Introduction on CFD in hemodynamics

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• Implementation in Ansys Fluent: CFD model setup
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CFD introduction

- What is CFD
- How is implemented in hemodynamics
- Why is useful in hemodynamics
- How should I use it
Computational fluid dynamics: CFD

• Fluid dynamics: physics of fluids
• Computational: numeric involved in solving the equation describing the motion of the fluid

There is a strong interplay between math concepts, physics knowledge and technological tools and environments used to implement a CFD model

• No general rules for specific model setup
• Need of a-priori knowledge on the fluid behavior
• If possible experimental (or theoretical) data to validate CFD results
Computer aided engineering workflow

- **PRE-PROCESSING**
- **COMPUTATION**
- **POST PROCESSING**

**COMPUTATIONAL**

**PHYSICS**

**MODEL**

**SOLVING**

**HPC ENVIRONMENT**

**VISUALIZATION**

**RESULTS**
From physics to model by means of measures

- In vitro
- Animal models
- In vivo

Measures are necessary to build reliable CAE models
In vitro models

Bicuspid porcine valve setup mock
Performed by Riccardo Vismara (Politecnico di Milano)
at the ForcardioLab
http://www.forcardiolab.it/
Animal models

PTFE implant device in sheep
Performed by
Fabio Acocella and Stefano Brizzola
Dipartimento Di Scienze Cliniche Veterinarie
Facolta' Di Medicina Veterinaria
Universita’ Degli Studi Di Milano
In vivo image based measures

Phase contrast MRI acquisition (3D, 3 velocity encoding directions)
Performed by
Giovanna Rizzo (IBFM-CNR) and
Marcello Cadioli (Philips Italia)
Computational model

1. Image processing or CAD tools
2. Geometry modeler
3. Meshing tools
4. CFD solvers
CFD solver

Codes
- Open Source
  - Academic
  - In house
- Commercial

Methods
- Finite Volumes
- Finite Elements
- Spectral
- Lattice Boltzmann
The CFD approach

- THE FLUID DYNAMIC APPROACH uses the geometry and mechanical properties of the vasculature and the principles of conservation of mass and momentum to obtain the blood flow-pressure relation.
- The solution of such equations yields information on instantaneous velocity and pressure distributions.
Domain-mesh-cell
Discretization

- Domain is discretized into a finite set of control volumes or cells. The discretized domain is called the “grid” or the “mesh.”
- General conservation equations for mass and momentum are discretized into algebraic equations and solver for each and all cells in the discretization

(physic --> math --> numeric --> sw)
In theory:
If \( \# \text{cells} \to \infty \) then the numerical solution \( \to \) 'exact'
and this will be independent from the numerical scheme adopted.

In practice:

\#\text{cells} if finite then the numerical solution \( \to \) ‘OK’
and this will be dependent from the properties of the numerical scheme adopted
(Exact) Analytical solution is not available:
Numerical/Algebraic (Approximated) solution of the problem

a tasking environment
A tasking environment: geometry
A tasking environment: physics

Time dependent flow waveforms

Spatial/temporal dependent velocity profiles
A tasking environment: knowledge

Limited ‘experimental’ knowledge on:

- Wall-properties (Young’s modulus?)
- Fluid-to-wall interaction (wall displacements?)
- Spatial/temporal velocity profiles distribution (accuracy of the measures in space & time?)
A tasking environment: math/numeric and tech

- Convergence
- Consistency
- Stability

- Boundedness
- Conservativeness
- Transportiveness

Math || Numeric
How should I use my computational tools

CFD can be helpful (and economically inexpensive) for:

• System analysis (and optimization) (example blood filter)


• Detailed measures (3D, high resolution space/time) (CFD Arch AO compared to PC MRI resolution)


• Hypothesis testing


• Validation of clinical practice (Doppler series)


• Implantable devices (FSI)


Blood fluid dynamics:
theory, equations and examples

• Physic of blood
• Working hypothesis in vessels
• Conservation laws
• Implementation in Ansys Fluent
• Notes on convergence
• Notes on source of errors
Physic of blood

- The main functions of the **blood** are the transport, and delivery of oxygen and nutrients, removal of carbon dioxide and waste products of metabolism, distribution of heat and signals of immune system.
- The **blood** flow resistance is influenced by the complicated architecture of the vascular network and flow behaviour of **blood** components - **blood** cells and plasma.
- At a macroscopic level the **blood** appears to be a liquid material, but at a microscopic level the **blood** appears to be a material with microscopic solid particles of varying size - various **blood** cells.
Density is a fluid property and is defined as:

\[ \rho = \frac{\text{Mass}}{\text{Volume}} \]

