CFD simulations – some information about scientific computing.

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CFD simulations.

Overview.

- What is CFD simulation?
- Why should we use CFD simulations.
- CFD simulation – important aspects.
- Start with simple convection – diffusion example:
  - Finite volume discretization and solution of discrete system.
  - Simulation examples.

What is CFD simulation.

Weak definition.

- Computational Fluid Dynamics or CFD is the analysis of systems involving fluid flow, heat transfer and associated phenomena such as chemical reactions by means of computer-based simulation. The technique is very powerful and spans a wide range of industrial and non-industrial application areas (*).
- Some examples are:
  - aerodynamics of aircraft and vehicles: lift and drag
  - turbomachinery: flows inside rotating passages, diffusers etc.
  - electrical and electronic engineering: cooling of equipment including micro- circuits
  - chemical process engineering: mixing and separation, polymer molding, foam expansion flows.
  - external and internal environment of buildings: wind loading and heating/ ventilation
  - meteorology: weather prediction
  - biomedical engineering: blood flows through arteries and veins

(*) An introduction to computational fluid dynamics. The finite volume method. H.K.Versteeg, W.Malalasekera.

CFD simulations.

Why we should use it.

- Computers are becoming more and more powerful.
- CFD simulations allows us to:
  - Fast prediction of flow behavior (depending on problem formulation).
  - Help the engineers to develop new products
  - The simulation enables the inspection of product parts that are not visible in the test setup.
  - Simulation enables engineers to make faster and better decisions.
  - Simulation improves product quality, durability, safety, and performance.
  - Simulation may reduce development time and costs significantly.
  - This speed leads to increased productivity and more efficient use of engineering resources.
- Don’t forget: CFD simulation is fun ☺

CFD simulations.

Important issues.

- CFD is by its nature complex because it combines several components, each of which is a challenge in its own right:
  - fluid dynamics and physical modelling;
  - geometry and meshing;
  - numerical methods – discretization of equations and solution of discrete system;
  - data analysis;
  - computing and programming
- It is therefore difficult to achieve CFD competence, i.e. to have the confidence to perform CFD analyses repeatedly and on a timely basis according to a defined standard.
- Many people often underestimate the complexity of CFD and assume that the required competence can be reached simply by "learning the software package".

CFD simulations.

Important issues.

- CFD work layout:
  - Define your problem;
  - STEP 1: create mathematical model describing your process.
  - STEP 2: discretize your equations on a given mesh.
  - STEP 3: solve discrete equation (or system of equations).
  - STEP 4: visualize and analyze simulation results.
- For STEP 1 – STEP 3 we introduce errors.
  - STEP 1: assumptions in model description.
  - STEP 2: errors in discretization.
  - STEP 3: errors when solving discrete equation.
- Goal: try to minimize errors in all 3 steps.

Convection – diffusion equation.

Equation and meaning.

- We define following convection – diffusion equation:

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

- Where ϕ is variable to solve, ρ – density, Γ – diffusion coefficient, u – velocity, S_ϕ - source term.
- Meaning of the terms:

Rate of increase of ϕ of fluid element	+	Net rate of flow of ϕ out of fluid element	=	Rate of increase of ϕ due to diffusion	+	Rate of increase of ϕ due to sources

Convection – diffusion equation.

Discretization.

- There are various methods for discretizing the governing equations called discretization methods.
- Some popular discretization methods used in CFD tools are
  - the finite element method,
  - the finite volume method
  - the finite difference method
- For CFD simulations most popular is Finite Volume Method (FVD).
- Advantages of FVM:
  - The FVM is a natural choice for solving CFD problems because the PDEs you need to solve for CFD are conservation laws
  - The biggest advantage of the FVM is that it only must perform a flow evaluation for the cell boundaries.
  - FVM conserves the quantities.

Convection – diffusion equation.

Discretization.

- We integrate equation over control volume (CV). CV can be associated to single mesh element.

$$\int_{CV} \frac{\partial(\rho\phi)}{\partial t} dV + \int_{CV} div(\rho\phi\mathbf{u})dV = \int_{CV} div(\Gamma\ grad\ \phi)dV + \int_{CV} S_\phi dV$$

- Now we make use of Gauss divergence theorem

$$\int_{CV} div\ \mathbf{a}dV = \int_{A} \mathbf{n}\ .\ \mathbf{a}dA$$

- where A denotes surface of control volume and n – normal to surface vector.

Convection – diffusion equation.

Discretization.

- Using Gauss divergence theorem we convert our equation to:

$$\frac{\partial}{\partial t}\left(\int_{CV} \rho\phi dV\right) + \int_A \mathbf{n}\,.\,(\rho\phi\mathbf{u})dA = \int_A \mathbf{n}\,.\,(\Gamma\ grad\ \phi)dA + \int_{CV} S_\phi dV$$

- terms meaning:

Rate of increase of ϕ	+	Net rate of decrease of ϕ due to convection across the boundaries	=	Rate of increase of ϕ due to diffusion across the boundaries	+	Net rate of creation of ϕ

- In discrete form we write equation volumetric terms as:
  - Time derivative term:

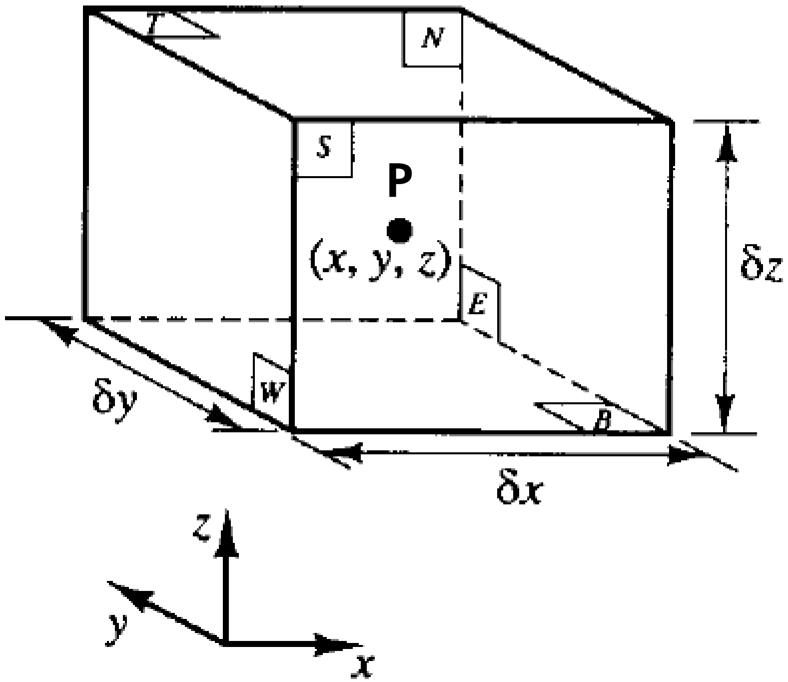
$$\frac{\partial}{\partial t}\left(\int_{CV} \rho\phi \, dV\right) = \frac{\partial(\rho\phi)}{\partial t}\delta CV$$

  - Source term:

$$\left(\int_{CV} S_\phi \, dV\right) = S_\phi \delta CV$$

$$\delta CV = \delta x \delta y \delta z$$

Control volume (CV)



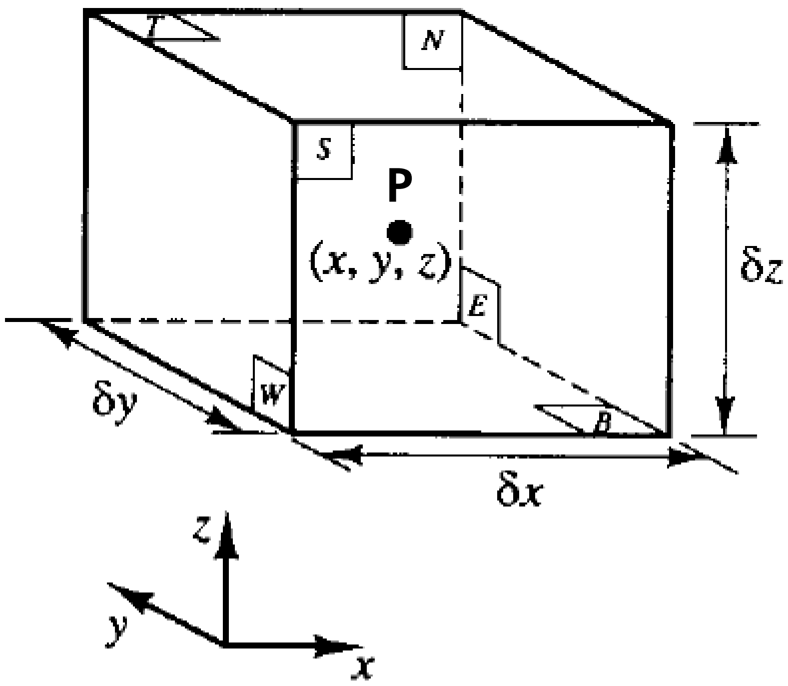
- In discrete form we write equation surface terms as:
  - Convection term:

$$\int_A n(\rho\phi u)\, dA = \sum_{f=\{e,w,n,s,t,b\}} n_f A_f \rho_f \phi_f u_f$$

  - Diffusion term:

$$\int_A n\,(\Gamma\,\nabla\phi)\, dA = \sum_{f=\{e,w,n,s,t,b\}} n_f A_f \Gamma_f \nabla\phi_f$$

Control volume (CV)



$$A_e = A_w = \delta y \delta z$$
$$A_n = A_s = \delta x \delta z$$
$$A_t = A_b = \delta x \delta y$$

$$n_e = n_n = n_t = 1$$
$$n_w = n_s = n_b = -1$$

Convection – diffusion equation.

Space discretization.

