionally stable



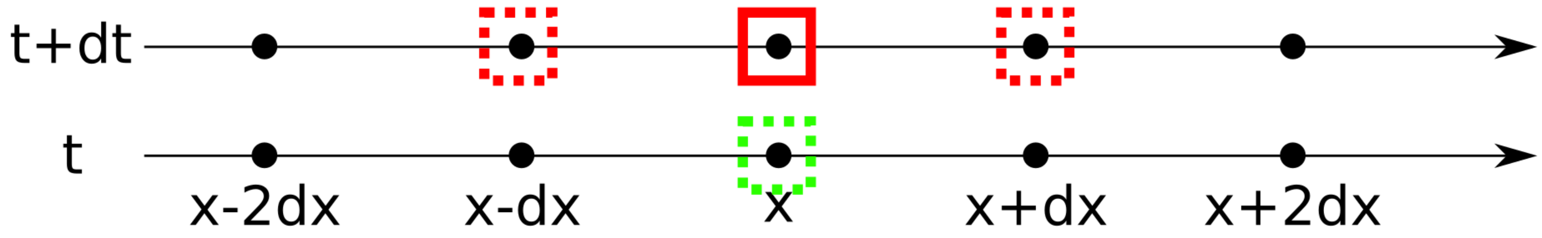
Example for implicit time discretization

- 1d GW flow: $S \frac{\partial h(x,t)}{\partial t} = T \frac{\partial^2 h(x,t)}{\partial x^2}$

- Finite difference discretization in time and space

$$S \frac{h(x,t+dt) - h(x,t)}{dt} = T \frac{h(x+dx,t+dt) \; - 2\, h(x,t+dt) + h(x-dx,t+dt)}{dx^2}$$

$$h(x,t+dt)\left(\frac{Sdx^2}{Tdt} + 2\right) - h(x+dx,t+dt) - h(x-dx,t-dt) = \frac{Tdt}{Sdx^2} h(x,t)$$



Time discretization schemes

- Euler forwards: The shown explicit scheme
- Euler backward: The shown implicit scheme
- Leap frog: A two step method (=higher order scheme)

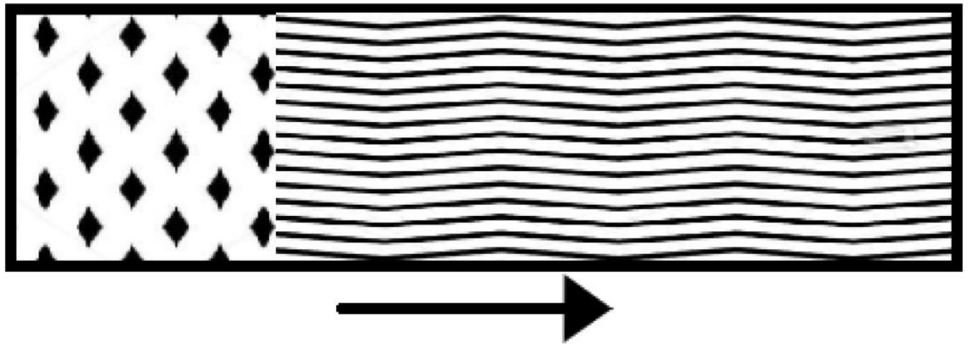
$$\frac{\partial h(x,t)}{\partial t} = \frac{h(x,t+dt) - h(x,t-dt)}{2dt}$$

