



Other topics

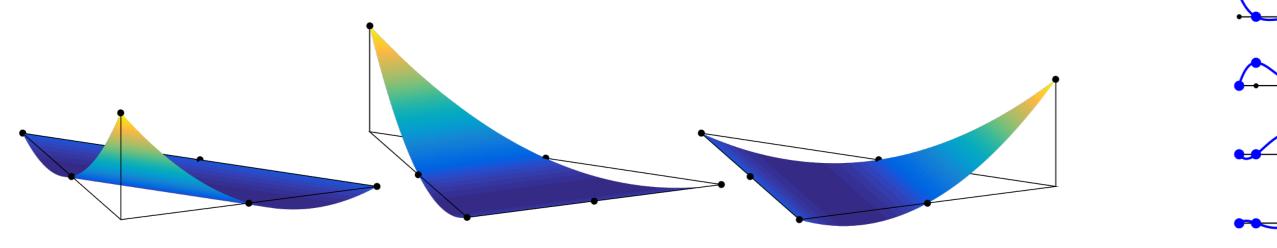
Numerical Flow Simulation

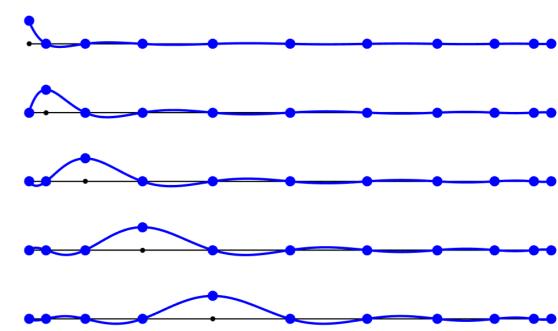
École polytechnique fédérale de Lausanne

Edouard Boujo Fall 2024

This week's lecture

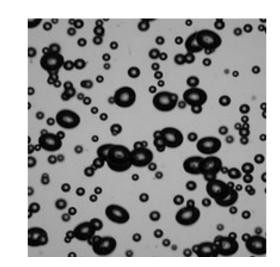
- Brief overview of 2 topics:
 - 1. Discretization/computation methods (other than FVM)





2. Techniques for handling fluid interfaces







Numerical Flow Simulation

Discretization/computation methods (reminder)

Some software (Commercial – Free/open)

(Mostly academic)

Fluent, Star-CCM+, OpenFOAM...

Comsol, FreeFEM++, AVBP....

Nek5000...

(Mostly academic)

SPH-flow, Fluidix...

PowerFLOW...

- Finite difference method (FDM)
- Finite volume method (FVM)
- Finite element method (FEM)
- Spectral element method (SEM)
- Spectral methods
- Particle-based methods
- Lattice Boltzmann methods (LBM)

Discretization/computation methods (reminder)

- Finite difference method (FDM)
- Finite volume method (FVM)
- Finite element method (FEM)
- Spectral element method (SEM)

Applicable to **any PDE** (electrodynamics, thermodynamics, pattern formation, quantum mechanics, statistical mechanics, economics...)

- Spectral methods
- Particle-based methods

Lattice Boltzmann methods (LBM)

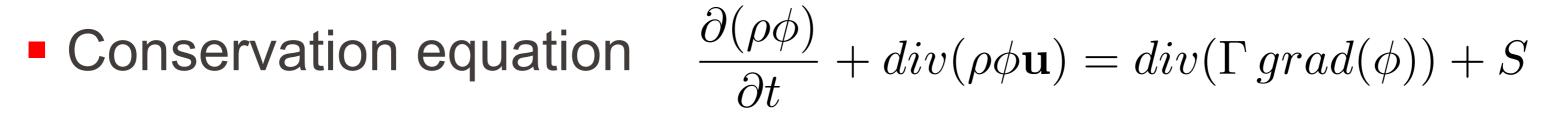
Specific to continuum media (solid / fluid)

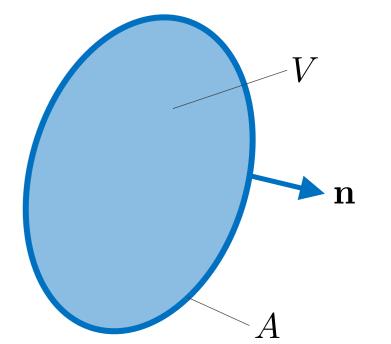
Specific to **fluid**

Discretization/computation methods

- Finite difference method (FDM)
- Finite volume method (FVM)
- Finite element method (FEM)
- Spectral element method (SEM)
- Spectral methods
- Particle-based methods
- Lattice Boltzmann methods (LBM)

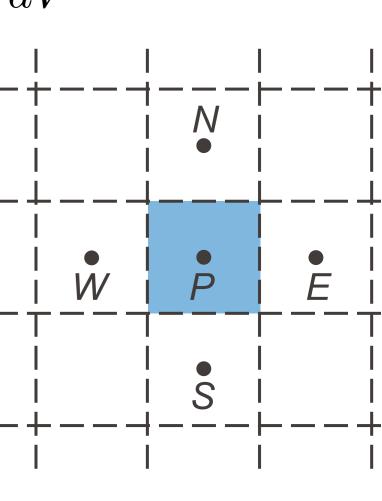
Finite volume method (reminder)

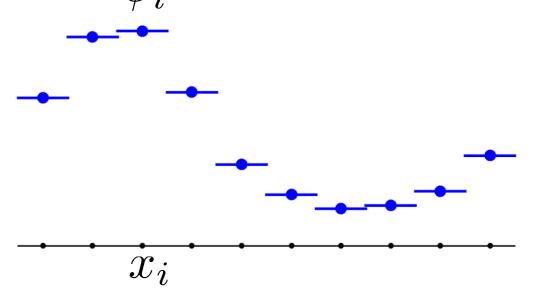




■ Integral form:
$$\frac{\partial}{\partial t} \int_V \rho \phi \, dV + \oint_A \rho \phi \mathbf{u} \cdot \mathbf{n} \, dA = \oint_A \Gamma \, grad(\phi) \cdot \mathbf{n} \, dA + \int_V S \, dV$$

- Divide the domain into a partition of control volumes
- Discretize the solution as nodal values: $\phi = (\phi_1, \phi_2, \dots, \phi_i, \dots, \phi_n)$
- Approximate volume integrals as functions of nodal values, and surface integrals as functions of face values
- Algebraic system of equations $\mathbf{A}(\phi) = \mathbf{0}$
- Note: solution defined at the nodes. No information between nodes, only information about averaged value in each CV (integral formulation).

