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HPC Training Series

An introduction to CFD

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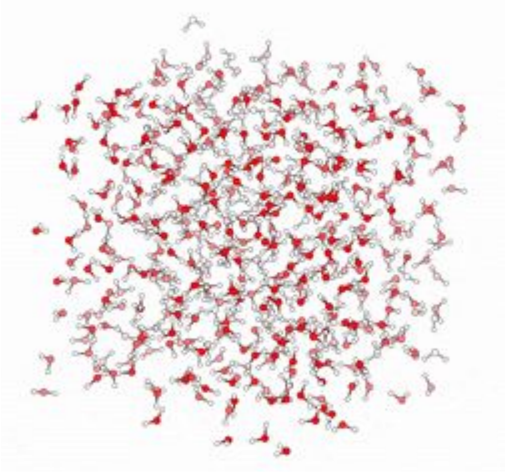
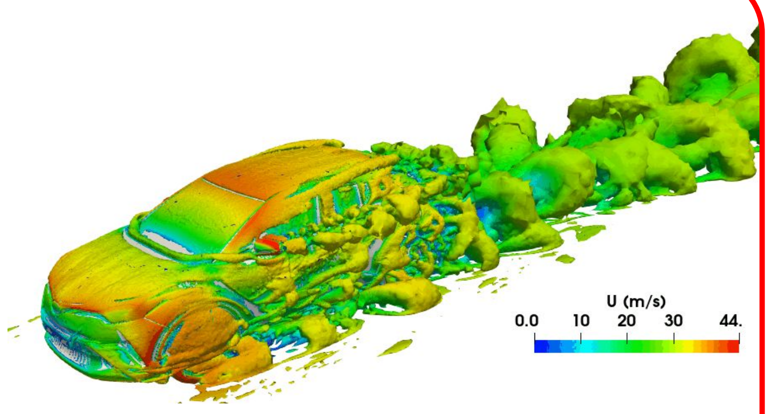
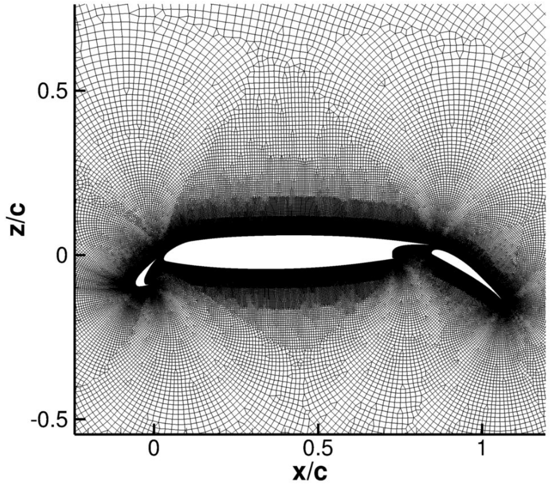
What scales are we simulating with CFD?



Molecular dynamics
- Discrete points in space (atoms and molecules)
- Interactions are modelled through solving Newton's equation of motion
- "Small" length and time scales



Continuum mechanics
- The material is assumed to be continuous
- The equations being solved are usually conservation laws (mass, momentum energy, etc)
- "Large" length and time scales



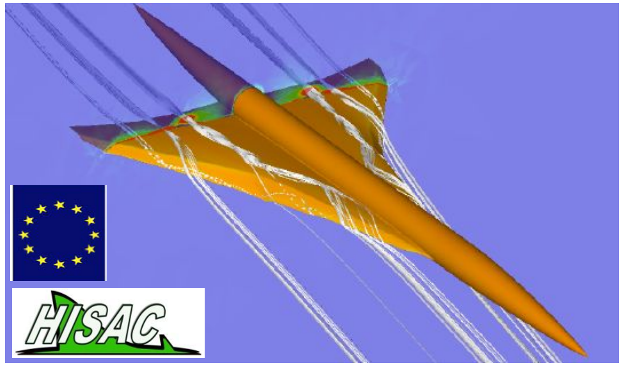
Continuous space needs to be discretized before we solve the underlaying equations □ *meshing!*

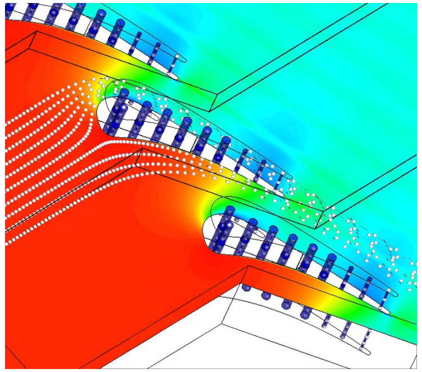
Compressible fluid flows (Air)

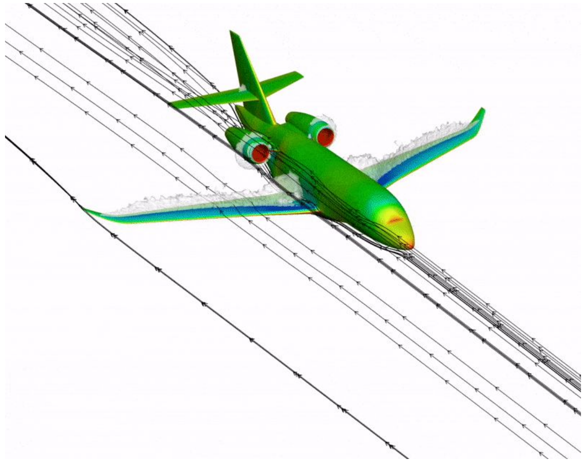
- Continuity eq.
- Momentum eq.
- Energy eq.
- Fluid's state eq.

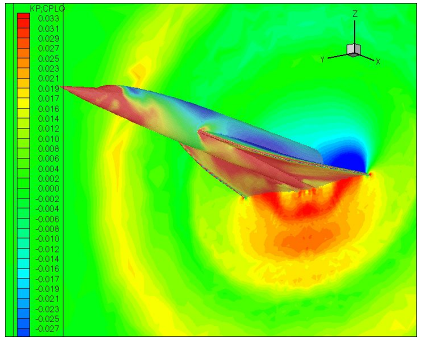
→

- Conservation of mass
- 2nd law of Newton
- Conservation of energy
- Perfect gas equation