  - Benefit: e.g. increased accuracy, conservative (for a selection of problems),…

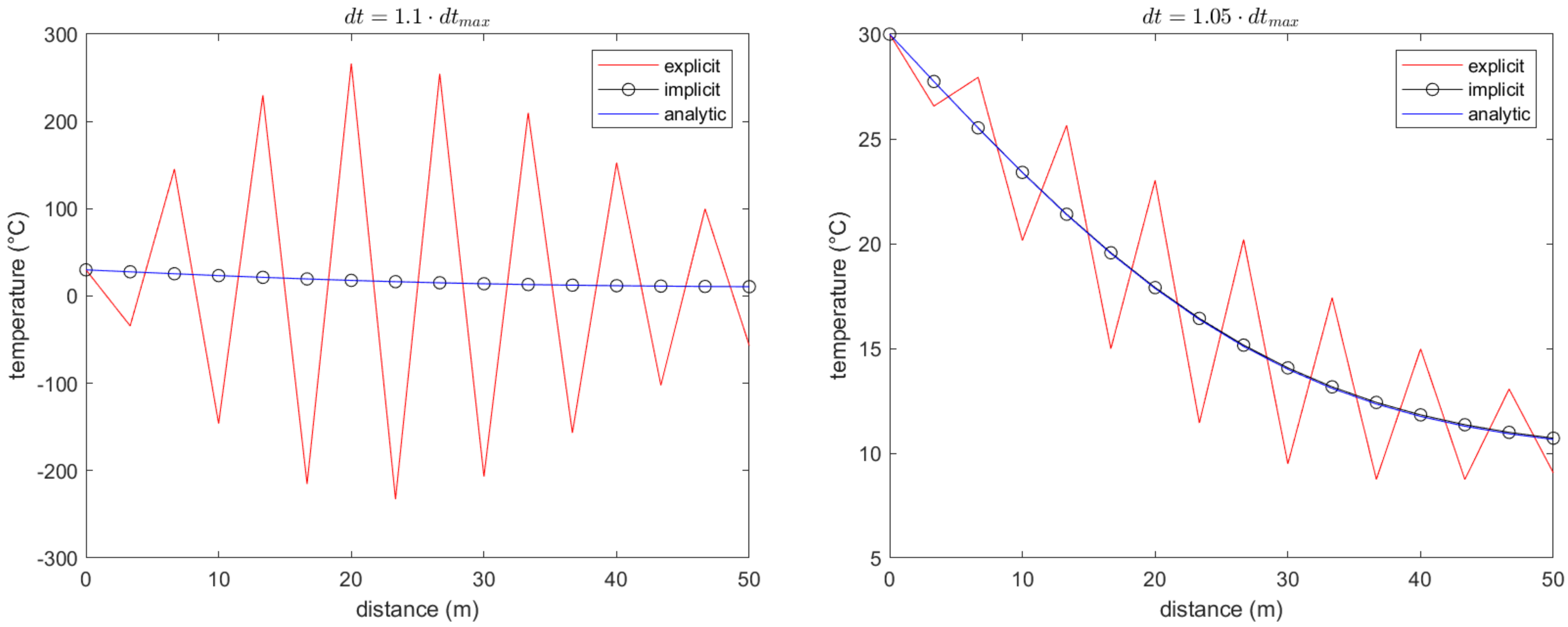
- There are many, many more schemes with benefits/drawbacks!

Example for comparison of explicit/implicit

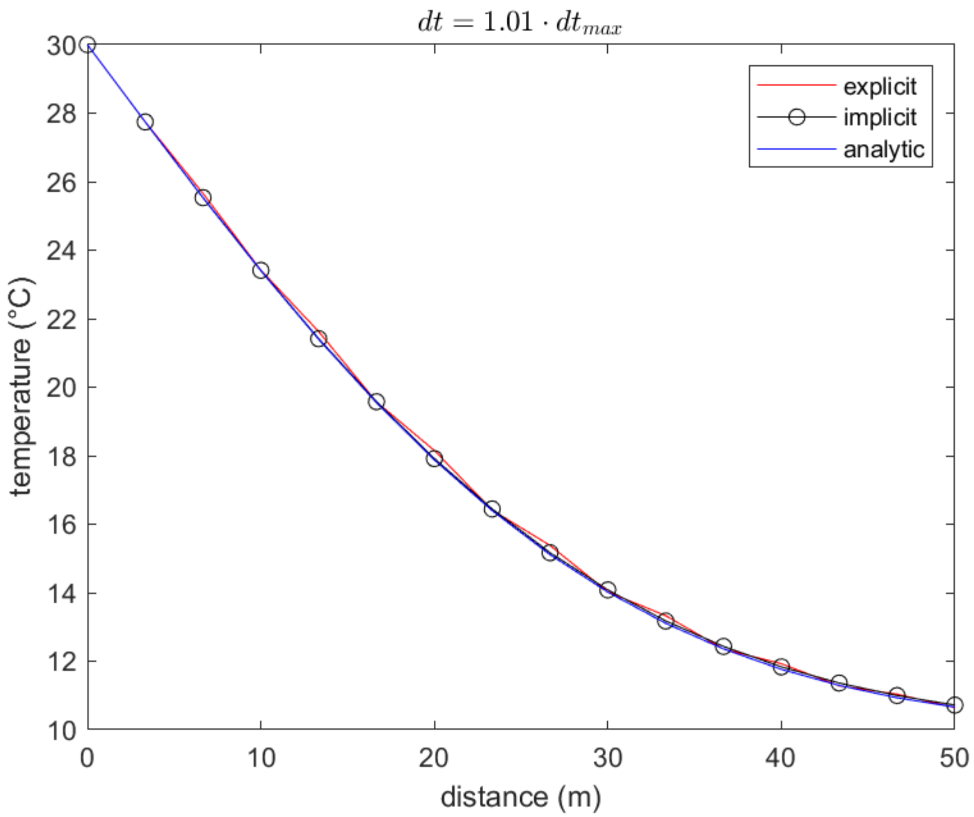
- Scenario:
  - Injection of warm water, e.g., industrial waste heat, into a low permeable aquifer
  - Assume that flow velocity is negligible
  - Homogeneous and isotropic aquifer properties
- Conceptual model:
  - 1D heat diffusion (no advection)

