

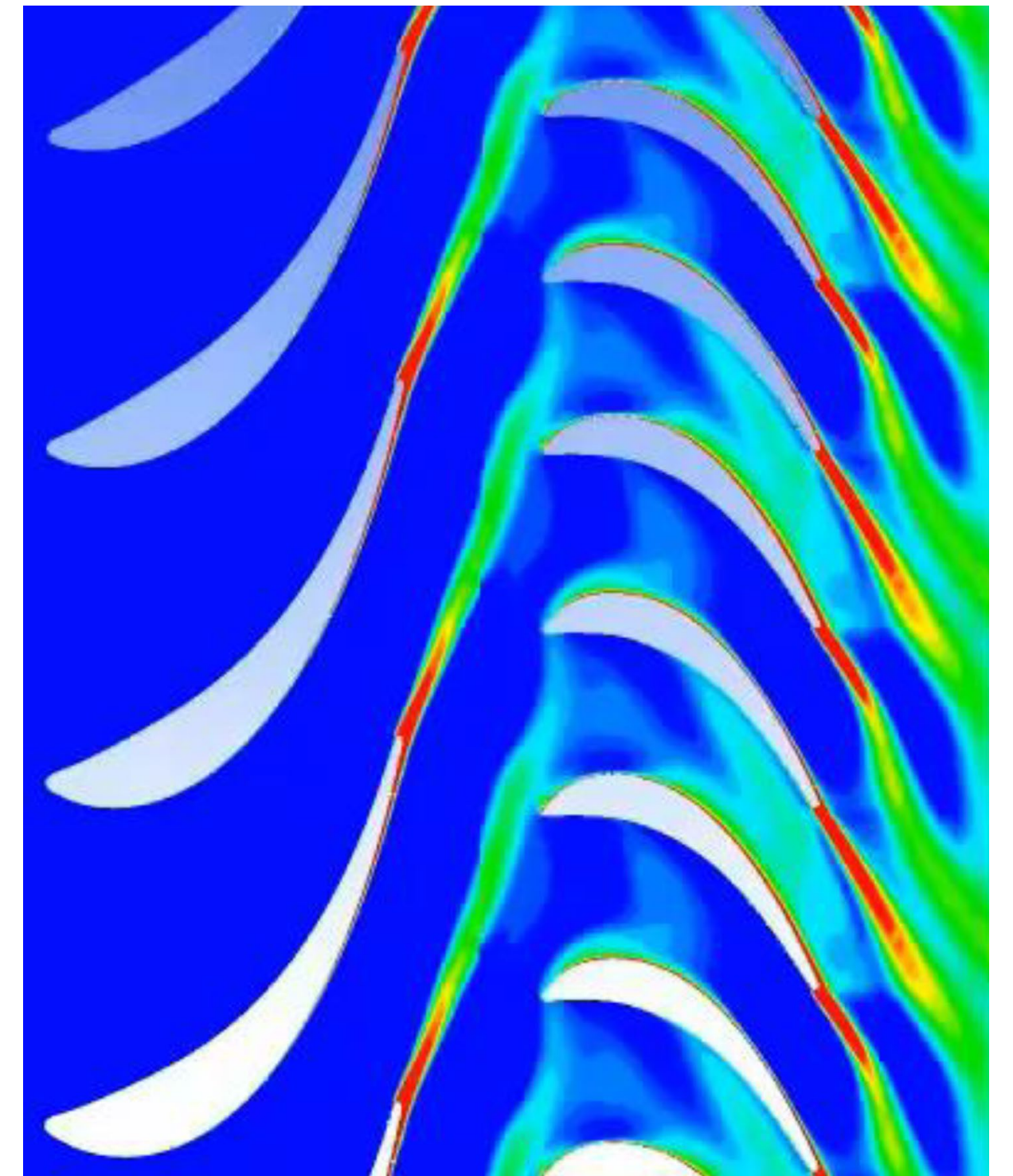
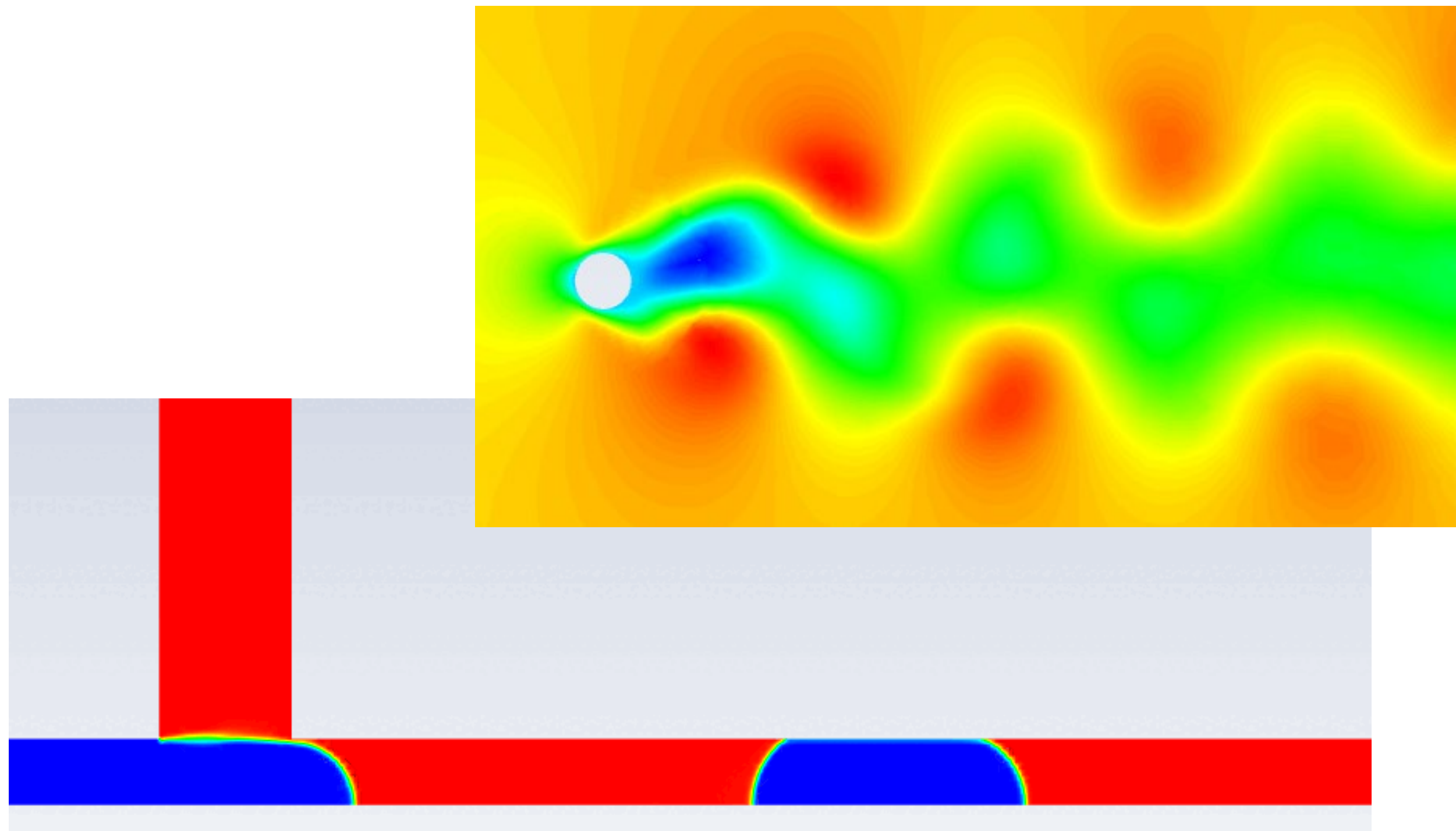
Time integration

Numerical Flow Simulation

Unsteady flows

- Ubiquitous in nature and engineering: instabilities, moving or deforming boundaries, natural convection, multiphase flows, turbulent flows...

Numerical Flow Simulation

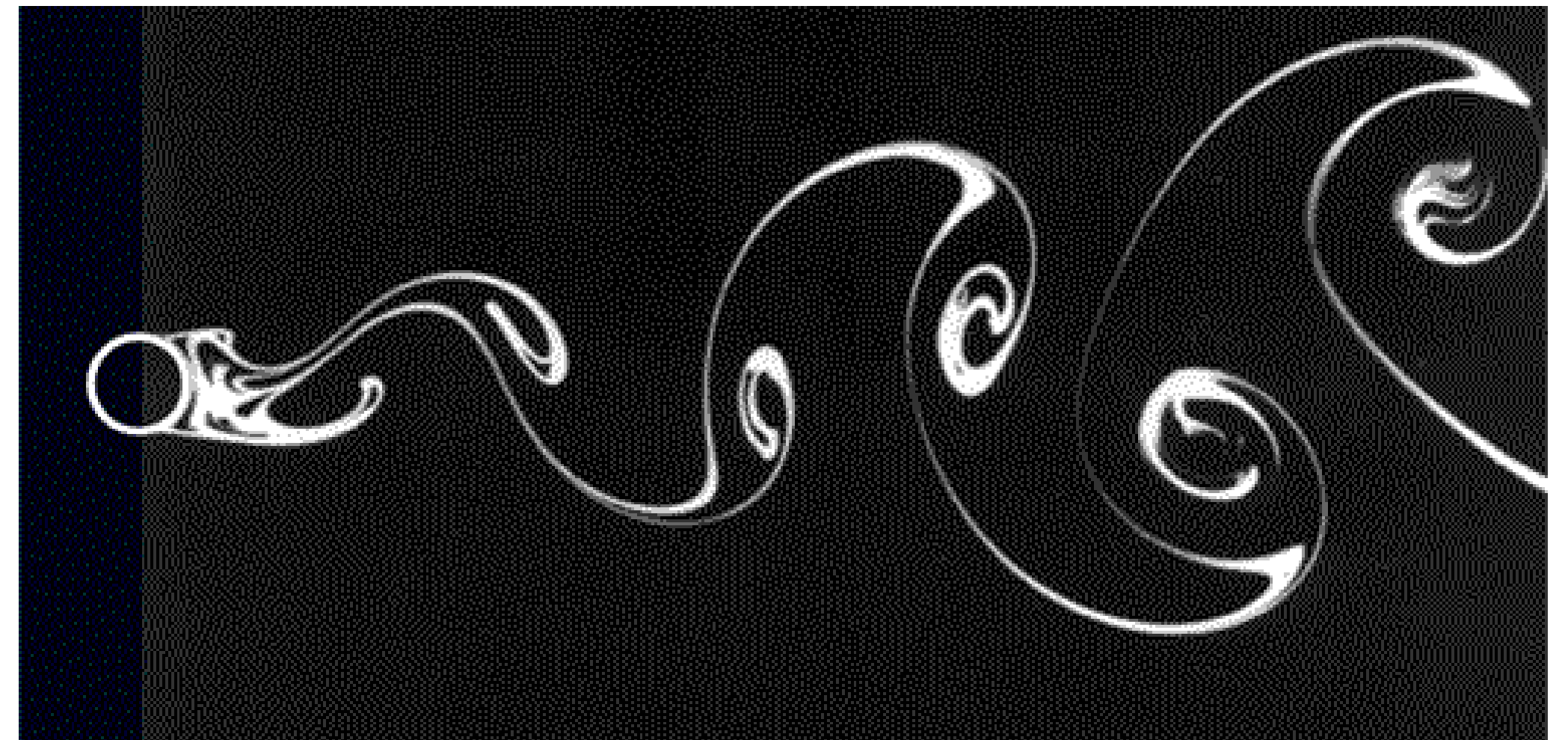


Unsteady flows

- Need to integrate the equations in time.



Steady flow: solution $\mathbf{u}(\mathbf{x})$, $p(\mathbf{x})$
depends on space only.



Unsteady flow: solution $\mathbf{u}(\mathbf{x},t)$, $p(\mathbf{x},t)$
depends on both space and time.

Simple “model” equations

- General conservation equation:

$$\boxed{\frac{\partial(\rho\phi)}{\partial t}} + \boxed{div(\rho\phi\mathbf{u})} = \boxed{div(\Gamma grad(\phi))} + \boxed{S}$$

unsteadiness convection diffusion source

- Steady/unsteady diffusion:

$$\boxed{\frac{\partial(\rho\phi)}{\partial t}} = \boxed{div(\Gamma grad(\phi))} + S = 0$$

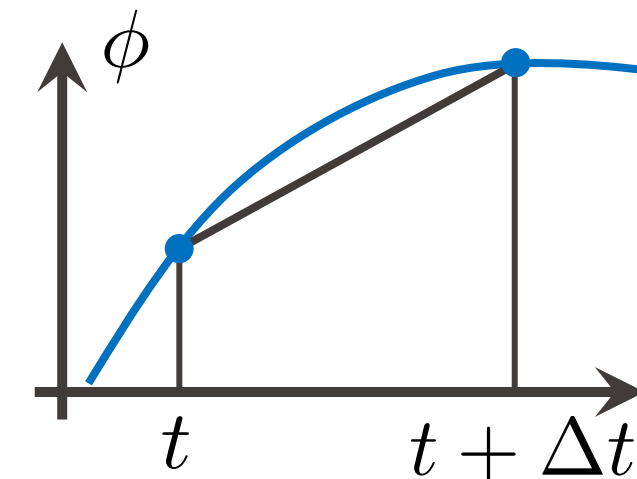
- Steady convection-diffusion, unsteady convection:

$$\boxed{\frac{\partial(\rho\phi)}{\partial t}} + \boxed{div(\rho\phi\mathbf{u})} = \boxed{div(\Gamma grad(\phi))}$$

Reminder: ordinary differential equations (ODE)

- Unknown $\phi(t)$ depends on **time only**. The RHS may depend explicitly on time, and may be nonlinear in ϕ :

$$\frac{d\phi}{dt} = f(t, \phi) \quad \phi(0) = \phi_0$$



- Simplest methods: linear approximation of time derivative: $\frac{d\phi}{dt} \approx \frac{\phi^{n+1} - \phi^n}{\Delta t}$

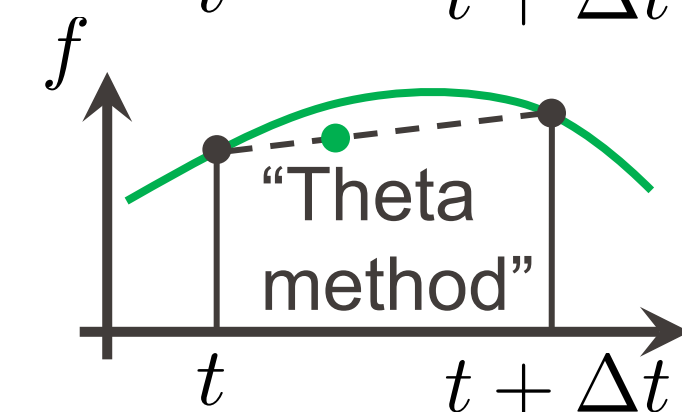
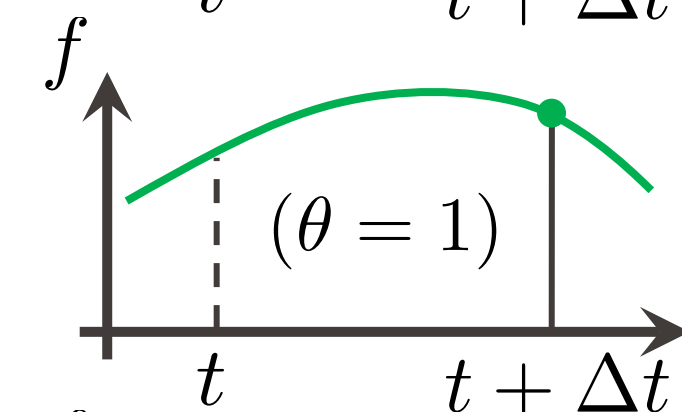
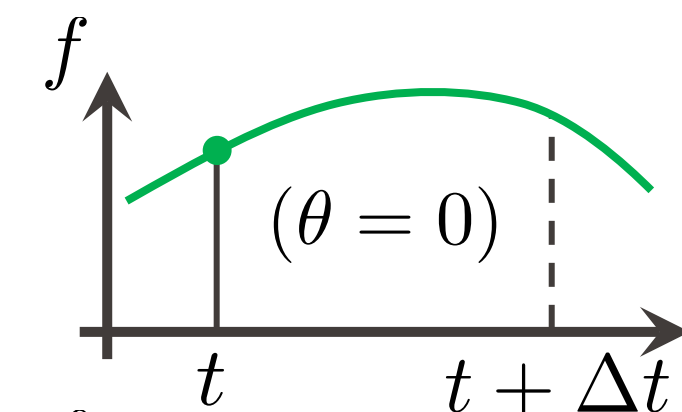
- Can evaluate the RHS at different times:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = f^n \Rightarrow \phi^{n+1} = \phi^n + \Delta t f^n$$

