GIAN Course on

Rarefied & Microscale Gases and Viscoelastic Fluids: a Unified Framework

Lecture 2
Introduction to (Physical & Mathematical) Fluid Dynamics and CFD

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Content

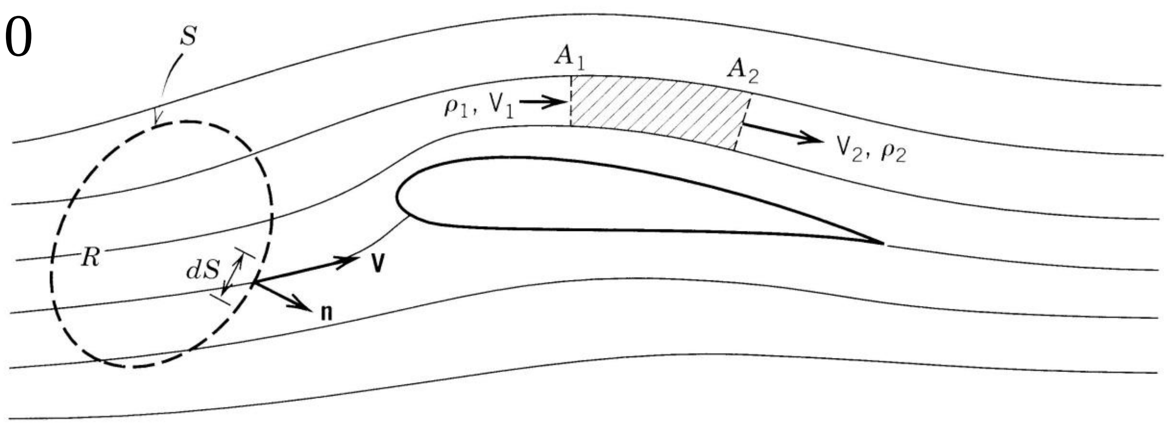
I. Fluid dynamics: Eulerian vs. Lagrangian

- Eulerian description of the fluid motion:
  Properties are function of space and time
  Imaginary volume of a properly selected shape, fixed in space
  V.**n***dS* represents in and out through the control surface
- Lagrangian approach: properties that are moving with the fluid (suitable for moving boundary problems)
- Conservation (neither be created nor destroyed): The sum of the time rate of mass within the region and the net flux of mass through a closed surface is zero

$$\frac{\partial}{\partial t}\int_R \boldsymbol{U} dV + \oint_S \boldsymbol{F}\cdot\boldsymbol{n} dS = 0$$

$\boldsymbol{U}$ conserved variable

$\boldsymbol{F}$ flux



I. Fluid dynamics: conservation laws

- **Conservation laws for mass, momentum and energy, in conjunction with the 2nd law of thermodynamics and the equation of state (EOS)**

$$\frac{\partial}{\partial t}\int_R \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{bmatrix} dV + \oint_S \begin{bmatrix} \rho \mathbf{u} \\ \rho \mathbf{u}\mathbf{u} + p\mathbf{I} + \mathbf{\Pi} \\ (\rho E + p)\mathbf{u} + (\mathbf{\Pi}\cdot\mathbf{u} + \mathbf{Q}) \end{bmatrix} \cdot \mathbf{n} dS = 0,$$

$$p = \rho R T$$

where $\mathbf{\Pi}$ is viscous shear stresses (tensor) and

$\mathbf{Q}$ is heat flux (vector)

No approximations introduced so far!