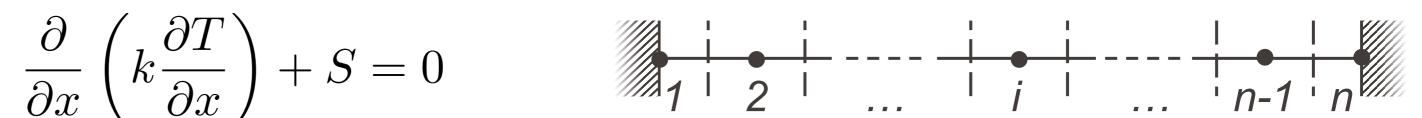




Finite volume method (reminder)

Example: 1D steady diffusion (e.g. heat conduction)

$$\frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + S = 0$$

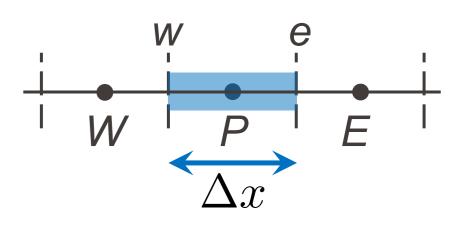


- Discretize into *n* CVs, *n* nodes: $T(\mathbf{x}) \to \mathbf{T} = (T_1, T_2, \dots, T_i, \dots, T_n)$
- Integration over CV + divergence theorem:

$$0 = \left(k\frac{\partial T}{\partial x}\right)_e - \left(k\frac{\partial T}{\partial x}\right)_w + \int_{x_w}^{x_e} S \, dx$$

Approximation as function of nodal values (CD):

$$0 \approx k_e \frac{T_E - T_P}{\delta x_{PE}} - k_w \frac{T_P - T_W}{\delta x_{WP}} + S_P \Delta x$$

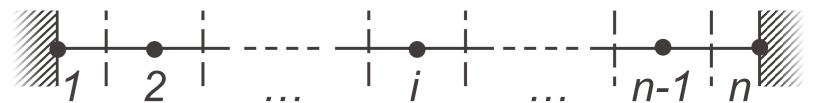


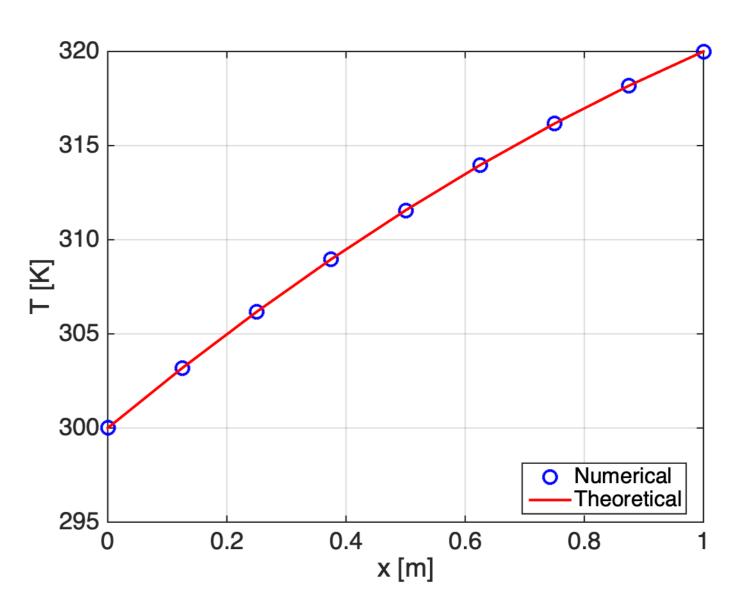
- Linear algebraic equation: $a_P T_P = a_W T_W + a_E T_E + b = \sum a_{nb} T_{nb} + b$
- Linear system (sparse matrix): AT = b

Finite volume method (reminder)

Example: 1D steady diffusion (e.g. heat conduction)

```
L = 1;
Ta = 300;
Tb = 320;
k = 400;
Sc = 5000;
n = 9; x = linspace(0, L, n); dx = L/(n-1);
%--- Matrix and boundary conditions
A = zeros(n,n); b = zeros(n,1);
for i=2:n-1
    A(i, i-1:i+1) = k*[-1 2 -1]/dx;
    b(i)
                = Sc*dx;
end
A(1,1) = 1; b(1) = Ta;
A(n,n) = 1; b(n) = Tb;
%--- Numerical solution
T = A \setminus b;
%--- Plot
figure('color','w'), hold on, grid on, box on,
plot(x,T,'bo')
%--- Theoretical solution
T theo = -Sc/(2*k)*x.^2 + ((Tb-Ta)/L+Sc*L/(2*k))*x + Ta;
plot(x,T_theo,'r-')
```





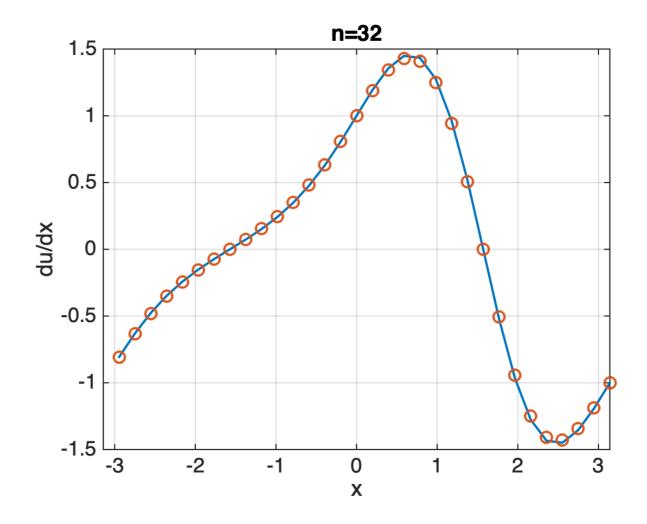
Finite volume method

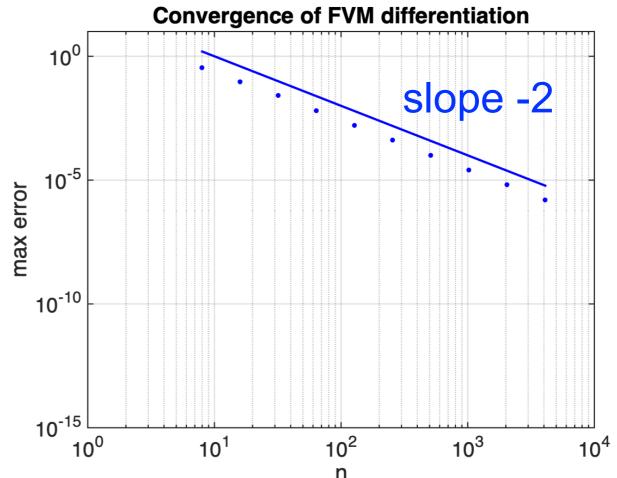
Focus on differentiation: 1st derivative

```
nvec = 2.^{(3:12)}; % Number of grid points
figure, hold on, box on, grid on
for n = nvec
    dx = 2*pi/n; x = -pi + dx*(1:n)'; % Grid generation
    %--- Differentiation matrix
    D = zeros(n,n);
    for i=2:n-1
        D(i, i-1:i+1) = [-1/2 \ 0 \ 1/2]/dx;
    end
                    = [0 \ 1/2]/dx; D(1,end) = -1/2/dx;
   D(1,1:2)
   D(end, end-1:end) = [-1/2 \ 0]/dx; D(end, 1) = 1/2/dx;
    D = sparse(D);
    u = \exp(\sin(x)); % Function
   uprime = cos(x).*u; % Analytical derivative
    uprime num = D*u; % Numerical derivative
    %--- Error
    err = norm(uprime-uprime num, inf);
    plot(n,err,'b.','markersize',15),
end
set(gca,'xscale','log'), set(gca,'yscale','log')
xlabel n, ylabel('max error'),
plot(nvec, 100./nvec.^2, 'b')
```