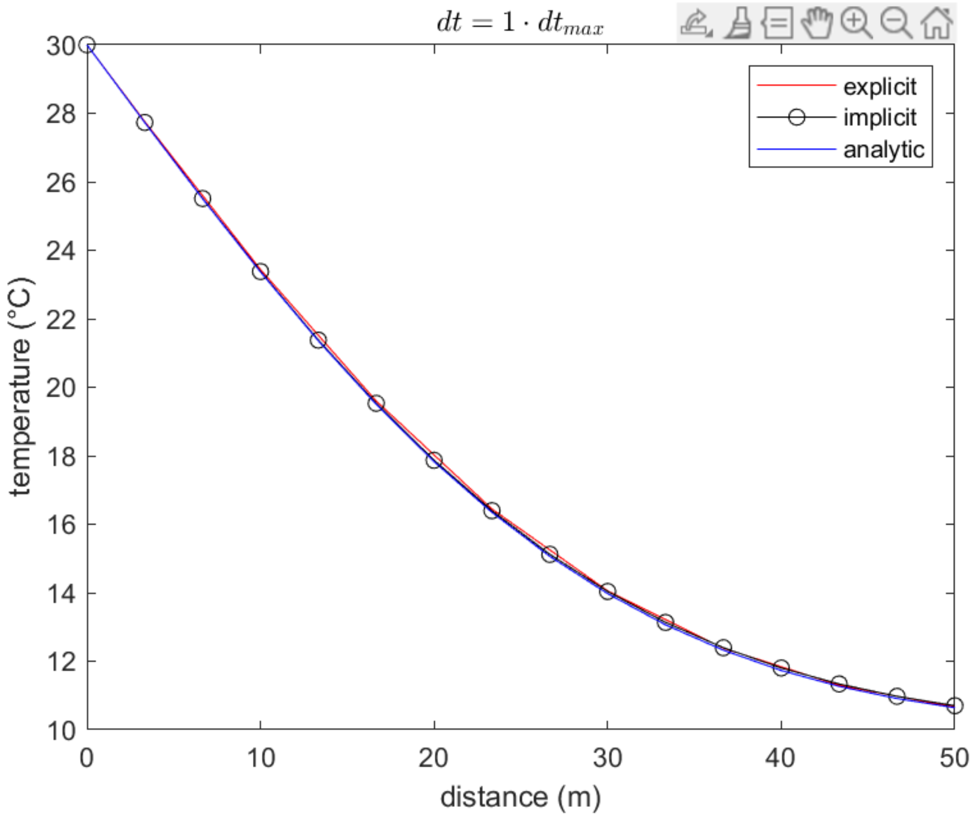


Comparison of explicit/implicit schemes



Comparison of explicit/implicit schemes





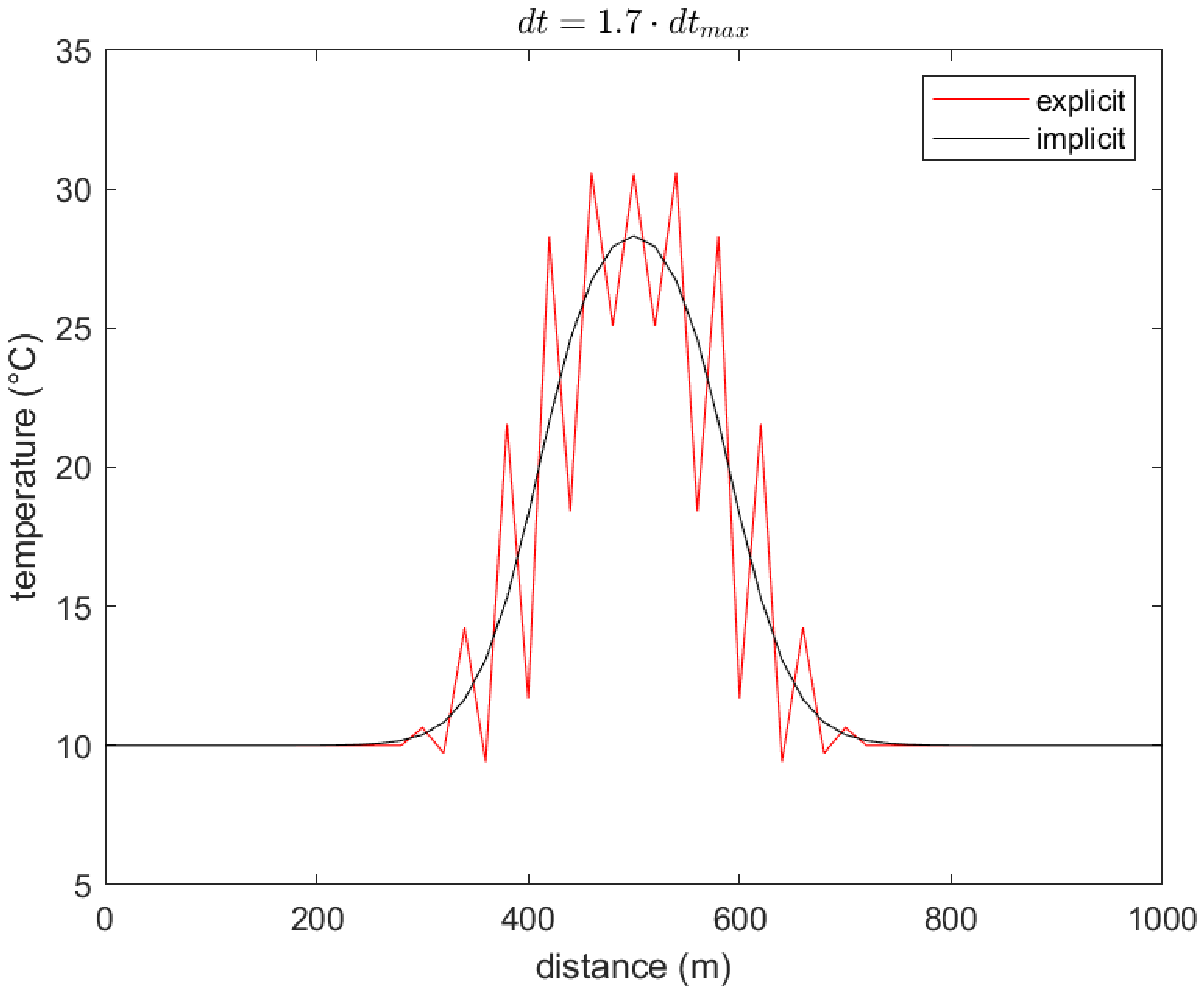
Comparison of explicit/implicit scheme

- Implicit schemes:
    - Unconditionally stable
    - Numerical cumbersome: Requires solution of LSE or finding of roots
- Explicit schemes:
    - Stability might require a very small time step
    - Quick and easy to solve
- Accuracy is independent of chosen scheme!
- There are schemes that are always unstable for different PDE types!