I. Fluid dynamics: dimensionless numbers

- **Dimensionless parameters (measuring relative importance of terms) in the stationary momentum equation**

  Viscous force (V) Inertial (I), Pressure (P)

- **Basis for model reduction and scaling laws**

$$\text{Reynolds no. Re} = \frac{\text{I}}{\text{V}} = \frac{\rho V^2}{\eta V / L} = \frac{\rho V L}{\eta}$$

$$\text{Mach no. M}^2 = \frac{\text{I}}{\text{P}} = \frac{\rho V^2}{p} = \left(\frac{V}{\sqrt{RT}} \right)^2$$

I. Fluid dynamics: integral and differential forms

- **Governing equations in integral and differential forms**
  - Defined for volume and enclosed surface

$$\frac{\partial}{\partial t}\int_R \mathbf{U}\,dV + \oint_S \mathbf{F}\cdot\mathbf{n}\,dS = 0$$

$$\Updownarrow \qquad \oint_S \mathbf{F}\cdot\mathbf{n}\,dS = \int_R \nabla\cdot\mathbf{F}\,dV; \quad \text{Gauss' theorem}$$

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla\cdot\mathbf{F} = 0$$

  - Defined for infinitesimal element

II. Navier-Stokes-Fourier

$$\frac{\partial}{\partial t}\begin{bmatrix}\rho\\ \rho\mathbf{u}\\ \rho E\end{bmatrix}+\nabla\cdot\begin{bmatrix}\rho\mathbf{u}\\ \rho\mathbf{u}\mathbf{u}+\dfrac{1}{\gamma M^2}p\mathbf{I}\\ \left(\rho E+\dfrac{1}{\gamma M^2}p\right)\mathbf{u}\end{bmatrix}+\frac{1}{\mathrm{Re}}\nabla\cdot\begin{bmatrix}0\\ \mathbf{\Pi}\\ \mathbf{\Pi}\cdot\mathbf{u}+\dfrac{1}{Ec\,\mathrm{Pr}}\mathbf{Q}\end{bmatrix}=0$$

Non-conserved variables

$$\mathbf{\Pi}=-2\eta\left[\nabla\mathbf{u}\right]^{(2)},\ \mathbf{Q}=-k\nabla T$$

$\Rightarrow$ $\mathbf{U}(t,x,y,z)$ or $\rho(t,x,y,z),\mathbf{u}(t,x,y,z),p(t,x,y,z)$

$\Rightarrow$ Drag $= x$ component of $\oint_S p_w\mathbf{n}dS+\oint_S \mathbf{\Pi}_w\mathbf{n}dS+\oint_S \mathbf{\Pi}_w\mathbf{s}dS$

$\Rightarrow$ $C_D\equiv F_D/(0.5\rho V^2 S)=fn(\mathrm{Re},M)$

II. Navier-Stokes-Fourier

Navier (1822) $\mathbf{\Pi} = -2\eta\left[\nabla\mathbf{u}\right]^{(2)}$

Fourier (1822) $\mathbf{Q} = -k\nabla T$

$$\begin{bmatrix} \Pi_{xx} & \Pi_{xy} \\ \Pi_{yx} & \Pi_{yy} \end{bmatrix} \leftarrow -2\eta(T)\begin{bmatrix} u_x - (u_x + v_y)/3 & (u_y + v_x)/2 \\ (v_x + u_y)/2 & v_y - (u_x + v_y)/3 \end{bmatrix}$$

$$\text{with } \Pi_{xx} + \Pi_{yy} + \Pi_{zz} = 0$$

$u_x(\equiv \partial u/\partial x)$ case (compression and expansion)

$$-2\eta(T)\begin{bmatrix} 2u_x/3 & 0 \\ 0 & -u_x/3 \end{bmatrix}$$

Newtonian or linear

Not like $(u_x)^2$

$u_y(\equiv \partial u/\partial y)$ case (velocity shear only)

$$-2\eta(T)\begin{bmatrix} 0 & u_y/2 \\ u_y/2 & 0 \end{bmatrix}$$

Uncoupled

Always vanishing normal stress Π_{xx} or Π_{yy}

$$\begin{bmatrix} Q_x \\ Q_y \end{bmatrix} \leftarrow -k(T)\begin{bmatrix} T_x \\ T_y \end{bmatrix}.$$