Example on a periodic domain:

$$u(x) = e^{\sin(x)} \longrightarrow u'(x) = \cos(x)u(x)$$





Discretization/computation methods

- Finite difference method (FDM)
- Finite volume method (FVM)
- Finite element method (FEM)
- Spectral element method (SEM)
- Spectral methods
- Particle-based methods
- Lattice Boltzmann methods (LBM)

j-1 • • • i+1 i+2 j-1 • • Δy j

- Solution discretized at grid points
- Derivatives expressed by combining Taylor expansions:

$$f_{i\pm 1} = f_i \pm \Delta x \left. \frac{\partial f}{\partial x} \right|_i + \left. \frac{\Delta x^2}{2!} \left. \frac{\partial^2 f}{\partial x^2} \right|_i \pm \left. \frac{\Delta x^3}{3!} \left. \frac{\partial^3 f}{\partial x^3} \right|_i + O(\Delta x^4)$$

$$f_{i\pm 2} = f_i \pm \dots$$

$$f_{i+3} = f_i \pm \dots$$

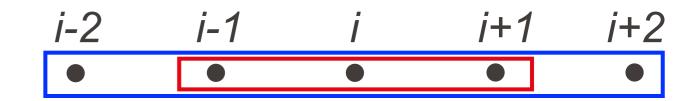
For example, 2nd-order approximations of 1st and 2nd derivatives:

$$f_{i+1} - f_{i-1} = 2\Delta x \left. \frac{\partial f}{\partial x} \right|_{i} + O(\Delta x^{3}) \quad \Rightarrow \quad \left. \frac{\partial f}{\partial x} \right|_{i} = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + O(\Delta x^{2})$$

$$f_{i+1} + f_{i-1} = 2f_{i} + \Delta x^{2} \left. \frac{\partial^{2} f}{\partial x^{2}} \right|_{i} + O(\Delta x^{4}) \quad \Rightarrow \quad \left. \frac{\partial^{2} f}{\partial x^{2}} \right|_{i} = \frac{f_{i+1} - 2f_{i} + f_{i-1}}{\Delta x^{2}} + O(\Delta x^{2})$$

Numerical Flow Simulation

Finite difference method



Can increase the order of accuracy by widening the stencil (i.e. using more neighbors). For example (on a uniform grid):

Derivative	Accuracy	- 5	-4	-3	-2	-1	0	1	2	3	4	5
1	2					-1/2	0	1/2				
	4				1/12	-2/3	0	2/3	-1/12			
	6			-1/60	3/20	-3/4	0	3/4	-3/20	1/60		
	8		1/280	-4/105	1/5	-4/5	0	4/5	-1/5	4/105	-1/280	
2	2					1	-2	1				
	4				-1/12	4/3	-5/2	4/3	-1/12			
	6			1/90	-3/20	3/2	-49/18	3/2	-3/20	1/90		
	8		-1/560	8/315	-1/5	8/5	-205/72	8/5	-1/5	8/315	-1/560	
3	2				-1/2	1	0	-1	1/2			
	4			1/8	-1	13/8	0	-13/8	1	-1/8		
	6		-7/240	3/10	-169/120	61/30	0	-61/30	169/120	-3/10	7/240	
4	2				1	-4	6	-4	1			
	4			-1/6	2	-13/2	28/3	-13/2	2	-1/6		
	6		7/240	-2/5	169/60	-122/15	91/8	-122/15	169/60	-2/5	7/240	

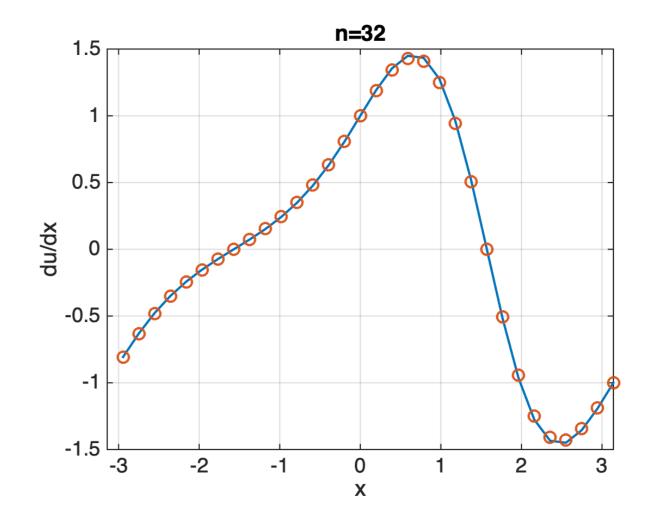
Focus on differentiation: 1st derivative

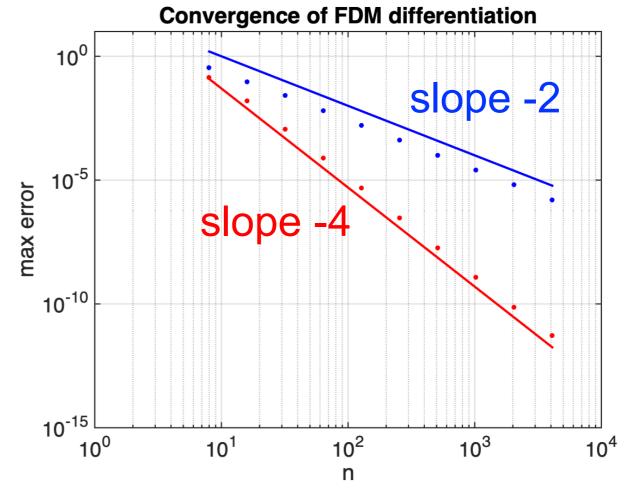
```
nvec = 2.^{(3:12)}; % Number of grid points
figure, hold on, box on, grid on
for n = nvec
    dx = 2*pi/n; x = -pi + dx*(1:n)'; % Grid generation
    %--- Differentiation matrix
    e = ones(n, 1);
    D = sparse(1:n, [2:n 1], 2*e/3, n, n)...
       -sparse(1:n,[3:n 1 2],e/12,n,n);
    D = (D-D')/dx;
   u = \exp(\sin(x)); % Function
    uprime = cos(x).*u; % Analytical derivative
    uprime num = D*u; % Numerical derivative
    %--- Error
    err = norm(uprime-uprime num, inf);
    plot(n,err,'r.','markersize',15),
end
set(gca,'xscale','log'), set(gca,'yscale','log')
xlabel n, ylabel('max error'),
plot(nvec, 500./nvec.^4, 'r')
```

↑ Example code: 4th-order FD. (In 1D, 2nd-order FD similar to 2nd-order FV.)

Example on a periodic domain:

$$u(x) = e^{\sin(x)} \longrightarrow u'(x) = \cos(x)u(x)$$







- Wide stencils are not ideal. In practice, accuracy not better if solution not smooth enough at the scale of the grid.
- Alternatively, can increase the order of accuracy with "compact FD": introduce additional degrees of freedom by combining Taylor expansions that involve the unknown derivative at other grid points.
- For example, for a 4th-order approximation of the 1st derivative, instead of looking for the standard expression

$$f_i' = \frac{af_{i-2} + bf_{i-1} + cf_i + df_{i+1} + ef_{i+2}}{\Delta x}$$

look for a compact expression of the form

$$\alpha f'_{i-1} + \beta f'_i + \gamma f'_{i+1} = \frac{af_{i-1} + bf_i + cf_{i+1}}{\Delta x}$$

and find in this case:

$$f'_{i-1} + 4f'_i + f'_{i+1} = \frac{3f_{i-1} - 3f_{i+1}}{\Delta x}$$

Example:

$$f'_{i-1} + 4f'_i + f'_{i+1} = \frac{3f_{i-1} - 3f_{i+1}}{\Delta x}$$

• Denoting the discretized solution $\mathbf{f} = (f_1, f_2, \dots, f_i, \dots f_n)$, this can be written as a linear system, to be solved for the derivative:

$$Af' = Bf$$

• When solving a PDE, e.g. $\frac{\partial f}{\partial t} + c \frac{\partial f}{\partial x} = 0$,

standard FD yields

$$\frac{\partial \mathbf{f}}{\partial t} + c\mathbf{D}\mathbf{f} = 0$$

while compact FD yields
$$\frac{\partial \mathbf{f}}{\partial t} + c\mathbf{f}' = 0 \Rightarrow \mathbf{A} \frac{\partial \mathbf{f}}{\partial t} + c\mathbf{B}\mathbf{f} = 0$$

to be solved for **f**, and where **A**, **B** have a narrower stencil than **D**.