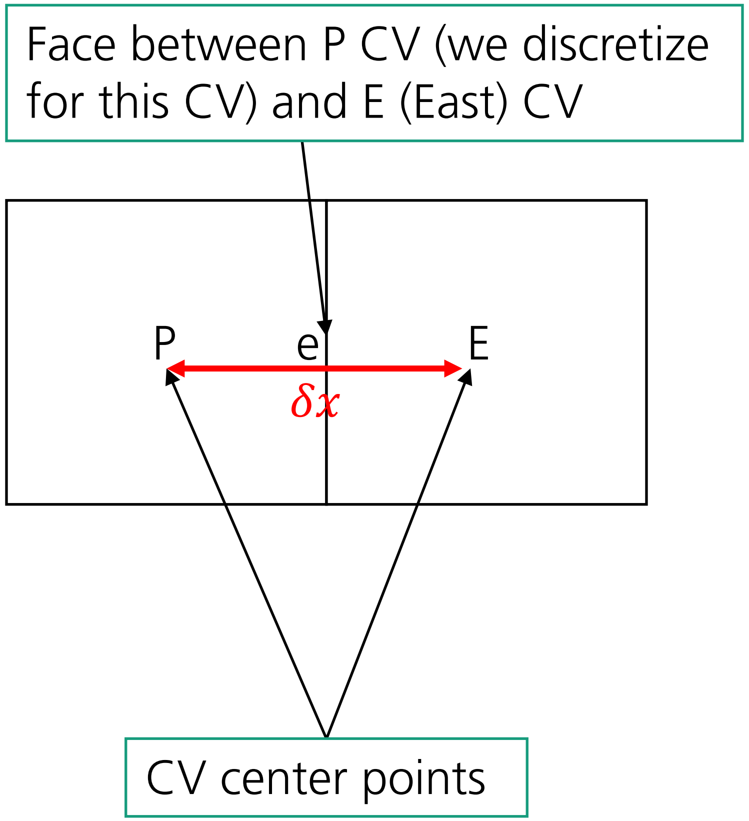
- We restrict discretization to x-axis (faces e,w) and assume constant density ρ :
  - Convection term, many different schemes could be used.
  - Simple 1st order accuracy in space $O(\delta x)$ scheme UPWIND reads as:

$$A_e \rho_e \phi_e u_e = \begin{cases} \rho A_e \phi_P u_e & if u_e \geq 0 \\ \rho A_e \phi_E u_e & if u_e < 0 \end{cases}$$

  - Diffusion scheme:

$$A_e \Gamma_e \nabla \phi_e = A_e \Gamma_e \frac{\phi_E - \phi_P}{\delta x} \qquad \Gamma_e = \frac{\Gamma_E + \Gamma_P}{2}$$

  - Gradient approximated by truncated Taylor expansion (second order space accuracy $O(\delta x^2)$). Arithmetic average for diffusion coefficient could be used.



Convection – diffusion equation.

Time discretization.

- Let assume time space is in steps with time step dt, we denote "new" time step values with superscript "$t+1$" and previous time step values with superscript "t"
  - Time derivative term is now approximated with backward Euler 1st order time approximation $O(\delta t)$:

$$\frac{\partial(\rho\phi)}{\partial t}\delta CV = \rho\frac{\phi_P^{t+1} - \phi_P^t}{dt}\delta CV$$

- Final decision is which scheme to use:
  - Explicit – all discretized terms used from previous time step, all ϕ values used as ϕ_P^t, ϕ_E^t
  - Implicit – all discretized term used in new time step, all ϕ values used as ϕ_P^{t+1}, ϕ_E^{t+1}
- Explicit scheme straightforward to implement, however such schemes require time step stability restrictions:
  - Convection: The Courant–Friedrichs–Lewy (CFL) condition: $\mathrm{CFL} = \frac{dt \cdot u}{dx} < 1$
  - Diffusion: $dt < \frac{1}{2}\frac{dx^2}{\Gamma}$

Convection – diffusion equation.

Implicit time discretization and linear algebra solutions.

- Fully implicit time discretization is unconditionally stable.
- However, it requires solution of linear algebra systems.
- We convert discretized system into algebraic system of the form: $\bar{A} \cdot x = b$
- Coefficients appearing in all discretized term build up matrix $\bar{A}$
- Source term, time step part (with ϕ_P^t) and discretized terms from outer geometry boundary parts build up vector b
- Vector $x = \{\dots, \phi_W^{t+1}, \phi_P^{t+1}, \phi_E^{t+1}, \dots\}$
- Many different methods to solve such systems, like iterative methods (CG, GMRES, BiCGstab, multigrid)
- To speedup solution of linear algebra systems preconditioners used. Here one tries to approximate $\mathrm{M} \approx \bar{A}$, where matrix M is easily invertible. Then one solves $\mathrm{M}^{-1}\bar{A} \cdot x = \mathrm{M}^{-1}b$. Note that $\mathrm{M}^{-1}\bar{A}$ has lower condition number, which results in faster convergence.

Convection – diffusion equation.

Implicit vs explicit discretization summary.

- Fully implicit time discretization:

$$\rho \frac{\phi_P^{t+1} - \phi_P^t}{dt} \delta CV + \sum_{f=\{e,w,n,s,t,b\}} n_f A_f \rho_f \phi_f^{t+1} u_f = \sum_{f=\{e,w,n,s,t,b\}} n_f A_f \Gamma_f \nabla \phi_f^{t+1} + S_\phi \delta CV$$

- Fully explicit discretization:

$$\rho \frac{\phi_P^{t+1} - \phi_P^t}{dt} \delta CV + \sum_{f=\{e,w,n,s,t,b\}} n_f A_f \rho_f \phi_f^{t} u_f = \sum_{f=\{e,w,n,s,t,b\}} n_f A_f \Gamma_f \nabla \phi_f^{t} + S_\phi \delta CV$$

- Mixed implicit – explicit discretization possible.

Convection – diffusion equation.

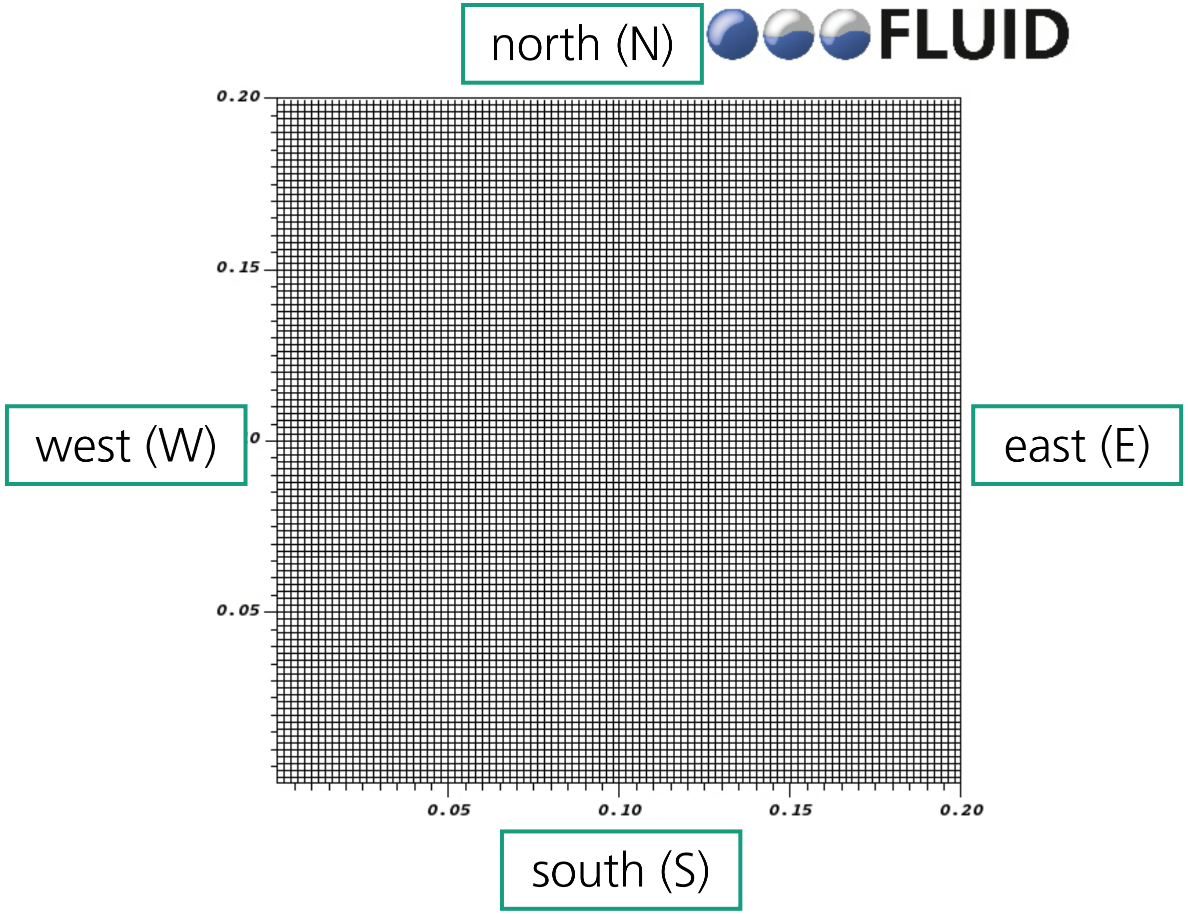
Boundary conditions.

- We will consider 3 different boundary conditions:
  - Dirichlet boundary: $\phi_{wall} = \bar{\phi}$, here we fix value at the boundary "wall" to pre-defined $\bar{\phi}$
  - Neumann boundary: $\frac{\partial \phi_{wall}}{\partial n} = \bar{\bar{\phi}}$, here we fix normal gradient at the boundary wall to pre-defined $\bar{\bar{\phi}}$. Note: when $\bar{\bar{\phi}}$=0, we assume no change of ϕ in the wall direction.
  - Flux condition: $\Gamma \nabla \phi \cdot n = \alpha_w (\phi_{wall} - \phi_{ext}) \cdot n$, here be balance fluxes from internal geometry part with flux from outside computational part by assuming external value ϕ_{ext} and parameter α_w. Note, for very high values of α_w this boundary condition approaches Dirichlet boundary (with value ϕ_{ext}) and for very low values of α_w we approach zero Neumann boundary condition.