Usually blood density is assumed to be similar (equal) to water density at T=300 K and P=10^5 Pa

\[ \rho = 1060 \ [\text{Kg/m}^3] \]
Blood viscosity

For viscous flow if the relationship between viscous forces (tangential component) and velocity gradient is linear then the fluid is called Newtonian and the slope of the line is a measure of a fluid property called viscosity (dynamic).

\[ S_y = \mu \frac{dv}{dx} \]
Also a cinematic viscosity can be defined by:
\[ \nu = \frac{\mu}{\rho} \]
Typical values are:
\[ \mu_{\text{blood}} = 0.0035 \text{ [kg/ms]} \quad (\nu_{\text{blood}} = 3.3 \times 10^{-6} \text{ [m}^2/\text{s]})) \]
Blood is Newtonian and non Newtonian

Shear stress
[Pa]

Shear rate (du/dx) [1/s]

\[ \tan(\alpha) = \mu \]  
(dynamic viscosity)  
[Pa s]
Reynolds number

- The Reynolds number $Re$ is defined as:

$$Re = \frac{r V L}{m}.$$ 

Here:

- $L$ is a characteristic length (say $D$ in tubes)
- $V$ is the mean velocity over the section ($\frac{Q}{Area}$)
- Density and viscosity are: $r, m$

- If $Re >> 1$ the flow is dominated by inertia.
- If $Re << 1$ the flow is dominated by viscous effects.
Effect of Reynolds number

Laminar flow

Turbulent flow
Effect of Reynolds number

Blood flow regimen

Re = 0.05

Re = 10

Re = 200

Re = 3000
Womersley number

- The Womersley number $W$ (or $Wo$ or $\alpha$) is defined as:
  \[ W = L(2\pi f r/m)^{1/2}. \]

Here:
- $L$ is a characteristic length (say $D/2$ in tubes)
- $f$ is the frequency of the flow waveform (1/period)
- density and viscosity are: $r$, $m$

- If $W \neq 0$ (< 1) the flow is dominated by viscous effect (similar to a poiseuille flow).
- If $W >> 1$ the flow is dominated by transient effect
Effect of Womersley number

Some typical values for the Womersley number in the cardiovascular system for a canine at a heart rate of 2Hz are:

Ascending Aorta -- 13.2
Descending Aorta -- 11.5
Abdominal Aorta -- 8
Femoral Artery -- 3.5
**Carotid Artery** -- 4.4
Arterioles -- 0.04
Capillaries -- 0.005
Venules -- 0.035
Interior Vena Cave -- 8.8
Main Pulmonary Artery -- 15
Womersley VS Reynolds

\[
\text{Re} = \frac{\text{convective inertia force}}{\text{viscous friction force}}
\]

\[
W = \frac{\text{transient inertia force}}{\text{viscous friction force}}
\]
Flow classifications

- Laminar vs. turbulent flow.
  - Laminar flow: fluid particles move in smooth, layered fashion (no substantial mixing of fluid occurs).
  - Turbulent flow: fluid particles move in a chaotic, “tangled” fashion (significant mixing of fluid occurs).

- Steady vs. unsteady flow.
  - Steady flow: flow properties at any given point in space are constant in time, e.g. $p = p(x,y,z)$.
  - Unsteady flow: flow properties at any given point in space change with time, e.g. $p = p(x,y,z,t)$. 
Steady laminar flow in a cylinder

- Steady viscous laminar flow in a horizontal pipe involves a balance between the pressure forces along the pipe and viscous forces.
- The local acceleration is zero because the flow is steady.
- The convective acceleration is zero because the velocity profiles are identical at any section along the pipe.