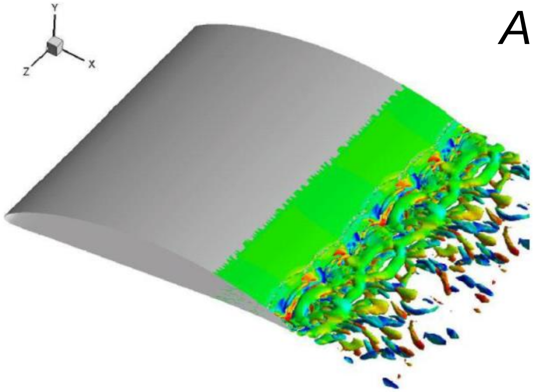
Not like $(T_x)^2$

III. Key issues: RMG vs turbulence

(Low Reynolds mesoscopic) fluid dynamics (RMG) is difficult because:

*It involves **microscopic** collisional interactions among fluid particles and their **interplay** with the kinematic motion of particles in the macroscopic framework. This challenge is vividly illustrated by the high Mach number shock singularity problem (HMNP)*. (R. S. Myong PoF 2014)

(High Reynolds) fluid dynamics is difficult because:



At extremely small scales, even turbulent flow is very simple. It is smooth and well behaved. At larger scales, however, a fluid is subject to very few constraints. It can develop arbitrary levels of complexity like the effect of turbulence on separation. (P. L. Roe, “Future developments in CFD,” ICAAT-GNU, May 2014)

III. Key issues: compressible vs incompressible

- **A common (but fatal when abused) logic**
  - Flow speed in typical micro- and nano-devices is low; that is, small *M*. Thus incompressible assumption and associated simplification like constant viscosity and thermal conductivity are well-justified.
- **Correct logic (Panton, *Incompressible Flow*, 2013, p. 248)**
  - When the temperature changes in the flow is finite, the flow must be considered; 1) (original) compressible, and 2) involving with the temperature dependence of transport coefficients, since

$$\eta / \eta_0 = 1 + \frac{d(\eta / \eta_0)}{d(T / T_0)} \left(\frac{T_w - T_0}{T_0} \right) \hat{T} + \cdots$$

IV. Introduction to CFD

- **CFD (Computational Fluid Dynamics)**

  A branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows

- **Computational physics vs numerical analysis**

  The computational physics, which concerns the study of computational models for a given physical problem, as opposed to the analysis of numerical methods for a given computational model, becomes a key issue during the initial phase of the study of CFD algorithms for RMG.

$x^2+2x=3$	vs	$x^2+2x=3$
$x^2+2x+1-1=3$		$x^2+2x-3=0$
$(x+1)^2=3+1=4$		$(x-1)(x+3)=0$
$x=-1\pm 2=1,-3$		$x=1,-3$

IV. CFD process

- Computational model & domain:
  - Boltzmann, Navier-Stokes-Fourier, etc.
- Geometry modeling
- Grid generation
- Flow solution
- Post-processing:
  - Contours, C_L, C_D, etc.
- Verification & validation