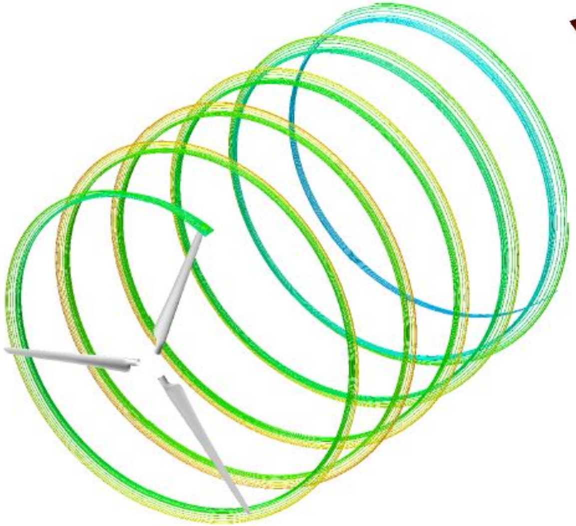


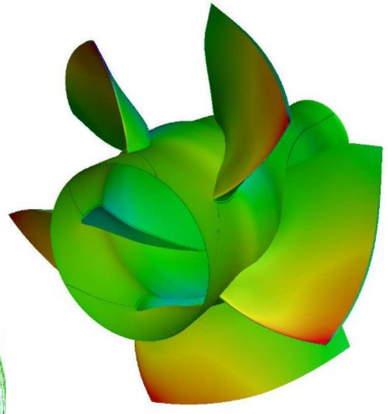


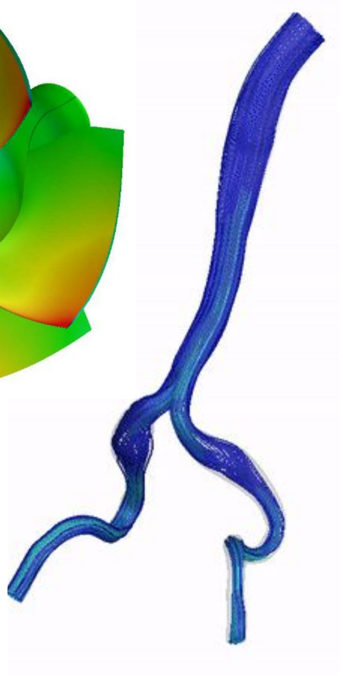


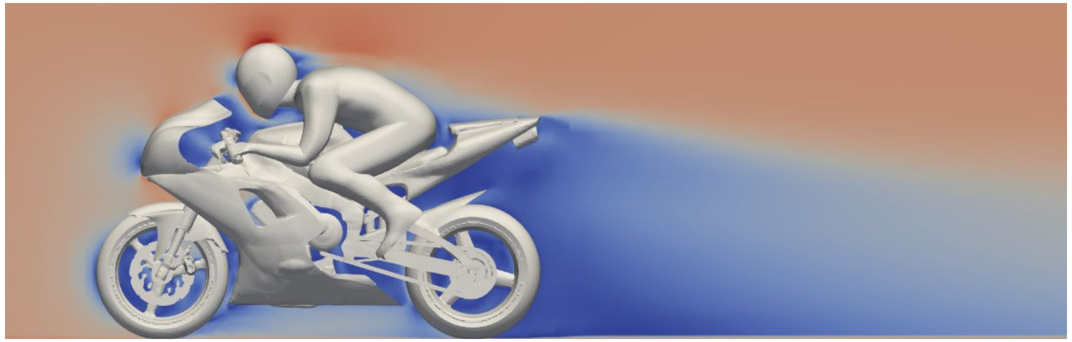
Incompressible fluid flows (Air/Water/Blood)

- Continuity eq.
- Momentum eq.







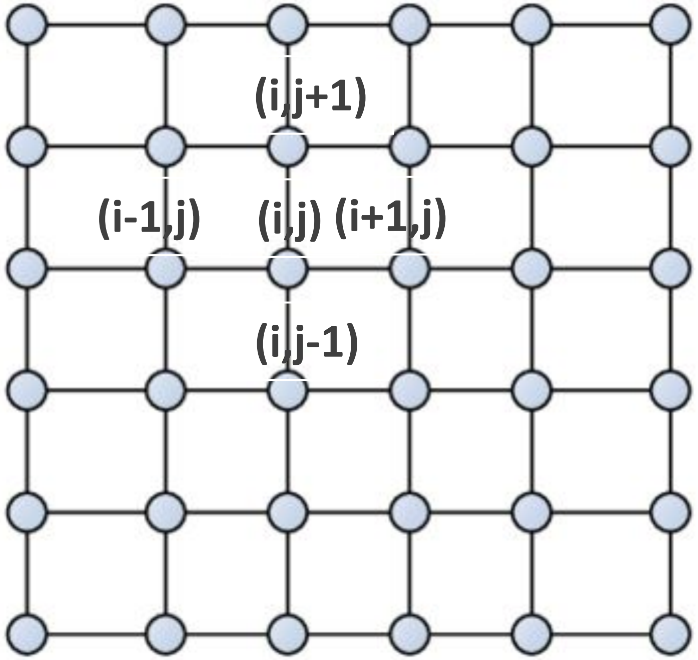


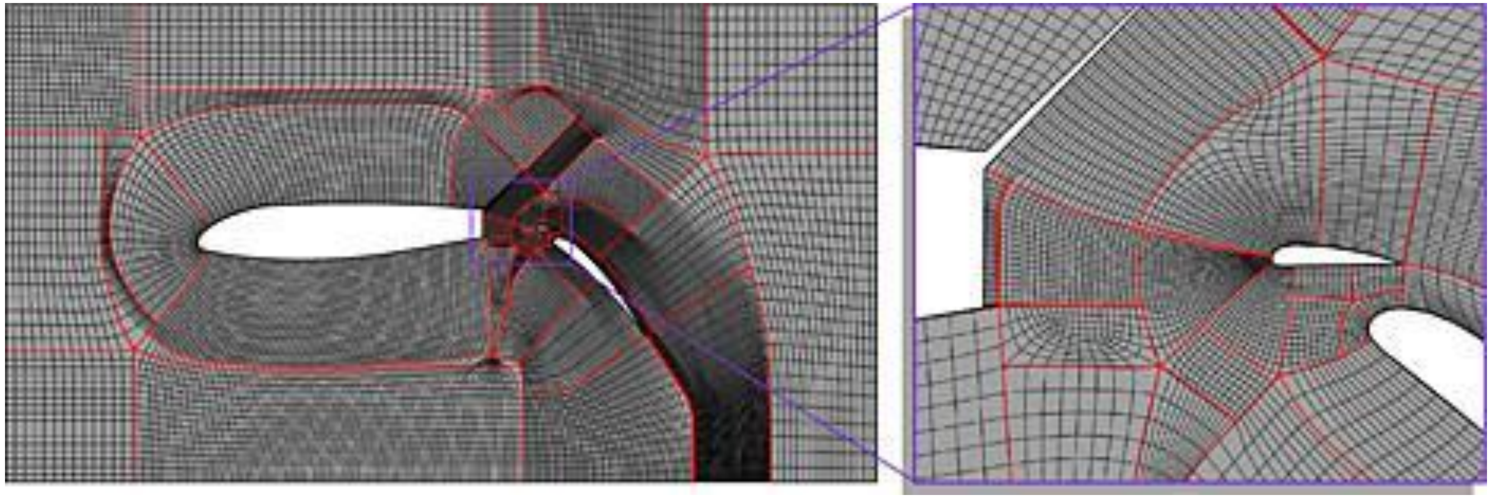
Discretization methodologies

- **Finite Differences (FD)**
- **Finite Element Method (FEM)**
- **Finite Volume Method (FVM)**

Discretization methodologies

- Finite Differences (FD)
  - Structured / multiblock structured meshes
  - High-order schemes → Aeroacoustics (CAA)





A crucial point: maintain discretization accuracy at block interfaces

- Finite Element Method (FEM)
- Finite Volume Method (FVM)

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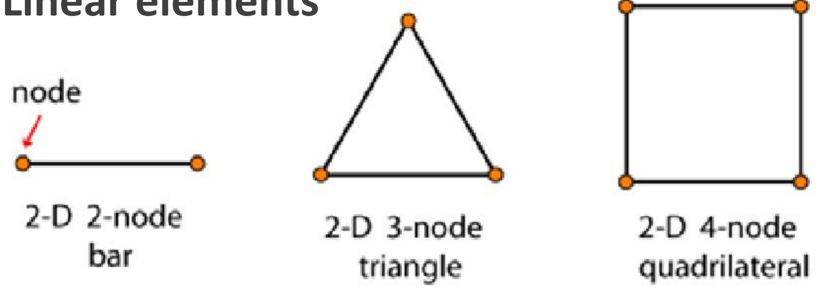
Discretization methodologies