Discretization/computation methods

- Finite difference method (FDM)
- Finite volume method (FVM)
- Finite element method (FEM)
- Spectral element method (SEM)

Spectral methods

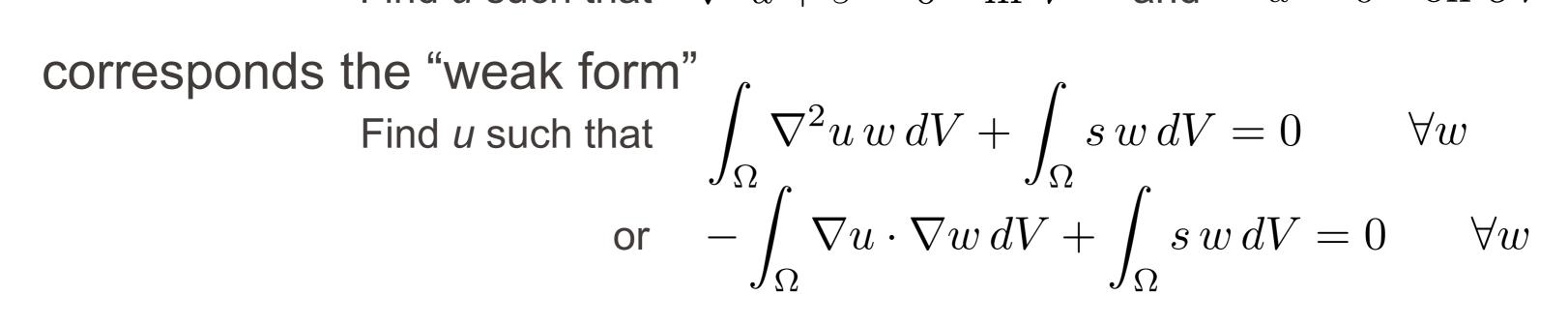
Particle-based methods

Lattice Boltzmann methods (LBM)

Finite element method

Transform the problem into its variational formulation ("weak form").
 For example, to the steady diffusion problem written in "strong form" as

Find u such that $\nabla^2 u + s = 0$ in V and u = 0 on ∂V

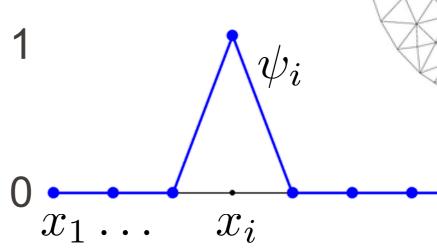


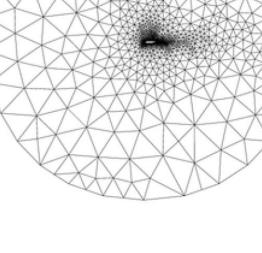


- Divide the domain into a partition of elements and nodes.
- Introduce basis functions (usually low-order polynomials) such that $\psi_i(x_i) = 1$ at node i,

 $\psi_i(x_j) = 0$ at other nodes j of the element.

(Piecewise def.: $\psi_i = 0$ on elements not containing node i)



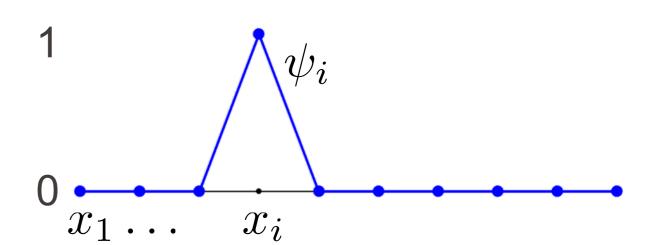


Numerical Flow Simulation

Finite element method

Discretize the solution u and test function w as combinations of basis functions:

$$u(x) = \sum_{i=1}^{n} u_i \psi_i(x)$$
 $w(x) = \sum_{i=1}^{n} w_i \psi_i(x)$



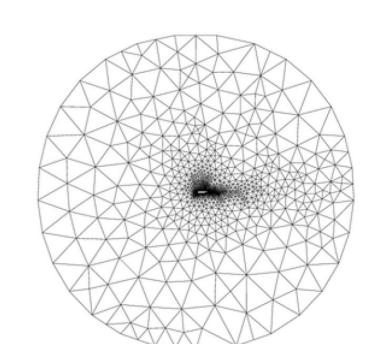
- Note: because of the properties of the ψ_i , the unknowns $\mathbf{u}=(u_1,u_2,\ldots,u_i,\ldots u_n)$ are nodal values: $u_i = u(x_i)$
- Insert into the weak form to obtain the discretized equation:

$$-\int_{\Omega} \nabla u \cdot \nabla w \, dV + \int_{\Omega} s \, w \, dV = 0 \qquad \forall w$$
$$\sum_{i} u_{i} \int_{\Omega} \nabla \psi_{i} \cdot \nabla \psi_{j} \, dV = \sum_{i} s_{i} \int_{\Omega} \psi_{i} \psi_{j} \, dV \quad \forall j$$