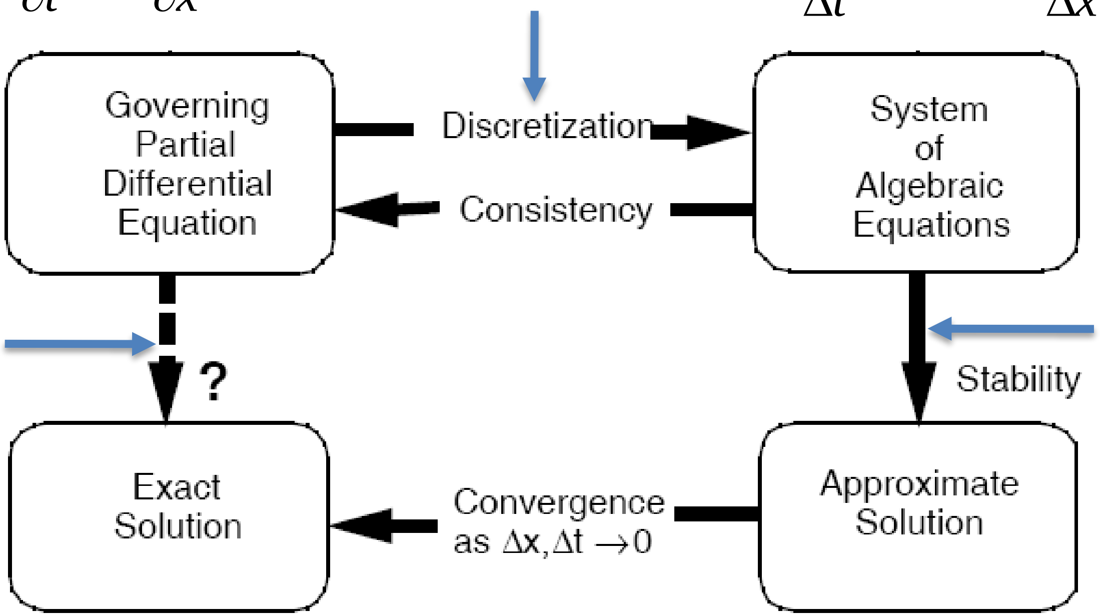
Memo

IV. Overall CFD solution procedure

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

Δx cell size, Δt time step
i node index, n time level

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$



Intial Condition

$u(t=0,x) = f(x)$

Boundary Condition

$u(t,x=L) = u_L$

Numerical IC

$u_1^1 = f(x_1), u_2^1 = f(x_2), \cdots$

Numerical BC

$u_{x=L}^1 = u_L, u_{x=L}^2 = u_L, \cdots$

$$u(x,t) = f(x-at)$$

$$u_i^n = u_1^2, u_2^2, \cdots, \\ u_1^3, u_2^3, \cdots, \\ \vdots$$

IV. Consistency, stability and accuracy of CFD

- **Truncation error: Expanding the solution using Taylor series**

$$u_i^{n+1} = u_i^n + \Delta t\left(\frac{\partial u}{\partial t}\right)_i^n + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)_i^n + \cdots, \quad u_{i-1}^n = u_i^n - \Delta x\left(\frac{\partial u}{\partial x}\right)_i^n + \frac{(\Delta x)^2}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i^n + \cdots$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0 \;\Rightarrow\; \left(\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x}\right)_i^n = -\frac{\Delta t}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)_i^n + \frac{a\Delta x}{2}\left(\frac{\partial^2 u}{\partial x^2}\right)_i^n + \cdots = O(\Delta t, \Delta x)$$

- **Consistent if the truncation error vanishes as the mesh is refined**

IV. Consistency, stability and accuracy of CFD

- **Stability: Errors (i.e. truncation, B.C.-related, round-off) do not grow as the calculation proceeds**

$$u_i^n = e^{at} e^{j\frac{m\pi}{L}x} \Rightarrow \frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$

$$\Rightarrow e^{a\Delta t} = f\left(\frac{a\Delta t}{\Delta x}, \frac{m\pi}{L}\Delta x\right);\ m \text{ no. of } \Delta x \text{ units; } L \text{ length}$$

- **The stability requirement is that the amplification factor** $\left|e^{a\Delta t}\right| \le 1$
- **Courant-Friedrichs-Lewy (CFL) condition on time step and mesh spacing**

$$\left|e^{a\Delta t}\right| \le 1 \Rightarrow \frac{a\Delta t}{\Delta x} \le 1$$