Stability

- During the solution the errors do not become larger
- For transient problems:
  - A stable model produces a bounded solution whenever the exact solution is bounded
- For iterative methods:
  - a stable method converges
- Stability does NOT imply accuracy – although instability implies inaccuracy!

Example of (in)stability



Stability criteria

- There are analytical criteria for stability
- Courant-Friedrich-Levy (CFL) / Courant number (C)

$$C = \frac{u\ dt}{dx} < C_{max}$$

  - With velocity u
  - If C > 1, the information is transported faster than allowed by the characteristics of the system

Example: CFL criteria for diffusion problem

- Use FD forward in time - centered in space scheme

$$h(x, t + dt) = h(x, t) + \frac{Tdt}{Sdx^2}(h(x + dx, t) - 2\,h(x, t) + h(x - dx, t))$$

$$C = \frac{T\,dt}{2\,S\,dx^2} < 1$$

$$dt < \frac{2\,S\,dx^2}{T}$$

Stability concerns

- The allowed time step becomes very small for
  - Large diffusivities
  - Small dx
- Consequence: Smaller dx increases numerical cost
  - Smaller dx = more cells to calculate
  - Smaller dt for stability necessary
- Stability analysis is a wide mathematical field
  - Advanced stability analysis based on eigenvalue analysis of the forward operator
  - Identify approaches that are always unstable for different kinds of PDE

Peclet number

- For advection-diffusion equation (solute/heat transport)

$$Pe = \frac{dx\ v}{D}$$

- Ratio of advection and diffusion
- Stable if Pe < 2 (depending on numerical method)
- If advection dominates, smaller grid size necessary
- Pe also helpful for choice of numerical scheme

Convergence

- Smaller time step / finer grid spacing = the numerical solution approaches a constant value (asymptotically)

- Example: Consider an iterative procedure
  - Termination criteria for iteration: a sufficient small change between iterations

- Convergence error: difference between approached value and numerical solution

Consistency

- Truncation error = the difference between exact and numerical solution
  - Depends on spatial discretization (time and space)

- Consistency = Truncation error approaches zero for dt and dx approaching zero

- In other words: For smaller dt and dx the numerical solution approaches the analytical solution.

Conservativity

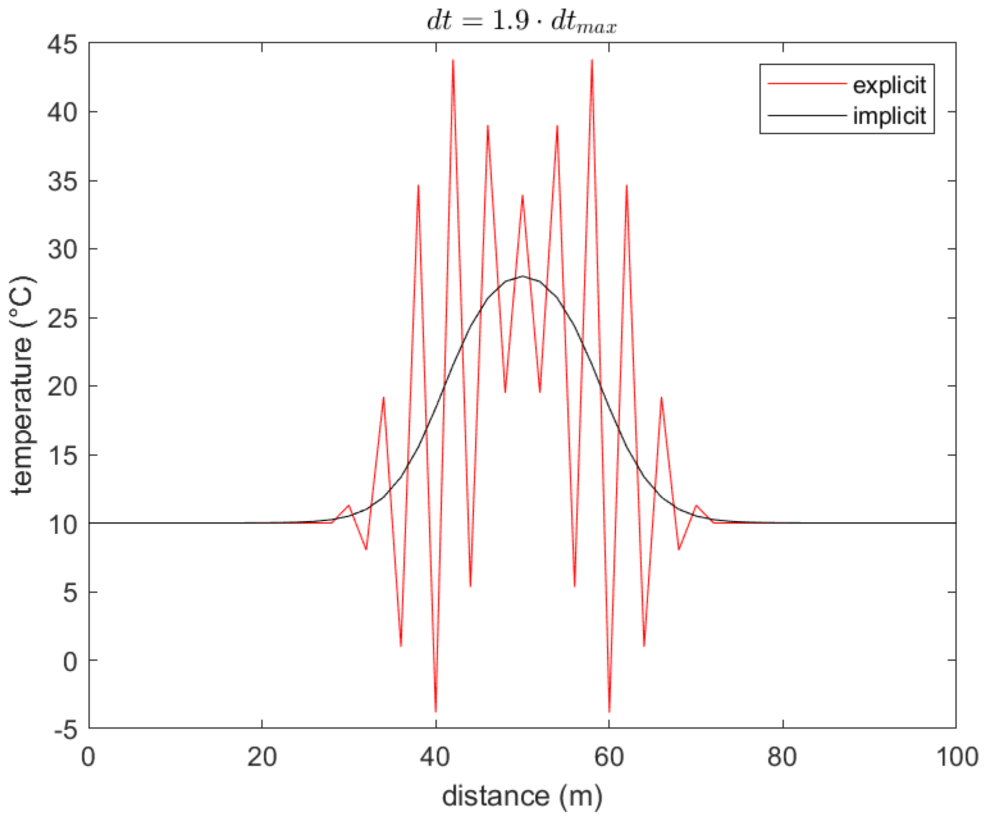
- Model equations represent balance equations for conserving physical quantities.
  - In groundwater flow: Fluid mass, temperature, solute concentration
- The total sum of e.g., mass or energy should always be conserved
- A conservative numerical scheme satisfies this statement on both a local and a global basis