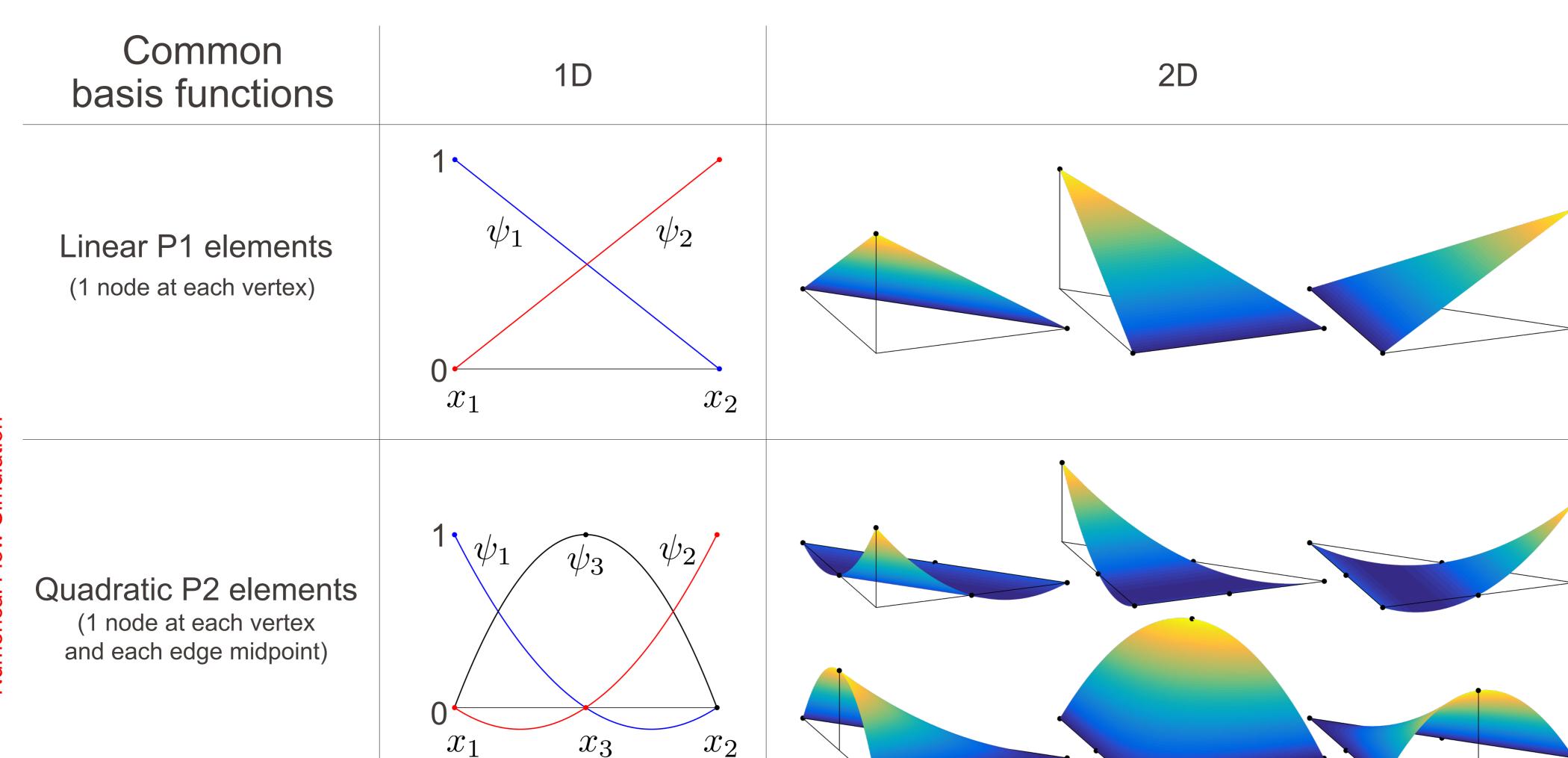


with (sparse) matrices:
$$\mathbf{A}_{i,j} = \int_{\Omega} \nabla \psi_i \cdot \nabla \psi_j \, dV$$
 $\mathbf{M}_{i,j} = \int_{\Omega} \psi_i \psi_j \, dV$

$$\mathbf{M}_{i,j} = \int_{\Omega} \psi_i \psi_j \, dV$$



Finite element method



Numerical Flow Simulation

Discretization/computation methods

- Finite difference method (FDM)
- Finite volume method (FVM)
- Finite element method (FEM)
- Spectral element method (SEM)

Spectral methods

Particle-based methods

Lattice Boltzmann methods (LBM)

Spectral methods

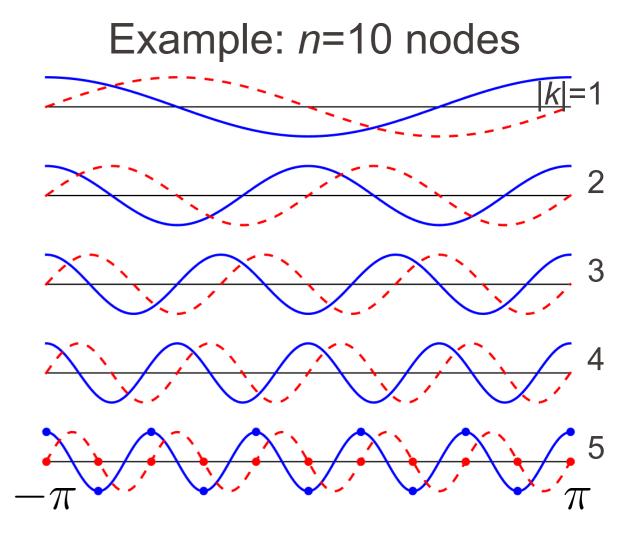
- Expansion on basis functions that are defined globally (over the whole domain)
- On periodic domains:
 - Basis functions: $\psi_k(x) = e^{ikx}$ (trigonometric polynomials) Expansion: Fourier series

$$u(x) = \sum_{k=-n/2}^{n/2-1} \hat{u}_k \psi_k(x) = \sum_{k=-n/2}^{n/2-1} \hat{u}_k e^{ikx}$$

- The unknowns $\hat{\mathbf{u}} = (\hat{u}_{-n/2}, \dots, \hat{u}_k, \dots)$ are the expansion coefficients (and are **not** nodal values).
- Differentiation becomes very easy: $\psi' = ik\psi$, and thus

$$u'(x) = \sum_{i \in \mathcal{U}} ik\hat{u}_k \psi_k(x)$$

- Can solve any PDE in Fourier space, and then come back to physical space.
- Can also derive (dense) differentiation matrices (e.g. ${\bf u}'={\bf D}{\bf u})$ and solve directly in physical space.



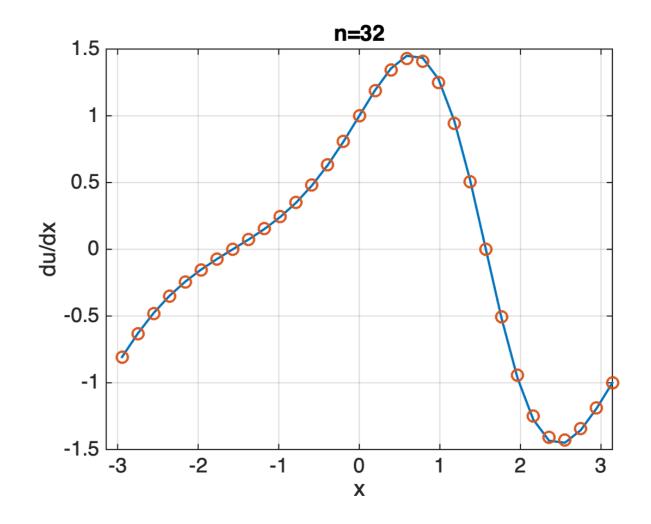
Spectral methods

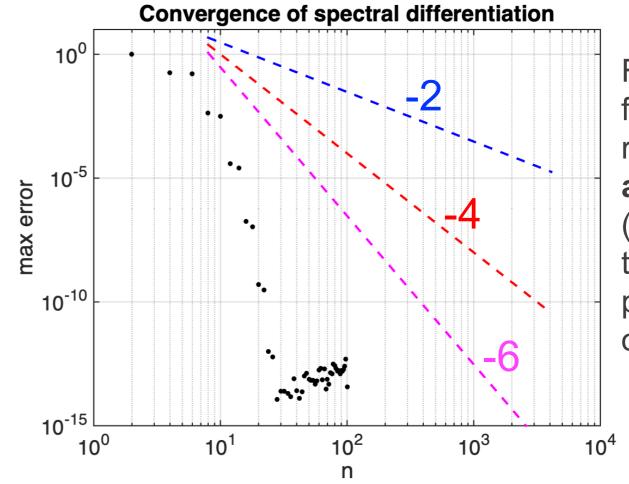
Focus on differentiation: 1st derivative

```
nvec = 2:2:100; % Number of grid points
figure, hold on, box on, grid on
for n = nvec;
    h = 2*pi/n; x = -pi + h*(1:n)'; % Grid generation
    %--- Differentiation matrix
    column = [0 .5*(-1).^(1:n-1).*cot((1:n-1)*h/2)];
    D = \text{toeplitz}(\text{column,column}([1 n:-1:2]));
    u = \exp(\sin(x)); % Function
    uprime = cos(x).*u; % Analytical derivative
    uprime num = D*u; % Numerical derivative
    %--- Error
    err = norm(uprime num-uprime, inf);
    plot(n,err,'k.','markersize',15),
end
set(gca,'xscale','log'),
set(gca, 'yscale', 'log')
xlabel n, ylabel('max error'),
```