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = f^{n+1} \Rightarrow \phi^{n+1} = \phi^n + \Delta t f^{n+1}$$

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \theta f^{n+1} + (1 - \theta) f^n \Rightarrow \phi^{n+1} = \phi^n + \Delta t (\theta f^{n+1} + (1 - \theta) f^n)$$

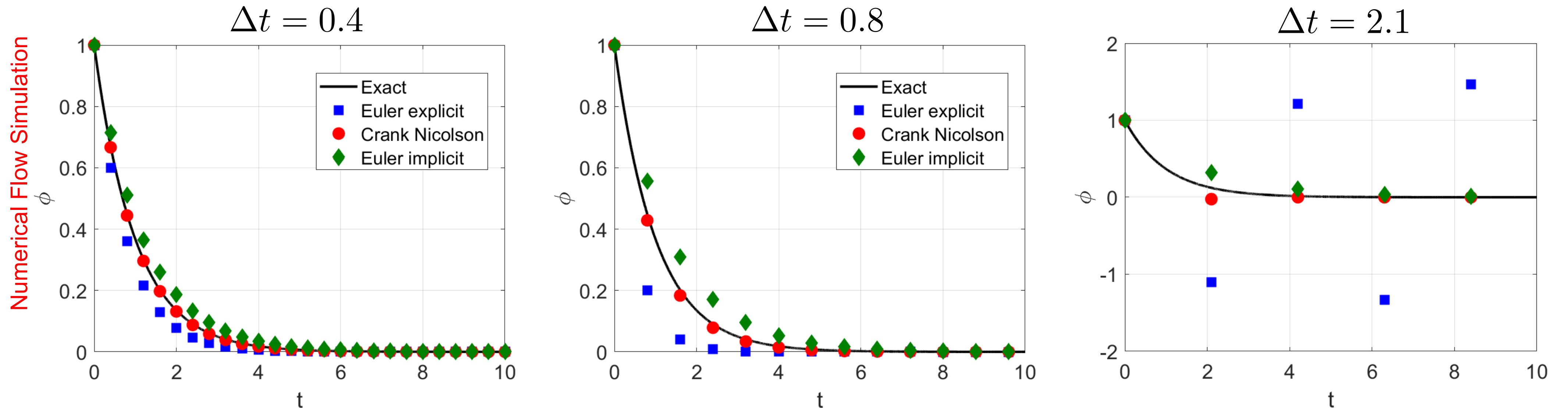
- If $\theta \neq 0$, must solve an **implicit** equation.



Reminder: ordinary differential equations (ODE)

- **Explicit Euler** (“forward Euler”): 1st-order accurate; can be unstable
- **Implicit Euler** (“backward Euler”): 1st-order accurate; unconditionally stable
- **Crank-Nicolson** ($\theta = 1/2$): 2nd-order accurate; unconditionally stable

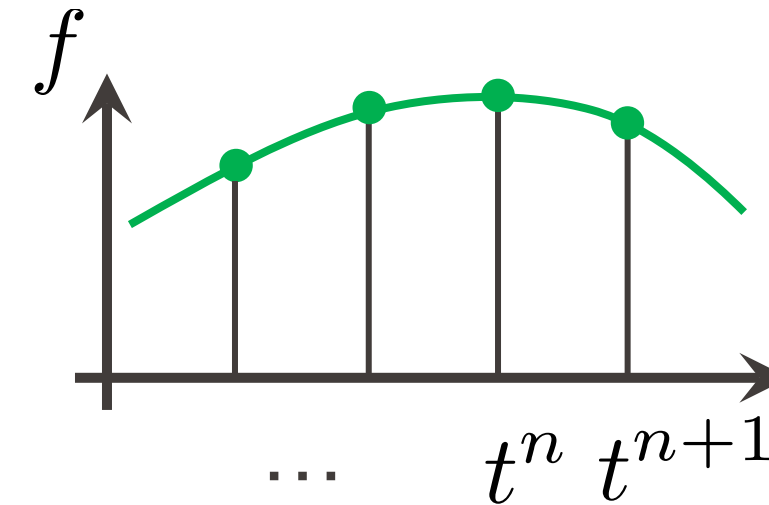
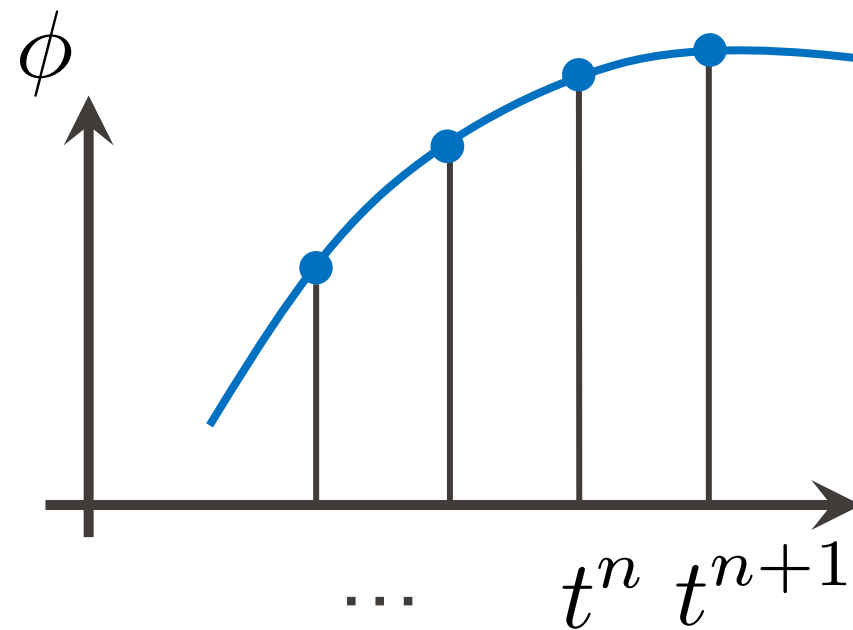
- Example: $\frac{d\phi}{dt} = -\phi \quad \rightarrow \quad \phi(t) = \phi_0 e^{-t}$



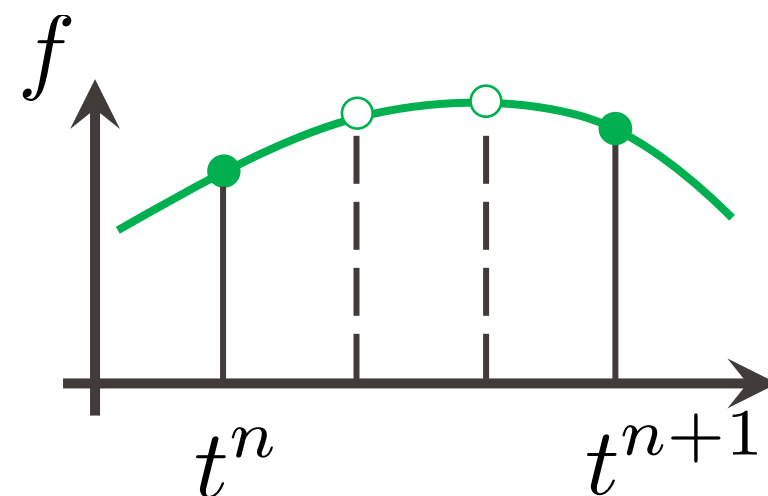
Reminder: ordinary differential equations (ODE)

- Other families of methods:

- 1. Linear multistep methods:** use more than 1 previous time step



- 2. Multistage methods:** evaluate f at intermediate stages between t and $t + \Delta t$



Reminder: ordinary differential equations (ODE)

1. **Linear multistep methods:** a s -step method uses the known solution at s previous time steps

$$\alpha_0 \phi^{n+1} + \alpha_1 \phi^n + \alpha_2 \phi^{n-1} \dots + \alpha_s \phi^{n+1-s} = \Delta t (\beta_0 f^{n+1} + \beta_1 f^n + \beta_2 f^{n-1} \dots + \beta_s f^{n+1-s})$$

- **Implicit** if $\beta_0 \neq 0$

- Adams family: LHS always $\frac{\phi^{n+1} - \phi^n}{\Delta t}$, i.e. $\alpha_0 = 1, \quad \alpha_1 = -1, \quad \alpha_j = 0 \quad \forall j > 1$

- Adams-Bashforth: explicit, accuracy s
- Adams-Moulton: implicit, accuracy $s+1$

- Backward-differentiation formula (BDF) family: RHS always f^{n+1} , i.e. $\beta_0 = 1, \quad \beta_j = 0 \quad \forall j > 1$

- Implicit, accuracy s

Reminder: ordinary differential equations (ODE)

1. Linear multistep methods

$$\alpha_0 \phi^{n+1} + \alpha_1 \phi^n + \alpha_2 \phi^{n-1} \dots + \alpha_s \phi^{n+1-s} = \Delta t \left(\beta_0 f^{n+1} + \beta_1 f^n + \beta_2 f^{n-1} \dots + \beta_s f^{n+1-s} \right)$$

Adams-Bashforth

s	accuracy	β_1	β_2	β_3	β_4
1	1	1			
2	2	3/2	-1/2		
3	3	23/12	-16/12	5/12	
4	4	55/24	-59/24	37/24	-9/24

(Explicit Euler)

Adams-Moulton

s	accuracy	β_0	β_1	β_2	β_3
0	1	1			
1	2	1/2	1/2		
2	3	5/12	8/12	-1/12	
3	4	9/24	19/24	-5/24	1/24

(Implicit Euler)

(Crank-Nicolson)

BDF

s	accuracy	α_0	α_1	α_2	α_3	α_4	β_0
1	1	1	-1				1
2	2	1	-4/3	1/3			2/3
3	3	1	-18/11	9/11	-2/11		6/11
4	4	1	-48/25	36/25	-16/25	3/25	12/25

(Implicit Euler)

Reminder: ordinary differential equations (ODE)

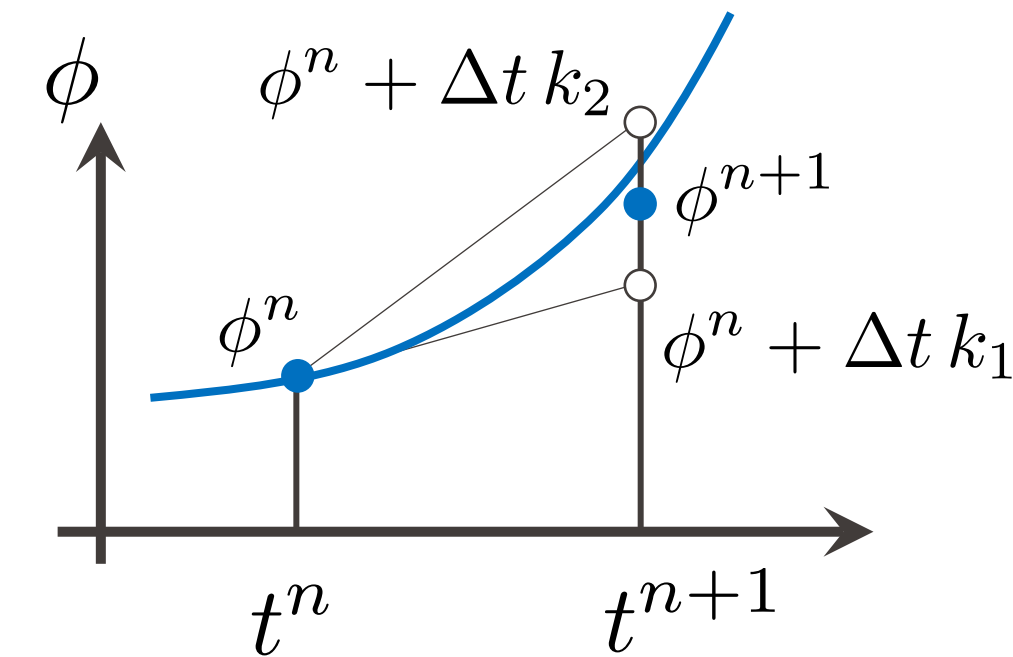
2. Multistage methods

- Most famous: explicit Runge-Kutta
 - RK2 (2nd-order accurate, 2 evaluations of the RHS per time step): estimate the new solution with the current slope
→ recompute the slope using this estimate → correct the estimate

$$\phi^{n+1} = \phi^n + \Delta t \frac{k_1 + k_2}{2}$$

$$k_1 = f(t^n, \phi^n)$$

$$k_2 = f(t^n + \Delta t, \phi^n + \Delta t k_1)$$



- RK4 (4th-order accurate, 4 evaluations of the RHS per time step): same idea, with intermediate values at time interval midpoint

$$\phi^{n+1} = \phi^n + \Delta t \frac{k_1 + 2k_2 + 2k_3 + k_4}{6}$$

$$k_1 = f(t^n, \phi^n)$$

$$k_2 = f\left(t^n + \frac{\Delta t}{2}, \phi^n + \frac{\Delta t}{2} k_1\right)$$

$$k_3 = f\left(t^n + \frac{\Delta t}{2}, \phi^n + \frac{\Delta t}{2} k_2\right)$$

$$k_4 = f(t^n + \Delta t, \phi^n + \Delta t k_3)$$

- More stable than explicit multistep methods, but more expensive per time step. 10

Partial differential equations (PDE)

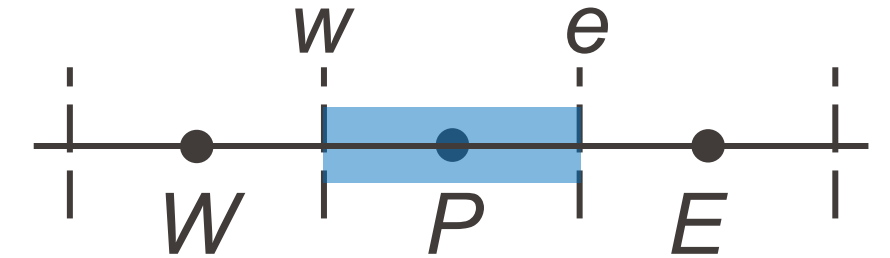
- Now the unknown $\phi(\mathbf{x}, t)$ depends on both **time and space**.
- The time-marching problem looks qualitatively similar, because spatial discretization turns the PDE into an ODE in time:

$$\left. \begin{aligned} \frac{\partial(\rho\phi)}{\partial t} + \text{div}(\rho\phi\mathbf{u}) &= \text{div}(\Gamma \text{grad}(\phi)) + S \\ \phi(\mathbf{x}, t) &\rightarrow \boldsymbol{\phi}(t) = (\phi_1(t), \phi_2(t) \dots) \end{aligned} \right\} \rightarrow \frac{\partial \boldsymbol{\phi}}{\partial t} = \mathbf{A}(\boldsymbol{\phi})$$

- However, not so simple: small spatial errors at each time step can accumulate and compromise accuracy / stability.