- Forthcoming simulation results are performed on 2D square geometry of size [0,0.2]x[0,0.2] (m)
- We start with simple diffusion equation:

$$\frac{\partial T}{\partial t} = \Gamma \Delta T$$

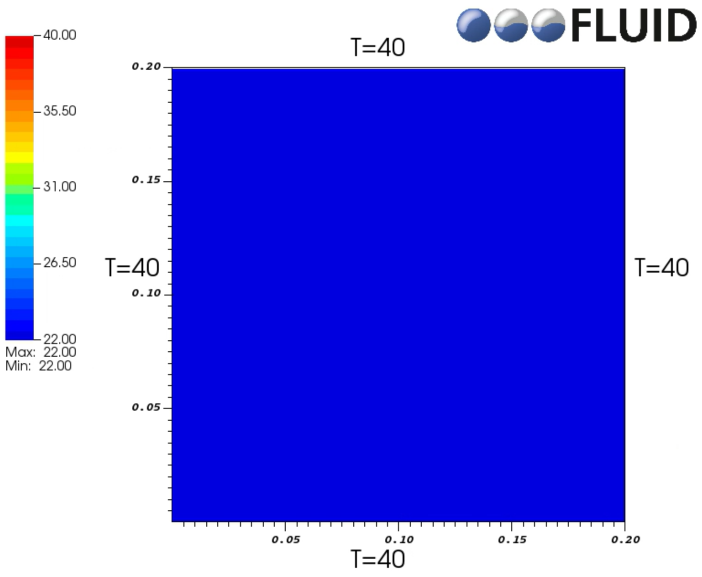
- We will test different:
  - Initial conditions
  - Boundary conditions (E,W,N,S)
  - Diffusivity values.

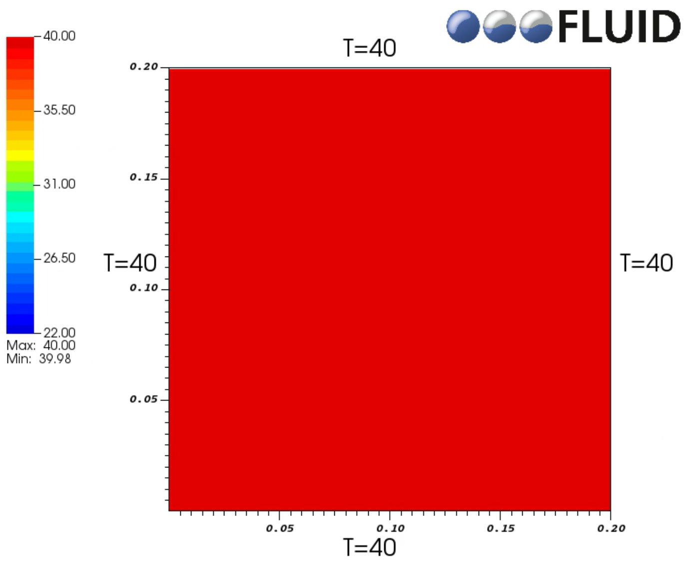


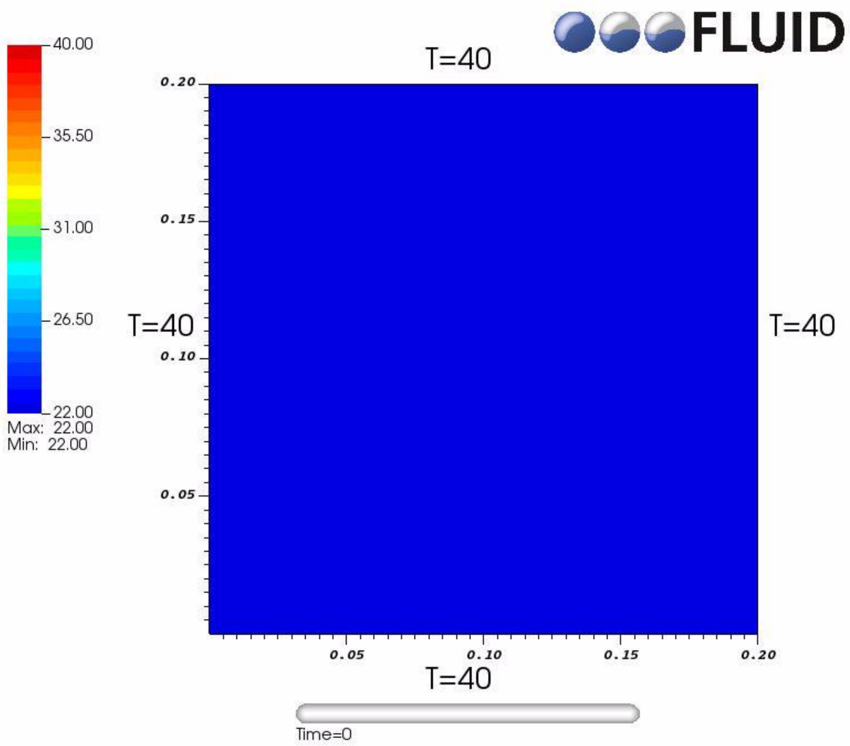
Simulation examples.

Diffusion equation.

- Case 1:
  - Diffusion value Γ=0.0001
  - Initial value 22;
  - Boundary condition (Dirichlet): T_W =40,T_E =40, T_N =40,T_S =40
- As expected, uniform steady state solution.

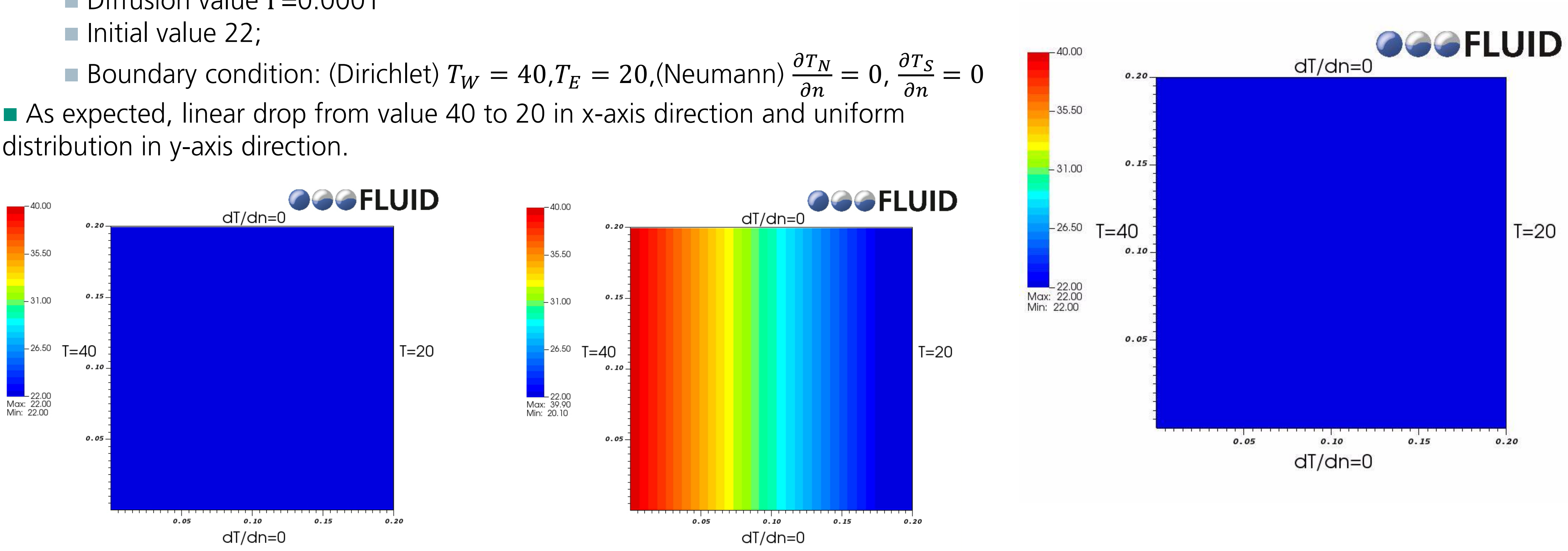




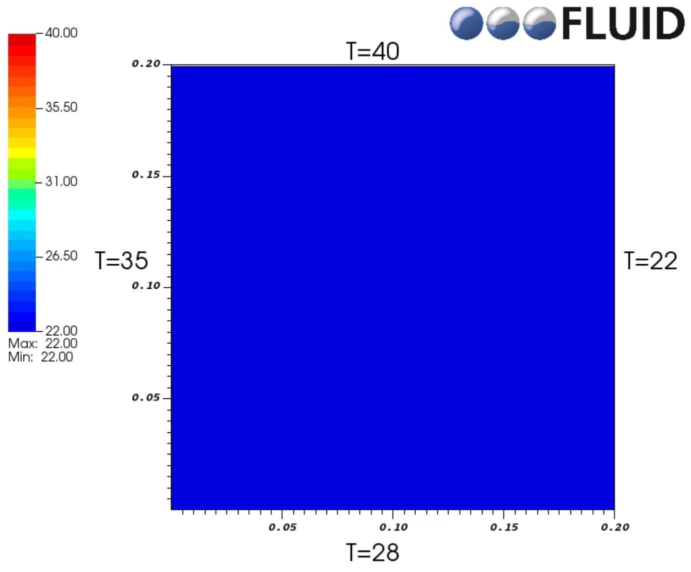


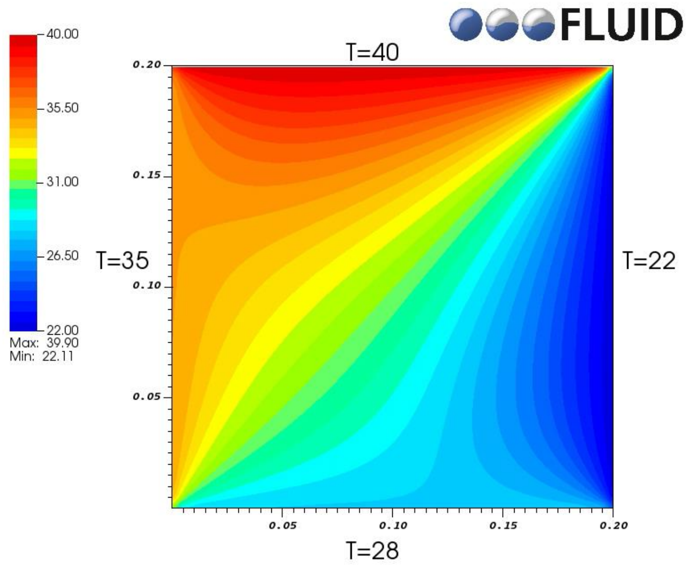
Simulation examples.
Diffusion equation.