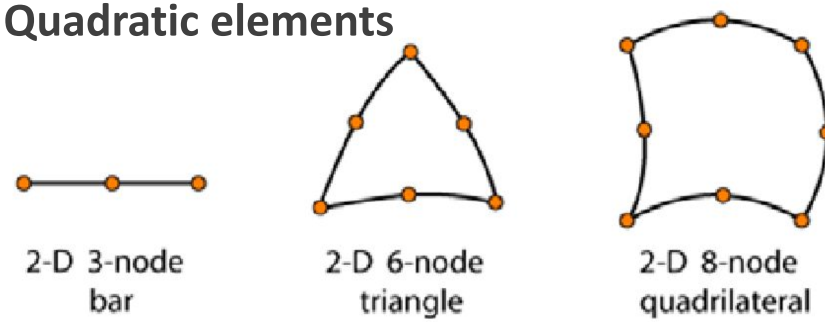
- Finite Differences (FD)
- Finite Element Method (FEM)

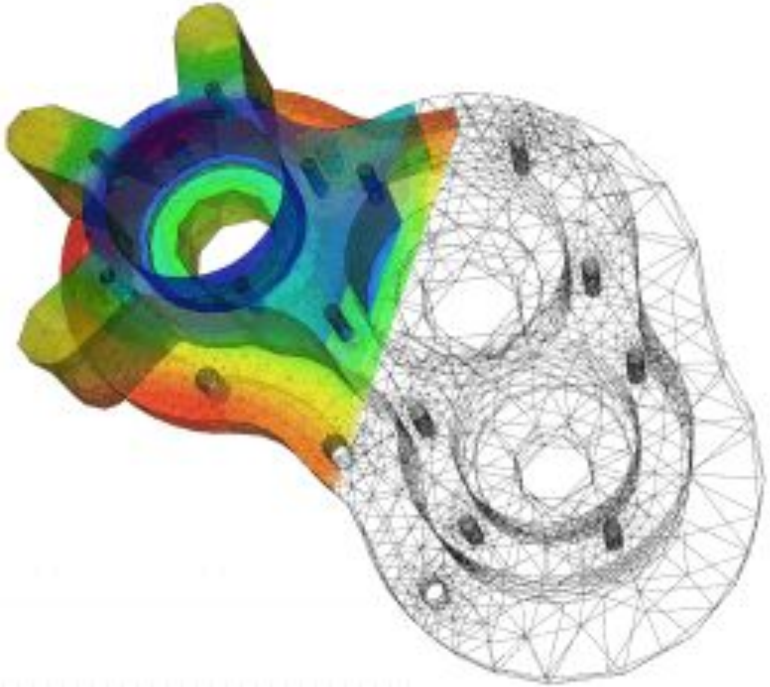
    Galerkin method → **Structural, heat transfer, electromagnetic engineering fields**

    Linear elements



Quadratic elements





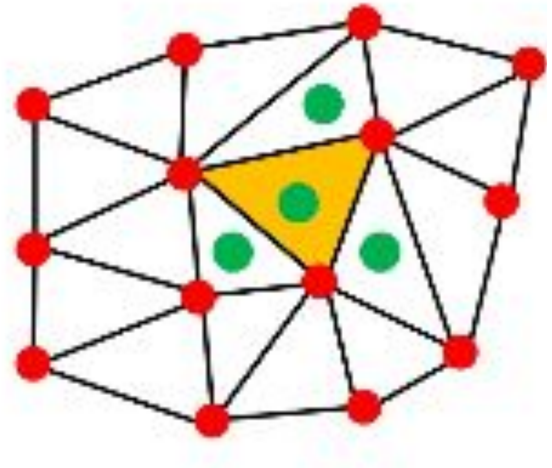
- Finite Volume Method (FVM)

Discretization methodologies

- Finite Differences (FD)
- Finite Element Method (FEM)
- Finite Volume Method (FVM)

Cell-centered approach

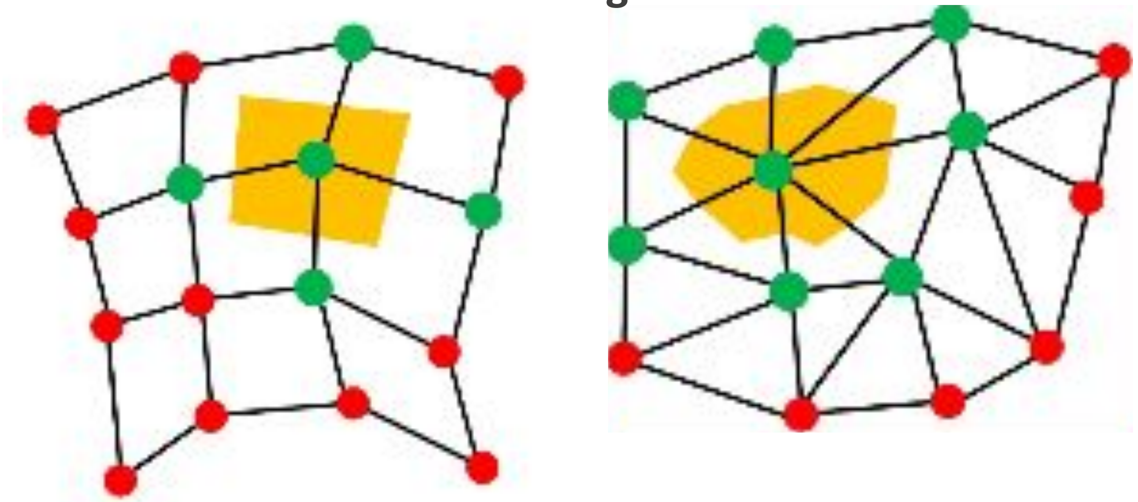
- Finite volumes = mesh elements
- Flow data stored at element centers
- Unstructured (hybrid) meshes
- Constant number of neighbors



OpenFOAM®

Vertex-centered approach

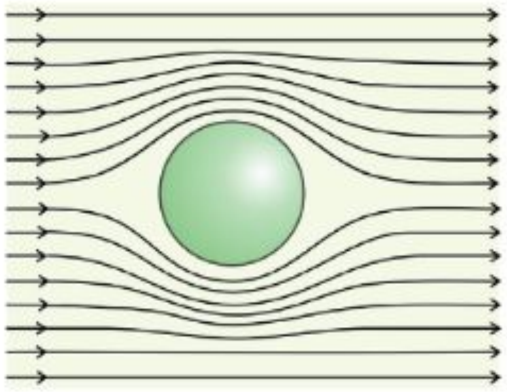
- The finite volumes are formed around the mesh vertices based on element and face barycenters (dual mesh)
- Flow data stored at mesh vertices
- Unstructured (hybrid) meshes
- Variable number of neighbors



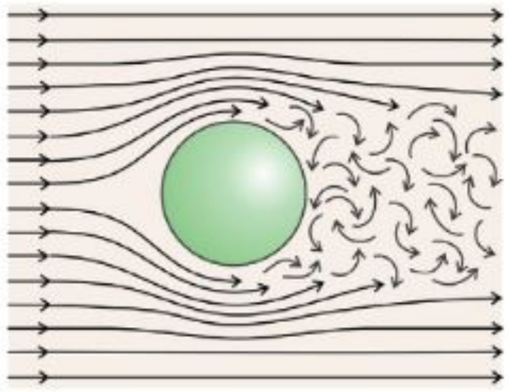
Turbulent flows

- Most of the industrial cases deal with interest include turbulent flows.
- Turbulence is the apparent chaotic motion of fluid flows. Fluid flows can be laminar and move in an orderly manner. Increasing the flow speed, the convective forces overcome the viscous ones and the laminar flow transitions into a turbulent one. The ratio between convective and viscous forces is called the Reynolds number. The higher that number is, the more turbulent the flow is.
- We need accurate modeling of turbulence.