- The shape of the spatial velocity profile is a parabola centered on the axis of the cylinder.
- The peak value is proportional to the pressure drop acting on the cylinder.
Unsteady flow in a cylinder

- Unsteady flow in a cylinder is governed by a balance among:
  - local acceleration,
  - convective acceleration,
  - pressure gradients
  - viscous forces
- In synthesis all the factors in the Navier-Stokes equations are relevant to determine the flow evolution.
- Thanks to the symmetry properties of the domain the solution of this problem can be analytically determined (Womersley solution)
- In general due to the shape of the domain this is not possible

Womersley solution
VS
PC MRI acquisition in a straight abdominal aorta section
Womersley solution
VS PC MRI acquisition in a straight abdominal aorta section
Incompressible vs. compressible flow

- Incompressible flow: volume of a given fluid particle does not change.
  - Implies that density is constant everywhere.
  - Essentially valid for all liquid flows.
- Compressible flow: volume of a given fluid particle can change with position.
  - Implies that density will vary throughout the flow field.
Single phase vs. multiphase flow &
homogeneous vs. heterogeneous flow

- Single phase flow: fluid flows without phase change (either liquid or gas).
- Multiphase flow: multiple phases are present in the flow field (e.g. liquid-gas, liquid-solid, gas-solid).
- Homogeneous flow: only one fluid material exists in the flow field.
- Heterogeneous flow: multiple fluid/solid materials are present in the flow field (multi-species flows).
Blood working hypothesis

1. Laminar flow (Reynolds < 2300)
2. Incompressible fluid
3. Unsteady behavior (Womersley ≠ 0)

The problem is described exactly by:
   – three Navier-Stokes equations
   – the equation of continuity

• BUT:
   – A general solution of such a system of nonlinear partial differential equations has not been achieved;
   – The physiological quantities which would arise in a treatment of blood flow in large arteries are not well known.

For both reasons it is necessary to work in terms of approximate models, which include the important features of the system under consideration and neglect unimportant features.
Important features of blood as fluid

1. Continuum hypothesis (molecular scales and or suspended particles are not relevant to study large arteries \(d > 1 \mu m\))
2. Laminar (Reynolds < 2000)
3. Unsteady (Womersely >> 1)
4. Incompressible (density \(\rho\) is constant \(\approx \rho_{water}\))
5. Isotropic (same behaviour in all directions)
6. Newtonian (viscosity (\(\mu\) and \(\lambda\)) are constant and do not depends on the shear rate)
Unimportant features of blood as fluid

- Viscosity depends on:
  - Temperature (energy eqn can be neglected)
  - % hematocrit
- Compressible (around $10^{-11}$[m$^2$/N] for low pressure)
- Transitional to turbulent under particular conditions and for certain vascular districts (valves, etc.)
Equations of conservation

Two general conservation equations:

1. Mass (divergence free)
2. Momentum: Newton’s second law: the change of momentum equals the sum of forces on a fluid particle
Navier-Stokes equations

\[ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \mu \nabla^2 \mathbf{v} + \mathbf{f} \]

Inertia (per volume)

\[ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) \]

Unsteady acceleration

Convective acceleration

Divergence of stress

- Pressure gradient
- Viscosity
- Other body forces
The rate of change over time (local acceleration) + Transport by convection = Pressure forces + Diffusion/viscous forces + Source terms

1. Non linear
2. Coupled (also in the continuity eqn)
3. Role of pressure (no equation of state for Newtonian incompressible fluids)
4. Second order derivatives
Blood in large vessels

- Local (unsteady) acceleration
- Convective acceleration
- Pressure gradients
- Viscous forces

The solver that are looking is like that:
- Pressure based solver (incompressible)
- Segregated solver (Mac number < 1)
- Laminar (Re < 2300)
- Unsteady (W > 0)
Segregated (pressure based) solver for viscous fluid under laminar unsteady flow regime in FLUENT
Iterative methods

All the issues abovementioned require numerical methods and techniques to build accurate and stable tools to integrate such equations.
Solvers in Ansys Fluent

- Density based: suitable for high speed and compressible fluids
- Pressure based: suitable for slow speed and incompressible fluids

For blood we will use the latter
Pressure-based solver: Coupled vs Segregated

• Coupled: more memory requirements, higher rate of convergence (thanks to coupling), not used for incompressible flow (but you can try). Limits on the time-stepping choice for unsteady flow (CFL).

• Segregated: default in Ansys Fluent, less memory requiring slower rate of convergence (de-coupled). No limits on the time-stepping for unsteady flows.
Segregated procedure

Solve a single equation at the time but for all cells in the domain

1. Initialized/Guessed-values
2. Solve momentum equations (x3 directions)
3. Solve continuity equation
4. Converged?
   - No
   - Yes
     - End
Coupled procedure

Solve all the equations at the time but for one cell and then iterate over all the cells in the domain.

- Initialized/Guessed-values
- Solve momentum equations (x3 directions) and continuity equation simultaneously
- Converged?
  - No
  - Yes
    - End
Unsteady flow chart: extra loop for time

Execute segregated or coupled procedure, iterating to convergence

Update solution values with converged values at current time

Requested time steps completed?