IV. Consistency, stability and accuracy of CFD

- **A consistent stable numerical scheme is convergent (Lax's Equivalence Theorem)**
- **Convergence means that the numerical solution approaches the true solution of the PDEs as the mesh is refined**

$$\begin{tikzcd}
\text{PDE} \arrow[r, leftrightarrow, "\text{consistency}"] \arrow[rr, leftrightarrow, bend right, "\text{convergence}"'] & \text{Discre. PDE} \arrow[r, leftrightarrow, "\text{stability}"] & \text{Num. PDE}
\end{tikzcd}$$

IV. Consistency, stability and accuracy of CFD

- **Truncation error:**
  - Usually 2nd-order accurate in space (and time)
    - Higher for wave propagation problems
  - Lower than 2nd-order accurate in practice (degradation by B.C.)
- **Grid refinement (convergence) study for error estimation:**
  - Numerical solutions on a series of grids (coarse, reference, fine) with different cell sizes

$$\text{Order of accuracy} = \frac{\ln\left[\left(\text{Soln}_{coarse} - \text{Soln}\right)\big/\left(\text{Soln} - \text{Soln}_{fine}\right)\right]}{\ln(\text{refinement ratio})}$$

V. Finite volume method

- **Discretization (explicit in time) of conservation laws in integral form**

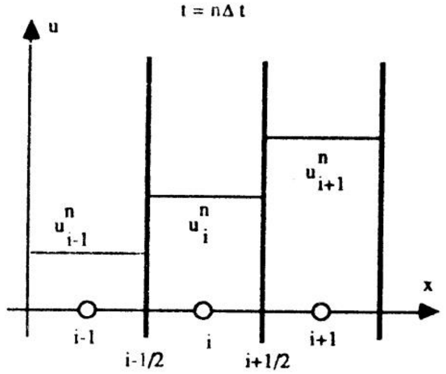
$$\overline{\mathbf{U}}_{i,j}^{n+1} = \overline{\mathbf{U}}_{i,j}^{n} - \frac{\Delta t}{A_{i,j}} \sum_{k=1}^{N(=4)} \mathbf{R}_k^{-1} \mathbf{F}_k^n \left(\mathbf{R}_k \mathbf{U}^n \right) \Delta L_k \xleftarrow{\text{FVM in 2-D}} \frac{\partial}{\partial t} \int_R \mathbf{U} dV + \oint_S \mathbf{F} \cdot \mathbf{n} dS = 0$$

$$\text{where } \overline{\mathbf{U}}_{i,j}^{n} \equiv \left(1/A_{i,j} \right) \int_R \mathbf{U}_{i,j}^n (\mathbf{r}, t) dA$$

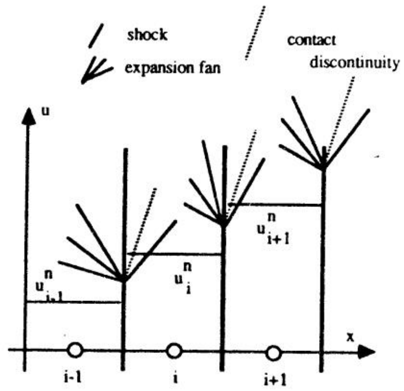
1-D

$$\overline{\mathbf{U}}_{i}^{n+1} = \overline{\mathbf{U}}_{i}^{n} - \frac{\Delta t}{\Delta x} \left[\mathbf{F}\left(\mathbf{U}_{i+1/2}^n \right) - \mathbf{F}\left(\mathbf{U}_{i-1/2}^n \right) \right]$$