Laminar



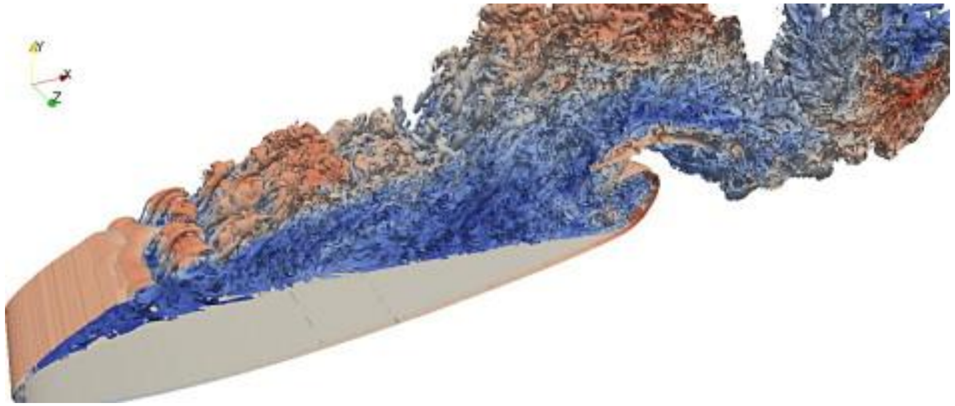
Turbulent



Turbulent flows

ACCURACY

- Direct Numerical Simulation (DNS)
  - Direct solution of the governing flow (Navier-Stokes) equations.
  - Extremely fine meshes & small times scales
  - Impossible for industrial applications.
  - Mainly used from academia to model simple flows (along with experiments).
  - DNS can be also used to improve the understanding of turbulence and to develop less expensive turbulence models predicting the main contribution of turbulence on the flow (AI).
- Large Eddy Simulation (LES)
- Reynolds-Averaged Navier Stokes (RANS)

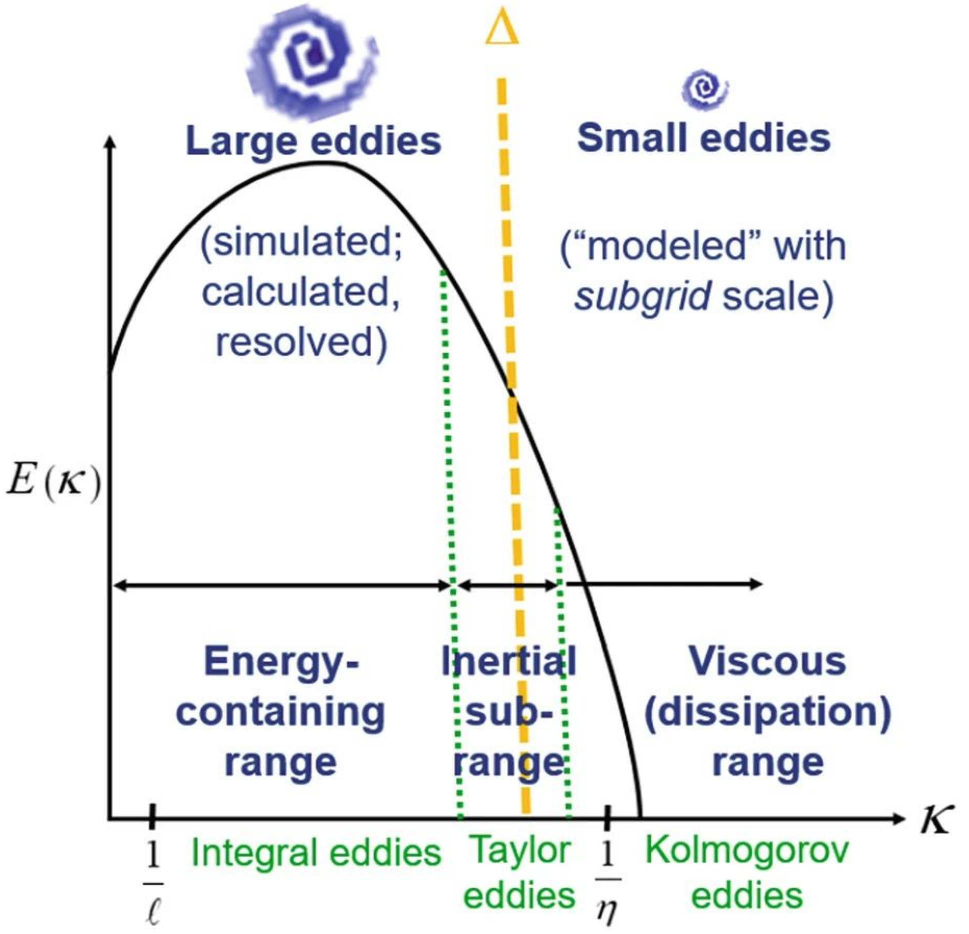


DNS on a stalled NACA0012 airfoil

Turbulent flows

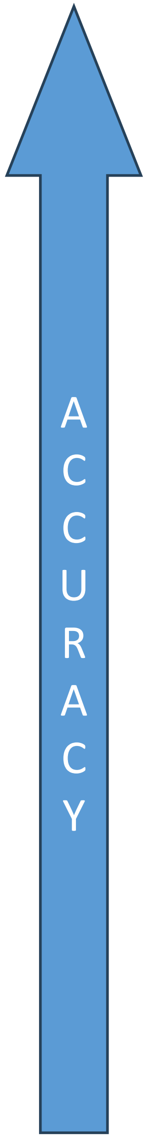
A C C U R A C Y

- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
  - The large eddies (most energy containing) are resolved directly, while the small ones are modeled.
  - Use of coarser meshes than DNS.
- Reynolds-Averaged Navier Stokes (RANS)

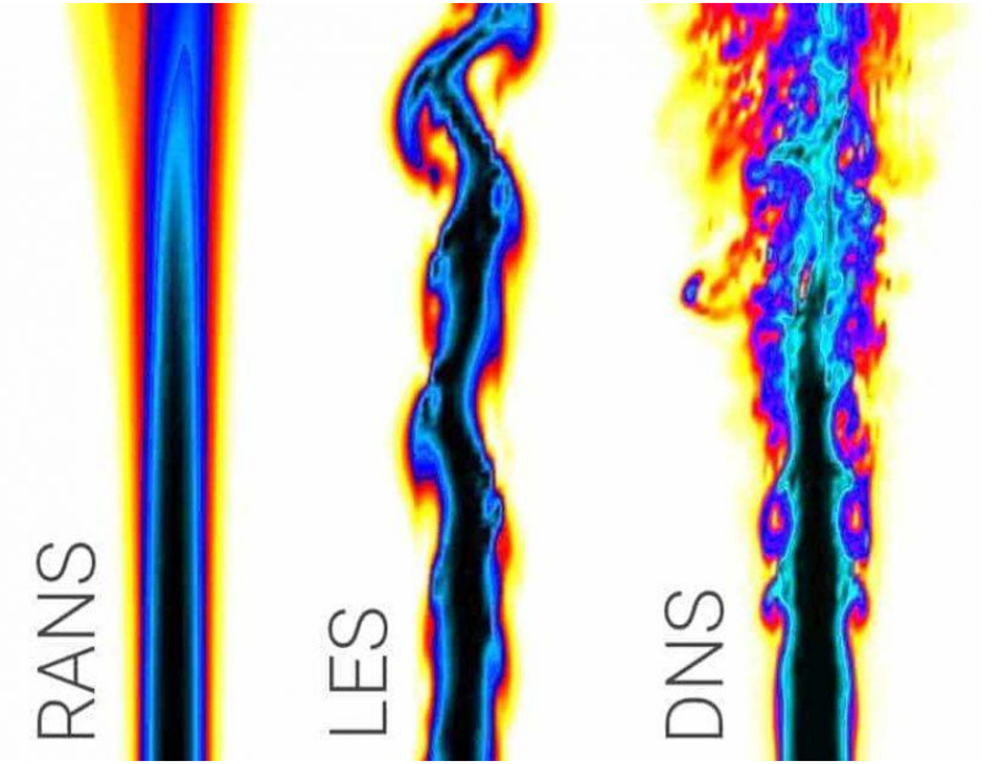


* Rodriguez, S LES and DNS Turbulence Modeling, Applied Computational Fluid Dynamics & Turbulence Modeling, pp 197–223, 2019