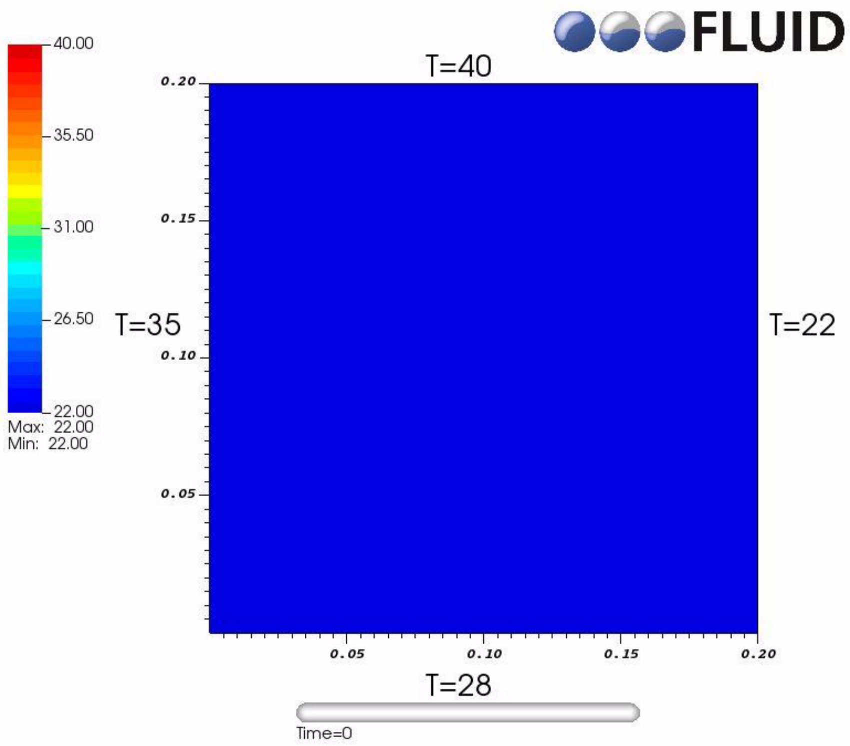
- Case 2:
  - Diffusion value Γ=0.0001
  - Initial value 22;
  - Boundary condition: (Dirichlet) $T_W = 40, T_E = 20$,(Neumann) $\frac{\partial T_N}{\partial n} = 0, \frac{\partial T_S}{\partial n} = 0$
- As expected, linear drop from value 40 to 20 in x-axis direction and uniform distribution in y-axis direction.



- Case 3:
  - Diffusion value Γ=0.0001
  - Initial value 22;
  - Boundary condition: $T_W = 35, T_E = 22$, $T_N = 40, T_S = 28$.

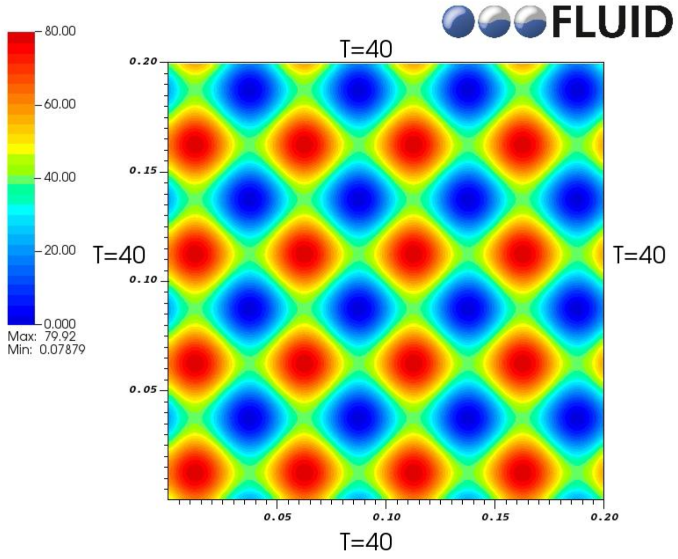


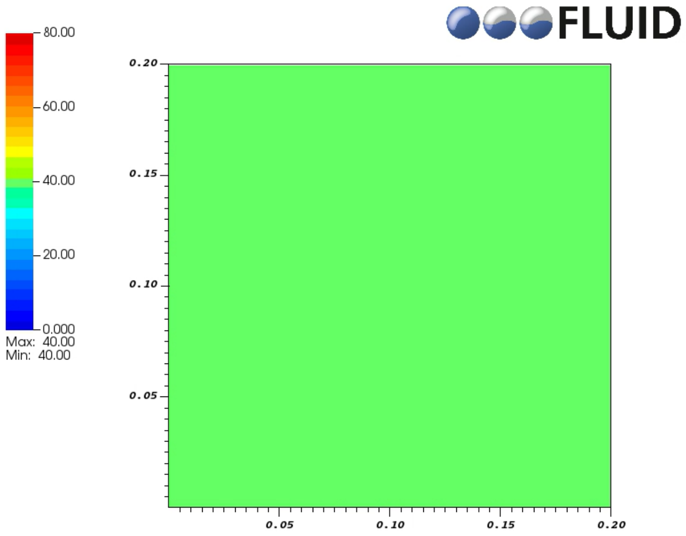


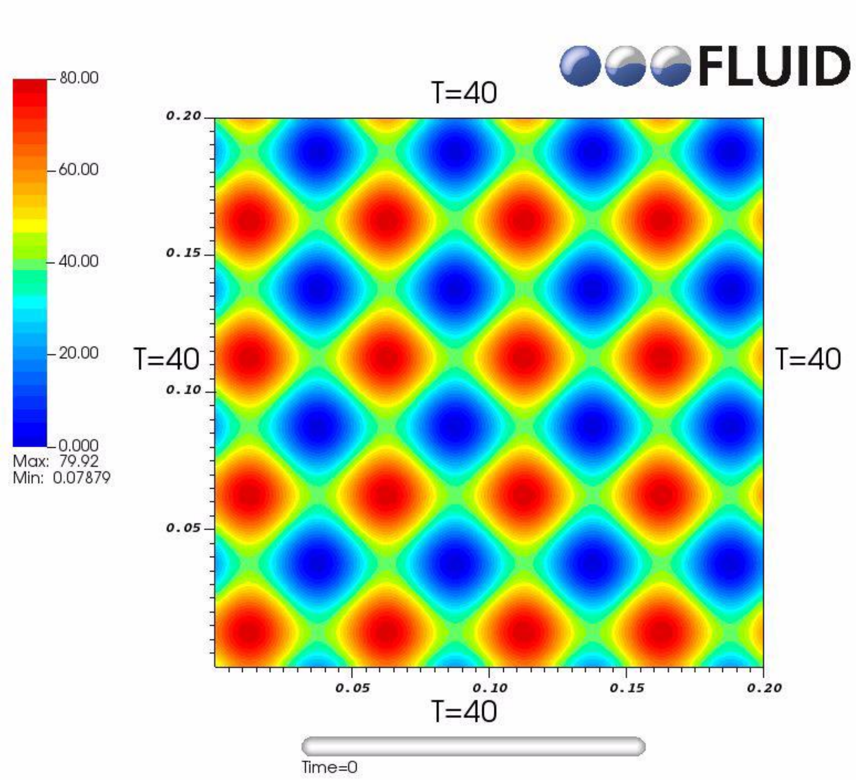


Simulation examples.
Diffusion equation.

- Case 4:
  - Diffusion value Γ=0.00001
  - Initial value: non-uniform;
  - Boundary condition: T_W =40,T_E =40, T_N =40,T_S =40.
- Uniform steady state solution.