Example on a periodic domain:

$$u(x) = e^{\sin(x)} \longrightarrow u'(x) = \cos(x)u(x)$$





For smooth functions: reach spectral accuracy (more accurate than any polynomial-order method)

Spectral methods

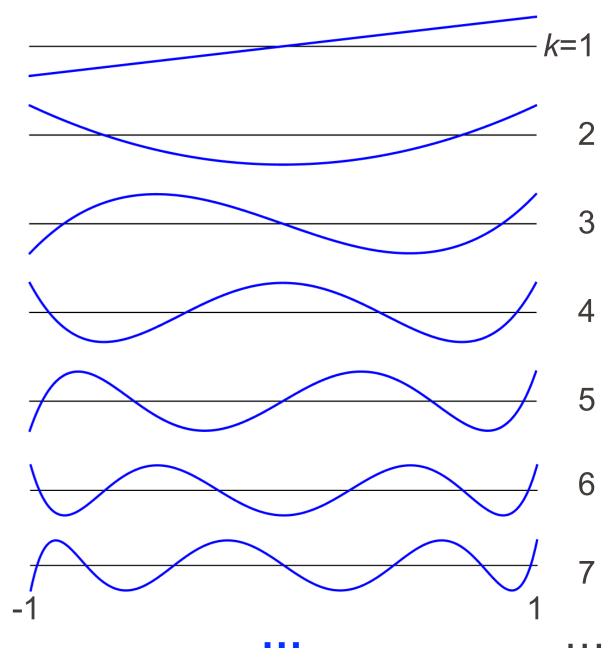
- Expansion on basis functions that are defined globally (over the whole domain)
- On non-periodic domains:
 - Basis functions: for ex. $T_k(x) = \cos(k\cos^{-1}(x))$ (Chebyshev polynomials). Expansion:

$$u(x) = \sum_{k=0}^{n} a_k T_k(x)$$

- The unknowns $\mathbf{a} = (a_0, a_1, \dots, a_k, \dots, a_n)$ are the expansion coefficients (and are **not** nodal values).
- Collocation method: enforce the governing equations on n+1 points. For ex.: Gauss-Chebyshev-Lobatto points:

$$x_j = \cos\left(\frac{j\pi}{n}\right)$$

 \rightarrow obtain an algebraic system for the a_k (dense matrix).

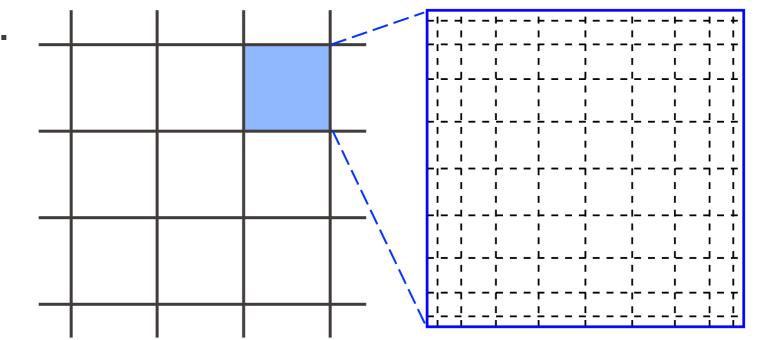


Discretization/computation methods

- Finite difference method (FDM)
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Spectral element methods

- One specific type of FEM, with high-order polynomials on each element:
 - Domain divided into a partition of elements and nodes.
 - Within each element, nodes are clustered near the boundaries (e.g. Gauss-Lobatto-Legendre points).
 - Piecewise basis functions: Lagrange polynomials such that $\psi_i(x_i) = 1$ at node i, $\psi_i(x_i) = 0$ at other nodes j of the element.

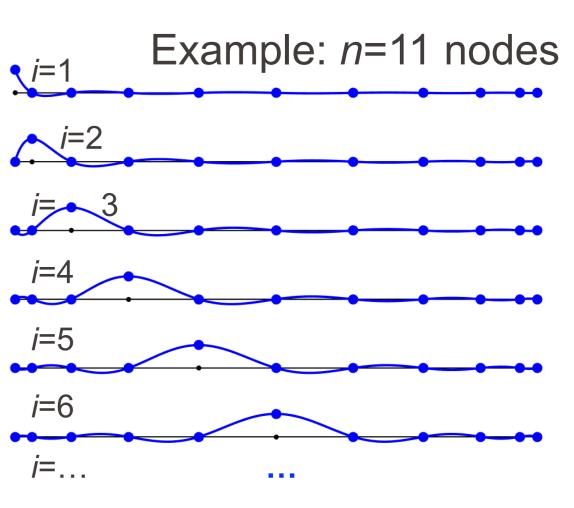


Discretize the solution *u* as combination of basis functions:

$$u(x) = \sum_{i=1}^{n} u_i \psi_i(x)$$

 In 2D/3D, basis functions are often a tensor product (separation of variables, unlike FEM):

$$u(x,y) = \sum_{i,j} u_{ij} \psi_i(x) \psi_j(y)$$



Combines flexibility of FEM (complex geometries) and spectral accuracy of SM.

Discretization/computation methods

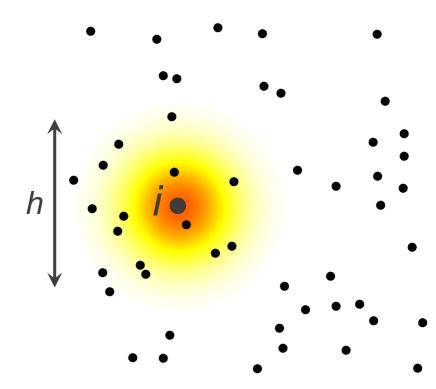
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Lattice Boltzmann methods (LBM)

Particle methods (here: smoothed-particle hydrodynamics, SPH)

- Mesh-free methods
- Lagrangian description: track a discrete set of fluid "particles"
- Mass conservation is automatically satisfied
- Any field f(x) is represented as a spatial average:

$$f(\mathbf{x}) = \int_{\Omega} f(\mathbf{x}') W(\mathbf{x} - \mathbf{x}', h) d\mathbf{x}' \approx \sum_{j} f(\mathbf{x}_{j}) W(\mathbf{x} - \mathbf{x}_{j}, h) V_{j}$$
V_j: volume of particle j



W: weighting function ("kernel") of characteristic size h ("smoothing length")

Solve NS eqs (in Lagrangian form) and track particles by solving

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mathbf{v}_i$$

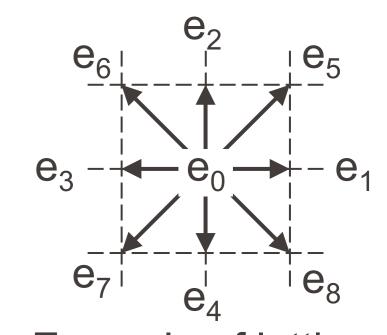
- No special treatment required for interfaces (free-surface flow, multiphase flows)
- High computational cost, but well suited to parallel computing
- Some boundary conditions difficult to define

Discretization/computation methods

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Lattice Boltzmann methods

- Do not solve the Navier-Stokes equations. Model the fluid as discrete fictive particles, that perform propagation and collision/relaxation steps.
- Fictive particles move in discrete directions (lattice). They transport density over space and time.
- LBM can also be understood as a discrete version of the Boltzmann equation (statistical/molecular description of a probability density function for the velocity and momentum).
- Under some assumptions, can re-derive the NS equations from the discrete LB equations.