Turbulent flows



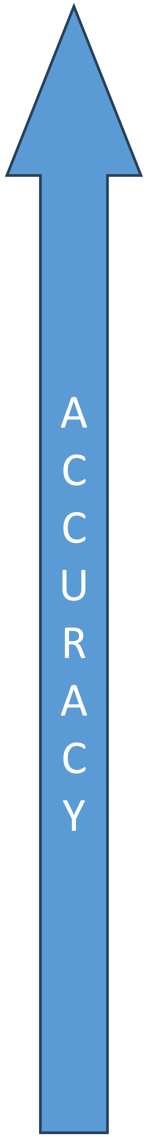
- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- **Reynolds-Averaged Navier-Stokes (RANS)**
  - **The Navier-Stokes (NS) equations are averaged forming the Reynolds-Averaged Navier-Stokes (RANS) ones.**
  - **RANS have the same form with NS including extra terms in the momentum equations (Reynolds stresses).**
  - **Turbulence models avoids computing the Reynolds stresses quantifying the effect of turbulence on the main flow field.**
  - **Some turbulence models:**
    - **Baldwin-Lomax (0-eq)**
    - **Spalart-Allmaras (1-eq)**
    - **k-ε (2-eqs)**
    - **k-ω (2-eqs)**
    - **…**



CFD modeling of turbulent jet

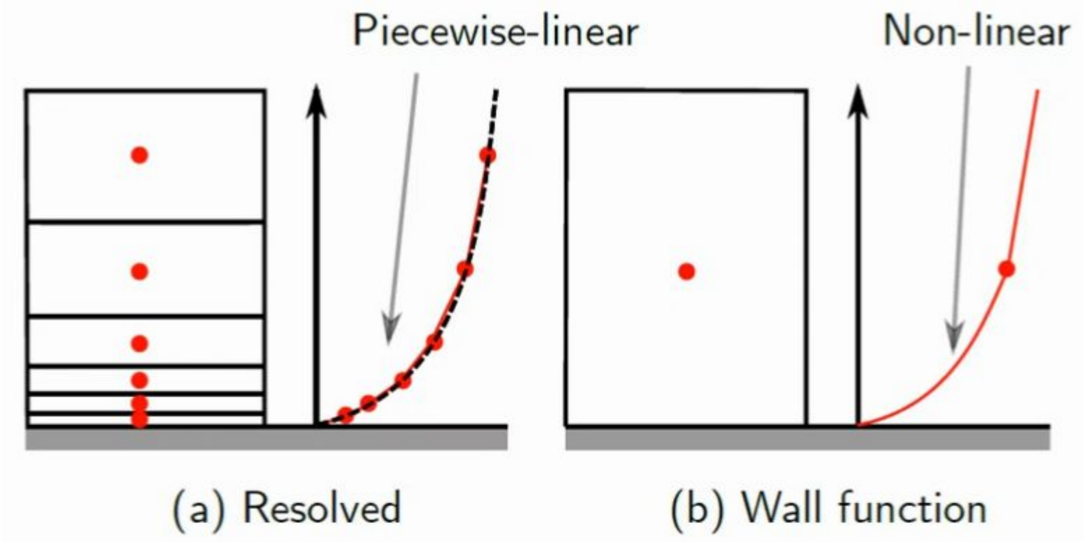
* https://www.idealsimulations.com/resources/turbulence-models-in-cfd

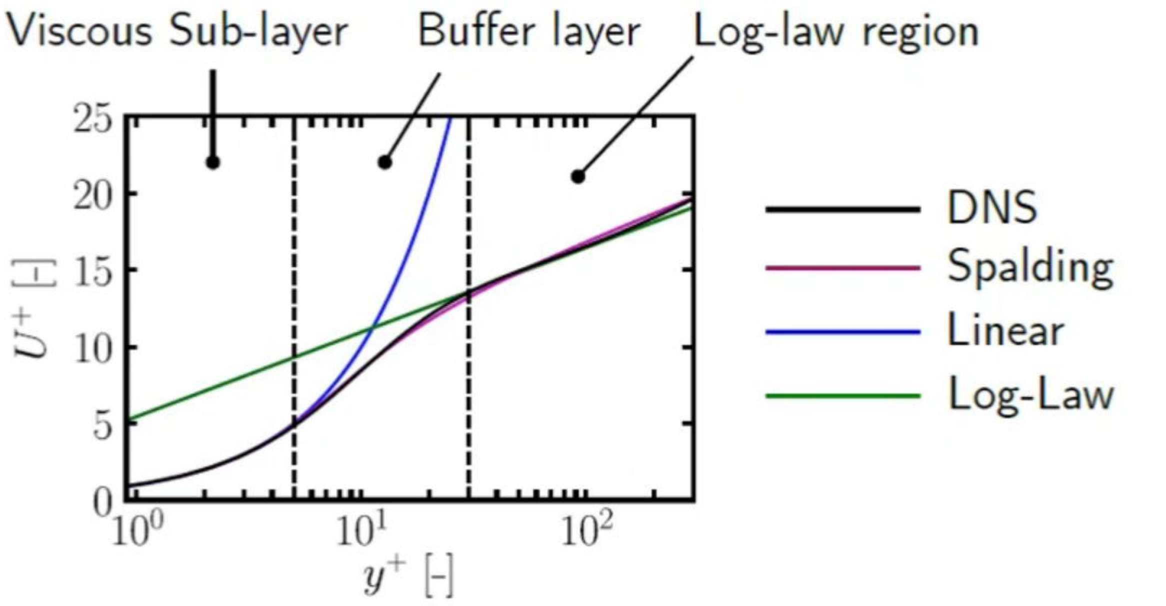
Turbulent flows



- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- **Reynolds-Averaged Navier-Stokes (RANS)**
  - **Wall functions**
    - **Use experimental information in computing wall shear stress**
    - **Enable the use of coarser meshes close to the wall**
    - **Accurate in regions with no flow separation**

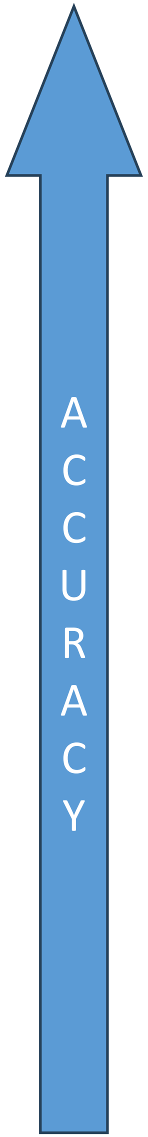
$$y^+ = y\frac{u_\tau}{\rho} \qquad u^+ = \frac{u}{u_\tau}$$