Take a time step

No

Yes

Stop
Guessed values and relaxation

• The iterative method to move from one iteration to the other uses guessed values.

• New values are found using the old value and a guessed one according to:

\[
\phi_P^{\text{new, used}} = \phi_P^{\text{old}} + U(\phi_P^{\text{new, predicted}} - \phi_P^{\text{old}})
\]

• Here U is the relaxation factor:
  – U < 1 is underrelaxation.
  – U = 1 corresponds to no relaxation. One uses the predicted value of the variable.
  – U > 1 is overrelaxation.
Spatial discretization: found adjacent cells values

- In order to solve the momentum equations we must make assumption on the values and the variation of the quantities across adjacent cells faces

- Under spatial discretization menu we have:
  - First-order upwind
  - Power-law scheme
  - Second-order upwind
  - QUICK
  - MUSCL
First order upwind

- Easy
- Stable
- Diffusive

A good starting point for the simulation setup
Second-order upwind

- More accurate than the first order upwind scheme
- Very popular

Flow direction

interpolated
Value uses the values of two cells ‘up’
Accuracy of numerical schemes

• The Taylor series polynomials for a certain quantity $\phi$ is:

$$
\phi(x_e) = \phi(x_p) + \frac{\phi'(x_p)}{1!}(x_e - x_p) + \frac{\phi''(x_p)}{2!}(x_e - x_p)^2 + \ldots + \frac{\phi^n(x_p)}{n!}(x_e - x_p)^n + \ldots
$$

• In the first order upwind we use only the constant and ignores the first derivative and consecutive terms (first order accurate)
• In the second order upwind scheme we use constant and the first order derivative (second order accurate)
Conservativeness

The conservation of the fluid property $\phi$ must be ensured for each cell and globally by the algorithm.
Boundedness

Iterative methods start from a guessed value and iterate until convergence criterion is satisfied all over the computational domain.

In order to converge math says that:

1. Diagonal dominant matrix (from the sys. of eqn.)
2. Coefficients with the same sign (positive)

Physically this means:

1. If you don’t have source terms the values are bounded by the boundary ones (if the pb is linear).
2. If a property increases its value in one cell then the same property must increase also in all the cells nearby.

Overshoot and undershoot present for certain algorithms is related to this property
Transportiveness

Directionality of the influence of the flow direction must be ‘readable’ by discretization scheme since it affects the balance between convection and diffusion.

So called ‘false-diffusion’ (i.e. numerically induced) is related to this property.
Pressure - velocity coupling

• For incompressible N-S eqn there is no explicit equation for P.
• P is involved in the momentum equations.
• V must satisfy also continuity equation.
• The so-called ‘pressure-velocity’ coupling is an algorithms used to obtain a valid relationship for the pressure starting from the momentum and the continuity equation.
• The oldest and most popular algorithm is the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) by Patankar and Spalding 1972.
Improvements on SIMPLE

- In order to speed-up the performances of the SIMPLE algorithm several versions have been derived:
  - SIMPLER (SIMPLE Revised)
  - SIMPLEC (SIMPLE Consistent)
  - PISO (Pressure Implicit with Splitting of Operators)
Simple vs Piso vs Coupled

For the same task (2 cycle of a Womersley problem on a 200m cells grid) using:
- the same settings except for the P-V coupling algorithm
- The same machine
- 8 computing cores

Elapsed times are:
Piso: 10h
Simple: 2h
Coupled: 7h
Simple-piso-coupled
What is convergence

• A flow field solution (P,V knowledge on all the cells in the domain) is considered ‘converged’ when the changes of the properties in the cells from one iteration to another are below a certain fixed value.
• General laws are missing; we have some good rules to understand when we are converged.

#1
Monitor the residuals
Residuals

- Residual: \( R_P = |a_p \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b| \)
- Usually scaled and normalized
Other convergence monitors

#2
Monitor ‘the other ‘ quantity on boundaries

#3
Monitor changes on quantities you are interest on
Source of errors and uncertainty

**Error:** deficiency in a CFD model.
Possible sources of error are:
- Numerical errors (discretization, round-off, convergence)
- Coding errors (bugs)
- User errors

**Uncertainty:** deficiency in a CFD model caused by a lack of knowledge.
Possible source of uncertainty are:
- Input data inaccuracies (geometry, BC, material properties)
- Physical model (simplified hypothesis for the fluid behavior)
Verification and Validation (V&V)

**Verification**: “solving the equation right” (Roache ‘98). This process quantify the errors.

**Validation**: “solving the right equations” (Roache ‘98). This process quantify the uncertainty.
Quantitative descriptors of arterial flows

- Blood flow data contain **valuable information for diagnosis, prognosis, and risk assessment of cardiovascular diseases**. Conventional inspection is insufficient to extract useful information. Thus, comprehensive visualization techniques are necessary to effectively communicate blood-flow dynamics and facilitate the analysis.