Unsteady 1D diffusion

$$\frac{\partial(\rho\phi)}{\partial t} = \frac{\partial}{\partial x} \left(\Gamma \frac{\partial\phi}{\partial x} \right)$$



- Assume the density is constant.
- Integration over CV, with CD scheme for diffusion term:

$$\rho \int_{x_w}^{x_e} \frac{\partial\phi}{\partial t} dx \approx \rho \frac{\partial\phi_P}{\partial t} \Delta x = \left(\Gamma \frac{\partial\phi}{\partial x} \right)_e - \left(\Gamma \frac{\partial\phi}{\partial x} \right)_w \approx \Gamma_e \frac{\phi_E - \phi_P}{\delta x_{PE}} - \Gamma_w \frac{\phi_P - \phi_W}{\delta x_{WP}}$$

- Linear approximation of the time derivative, theta method for the RHS:

$$\rho \frac{\phi_P^{n+1} - \phi_P^n}{\Delta t} \Delta x = \theta \left[\Gamma_e \frac{\phi_E^{n+1} - \phi_P^{n+1}}{\delta x_{PE}} - \Gamma_w \frac{\phi_P^{n+1} - \phi_W^{n+1}}{\delta x_{WP}} \right] + (1-\theta) \left[\Gamma_e \frac{\phi_E^n - \phi_P^n}{\delta x_{PE}} - \Gamma_w \frac{\phi_P^n - \phi_W^n}{\delta x_{WP}} \right]$$

- Algebraic equation for ϕ^{n+1} : $a_P \phi_P^{n+1} = a_W \phi_W^{n+1} + a_E \phi_E^{n+1} + b(\phi^n)$

- Assemble the system and march in time:

$$\mathbf{A} \phi^{n+1} = \mathbf{b}(\phi^n) \quad \rightarrow \quad \phi^{n+1} = \mathbf{A}^{-1} \mathbf{b}(\phi^n)$$

Unsteady 1D diffusion

- Algebraic equation: $a_P \phi_P^{n+1} = a_W \phi_W^{n+1} + a_E \phi_E^{n+1} + b(\phi^n)$

$$a_P = \frac{\rho \Delta x}{\Delta t} + \frac{\theta \Gamma_e}{\delta x_{PE}} + \frac{\theta \Gamma_w}{\delta x_{WP}} \quad a_E = \frac{\theta \Gamma_e}{\delta x_{PE}} \quad a_W = \frac{\theta \Gamma_w}{\delta x_{WP}}$$

$$b = \left(\frac{\rho \Delta x}{\Delta t} - \frac{(1-\theta)\Gamma_w}{\delta x_{WP}} - \frac{(1-\theta)\Gamma_e}{\delta x_{PE}} \right) \phi_P^n + \left(\frac{(1-\theta)\Gamma_e}{\delta x_{PE}} \right) \phi_E^n + \left(\frac{(1-\theta)\Gamma_w}{\delta x_{WP}} \right) \phi_W^n$$

- Explicit Euler** ($\theta = 0$):

$$a_P = \frac{\rho \Delta x}{\Delta t}, \quad a_W = 0, \quad a_E = 0$$

Each CV decoupled from neighbors.
No need to solve a system!

$$b = \left(\frac{\rho \Delta x}{\Delta t} - \frac{\Gamma_w}{\delta x_{WP}} - \frac{\Gamma_e}{\delta x_{PE}} \right) \phi_P^n + \left(\frac{\Gamma_e}{\delta x_{PE}} \right) \phi_E^n + \left(\frac{\Gamma_w}{\delta x_{WP}} \right) \phi_W^n$$

Boundedness criterion: all coefficients should have the same sign. Here, if uniform grid and constant Γ : $\Delta t < \frac{\rho(\Delta x)^2}{2\Gamma}$

ϕ_W^{n+1}	ϕ_P^{n+1}	ϕ_E^{n+1}
ϕ_W^n	ϕ_P^n	ϕ_E^n

Unsteady 1D diffusion

Each CV coupled to neighbors.

- **Crank-Nicolson** ($\theta = 1/2$):

Must solve a linear system at each iteration!

$$a_P = \frac{\rho\Delta x}{\Delta t} + \frac{\Gamma_e}{2\delta x_{PE}} + \frac{\Gamma_w}{2\delta x_{WP}}, \quad a_W = \frac{\Gamma_w}{2\delta x_{WP}}, \quad a_E = \frac{\Gamma_e}{2\delta x_{PE}}$$

$$b = \left(\frac{\rho\Delta x}{\Delta t} - \frac{\Gamma_w}{2\delta x_{WP}} - \frac{\Gamma_e}{2\delta x_{PE}} \right) \phi_P^n + \left(\frac{\Gamma_e}{2\delta x_{PE}} \right) \phi_E^n + \left(\frac{\Gamma_w}{2\delta x_{WP}} \right) \phi_W^n$$

Similar **boundedness criterion**: $\Delta t < \frac{\rho(\Delta x)^2}{\Gamma}$

- **Implicit Euler** ($\theta = 1$):

$$a_P = \frac{\rho\Delta x}{\Delta t} + \frac{\Gamma_e}{\delta x_{PE}} + \frac{\Gamma_w}{\delta x_{WP}}, \quad a_W = \frac{\Gamma_w}{\delta x_{WP}}, \quad a_E = \frac{\Gamma_e}{\delta x_{PE}}$$

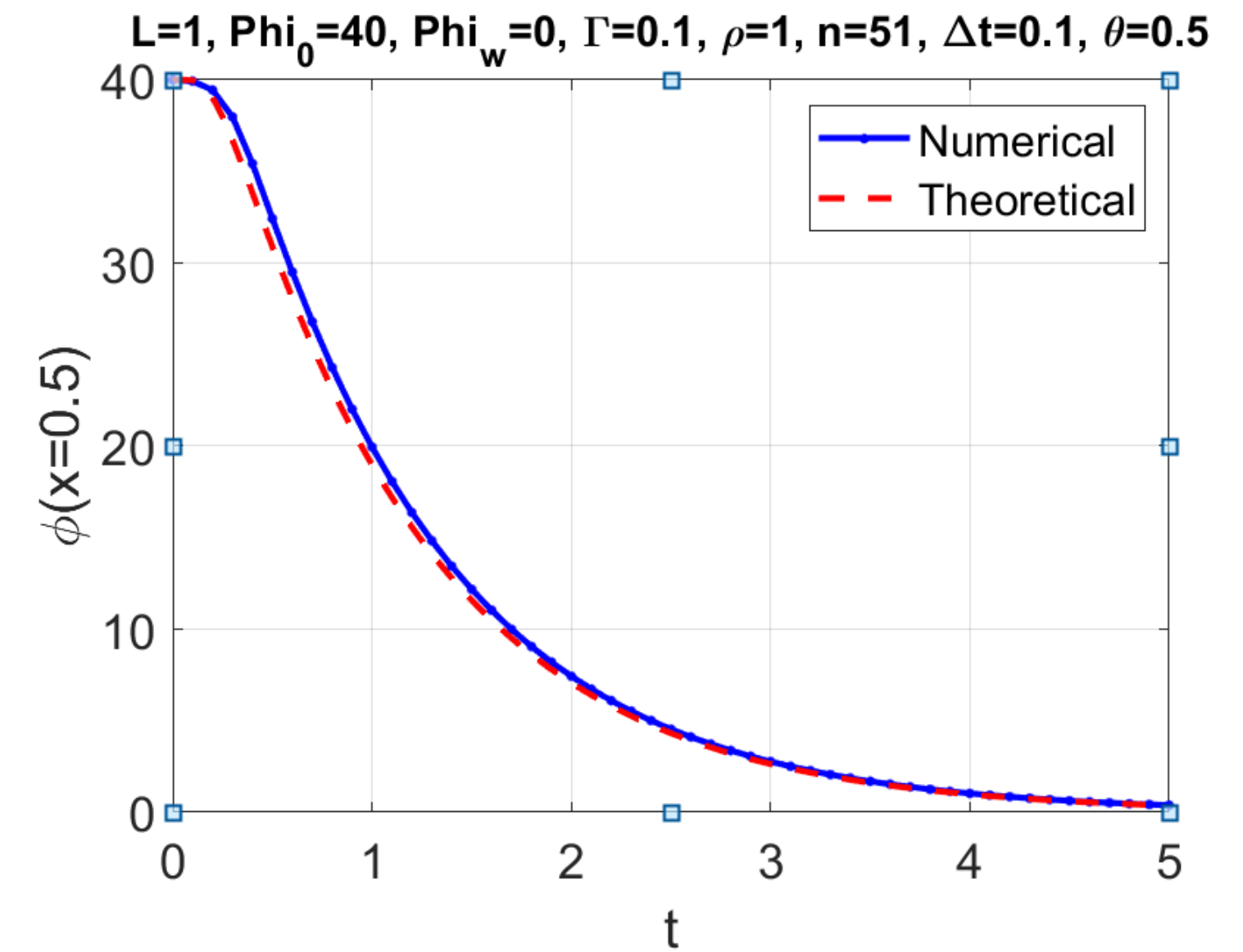
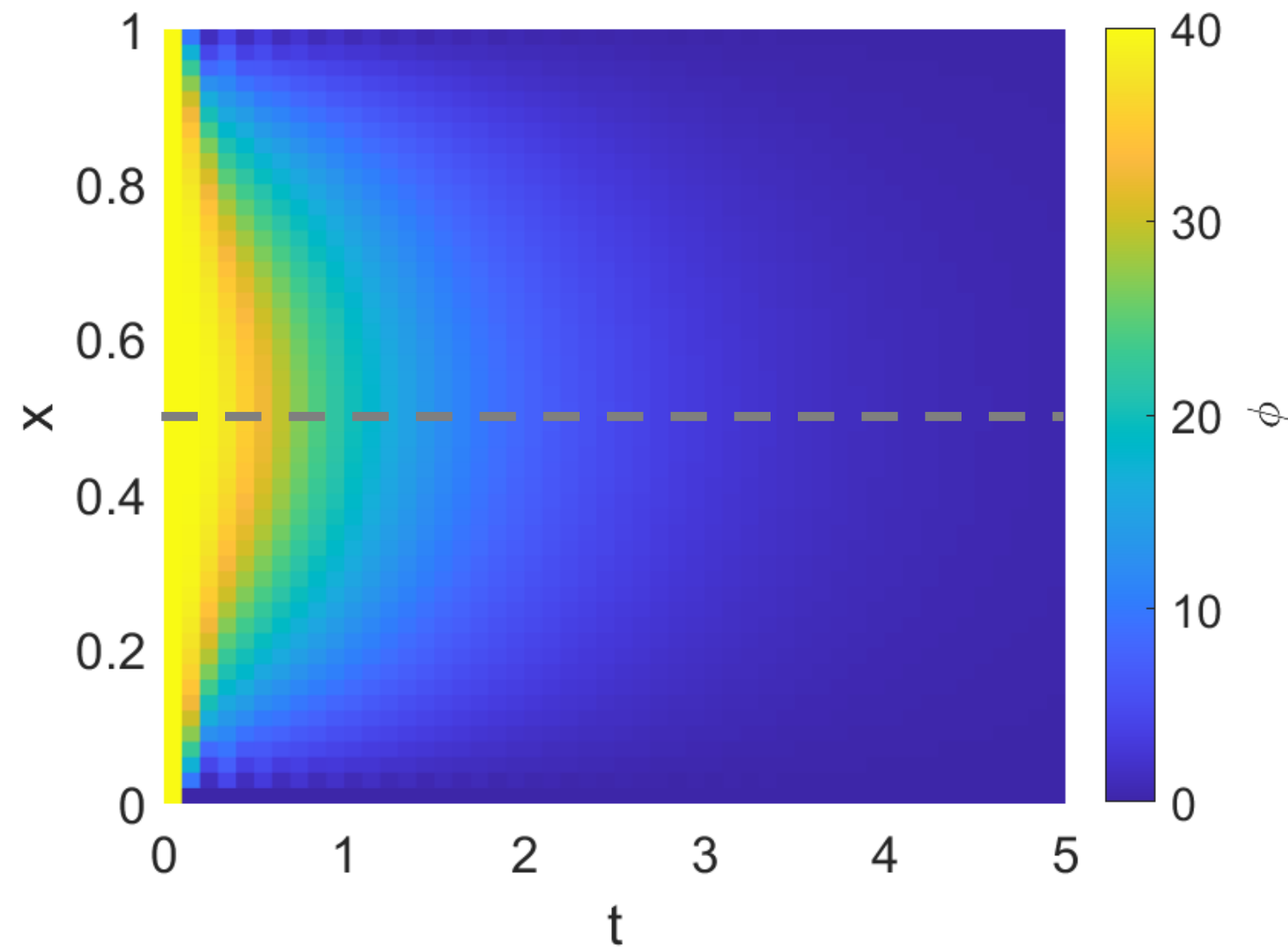
$$b = \left(\frac{\rho\Delta x}{\Delta t} \right) \phi_P^n$$

All coefficients always positive.

Unsteady 1D diffusion

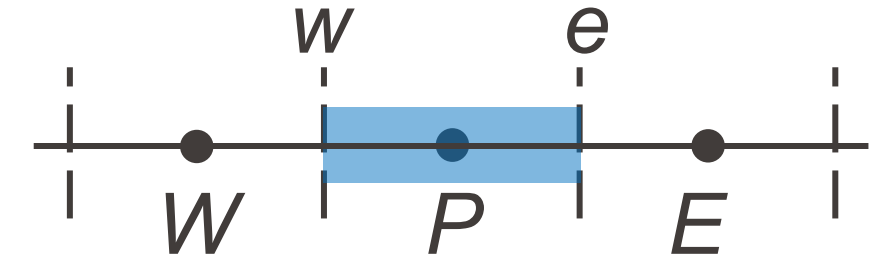
- Example

$$\rho=1, \Gamma=0.1$$



Unsteady 1D convection

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho\phi u)}{\partial x} = 0$$



- Assume the density and velocity are known.
- Integration over CV, with UD scheme for convection term ($u > 0$):

$$\rho \int_{x_w}^{x_e} \frac{\partial \phi}{\partial t} dx + (\rho\phi u)_e - (\rho\phi u)_w \approx \rho \frac{\partial \phi_P}{\partial t} \Delta x + (\rho u)_e \phi_P - (\rho u)_w \phi_W = 0$$

- Linear approximation of the time derivative, theta method for the RHS:

$$\rho \frac{\phi_P^{n+1} - \phi_P^n}{\Delta t} \Delta x + \theta [(\rho u)_e \phi_P^{n+1} - (\rho u)_w \phi_W^{n+1}] + (1-\theta) [(\rho u)_e \phi_P^n - (\rho u)_w \phi_W^n] = 0$$

- Algebraic equation for ϕ^{n+1} : $a_P \phi_P^{n+1} = a_W \phi_W^{n+1} + b(\phi^n)$

- Assemble the system and march in time:

$$\mathbf{A} \phi^{n+1} = \mathbf{b}(\phi^n) \rightarrow \phi^{n+1} = \mathbf{A}^{-1} \mathbf{b}(\phi^n)$$

Unsteady 1D convection

- Algebraic equation: $a_P \phi_P^{n+1} = a_W \phi_W^{n+1} + b(\phi^n)$

$$a_P = \left(\frac{\rho_P \Delta x}{\Delta t} + \theta (\rho u)_e \right), \quad a_W = \theta (\rho u)_w$$

$$b = \left[\frac{\rho_P \Delta x}{\Delta t} - (1 - \theta) (\rho u)_e \right] \phi_P^n + (1 - \theta) (\rho u)_w \phi_W^n$$

- Explicit Euler** ($\theta = 0$):

$$a_P = \frac{\rho_P \Delta x}{\Delta t}, \quad \boxed{a_W = 0} \quad \begin{array}{l} \text{Each CV decoupled from neighbors.} \\ \text{No need to solve a system.} \end{array}$$

$$b = \boxed{\left[\frac{\rho_P \Delta x}{\Delta t} - (\rho u)_e \right]} \phi_P^n + (\rho u)_w \phi_W^n$$

Boundedness criterion: all coefficients should have the same sign. Here, if constant density:

$$\Delta t < \frac{\Delta x}{u}$$

Courant–Friedrichs–Lewy (CFL) condition

Unsteady 1D convection

- **Crank-Nicolson** ($\theta = 1/2$):

$$a_P = \left(\frac{\rho_P \Delta x}{\Delta t} + \frac{1}{2} (\rho u)_e \right), \quad a_W = \frac{1}{2} (\rho u)_w$$

$$b = \left[\frac{\rho_P \Delta x}{\Delta t} - \frac{1}{2} (\rho u)_e \right] \phi_P^n + \frac{1}{2} (\rho u)_w \phi_W^n$$

Similar **boundedness criterion**: $\Delta t < 2 \frac{\Delta x}{u}$

- **Implicit Euler** ($\theta = 1$):

$$a_P = \left(\frac{\rho_P \Delta x}{\Delta t} + (\rho u)_e \right), \quad a_W = (\rho u)_w$$