Example of lattice: D2Q9 (2D, 9 directions)

Pros:

- Runs efficiently in parallel
- Suitable for multi-phase flows
- Handles well complex geometries

Cons:

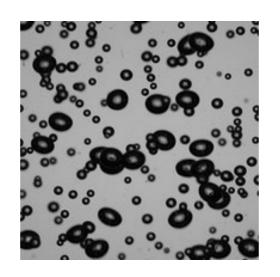
- High-Mach number flows
- Multi-phase limited to small density ratios

Summary: overview of some characteristics

	Main advantage	Meshing capability
 Finite difference (FDM) 	Very easy to implement	Simple geometries
Finite volume (FVM)	Conservation is enforced	Complex geometries
 Finite element (FEM) 	Strong mathematical foundation	Complex geometries
 Spectral element (SEM) 	Combines flexibility of FEM with accuracy of spectral methods	Rather complex geometries
 Spectral methods 	High accuracy (for smooth solutions)	Simple geometries
Particle-based methods	Suitable for multi-phase. Easily parallelizable	Complex geometries
 Lattice Boltzmann (LBM) 	Suitable for multi-phase. Easily parallelizable	Complex geometries

 Relevant to two-phase flows: immiscible liquids, liquid-gas free surface, bubbles, etc.

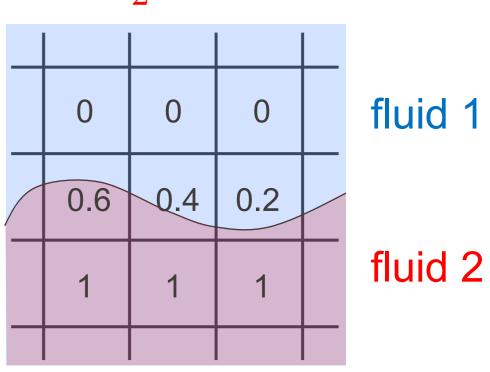






- In particle methods (mesh-free, Lagrangian): no additional treatment needed
- In other methods (mesh-based, Eulerian), several options:
 - 1. Volume of fluid (VOF)
 - 2. Level-set
 - 3. Deforming mesh

$\alpha_2 = \dots$



1. Volume of fluid (VOF)

- Each phase *i* characterized by its **volume fraction** α_i
 - $\alpha_i = 0$: the mesh cell is empty of fluid *i*,
 - $\alpha_i = 1$: the mesh cell is full of fluid *i*,
 - $0 < \alpha_i < 1$: the mesh cell contains the interface between fluid *i* and one or more fluids.
 - In each cell: $\sum_{i} \alpha_{i} = 1$ (the volume is constant)
- Appropriate properties and variables (e.g. density) are assigned to each cell (local weighted average): $f = \sum_i \alpha_i f_i$
- Additional transport equations for volume fractions: $\frac{\partial \alpha_i}{\partial t} + (\mathbf{u} \cdot \nabla)\alpha_i = 0$
- Interface not solved for, but approximately reconstructed.
- Pros: conserves volume; easy to implement.
- Cons: smears the surface; spatial derivatives (e.g. needed to compute the curvature for surface tension effects) difficult to compute (α_i discontinuous across the interface) $_{32}$

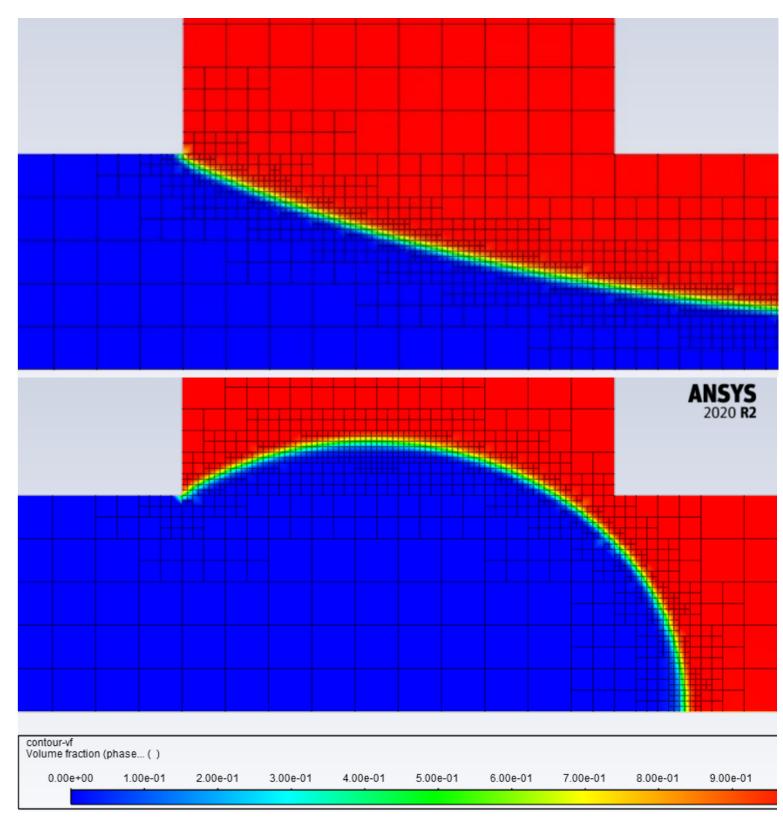
1. Volume of fluid (VOF)

 Volume fraction is a convenient quantity for dynamic mesh adaption: refine near the interface, coarsen far from it, update over time

→ accurate solution, efficient usage of resources.
(In Fluent: pre-defined adaption setting for VOF.)

 Example: "flow-focusing" microfluidic device for droplet production. Re << 1.



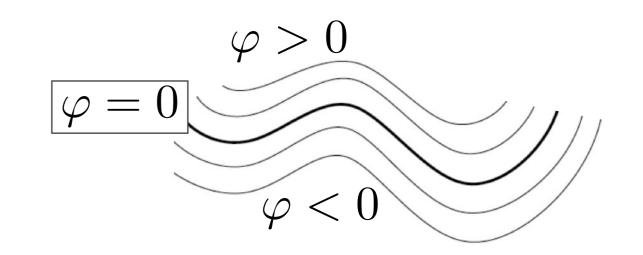


Numerical Flow Simulation

2. Level-set

- Interface = a certain iso-contour of a globally defined level-set function φ .
- For ex., φ = signed **distance** to the interface; interface: iso-contour $\varphi = 0$.