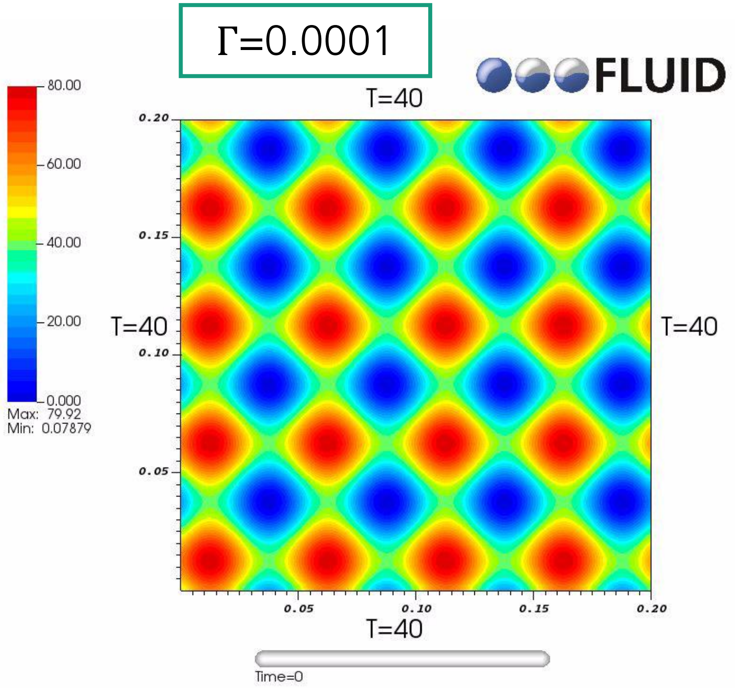


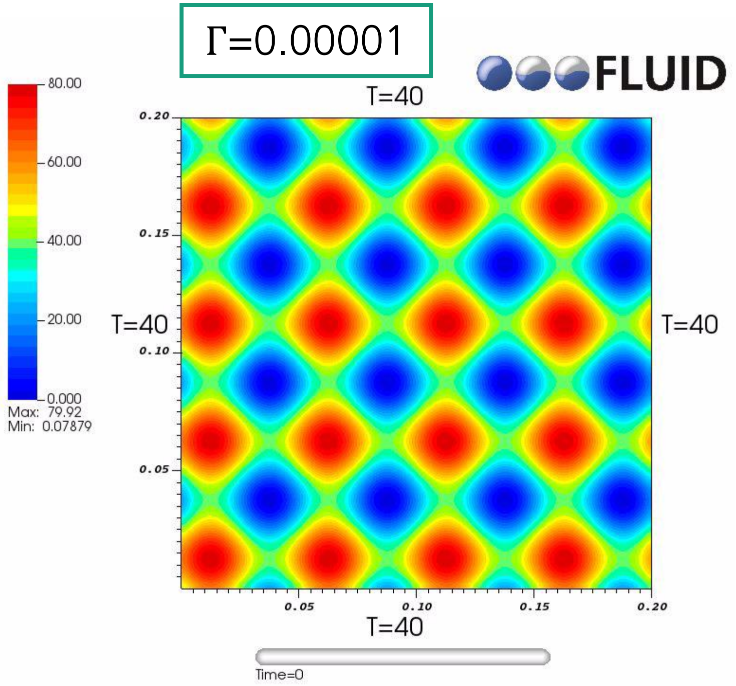


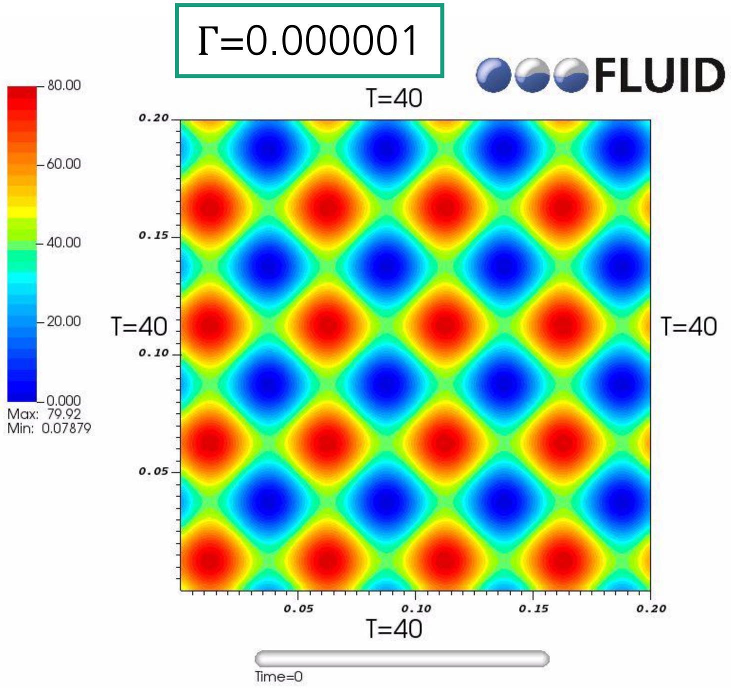
Simulation examples.

Diffusion equation.

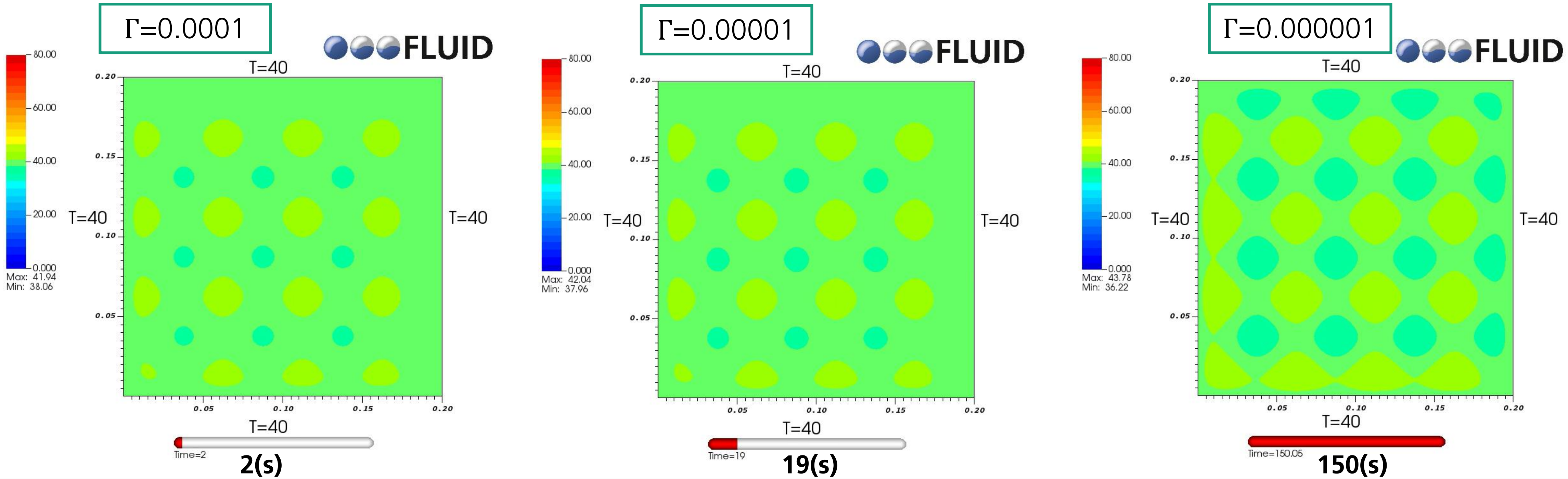
- Case 5:
  - Diffusion value Γ=0.0001,0.00001, 0.000001
  - Initial value: non-uniform;
  - Boundary condition: T_W =40,T_E =40, T_N =40,T_S =40.
- Diffusion parameter has impact on speed of diffusion.





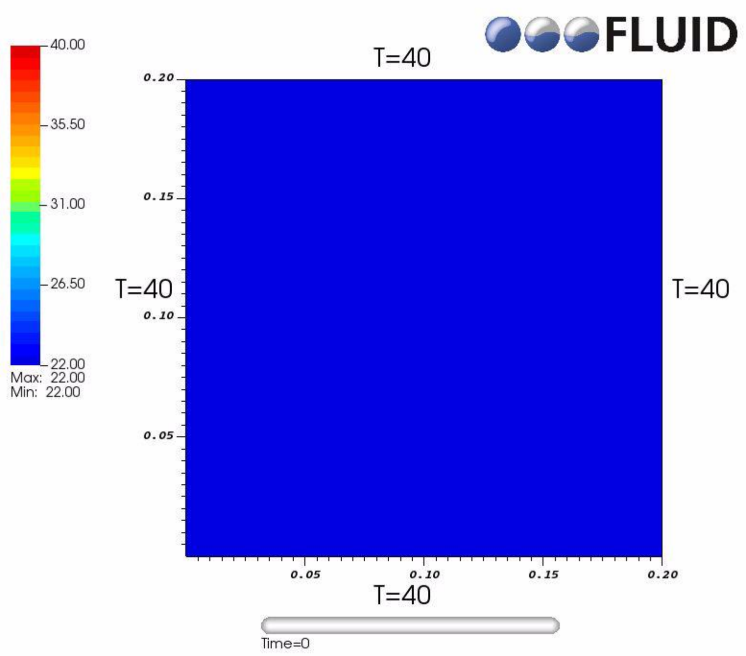


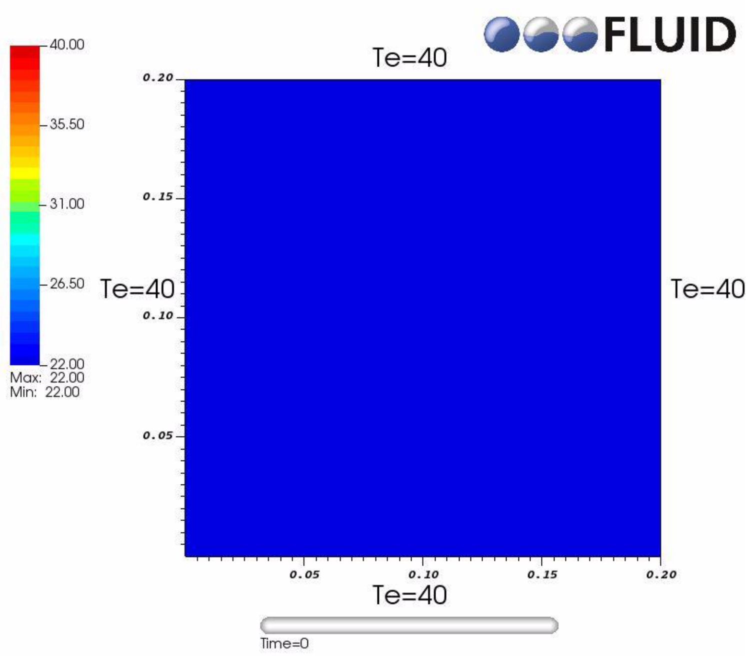
- Case 5:
  - Diffusion value Γ=0.0001,0.00001, 0.000001
  - Initial value: non-uniform;
  - Boundary condition: T_W =40,T_E =40, T_N =40,T_S =40.
- Diffusion parameter has impact on speed of diffusion and smooths out initial oscillations.



Simulation examples.
Diffusion equation.

- Case 6:
  - Diffusion value Γ=0.0001
  - Initial value: 22;
  - Boundary condition 1: T_W =40,T_E =40, T_N =40,T_S =40.
  - Boundary condition 2: Flux on all boundaries with α_w=0.5 and $T_{ext} = 40$
- Diffusion parameter has impact on speed of diffusion and smooths out initial oscillations.