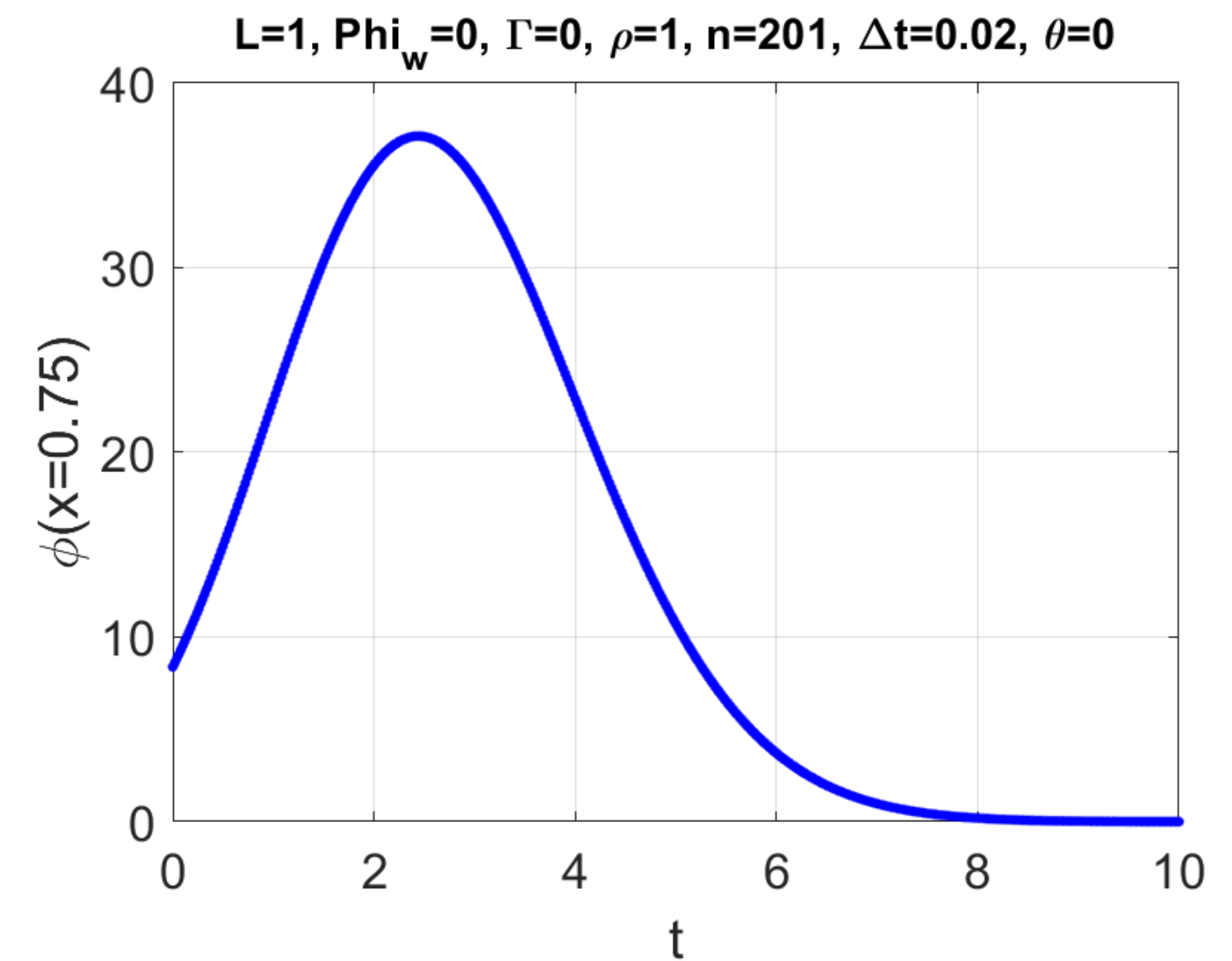
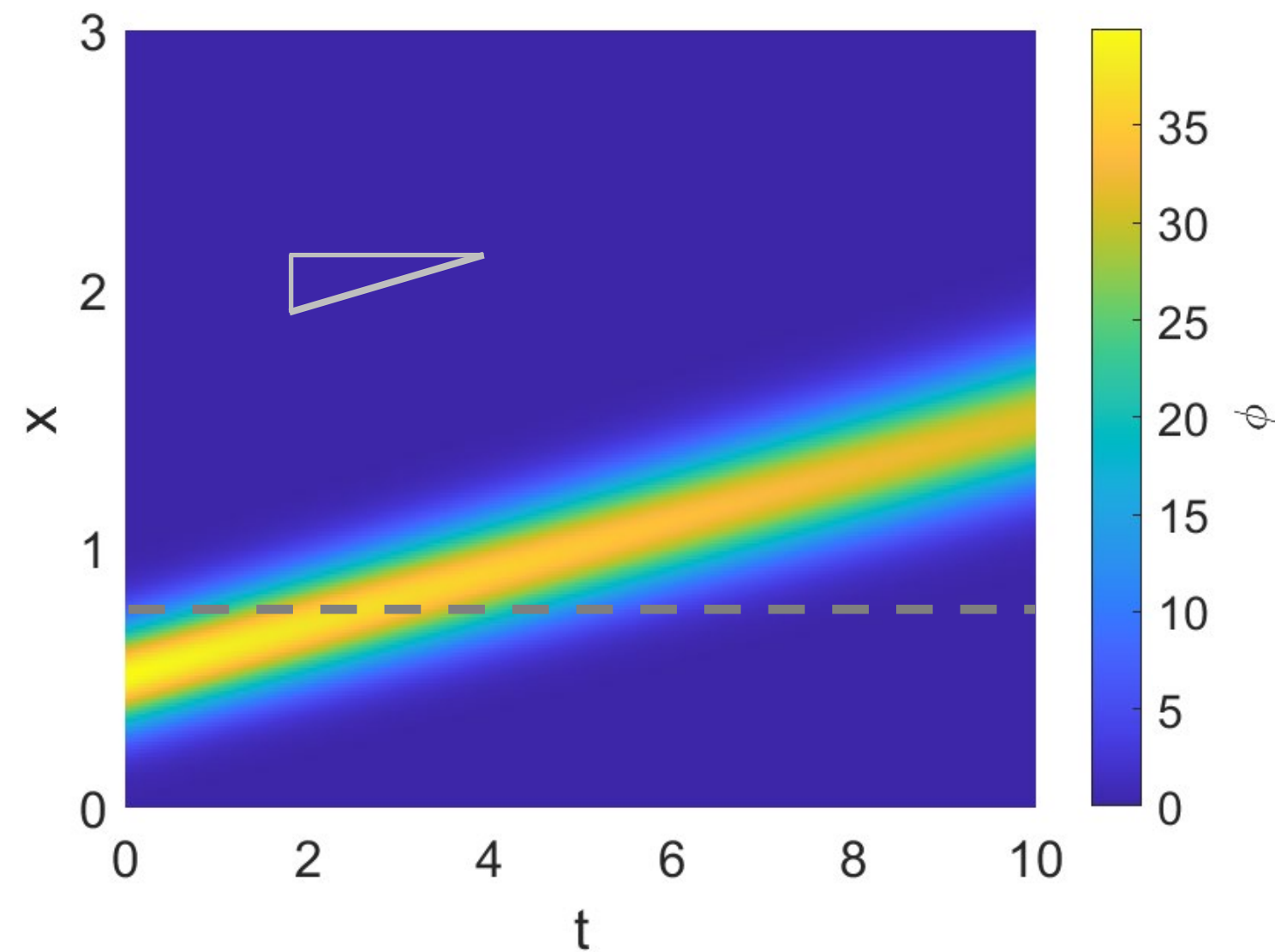
$$b = \left(\frac{\rho_P \Delta x}{\Delta t} \right) \phi_P^n$$

All coefficients always positive.

Unsteady 1D convection

- Example

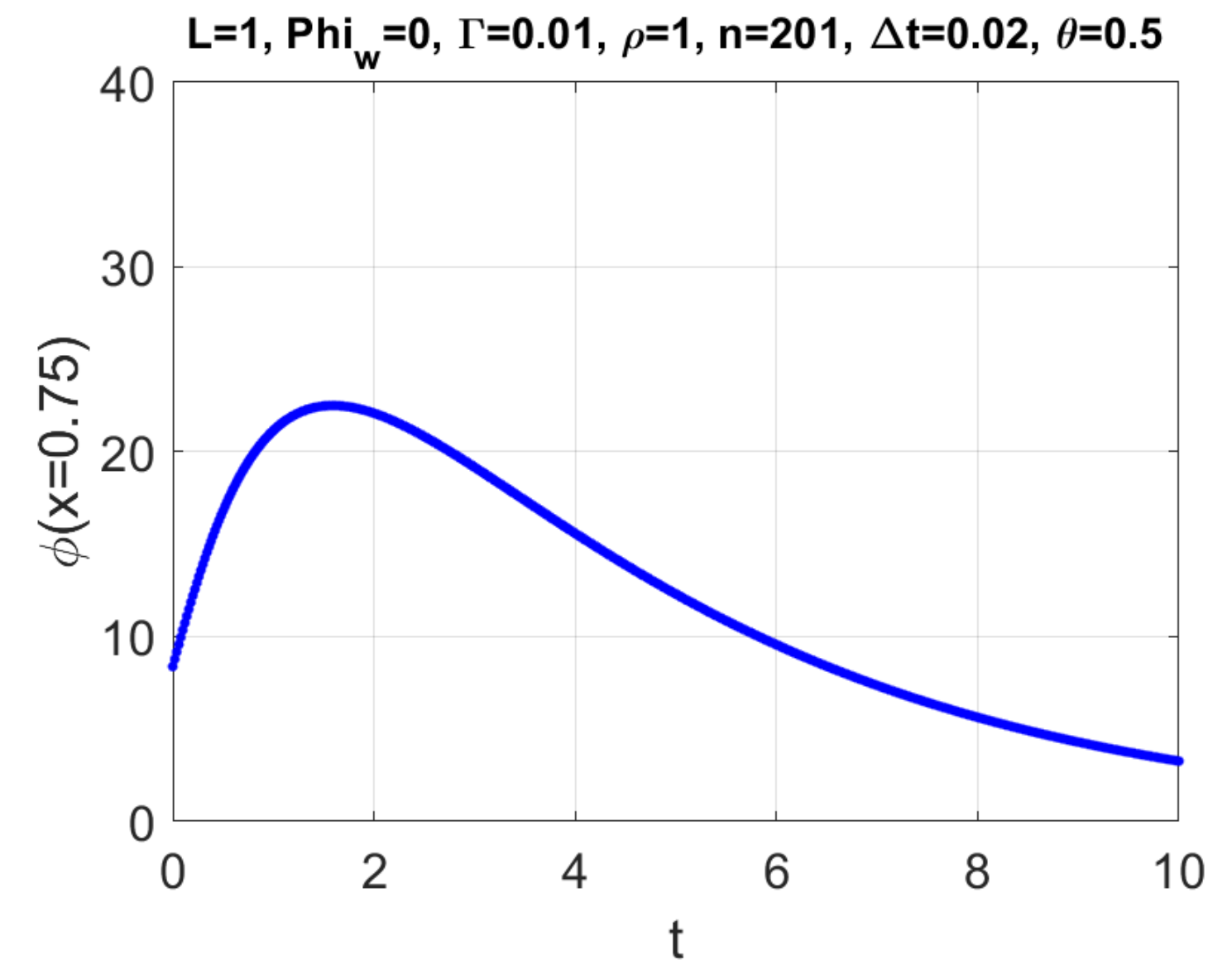
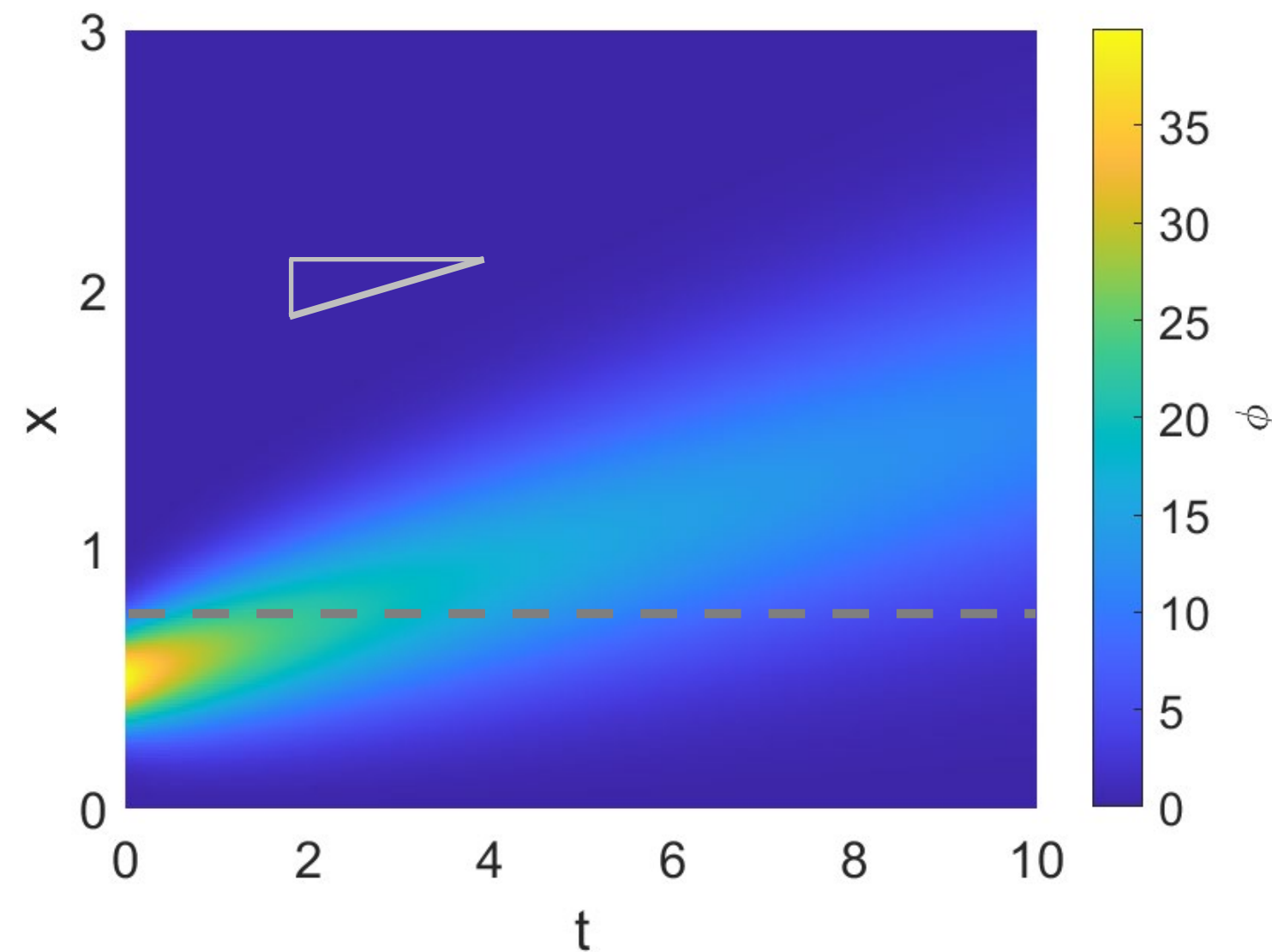
$$\rho=1, u=0.1$$



Unsteady 1D convection-diffusion

- Example

$$\rho=1, \Gamma=0.01, u=0.1$$



Boundedness criterion: physical interpretation

- For any partially explicit theta method ($\theta < 1$), the time step must satisfy:

$$\text{for pure diffusion: } \Delta t < O\left(\frac{\rho(\Delta x)^2}{\Gamma}\right),$$

$$\text{for pure convection: } \Delta t < O\left(\frac{\Delta x}{u}\right).$$

- Physically:
$$\frac{\partial(\rho\phi)}{\partial t} = \frac{\partial}{\partial x} \left(\Gamma \frac{\partial\phi}{\partial x} \right)$$

$$\sim \frac{\rho\phi}{T} \quad \sim \frac{\Gamma\phi}{L^2}$$

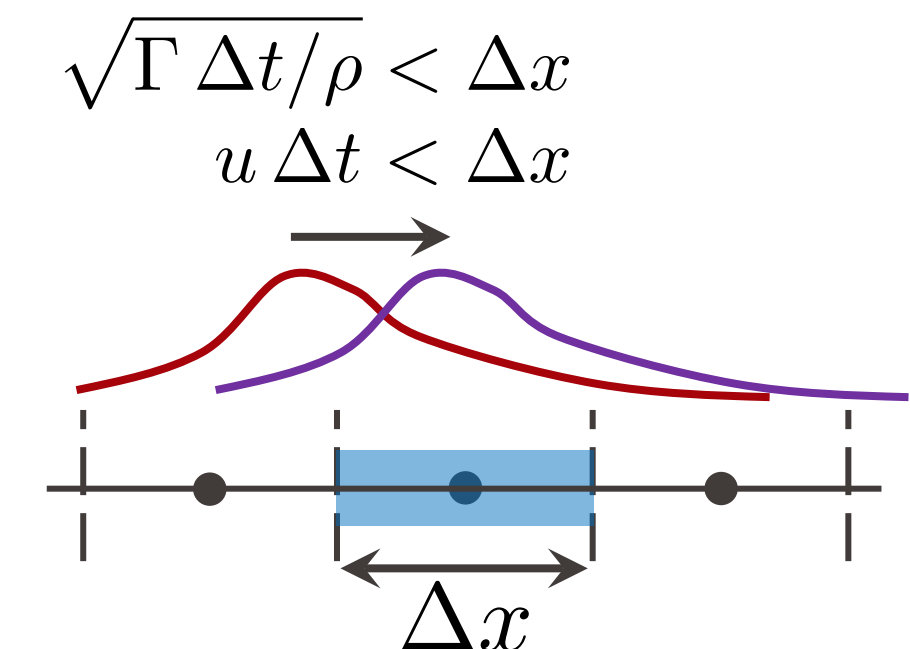
$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho\phi u)}{\partial x} = 0$$

$$\sim \frac{\rho\phi}{T} \quad \sim \frac{\rho\phi u}{L}$$

Characteristic diffusive length: $L \sim \sqrt{\frac{\Gamma T}{\rho}}$

Char. convective length: $L \sim u T$

- The time step Δt should be smaller than the time needed for the diffusive / convective process to travel over a distance Δx (one CV).