- Hemodynamics descriptors are used to **visualize disturbed flow**, to **perform quantitative comparisons** and to **measure hemodynamic performances** of surgical interventions, device optimization, follow-up studies.

- Effective flow visualizations **facilitates a better understanding of the physical phenomena** and also **open new venues of scientific investigation**.
Atherosclerosis

Focal Disease
Bends - Branches - Bifurcations

“Disturbed” Blood Flow

Endothelial Flow-Mediated Response
Atherosclerosis

Evidences suggest that initiation and progression of atherosclerotic disease is influenced by “disturbed flow”.

**Aggravating Flow Events**
- Flow Separation/Reattachment
- Low Oscillatory Wall Shear
- Vortical Flows
- Stagnation Point Flows
- High Shear Stress Regions
- Hypertension Flows
- Long Particle Residence Times

**Abnormal Biological Events**
- Endothelial Cell Dysfunction
- Injury of Endothelium
- Enhanced Wall Permeability
- Wall Influx of LDL and Monocytes
- Aggregation/Deposition of Platelets, Fibrin; SMC Proliferation

**Indicator Functions**
- Wall Shear Stress (WSS)
- Variations of WSS, i.e., Shear Index, Gradient, Angle Deviation, etc.
- Normal Pressure Gradient
- Particle Deposition Patterns
- Wall Particle Density (WPD)

**Blood Vessel Diseases**
- Atherosclerosis
- Hyperplasia
- Thrombosis
Hemodynamic factors

The role played by haemodynamic forces acting on the vessel wall is fundamental in maintaining the normal functioning of the circulatory system, because arteries adapt to long term variations in these forces. That is, arteries attempt to re-establish a physiological condition by:

- dilating and subsequently remodelling to a larger diameter in the presence of increased force magnitude
- remodelling to a smaller diameter, or thickening the intimal layer, in the presence of decreased force magnitude.

[Malek et al., 1999]
Wall Shear Stress - WSS

- The Wall Shear Stress (WSS), $\tau_w$, is given by:

$$\tau_w = \mu \left( \frac{\partial u}{\partial y} \right)_{y=0}$$

Where $\mu$ is the dynamic viscosity, $u$ is the velocity parallel to the wall and $y$ is the distance to the wall.

- Low and oscillating WSS has been proposed as a localizing factor of the development of atherosclerosis.
WSS on Endothelial Cells (ECs)

WSS can change the morphology and orientation of the endothelial cell layer: endothelial cells subjected to a laminar flow with elevated levels of WSS tend to elongate and align in the direction of flow, whereas in areas of disturbed flow endothelial cells experience low or oscillatory WSS and they look more polygonal without a clear orientation, with a lack of organization of the cytoskeleton and intercellular junctional proteins.

Left: F-actin organization in bovine aortic ECs before and after the application of a steady shear stress. Note extensive F-actin remodeling.
Right: Bovine aortic ECs before flow and after. The cells elongate and align in the direction of flow. [Barakat, 2013]
WSS on Endothelial Cells (ECs)

[Malek et al., 1999]
Tool for WSS descriptors: CFD

Imaging + Computational Fluid Dynamics (CFD): reconstruction of complex WSS patterns with a high spatial and temporal resolution.

[Steinman 2002]
WSS Descriptors:
Time Averaged WSS

• Time-Averaged Wall Shear Stress (TAWSS) can be calculated by integrating each nodal WSS vector magnitude at the wall over the cardiac cycle.
• Low TAWSS values (lower than 0.4 Pa) are known to stimulate a proatherogenic endothelial phenotype
• Moderate (greater than 1.5 Pa) TAWSS values induces quiescence and an atheroprotective gene expression profile.
• High TAWSS values (greater than 10-15 Pa, relevant from 25-45 Pa) can lead to endothelial trauma.

\[
TAWSS = \frac{1}{T} \int_{0}^{T} |WSS(s, t)| \cdot dt
\]