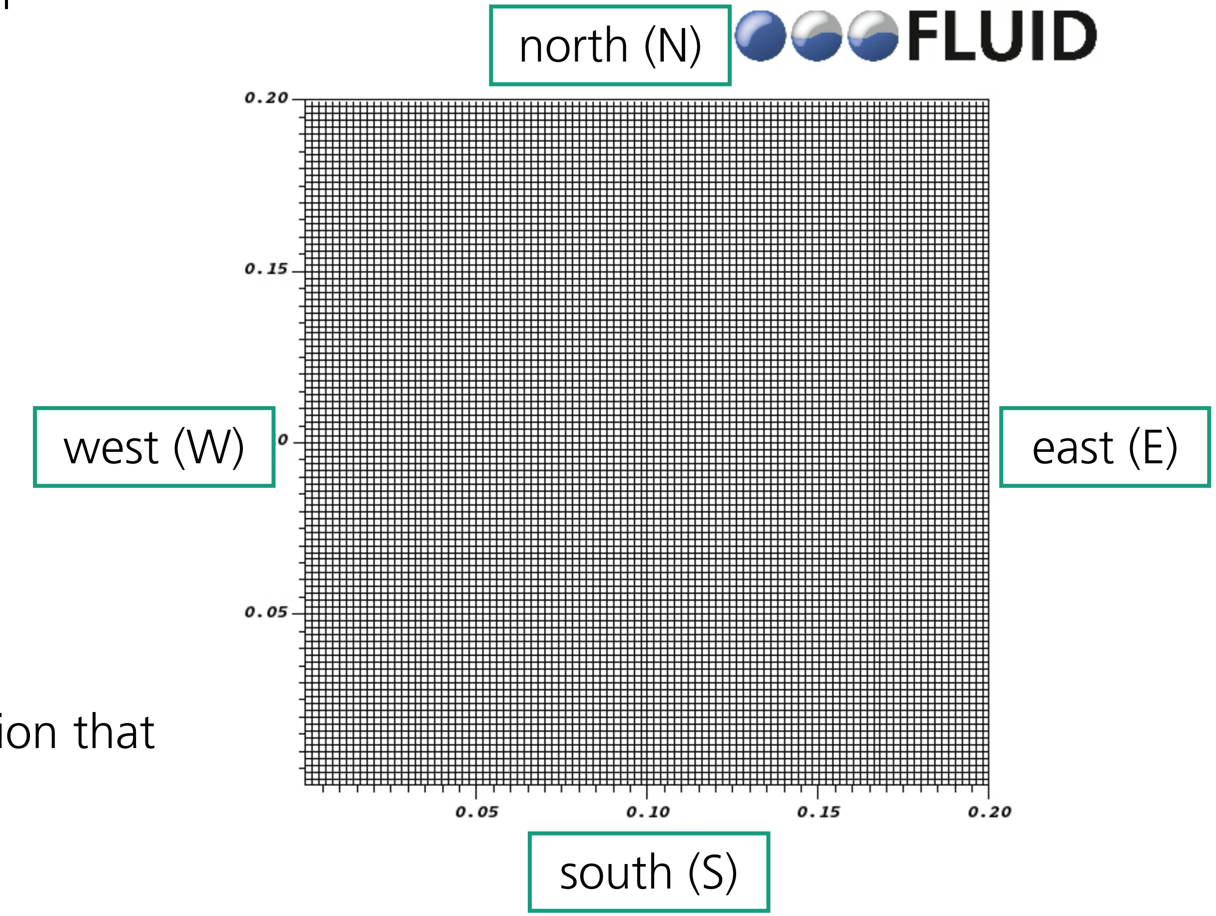
Simulation examples.

Convection equation.

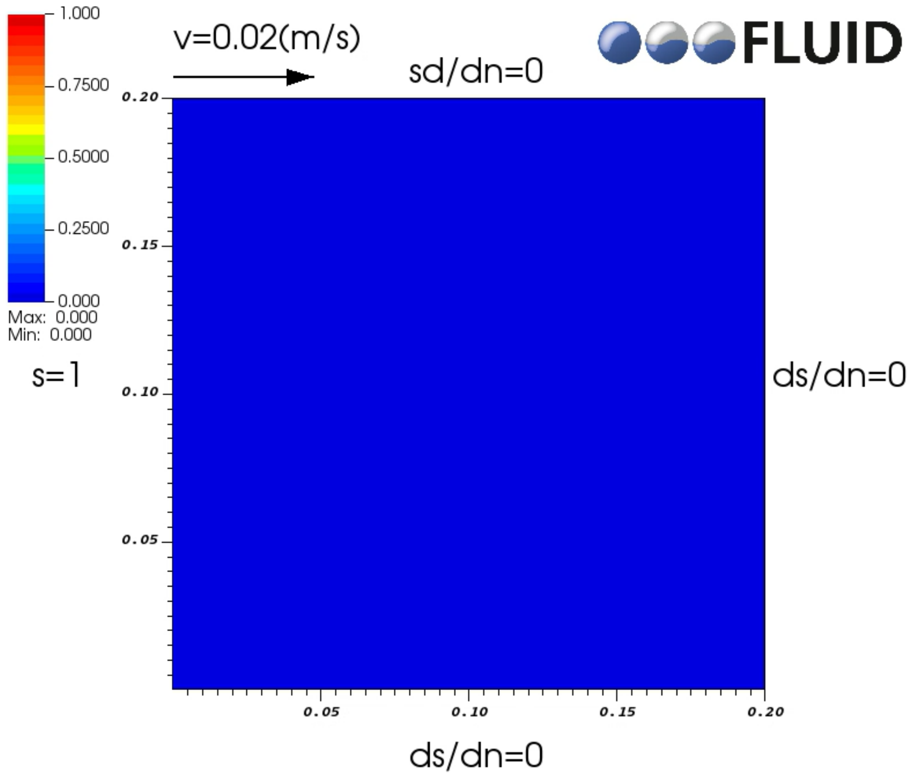
- Forthcoming simulation results are performed on 2D square geometry of size [0,0.2]x[0,0.2] (m)
- We consider simple convection equation:

$$\frac{\partial s}{\partial t} + u \cdot \nabla s = 0$$

- We will test different:
  - Initial conditions
  - Boundary conditions (E,W,N,S)
  - Velocity fields.
  - Different diffusion schemes.
- Note, that all convection schemes show artificial diffusion that may affect accuracy of the solution.



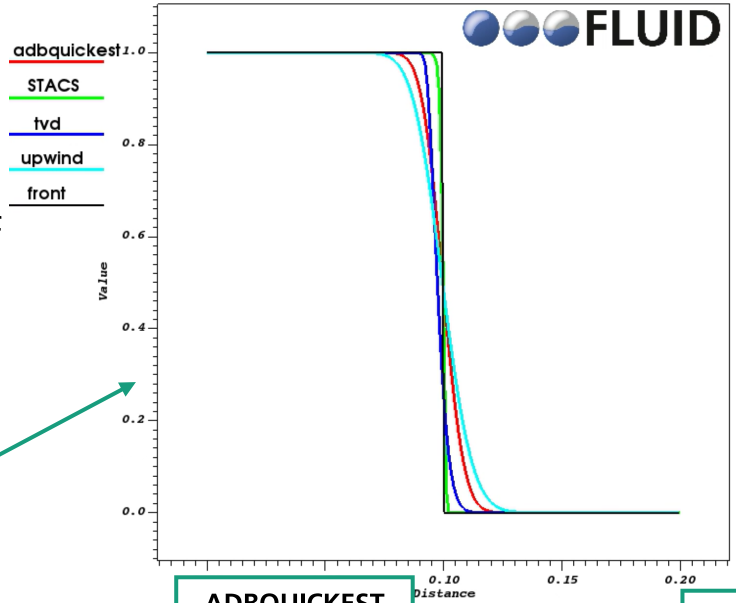
- Case 1:
  - Constant convection velocity: u = (0.02,0).
  - Initial value: s =0;
  - Boundary condition: $s_W = 1, \frac{\partial s_E}{\partial n} = 0, \frac{\partial s_N}{\partial n} = 0, \frac{\partial s_S}{\partial n} = 0.$
- 4 different convection schemes used.
  - Upwind
  - TVD superbee
  - ADBQUICKEST
  - STACS
- Note, we do not discuss in detail implementation issues for all those schemes.

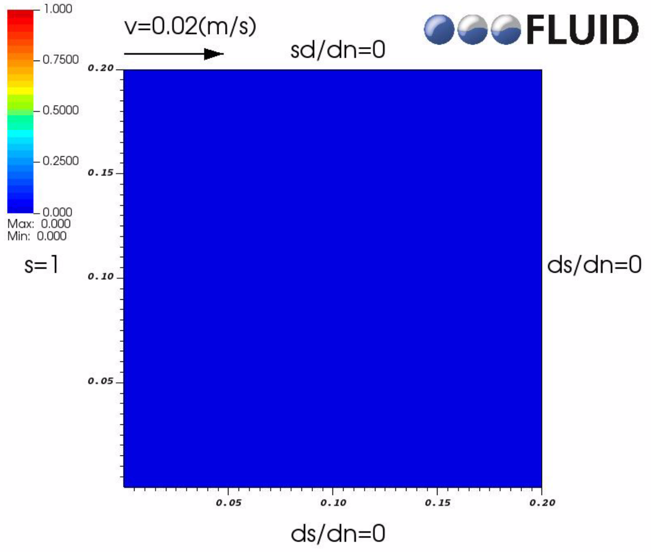


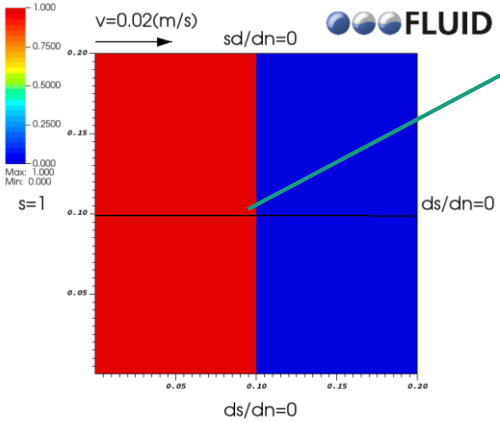
Simulation examples.

Convection equation.

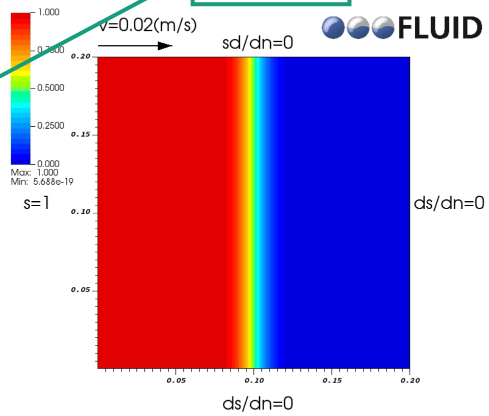
- Case 1:
- Simulated time: 5(s)
- Upwind scheme shows highest diffusivity of the front propagation.
- STACS shows smallest diffusivity.
- We use constant time step $dt = 0.0005\ (s)$



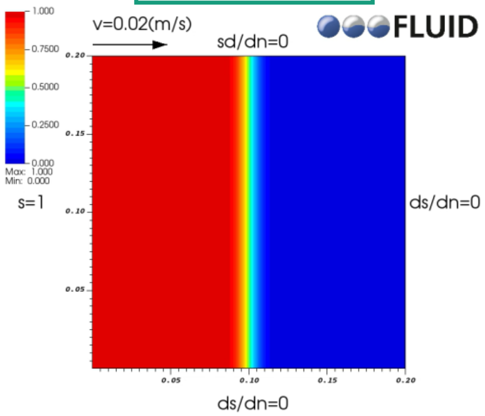




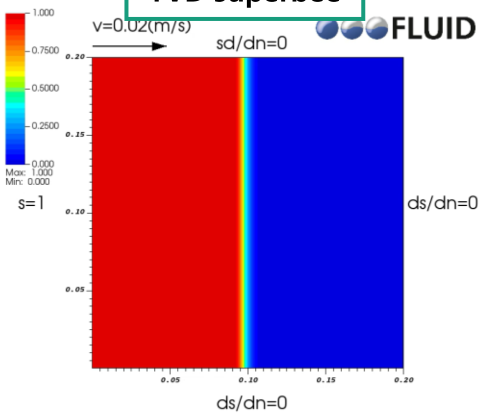
Upwind



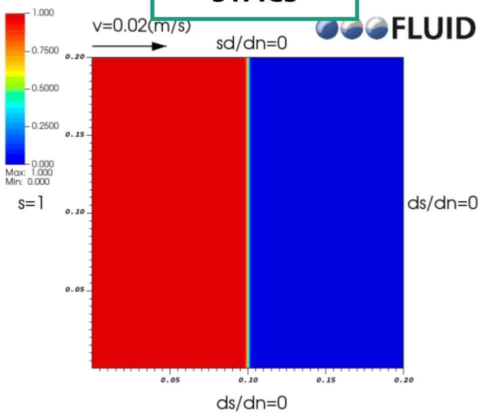
ADBQUICKEST



TVD superbee



STACS



Simulation examples.