Boundedness criterion: physical interpretation

- For any partially explicit theta method ($\theta < 1$), the time step must satisfy:

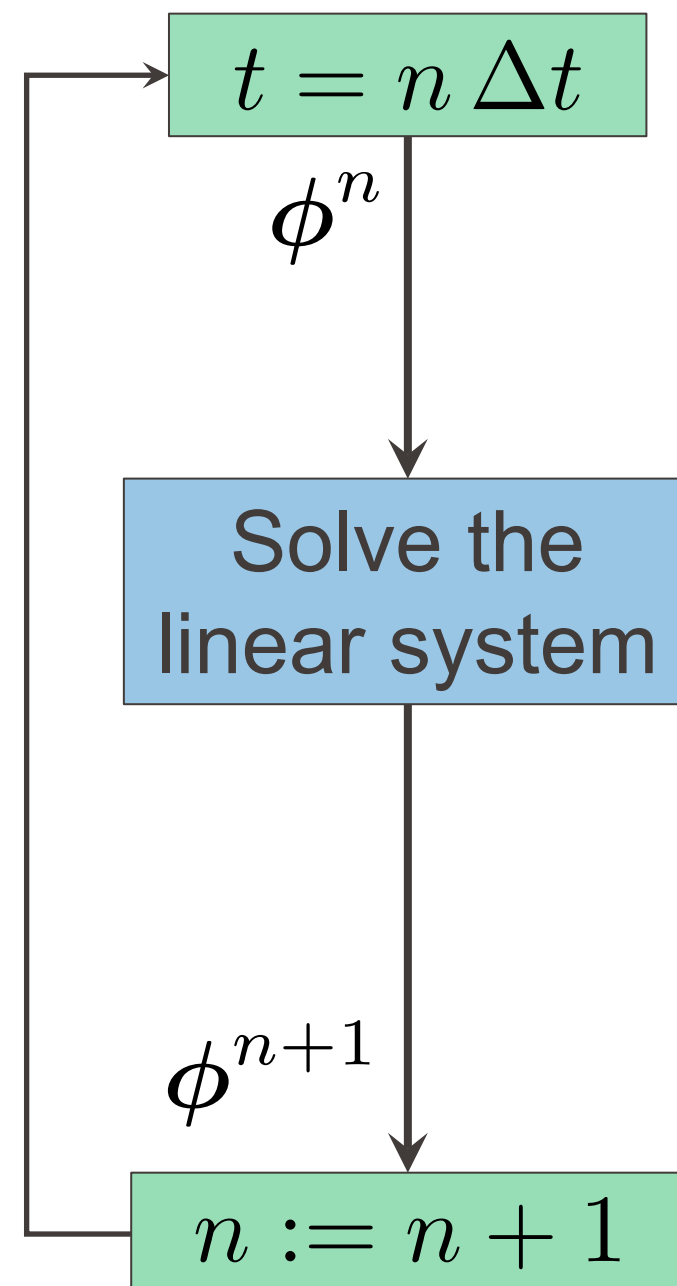
$$\text{for pure diffusion: } \Delta t < O\left(\frac{\rho(\Delta x)^2}{\Gamma}\right), \quad \left| \quad \text{for pure convection: } \Delta t < O\left(\frac{\Delta x}{u}\right).$$

- Note: when refining the mesh, the time step must also be reduced
→ simulations become more expensive for two reasons.

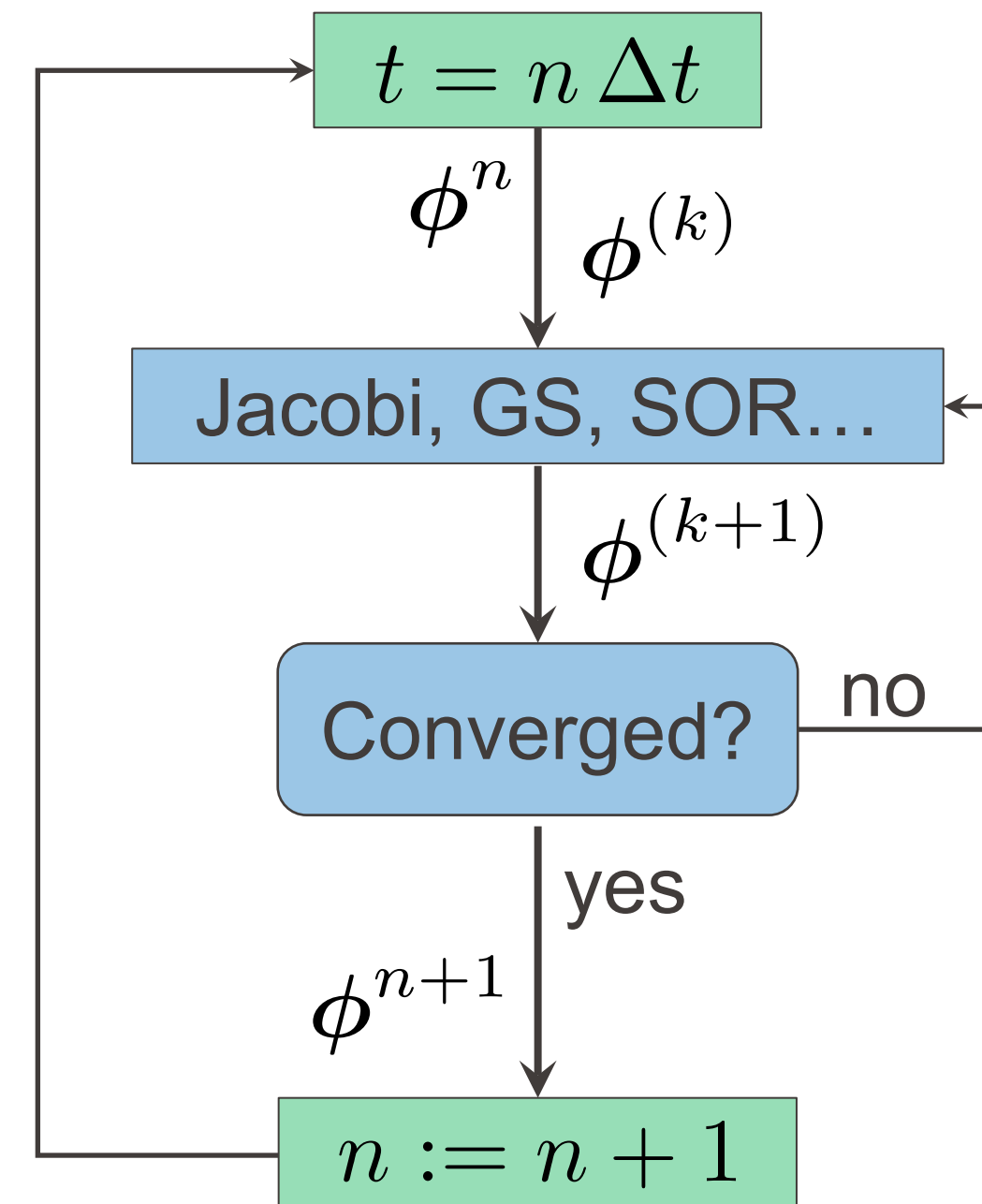
Schematic algorithms for unsteady simulation

- At **each time step**, must solve an algebraic system of equations.

Linear eq., direct method



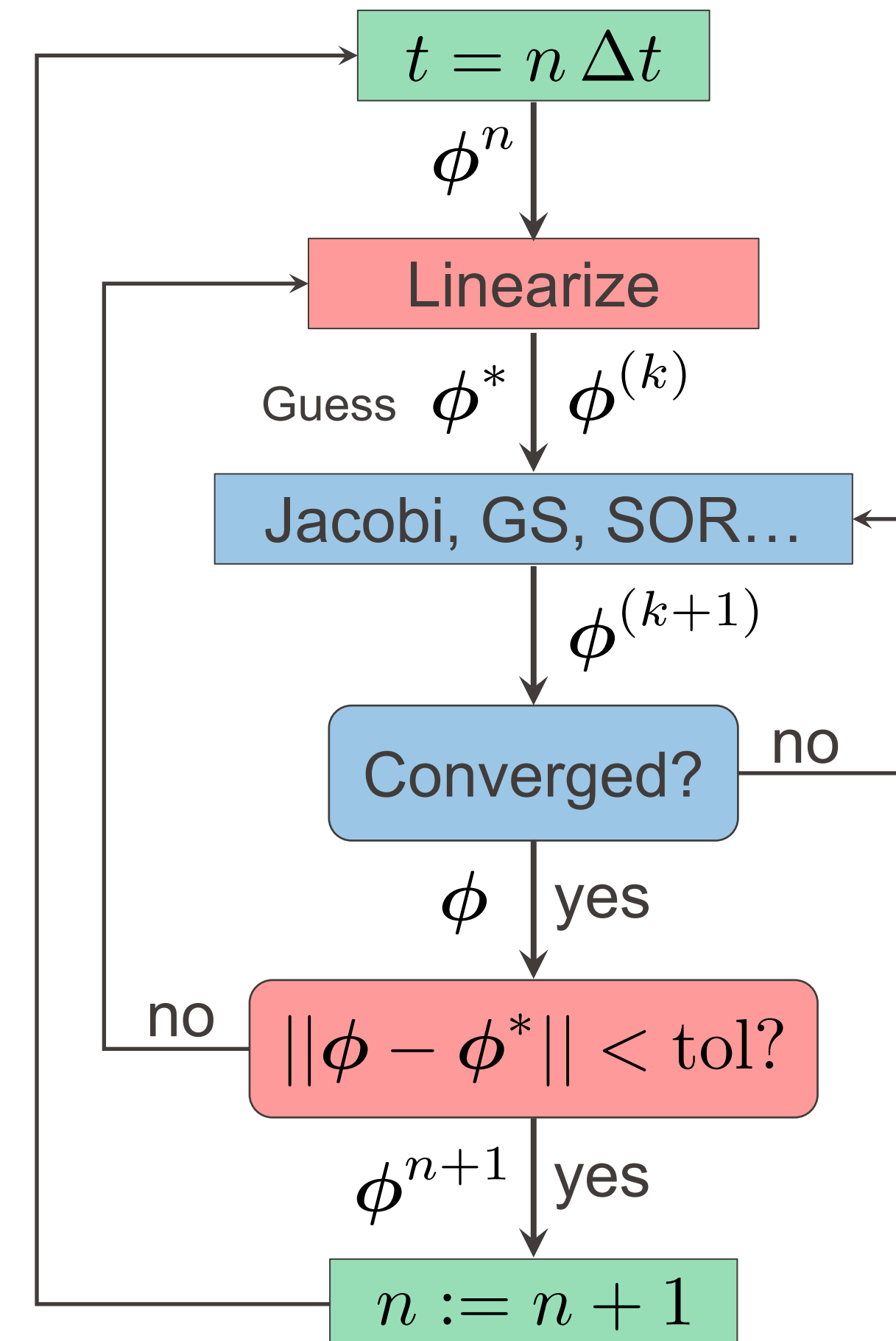
Linear eq., iterative method



Schematic algorithms for unsteady simulation

- So far (today), we have only dealt with **linear** governing equations. If the equations are **nonlinear**, one must linearize at **each time step**.