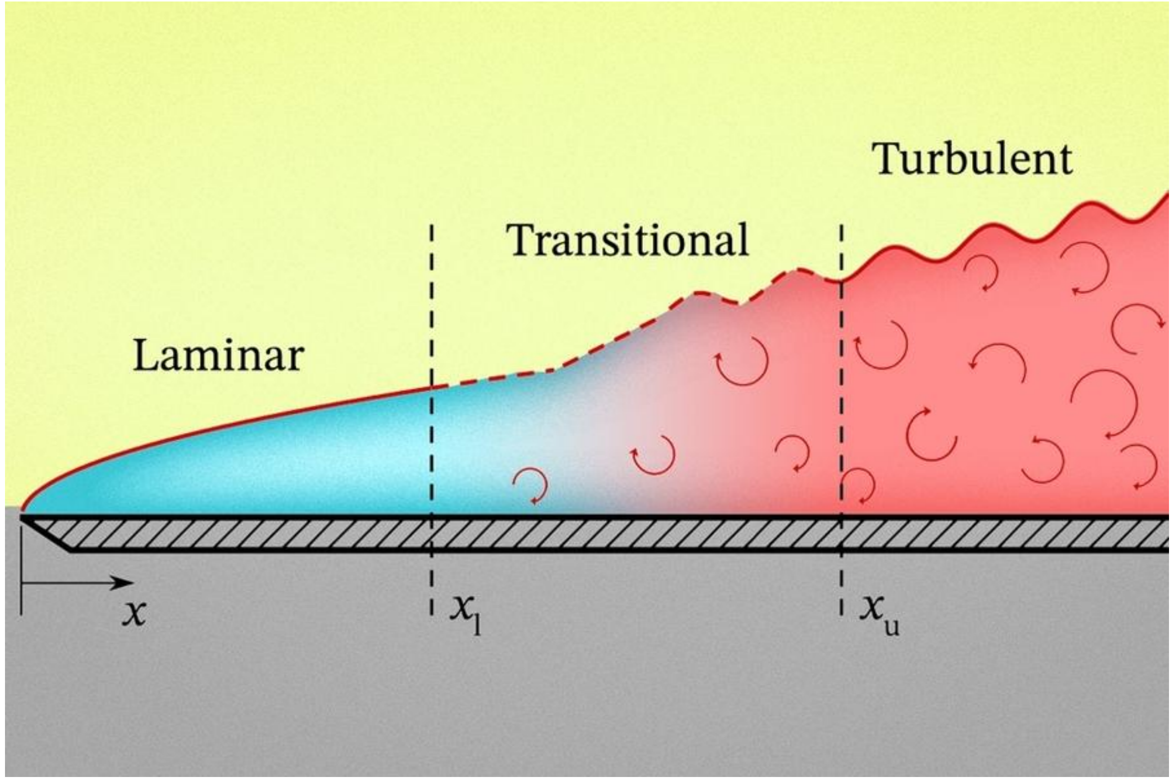


* https://cfd.blogs.upv.es/turbulence/wall-functions

Turbulent flows



- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- **Reynolds-Averaged Navier-Stokes (RANS)**
  - **Transition models:**
    - **γ-Re_θ (2-eqs)**
    - **…**

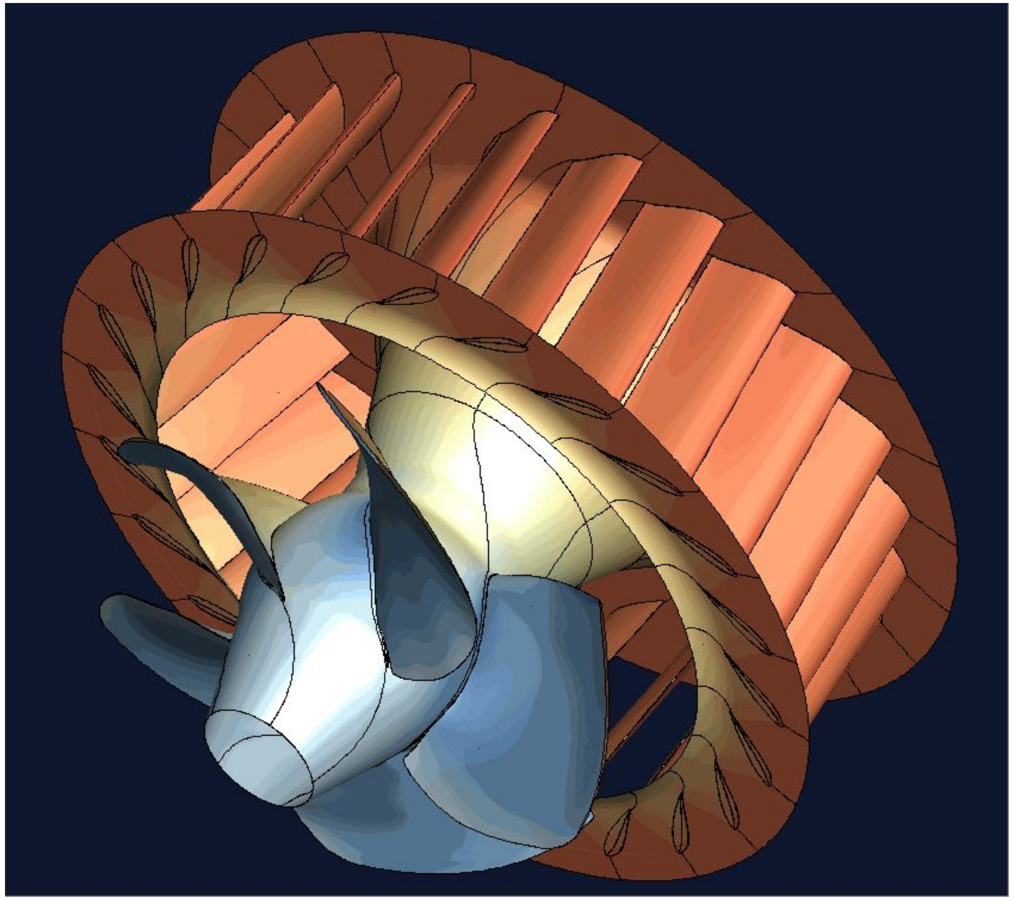


* https://news.mit.edu/2020/how-fluids-heat-cool-surfaces-0428

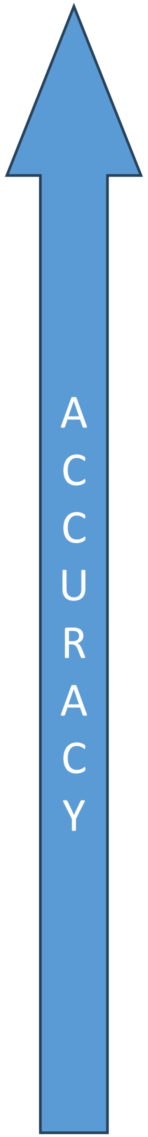
Turbulent flows

ACCURACY

- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- Reynolds-Averaged Navier-Stokes (RANS)
  - Unsteady - URANS