Convection equation – artificial diffusion for UPWIND scheme.

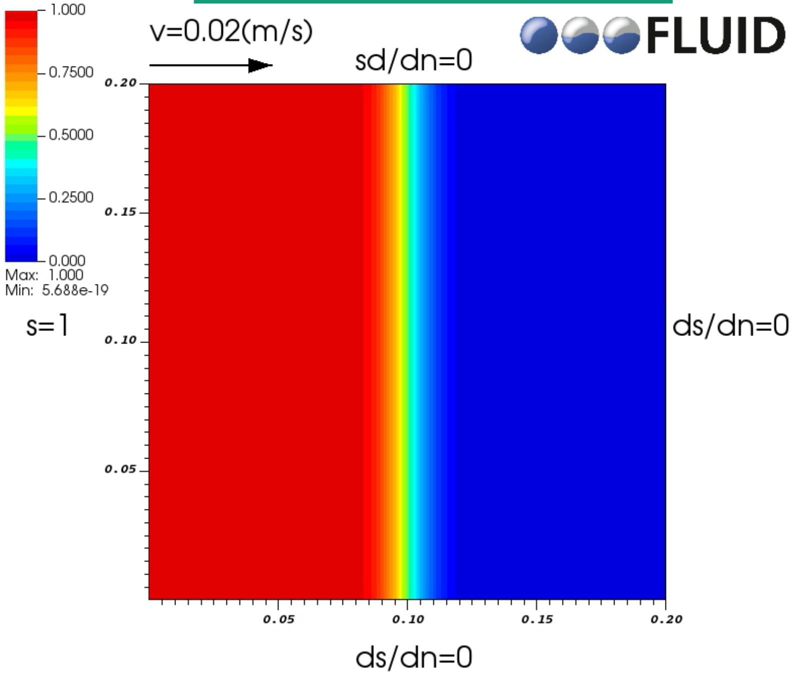
- We consider now Upwind scheme.
- Using Taylor expansion one can determine the local truncation error of discretization scheme.
- For upwind scheme one can show that dropping first order terms from Taylor expansion leads to artificial numerical diffusion term: $\frac{u \cdot dx}{2}(1 - CFL)\frac{\partial^2 s}{\partial x^2}$
- Recall, CFL is Courant–Friedrichs–Lewy value.
- This means that we can reduce numerical diffusion in 2 ways:
  - use finer mesh (reduction of dx)
  - use time step such that $CFL = 1$, however for explicit scheme this may lead to instabilities. For $CFL > 1$ explicit schemes are instable.

Simulation examples.

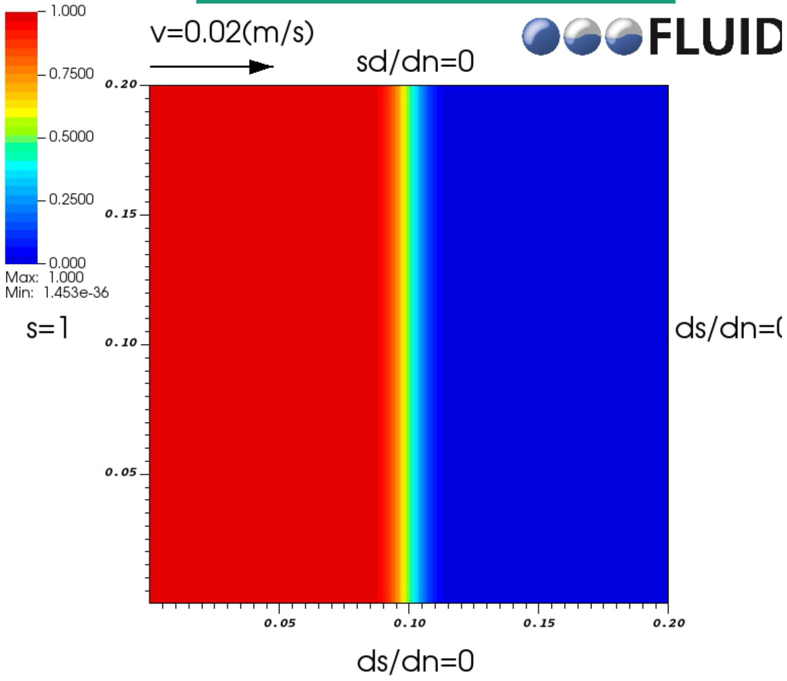
Convection equation – artificial diffusion for UPWIND scheme.

- We consider now Upwind scheme for different simulation setup.

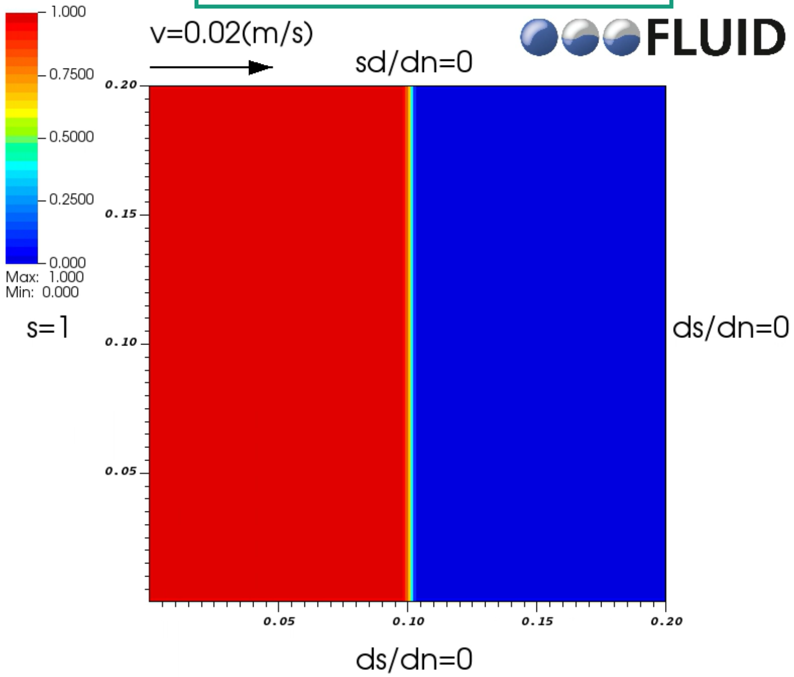
Dt=0.0005, dx = 0.001
CFL = 0.01



Dt=0.0005, dx = 0.0005
CFL = 0.02



Dt=0.0049, dx = 0.001
CFL = 0.98

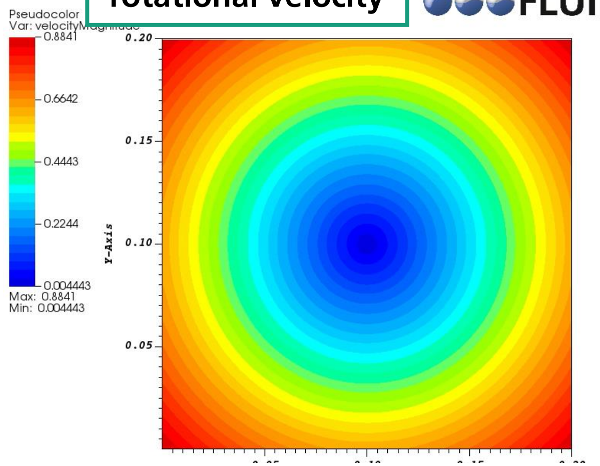


- Note that for fluid dynamics application no possible to choose time step to satisfy $CFL \approx 1$ in all grid elements.

- Case 2 so called Zalesak disc:
  - rotational velocity wit center of 0.1.
  - Initial value: disc with cut out located away from middle point (0.1,0.1);
  - Boundary condition: $\frac{\partial s_W}{\partial n}=0, \frac{\partial s_E}{\partial n} = 0, \frac{\partial s_N}{\partial n} = 0, \frac{\partial s_S}{\partial n} = 0.$
- 4 different convection schemes used.
  - Upwind
  - TVD superbee
  - ADBQUICKEST
  - STACS
- Simulation stops after one full revolution.