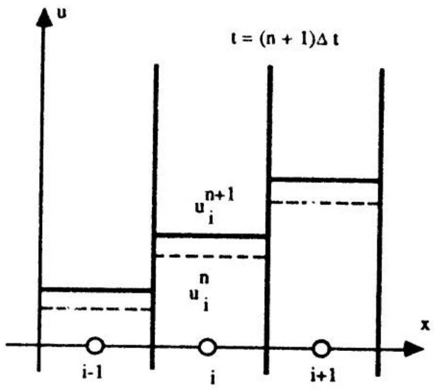
V. Finite volume method



Define a piecewise constant approximation of the solution at time nΔt



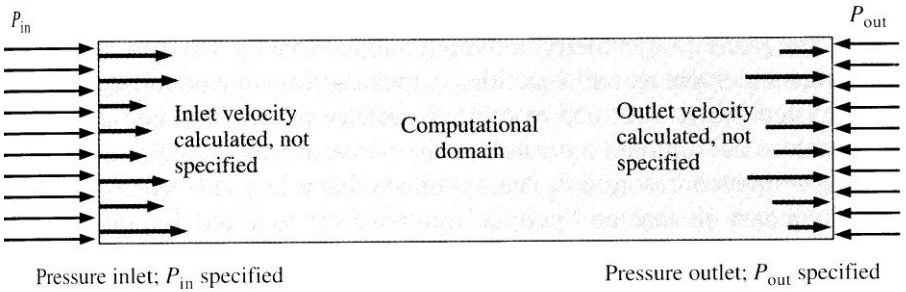
Obtain the solution for the local Riemann problem at the cell interfaces



Average the variables after a time interval Δt and repeat until convergence of residuals

V. Boundary Conditions

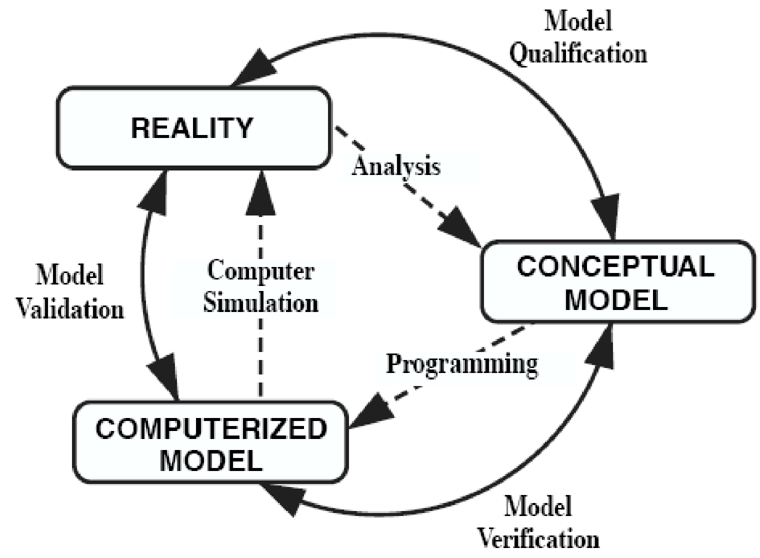
- Thinking fluid dynamics first (before CFD) is essential
- Types of boundary conditions
  - Solid wall: no slip, no penetration, wall roughness for turbulence, temperature or heat flux specified
  - Far-field in external flows: in or out, supersonic or subsonic
  - Inflow and outflow in internal flows: velocity or pressure specified
  - Flow symmetry; boundary between blocks; periodic boundary
- An example: As the CFD solution converges, the velocity adjust itself such that the prescribed pressure B.C. is satisfied



VI. Verification and validation (V & V)

- **Verification**: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.