Turbulent flows



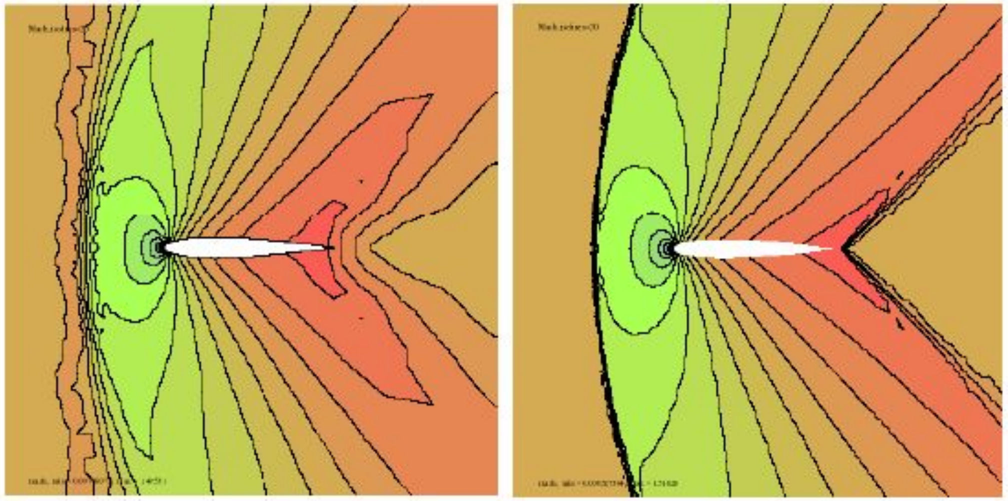
- Direct Numerical Simulation (DNS)
- Large Eddy Simulation (LES)
- **Reynolds-Averaged Navier-Stokes (RANS)**
  - **Two-phase flow models**
  - **Low-Mach number preconditioning technique**
  - **Pseudo-compressibility technique**

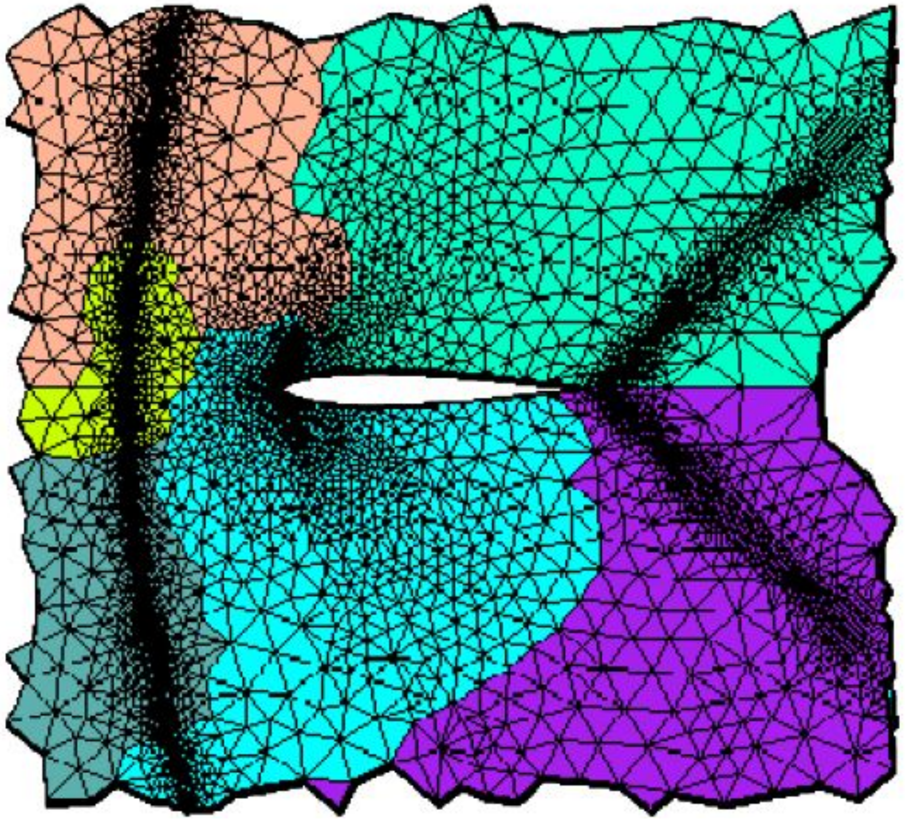
More on it, later

Mesh refinements

- Viscous layers
- Mesh refinement close to flow non-linearities (shock waves)