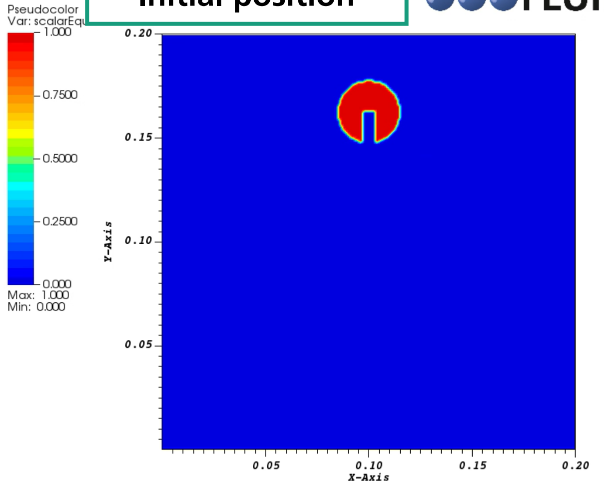
rotational velocity

FLUID



Initial position

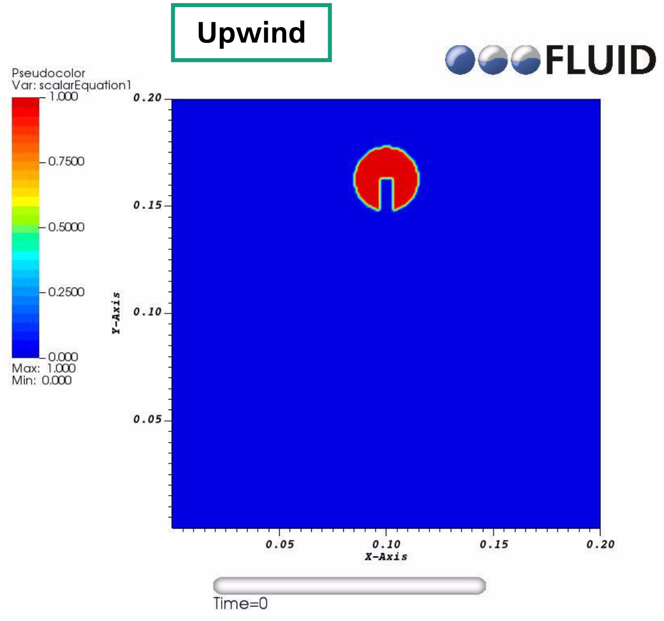
FLUID

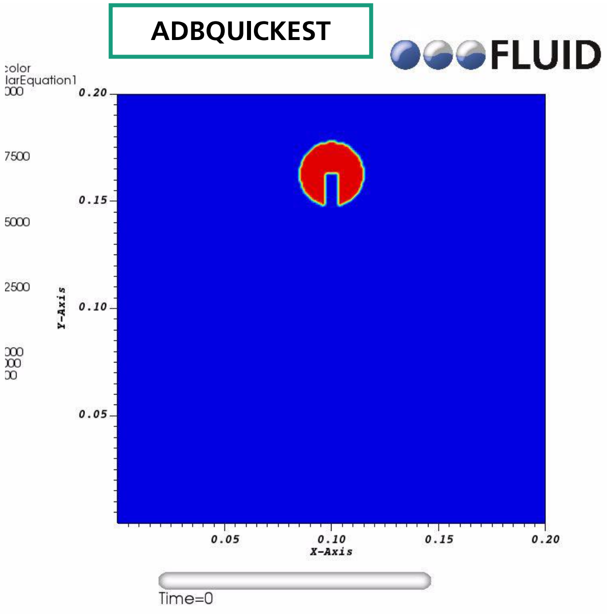


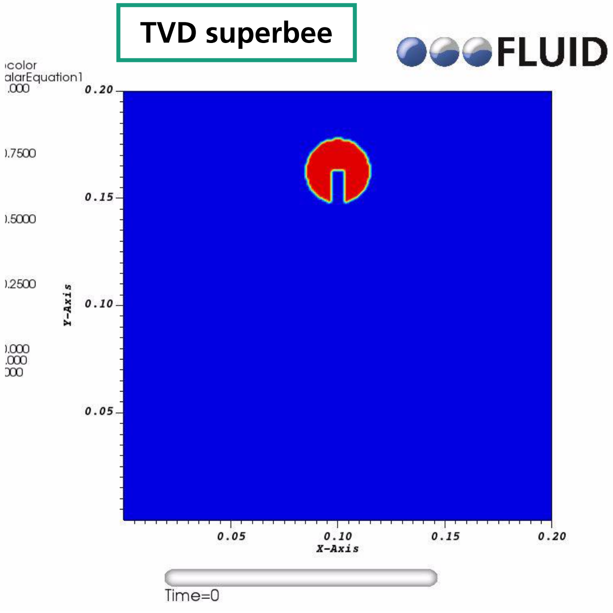
Simulation examples.

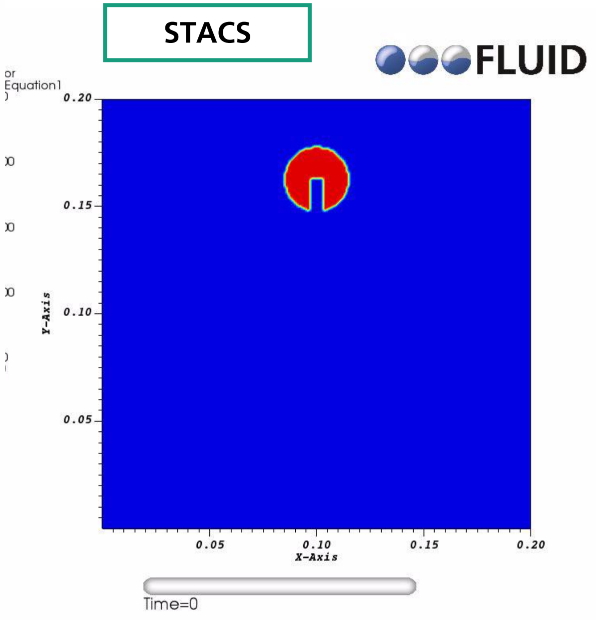
Convection equation.

- Case 2: Zalesak disc, one revolution
- Simulation time 1 (s).





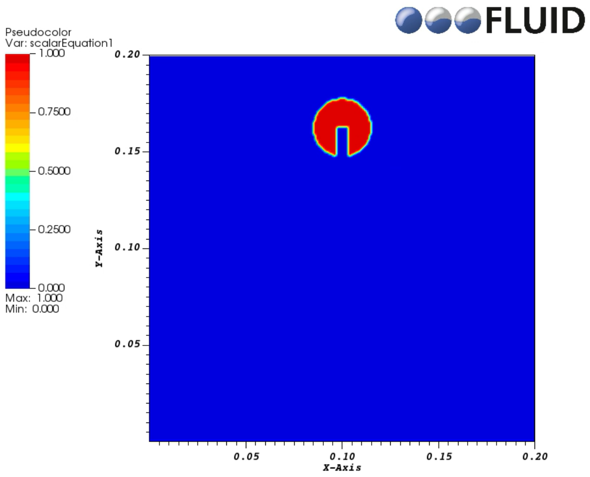


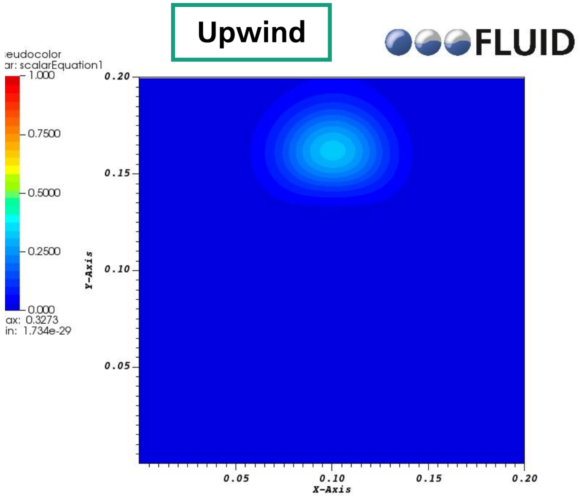


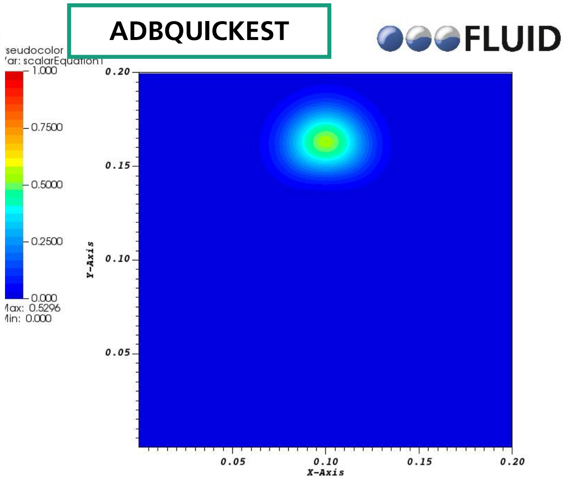
Simulation examples.

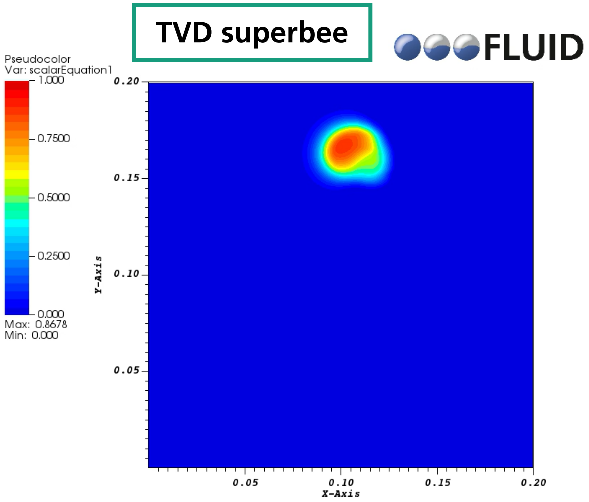
Convection equation.

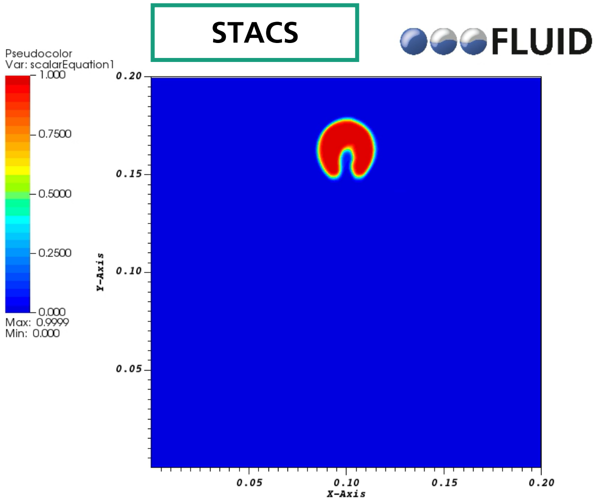
- Case 2:
- Simulated time: 1(s)
- Only STACS retains original shape after one revolution. However, also for STACS front diffuses as well.











Summary and outlook.

- Short introduction to scientific computing has been presented.
- Several simulation examples of convection, diffusion type have been showed and discussed.
- REMEMBER: Do not trust any simulation tool ! Always analyze simulation results to be more

confident that simulation provide correct output.

- Next lecture:
  - Some aspects of flow equations will be discussed.
  - Newtonian, non-Newtonian flows.
  - Industrial application examples.

Vielen Dank für Ihre Aufmerksamkeit

Fraunhofer
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