Nonlinear eq., iterative method



Schematic algorithms for unsteady simulation

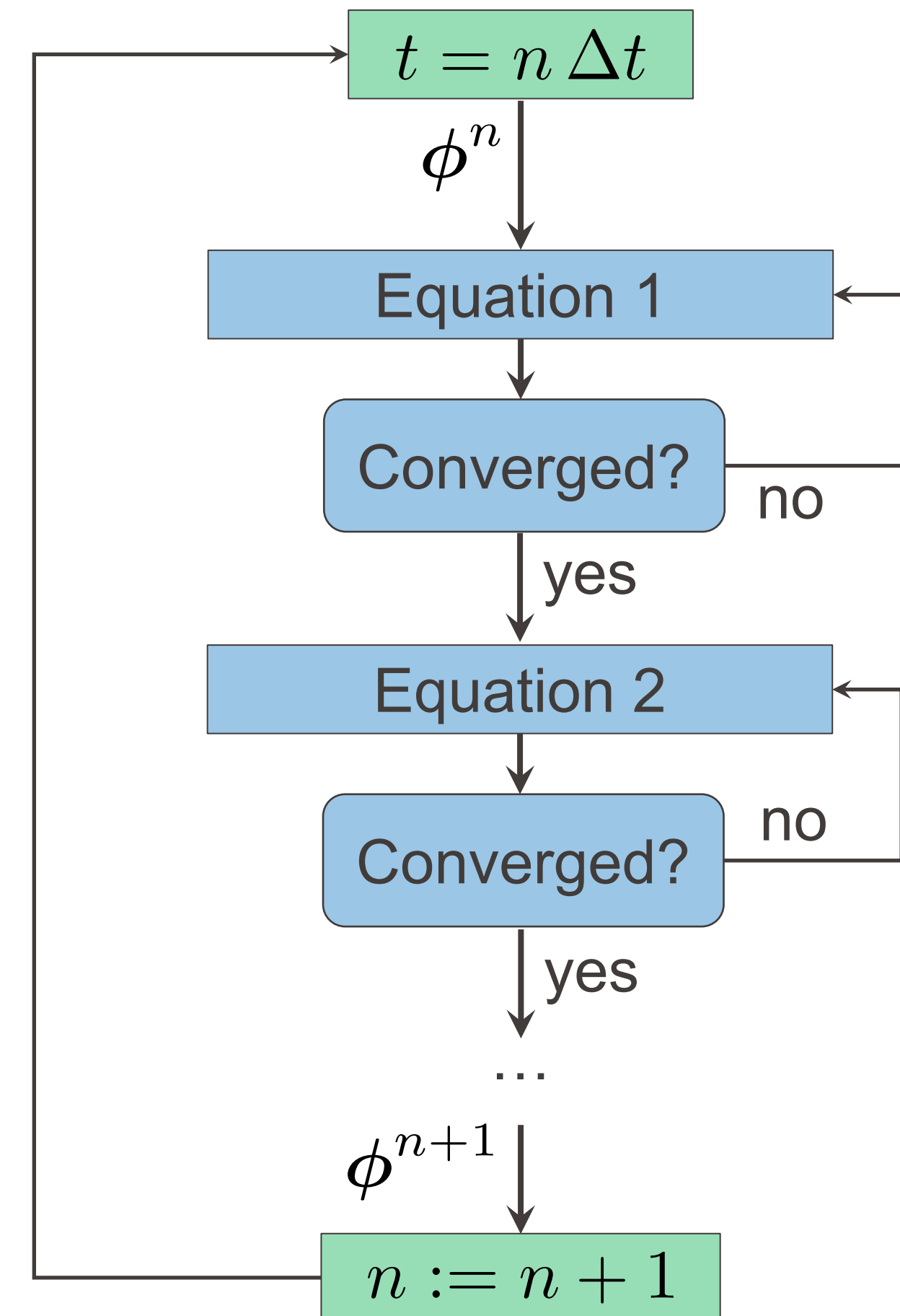
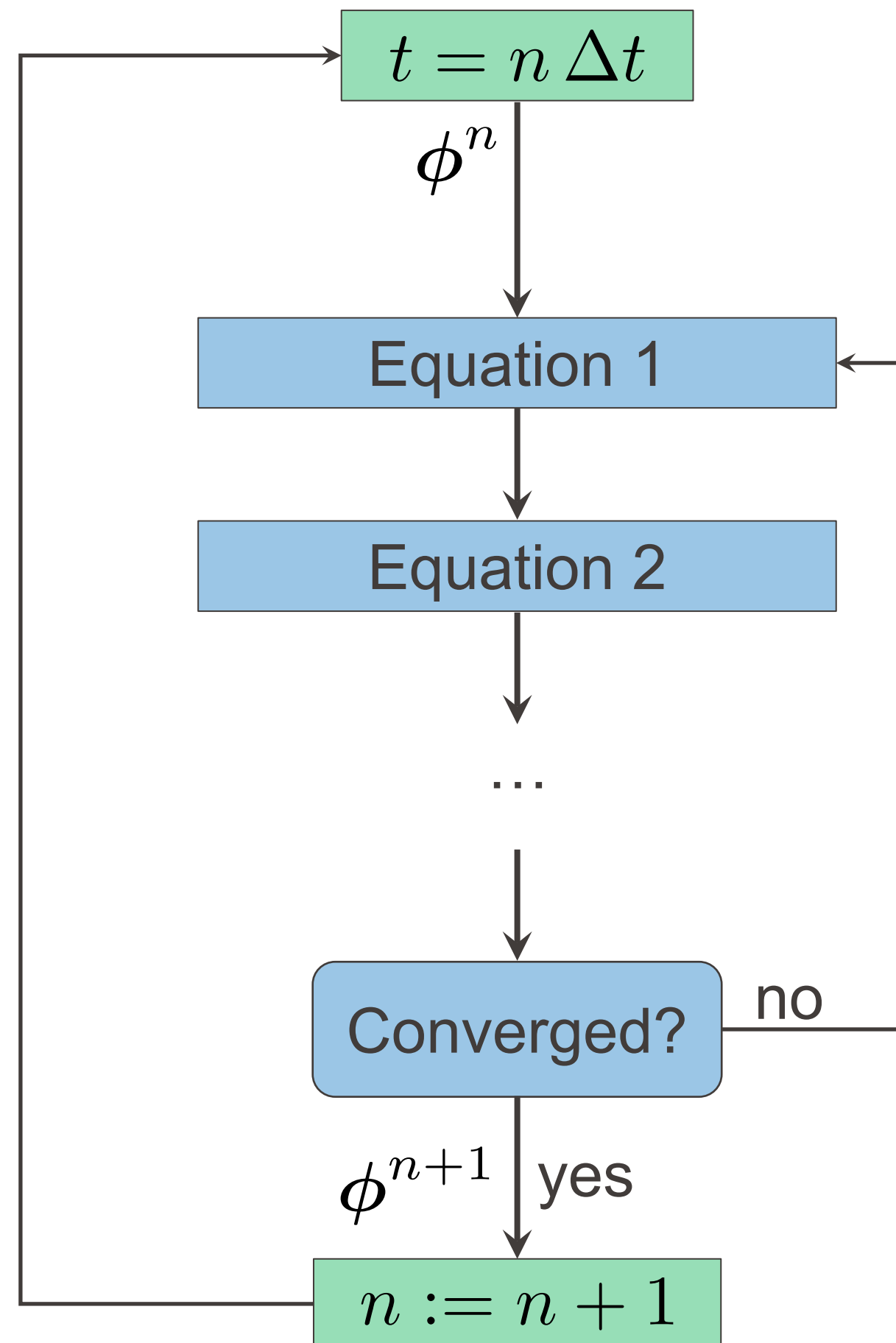
- Reminder: so far (today), we have only dealt with the solution of a **single** governing equation. If **several** equations are solved, 2 approaches (see also week 5 about the Navier-Stokes equations):
 1. **Coupled** approach: all equations solved **simultaneously** → one single large system (similar to previous slides). Requires more memory.
 2. **Segregated** approach: equations solved **separately**. Two options:
 - a) **iterative** scheme: solve each equation once, then repeat until global convergence;
 - b) **non-iterative** scheme: iterate each equation until individual convergence, then proceed to next equation.

Schematic algorithms for unsteady simulation

Segregated approach, iterative scheme

Segregated approach, non-iterative scheme

Numerical Flow Simulation

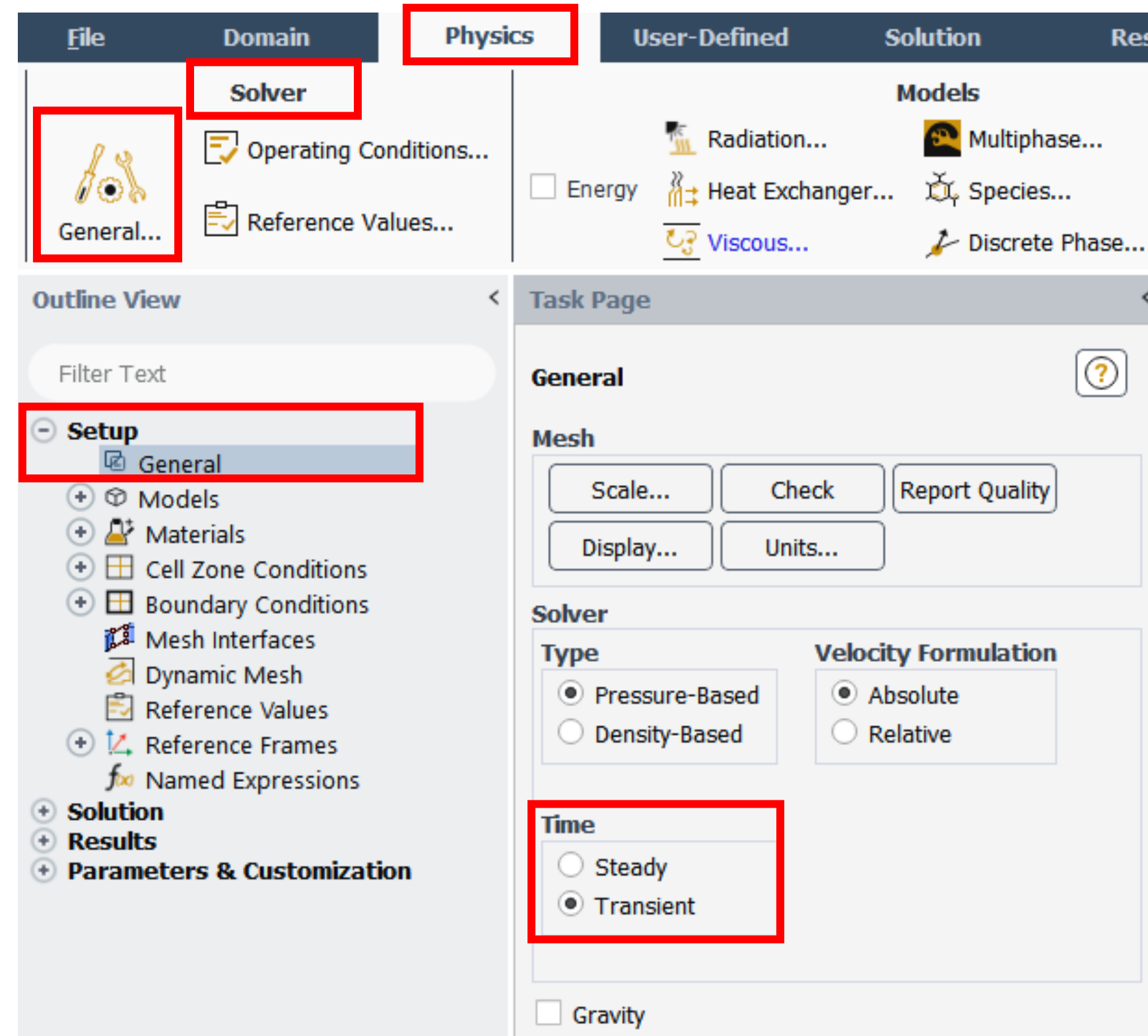


Summary and guidelines

- Unsteady simulations are much more **expensive** than steady ones (→ ask yourself if they are really needed).
- They also produce **a lot of data** (→ be careful with what you store).
- **Explicit** schemes: strong stability **limitation on the time step**.
- **Implicit** schemes: unconditionally stable (ODEs), BUT the time step must be small enough to:
 - avoid unphysical oscillations (PDEs),
 - resolve time-dependent features **accurately** (diffusion, convection, buoyancy...),
 - at the very least, converge the solution at each time step (→ check the residuals).
- The **initial condition** may be very important.

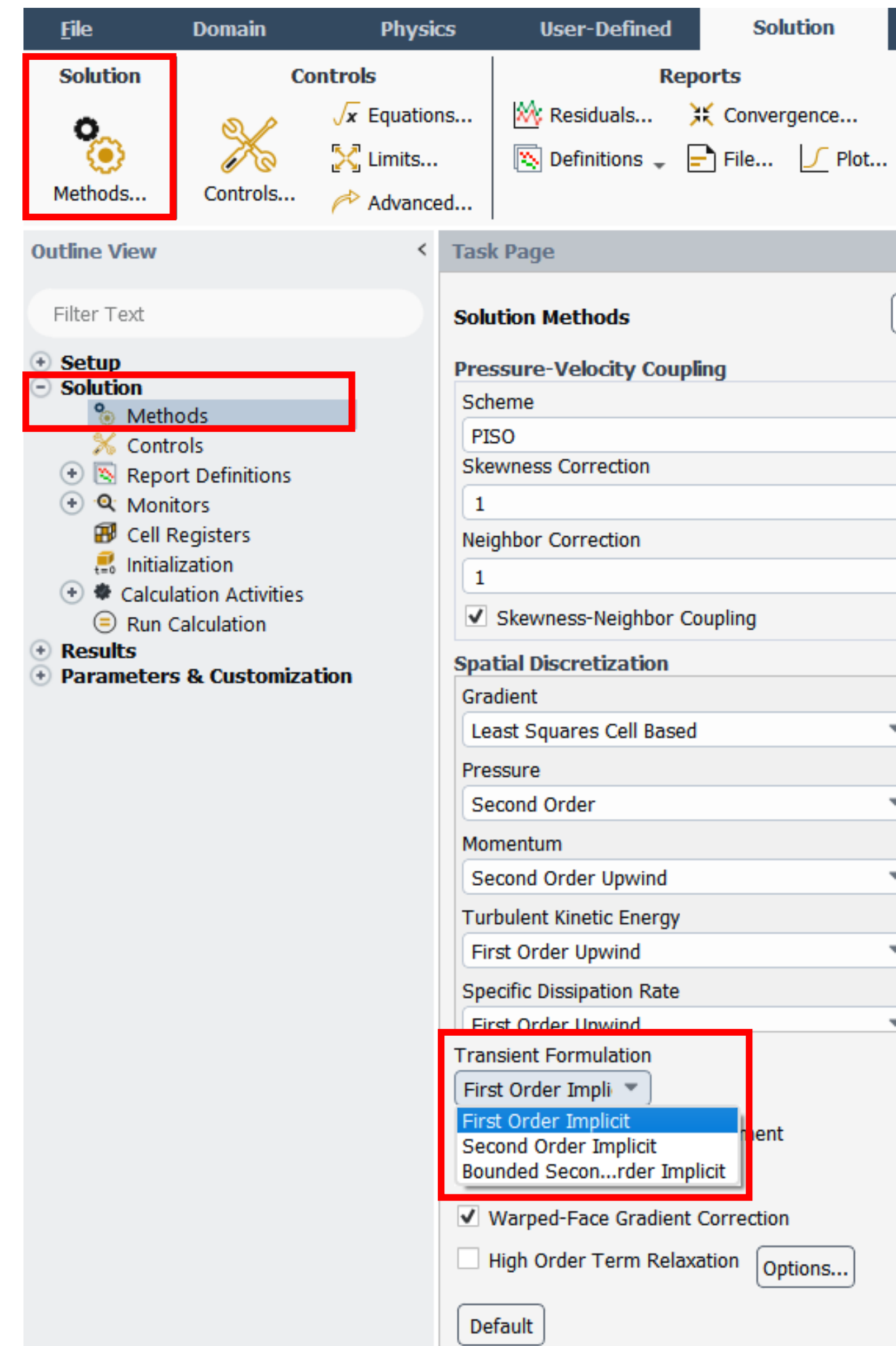
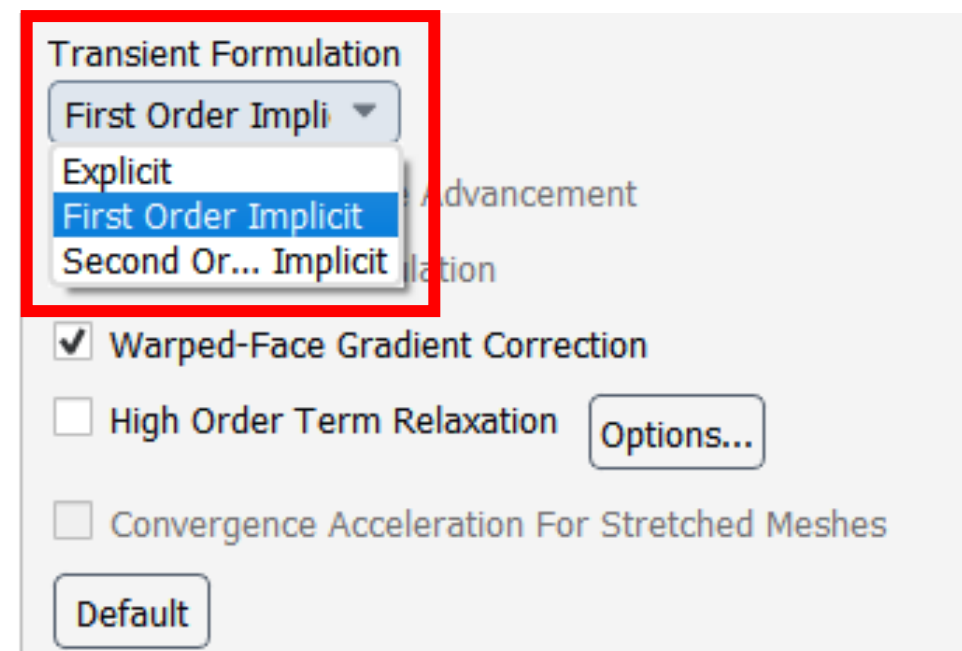
Fluent specifics

- Enable transient solver:



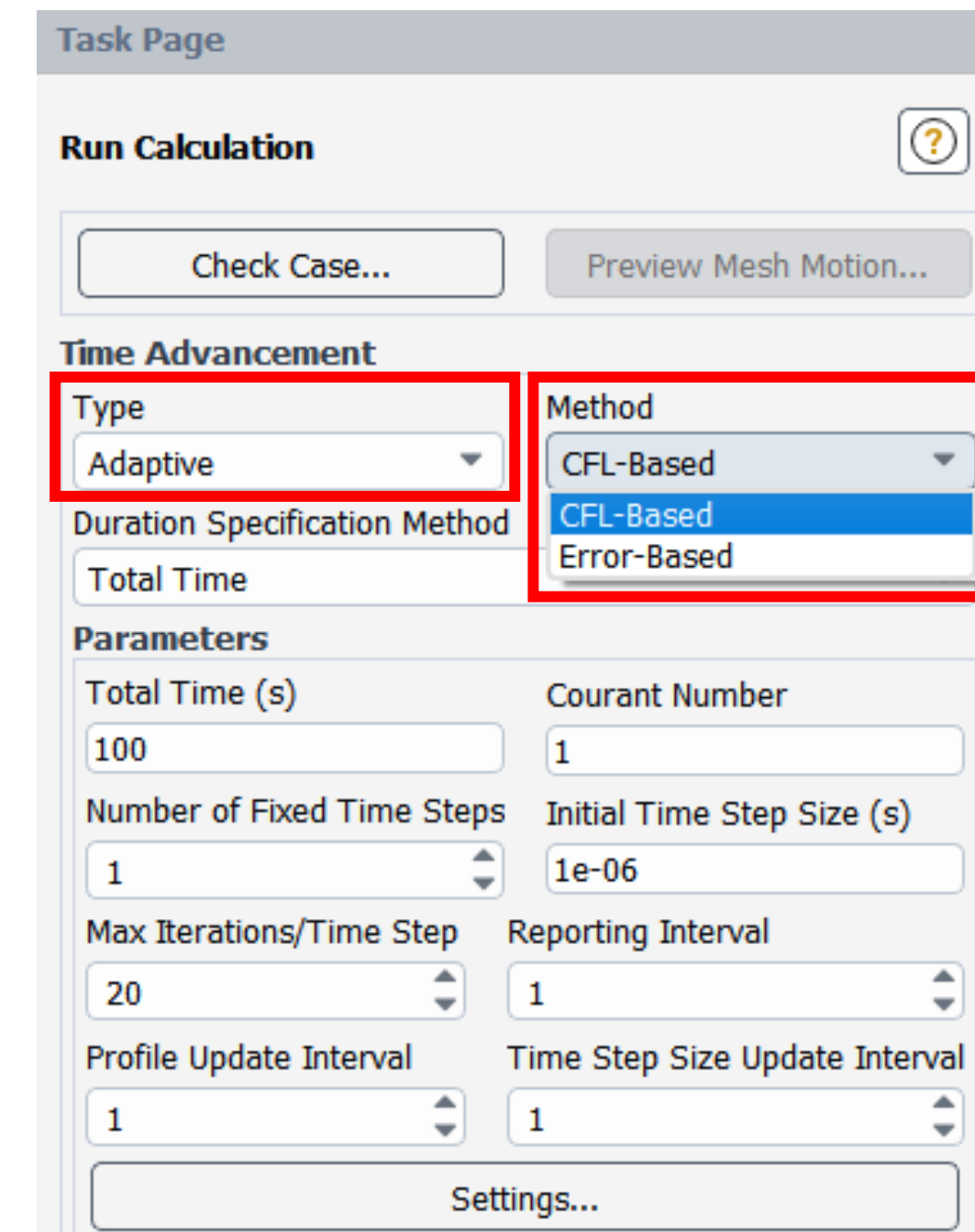
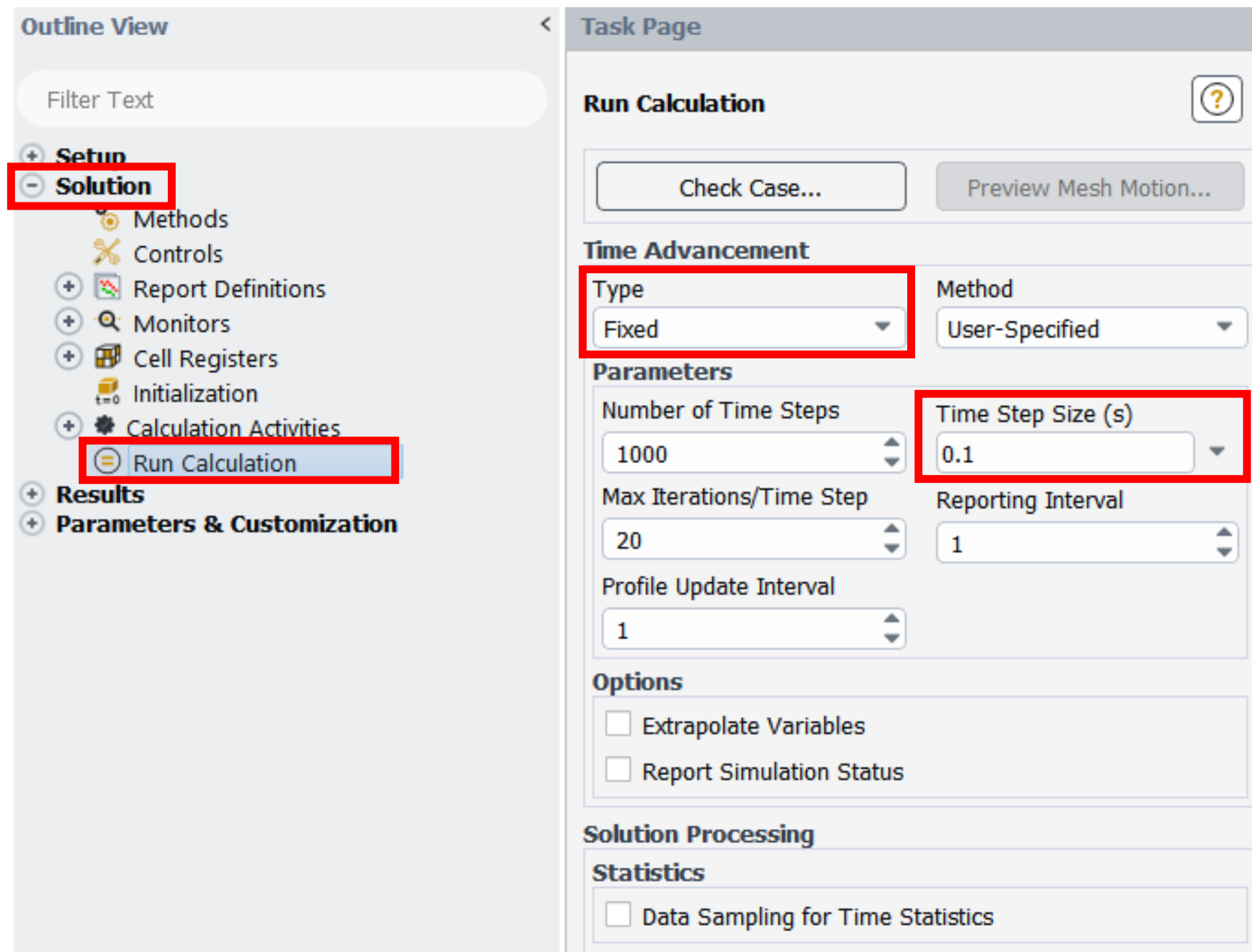
Fluent specifics

- **Pressure-based solver: implicit** schemes.
 - 1st order (implicit Euler): more stable but less accurate,
 - 2nd order (BDF2): more accurate but may produce oscillations,
 - Bounded 2nd order (weighted BDF2): eliminates oscillations.
- **Density-based solver: implicit** (1st / 2nd order) and **explicit** (Runge-Kutta) schemes.



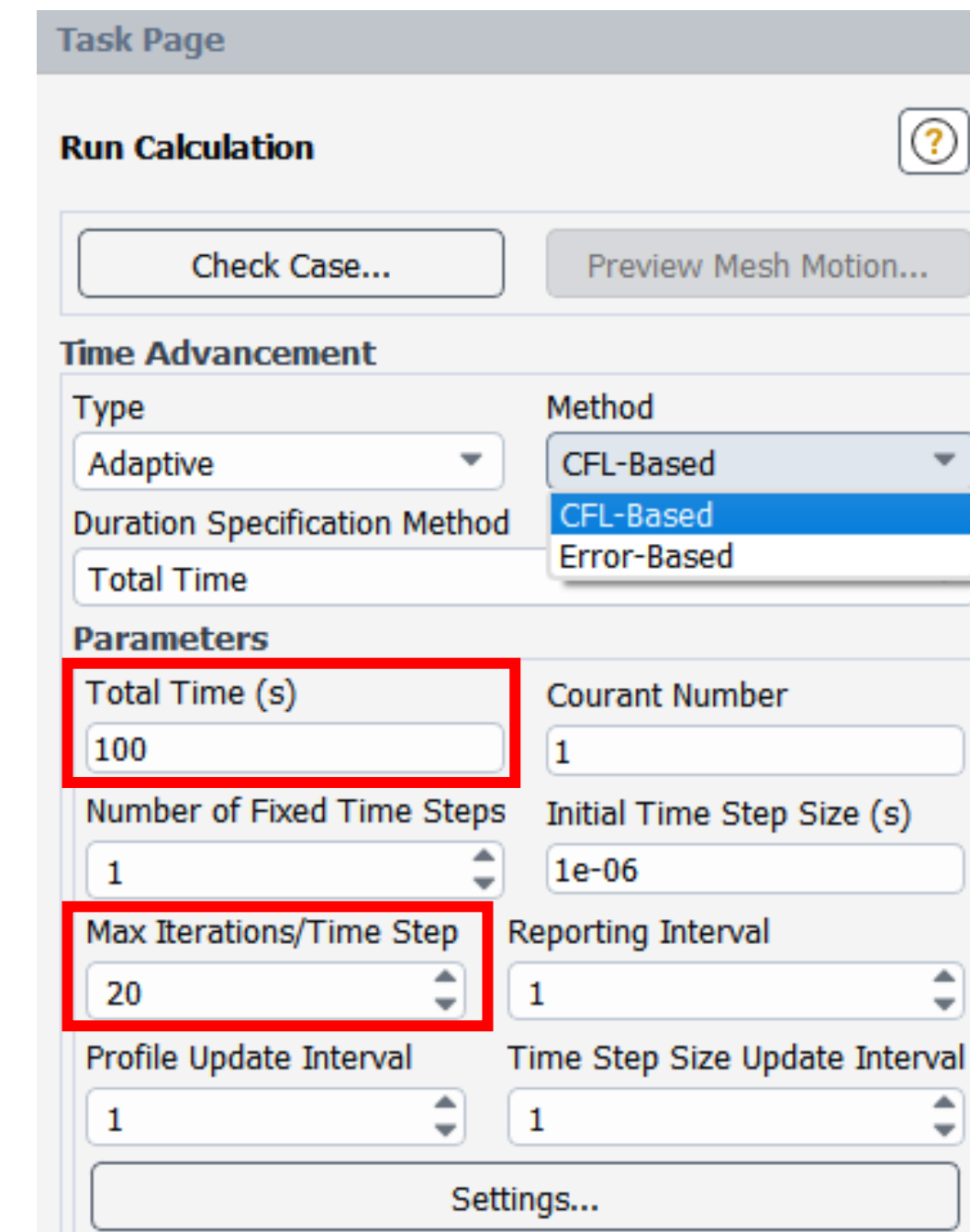
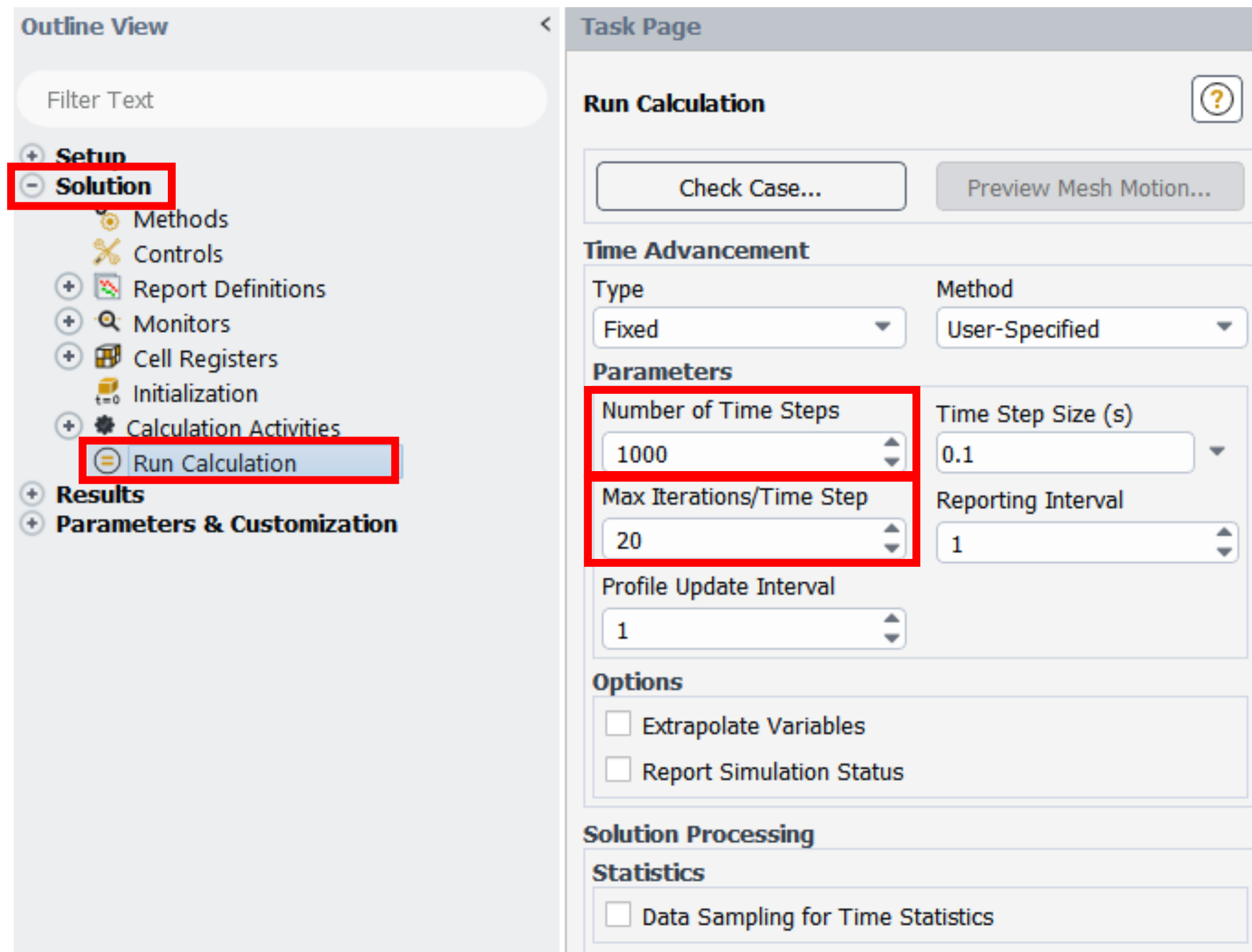
Fluent specifics

- Specify the **time step**:
 - **Fixed**: constant value
 - **Adaptive**: Fluent adjusts the time step to respect a target CFL number or a target truncation error (temporal error).