• Interface location explicitly solved for with a transport equation: $\frac{\partial \varphi}{\partial t} + (\mathbf{u} \cdot \nabla)\varphi = 0$

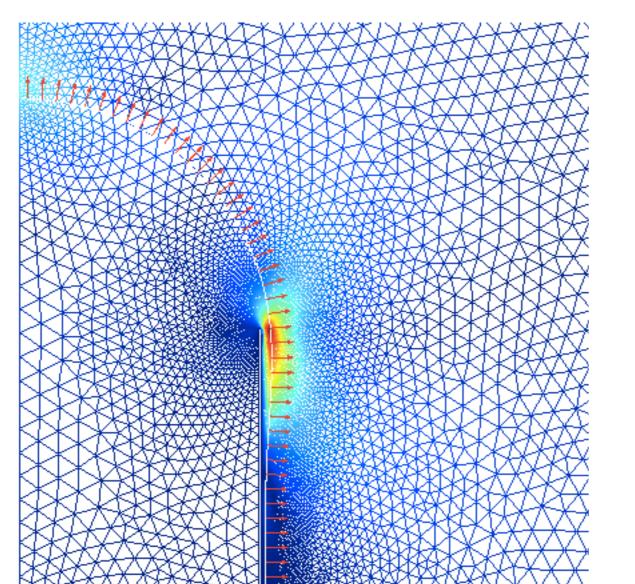


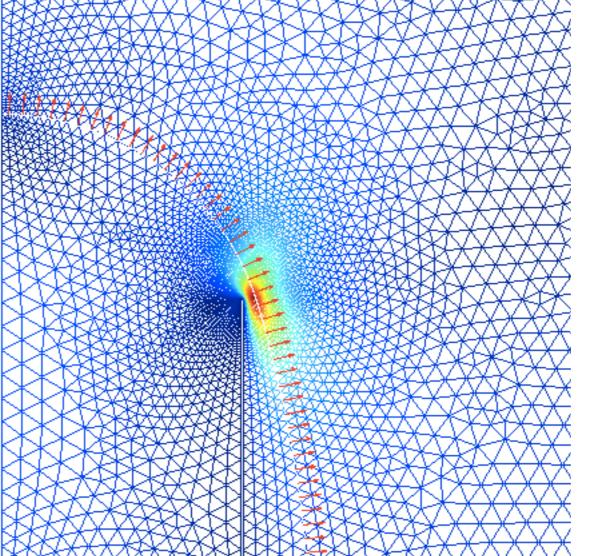
(In practice, additional source term for numerical stability.)

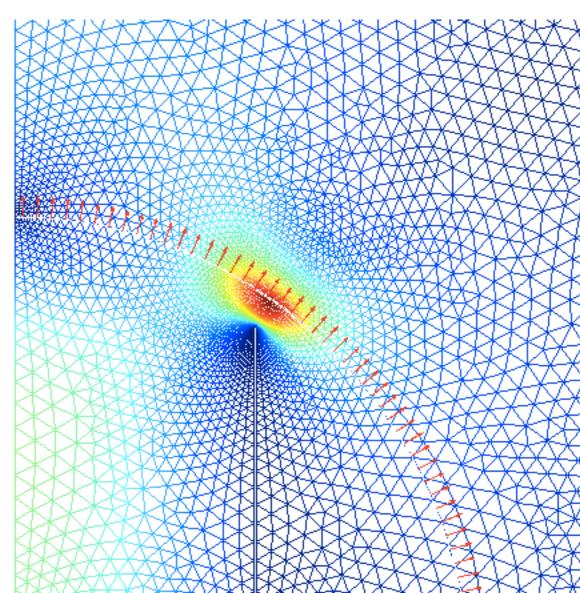
- Pros: smooth and continuous, spatial derivatives can be calculated accurately.
- Cons: does not conserve volume; numerically challenging (e.g. highly distorted interfaces).

3. Deforming mesh

- Solve flow in each phase with appropriate BC (involving stresses + surface tension).
- Move the interface with the fluid velocity.
- Deform the mesh: given the interface position, move interior mesh points according to a smoothing method (e.g. Poisson equation, or "material" behavior inspired by solid mechanics).
- Example: liquid jet in air, pre-wetted nozzle walls, small Weber number (surface tension >> inertia)







3. Deforming mesh

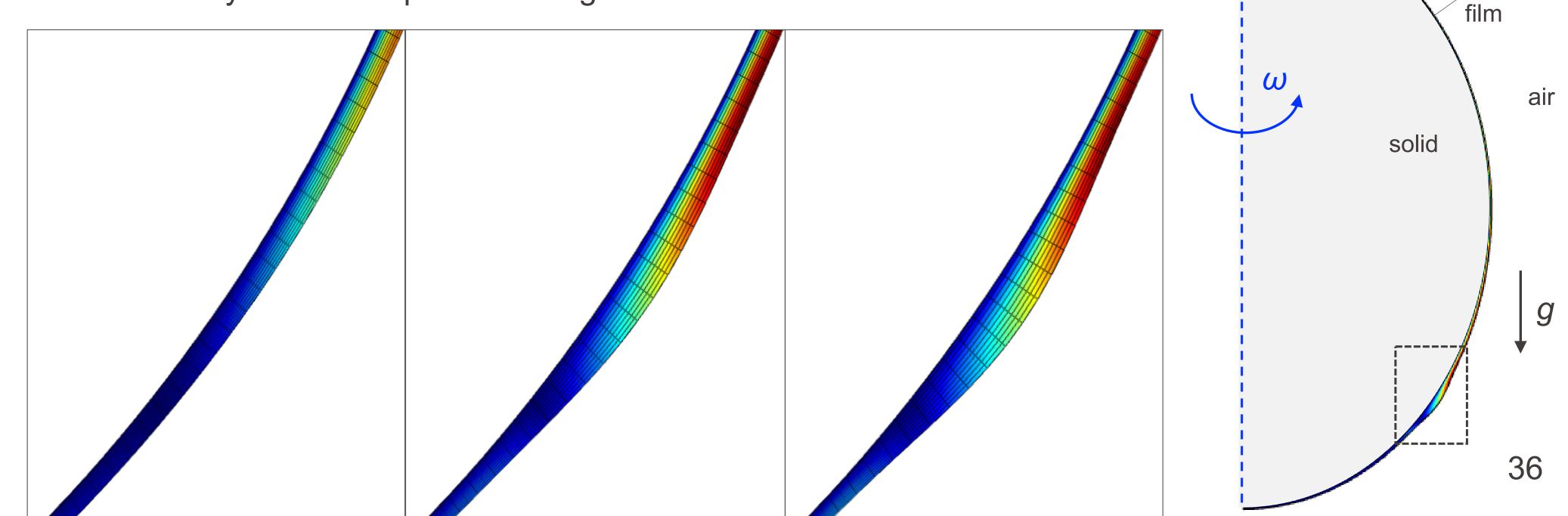
Numerical Flow Simulation

(Comsol)

 Useful to reduce the computational cost when the flow is of interest in one phase only (if can neglect the flow in other phases, and its effect on the interface): mesh and solve for the flow in that phase only.

thin liquid

• Example: gravity-driven coating of the outer surface of a solid axisymmetric ellipsoid rotating around its vertical axis. *Re* << 1.



Thank you for your attention!