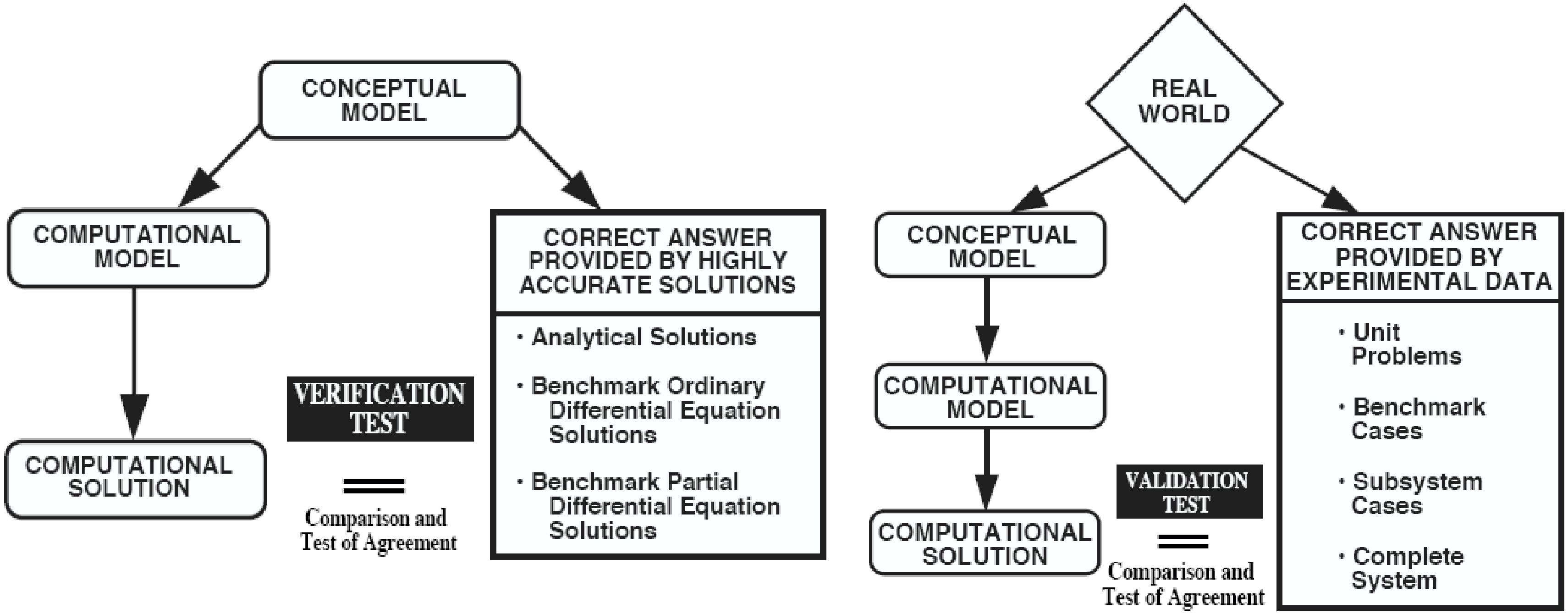
- **Validation**: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model



Oberkampf WL, Roy CJ. *Verification and Validation in Scientific Computing*. Cambridge University Press, 2010.

VI. Verification and validation (V & V)

- Verification & validation: role of analytic solutions and benchmark cases



VI. Validation process (sources of uncertainty)

- Sources of uncertainty in computational model:
  - Physical models: inviscid, viscous, incompressible
  - Auxiliary physical models: EOS, transport properties, turbulence model
  - Boundary conditions: Roughness, far-field, geometry representation
  - Initial conditions
  - Discretization, round-off, user errors
- Ingredients for validation of computational model:
  - Experimental data
  - Experimental uncertainty propagation
  - Computational model uncertainty propagation
  - Comparison error

VII. Tips in CFD practice

- "*It is a poor workman who blames his tools - the good man gets on with the job, given what he's got, and gets the best answer he can*" (R.W. Hamming, You and Your Research)
- Solve the simple problems first (physics and grids)
- Study the benchmark problems
- Think FD before CFD (it's a bunch of numbers until FD comes in)
- Do not trust perfect agreement too much (often qualitative aspects more useful)

VII. Some words on CFD

- Garbage in, garbage out: the results are only as good as the input data.
- Skilled CFD practitioners cleverly use CFD to predict trends, rather than to guarantee absolute values.
- No one believes the CFD results except the one who performed the calculation, and everyone believes the experimental results except the one who performed the experiment.
- Navier-Stokes vs lattice Boltzmann: will it change the landscape of CFD ? “It may create some turbulence in the CFD market…”

Q & A