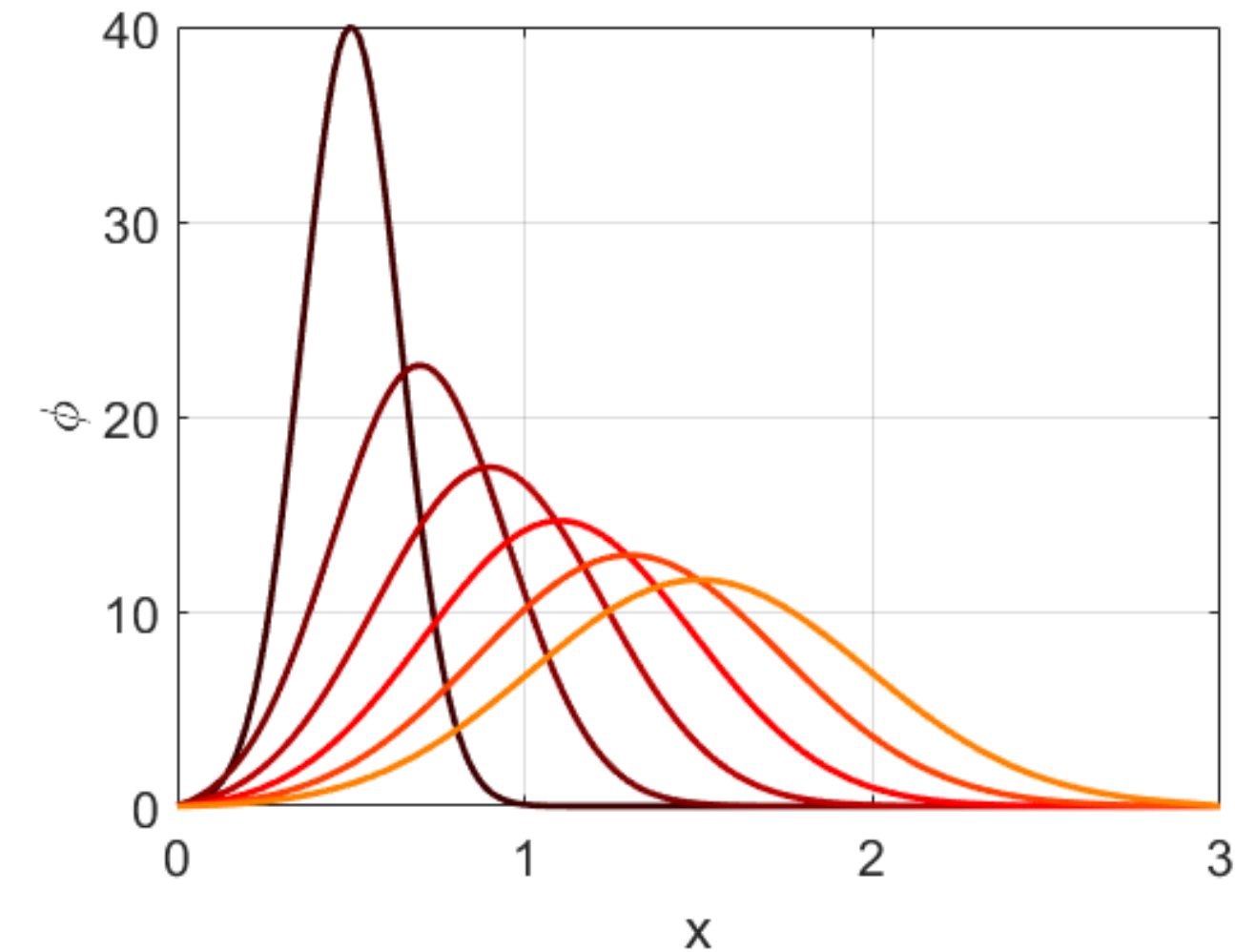
Fluent specifics

- Specify the **maximum number of iterations** allowed in each time step. Avoid too large values (better to reduce the time step).
- Specify the **number of time steps**, or the **physical time** to be simulated.

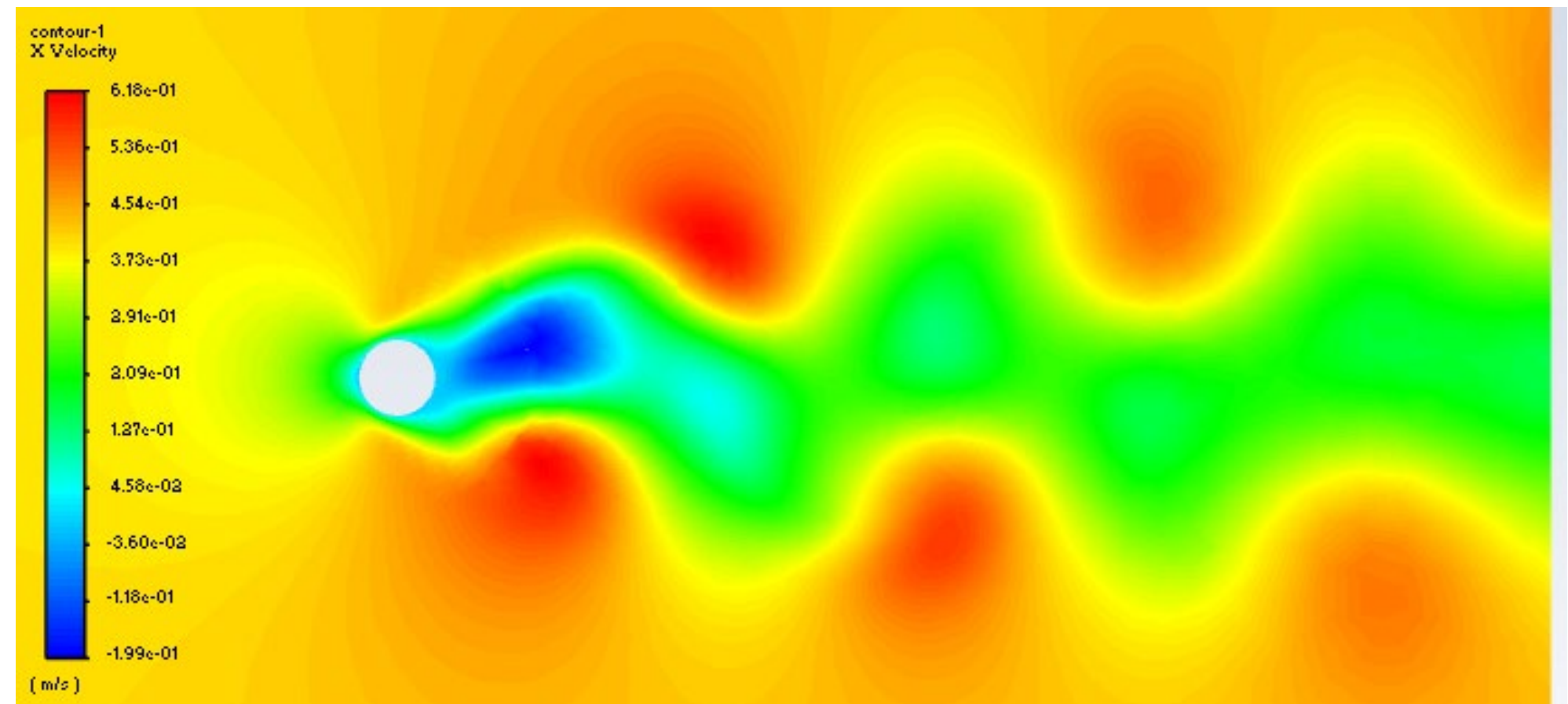


This week's exercise and tutorial

- Matlab exercise: convection-diffusion



- Fluent tutorial: vortex shedding



Appendix: pseudo-transient simulation (1/4)

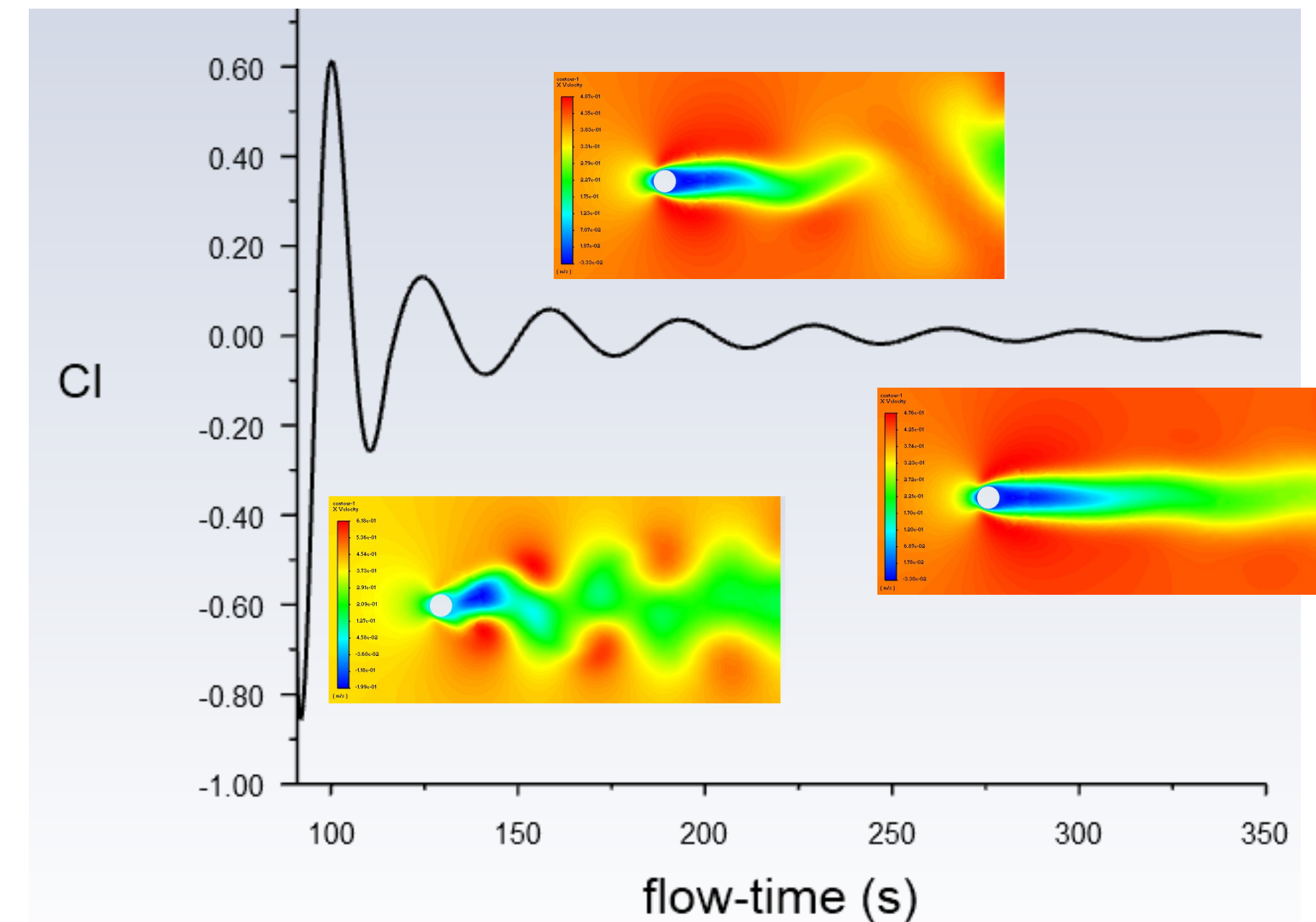
- For **steady** problems, most natural approach is to use a **steady** solver (weeks 2-5).
- In principle, one may also use an **unsteady** solver, simulate the physical process, and wait until reaching a steady state. However, this naive approach may be very slow because the flow may settle only very slowly (depending on the initial condition, the physical parameters, etc.).

Example: flow past a 2D cylinder, sudden reduction of Re from 100 (unsteady flow) to 40 (steady flow).

With an **unsteady** solver, need several vortex-shedding periods to reach the steady regime. Here:

- convective time (cylinder diameter divided by freestream velocity) = 1 s,
- physical time to reach steady state = $O(10^3)$ s,
- constant time step = 0.1 s

→ $O(10^4)$ iterations.



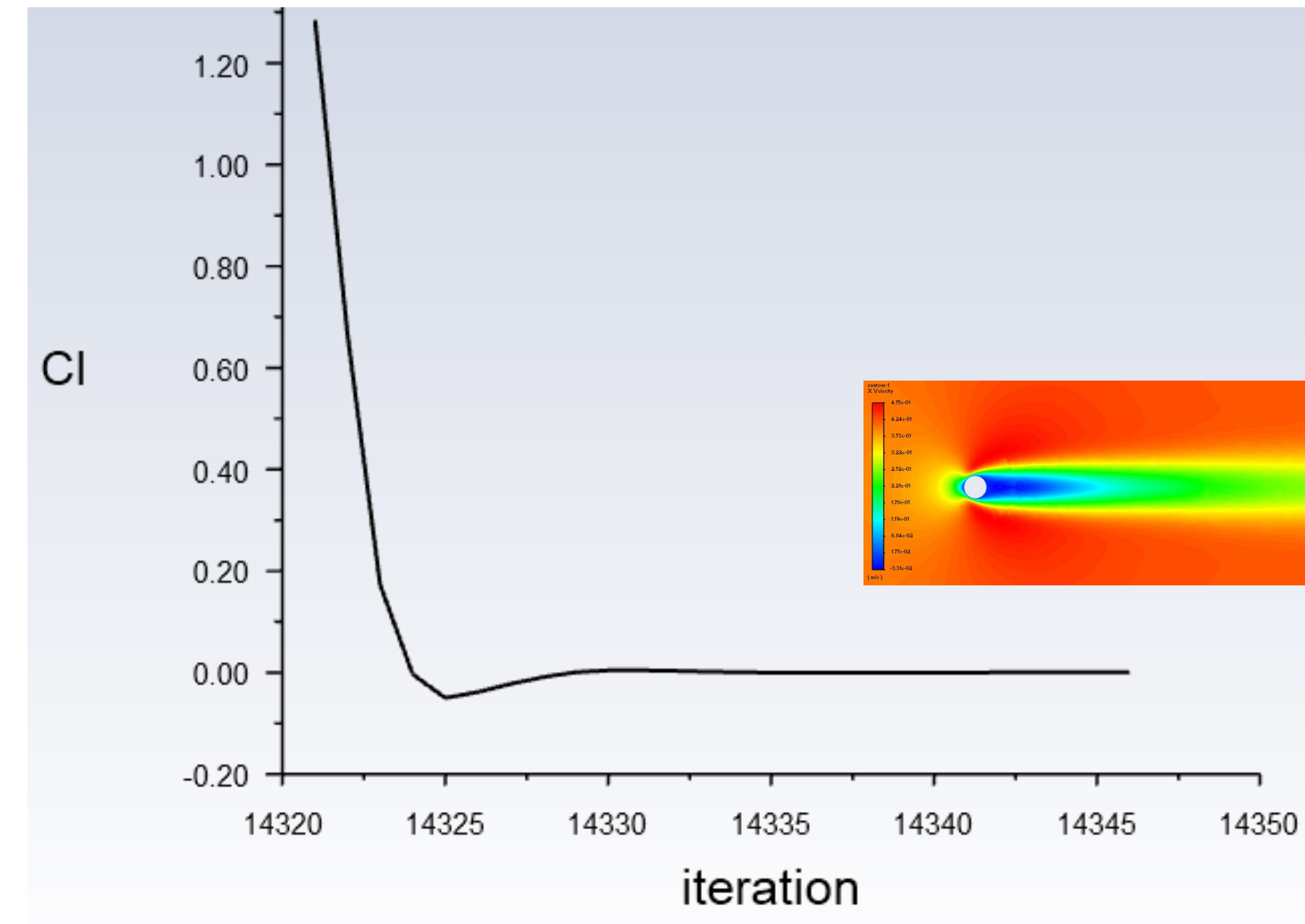
Appendix: pseudo-transient simulation (2/4)

- For **steady** problems, most natural approach is to use a **steady** solver (weeks 2-5).
- In principle, one may also use an **unsteady** solver, simulate the physical process, and wait until reaching a steady state. However, this naive approach may be very slow because the flow may settle only very slowly (depending on the initial condition, the physical parameters, etc.).

Example: flow past a 2D cylinder, sudden reduction of Re from 100 (unsteady flow) to 40 (steady flow).

With a **steady** solver: need only **30 iterations**.

Numerical Flow Simulation



Appendix: pseudo-transient simulation (3/4)

- One exception: so-called “pseudo-transient” simulation. An **unsteady** solver is used, but the time step does not correspond to a physical time step. Compare the following:

- **Unsteady solver**
(time integration;
this week):

$$\left(\tilde{a}_P + \frac{\rho_P \Delta x}{\Delta t} \right) \phi_P^{n+1} = \sum \tilde{a}_{nb} \phi_{nb}^{n+1} + \tilde{b}(\phi^n) + \frac{\rho_P \Delta x}{\Delta t} \phi_P^n$$

- **Steady solver**
(iterative method,
under-relaxation; week 3):

$$\left(\frac{\tilde{a}_P}{\alpha} \right) \phi_P^{(k+1)} = \sum \tilde{a}_{nb} \phi_{nb}^{(k+1)} + \tilde{b}(\phi^{(k)}) + \left(\frac{1 - \alpha}{\alpha} \right) \tilde{a}_P \phi_P^{(k)}$$

- Clear analogy: can identify $\frac{\rho_P \Delta x}{\Delta t} = \left(\frac{1 - \alpha}{\alpha} \right) \tilde{a}_P$
- Interpretation: pseudo-transient calculation equivalent to under-relaxed iterative steady calculation. The pseudo time step may be local (i.e. space-dependent).
- Useful in some cases, when stability problems in steady calculation.

Appendix: pseudo-transient simulation (4/4)

- **In Fluent:** available for pressure-based coupled solver, and density-based implicit solver. Can specify the pseudo time step, or leave the default automatic calculation. In both case, it is actually a global (not local) value.