- E.g.: no thermal energy might get lost or generated by the numerical scheme itself

Boundedness

- Numerical solutions should lie within proper bounds.
- Physically non-negative quantities (e.g., density, concentration, absolute temperature) must always be positive.
- Unbounded solutions can occur on too coarse meshes or too large time steps in form of wiggles exhibiting overshoots and undershoots of the solution.
- Wiggles are usually a signal that the spatial discretization is too coarse, and some refinements (at least locally) are required
- **Boundedness is a easy self-diagnosis property!**

Example for (violated) boundedness



Error sources

- Modeling error = errors embedded in the conceptual model
  - Cause: assumptions and simplifications made
  - Consequence: even if solved exactly, the solution is not a correct representation of reality.
- Discretization error = resulting from the use of numerical methods
  - Depending on numerical method and scheme used
  - More accurate approximations can dramatically increase numerical costs

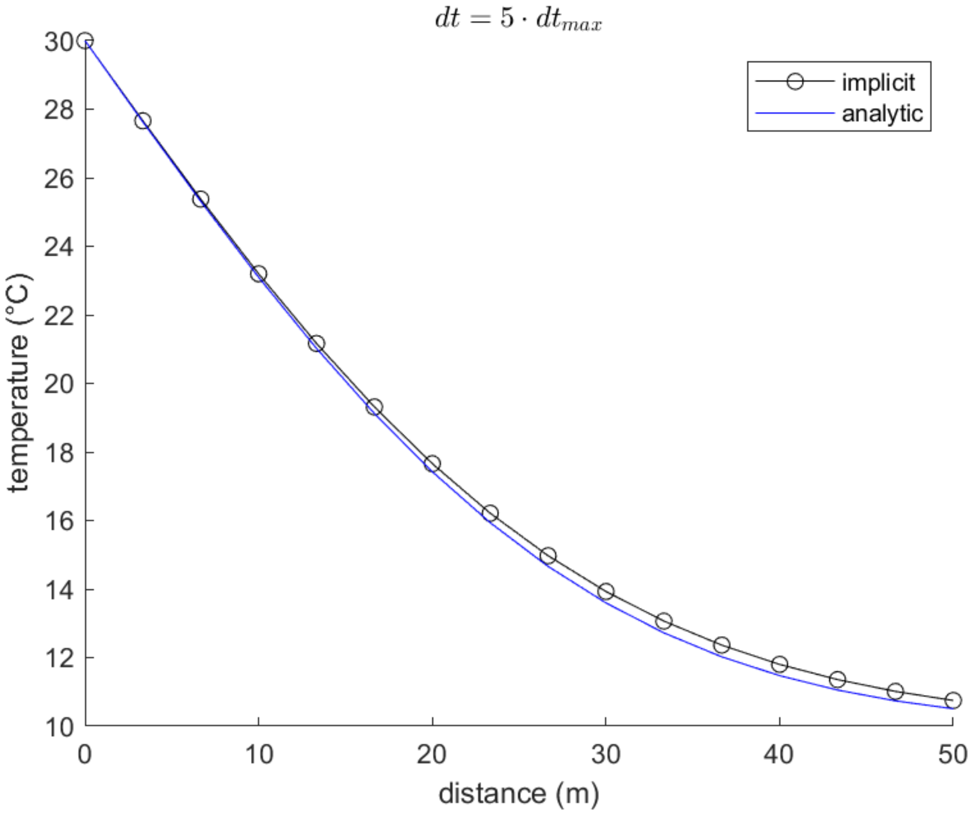
Accuracy

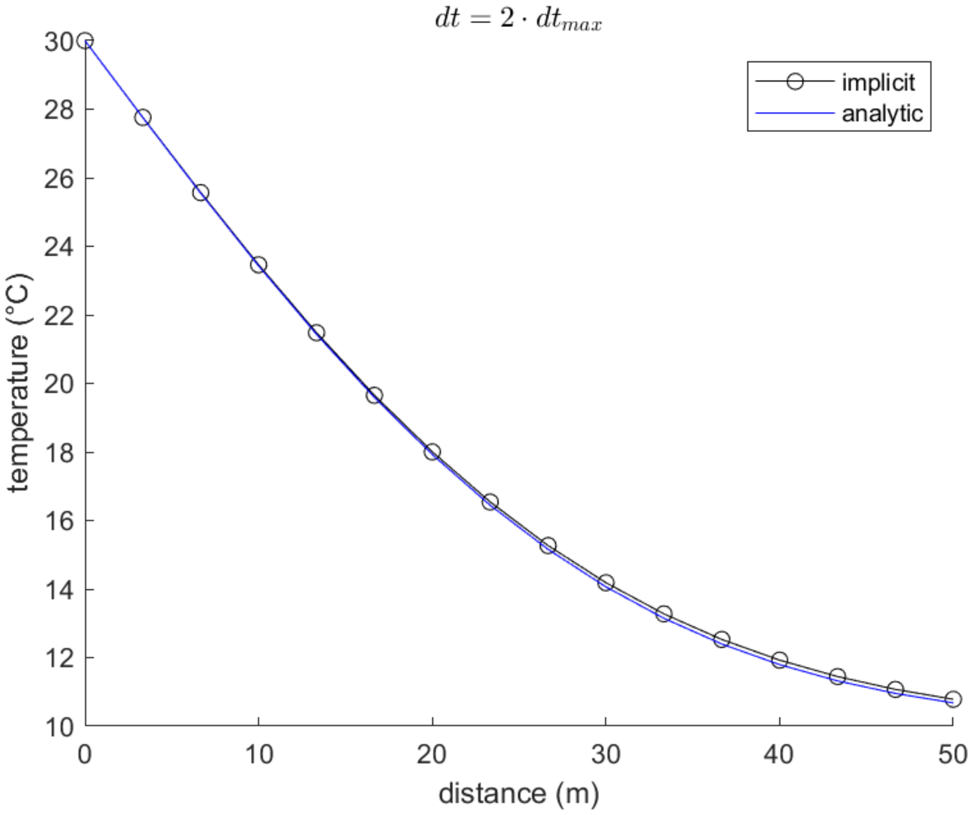
- A scheme works accurately if both the discretization and the convergence errors remain sufficiently small
- Modeling errors are an additional concern
- Errors may cancel each other
  - A solution obtained on a coarse mesh may agree much better with the experiment than on a finer mesh

Accuracy and validity

- Validity:
  - Are you solving the right equations for the specific problem?
- Accuracy:
  - Are the equations approximated corrected?
- Numerical simulations are always APPROXIMATIONS!

Example: Accuracy depending on time step





Catching errors

- Verification: compare with analytical solution
- Benchmark: compare basic model with other numerical solutions of accepted quality
- Validation: comparison with high quality experimental data

- Multiple sources:
  - E.g., improper model equations, wrong parameters, inconsistent boundary/initial conditions
- Measurements can possess their own errors (in lab and field).
- There is no sense in reducing the modeling error below the level of measurement accuracy.

Lessons learned

- Definition of stability and effects of instability
- Calculation stability criteria (CFL, Pe)
- Definitions of different properties of a numerical model
- Detection of violation of some properties