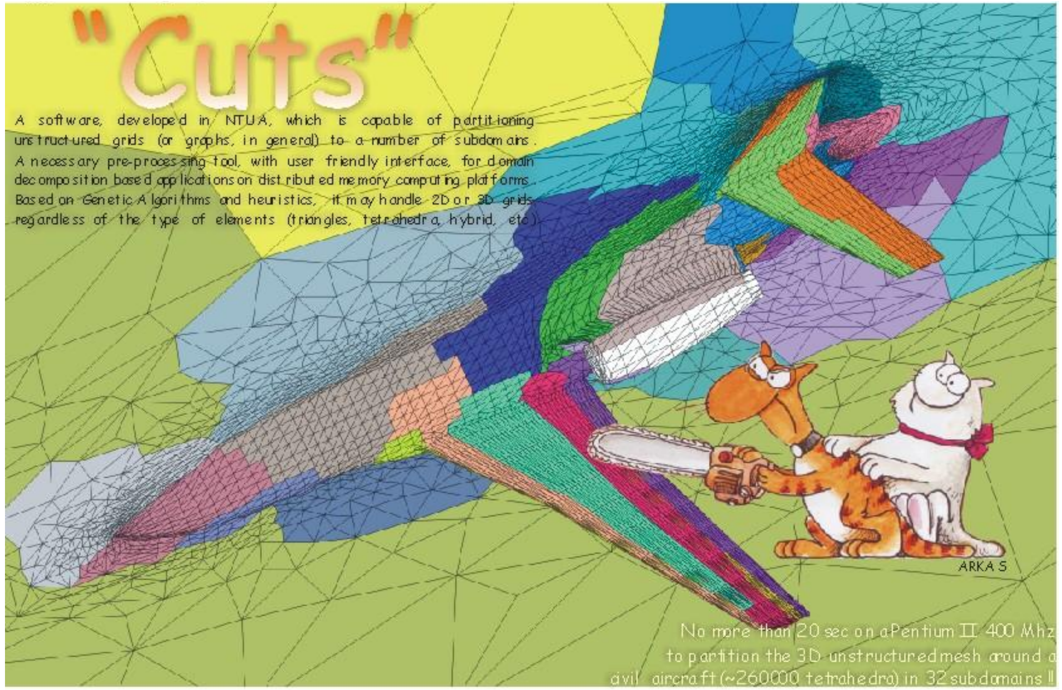
Initial mesh refined mesh





Modern CFD

- HPC clusters
- Sophisticated workflow managers

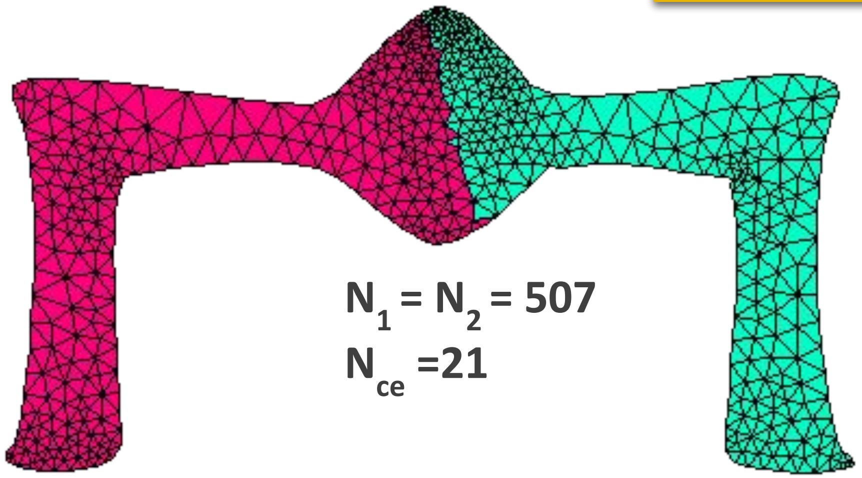


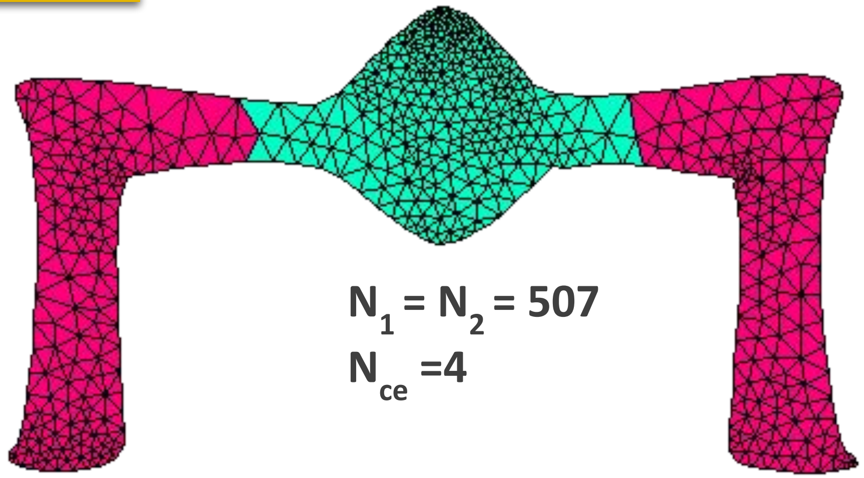
- Each compute node computes the flow field at a limited number of subdomains
- Use MPI to transfer data between the compute processes

Modern CFD

- Mesh partitioning
  - Create subdomains with equal number of elements
  - Minimize interface elements → Minimize MPI communications & Increase parallel efficiency

Computational mesh inside an artery model with aneurism





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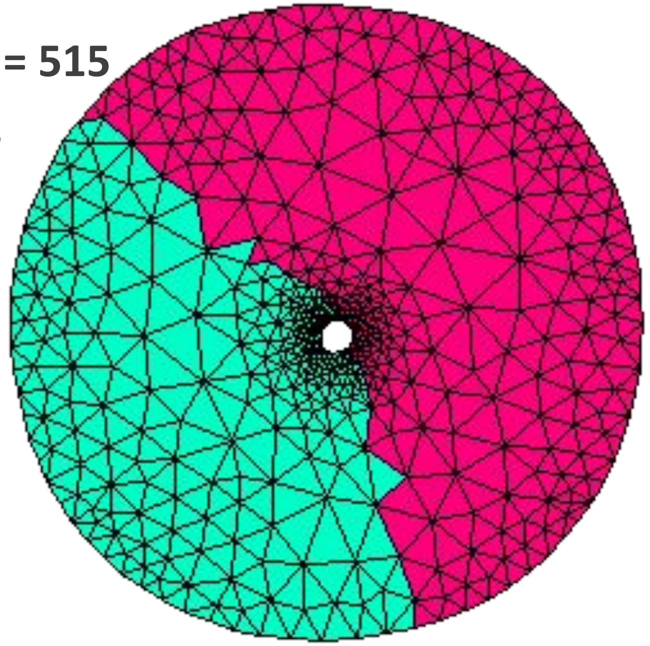
Modern CFD

- Mesh partitioning
  - Create subdomains with equal number of elements
  - Minimize interface elements → Minimize MPI communications & Increase parallel efficiency

Computational mesh around a 2D cylinder

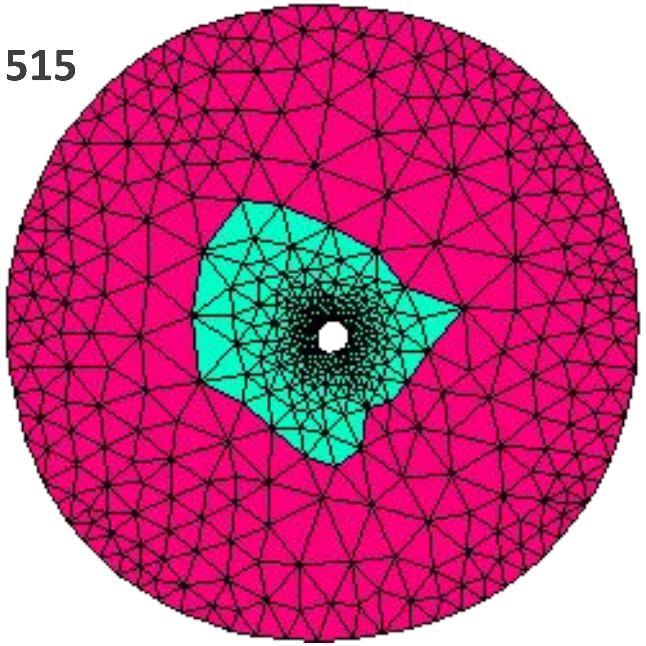
$N_1 = N_2 = 515$

$N_{ce} = 31$



$N_1 = N_2 = 515$

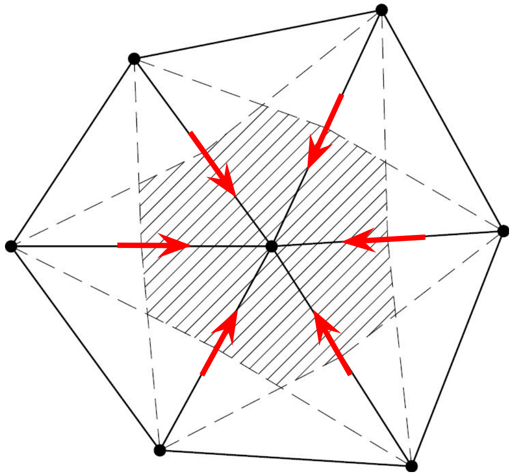
$N_{ce} = 19$

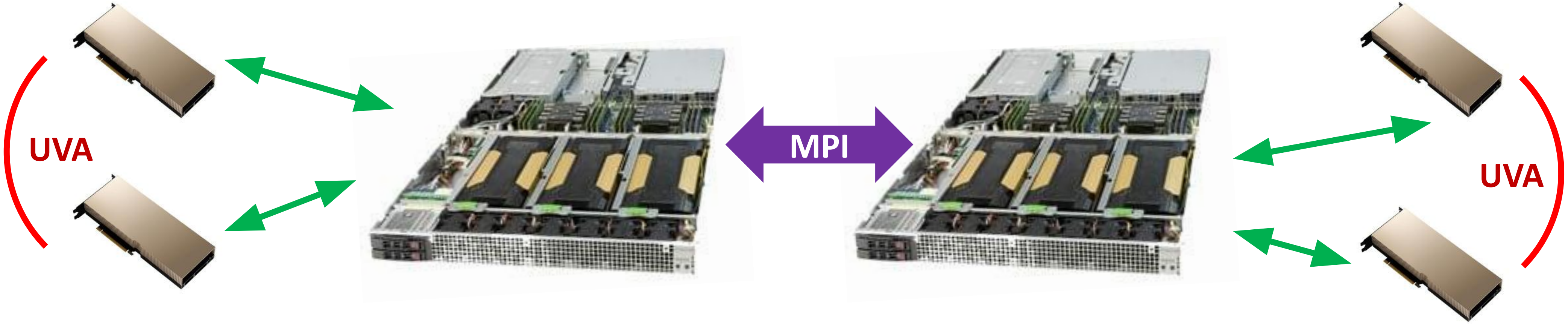


Modern CFD

- GPUs
  - Massively parallel CPU co-processors
  - High floating-point operations rate
  - Low latency
  - Energy efficient

- Multiple threads run in parallel in a single GPU executing the same function (kernel)
- Each thread can be assigned with one mesh node computing, for instance, its residual





Modern CFD

- **Quantum computing**