[Malek et al., 1999]
WSS Descriptors: 
Oscillatory Shear Index

- Oscillatory Shear Index (OSI) is used to identify regions on the vessel wall subjected to highly oscillating WSS directions during the cardiac cycle. These regions are usually associated with bifurcating flows and flow patterns strictly related to atherosclerotic plaque formation and fibrointimal hyperplasia.
- Low OSI values occur where flow disruption is minimal
- High OSI values (with a maximum of 0.5) highlight sites where the instantaneous WSS deviates from the main flow direction in a large fraction of the cardiac cycle, inducing perturbed endothelial alignment.

\[
\text{OSI} = 0.5 \left[ 1 - \left( \frac{\int_0^T \text{WSS} (s, t) \cdot dt}{\int_0^T |\text{WSS} (s, t)| \cdot dt} \right) \right] \quad 0 \leq \text{OSI} \leq 0.5
\]

[Ku et al., 1985]
WSS Descriptors:
Relative Residence Time

- Relative Residence Time (RRT) is inversely proportional to the magnitude of the time-averaged WSS vector (i.e., the term in the numerator of the OSI formula).
- Recommended as a robust single descriptor of “low and oscillatory” shear [Lee et al., 2009].

\[
RRT = \frac{1}{(1 - 2 \cdot OSI) \cdot TAWSS} = \frac{T}{\int_0^T \mathbf{WSS}(s,t) \cdot dt}
\]

[Himburg et al., 2004]
WSS Descriptors:
Gradient-based descriptors

- WSS spatial gradient (WSSG) is a marker of endothelial cell tension. It is calculated from the WSS gradient tensor components parallel and perpendicular to the time-averaged WSS vector (m and n, respectively) [Depaola et al., 1992].

\[
WSSG = \frac{1}{T} \int_0^T \sqrt{\left( \frac{\partial \tau_{w,m}}{\partial m} \right)^2 + \left( \frac{\partial \tau_{w,n}}{\partial n} \right)^2} dt
\]

- The WSS angle gradient (WSSAG) highlights regions exposed to large changes in WSS direction, irrespective of magnitude. This is done by calculating, for each element’s node (index j), its direction relative to some reference vector (index i, e.g. that at the element’s centroid) [Longest et al., 2000].

\[
WSSAG = \frac{1}{T} \int_0^T \left| \int \int \nabla \phi_j dA_i \right| dt, \quad \phi_j = \cos^{-1}\left( \frac{\tau_{w,i} \cdot \tau_{w,j}}{|\tau_{w,i}| |\tau_{w,j}|} \right)
\]

- WSS temporal gradient is the maximum absolute rate of change in WSS magnitude over the cardiac cycle.

\[
WSST = \max \left( \left| \frac{\partial |\tau_w|}{\partial t} \right| \right)
\]
WSS Descriptors: Harmonic-based descriptors

The harmonic content of the WSS waveforms can be a possible metric of disturbed flow. This statement is enforced by results revealing that endothelial cells sense and respond to the frequency of the WSS profiles.

- The time varying WSS magnitude at each node can be Fourier-decomposed, and the dominant harmonic (DH) is defined as the harmonic with the highest amplitude [Himburg & Friedman, 2006].

\[
DH = \max(F_w(n\omega_0)), \quad F_w = \text{FFT}(|\tau_w|), \quad \omega_0 = 2\pi/T
\]

- The harmonic index (HI) is defined as the relative fraction of the harmonic amplitude spectrum arising from the pulsatile flow components [Gelfand et al., 2006].

\[
HI = \frac{\sum_{n=1}^{\infty} F_w(n\omega_0)}{\sum_{n=0}^{\infty} F_w(n\omega_0)}
\]
And the bulk flow?

The need for a reduction of the complexity of highly four-dimensional blood flow fields, aimed at identifying hemodynamic actors involved in the onset of vascular pathologies, was driven by histological observations on samples of the vessel wall.

Disturbed flow within arterial vasculature has been primarily quantified in terms of WSS-based metrics.

This strategy was applied notwithstanding arterial hemodynamics is an intricate process that involves interaction, reconnection, and continuous re-organization of structures in the fluid!

The investigation of the role played by the bulk flow in the development of the arterial disease needs robust quantitative descriptors with the ability of operating a reduction of the complexity of highly 4D flow fields.

[Morbiducci et al., 2010]
Eulerian vs. Lagrangian

<table>
<thead>
<tr>
<th>Lagrangian</th>
<th>Eulerian</th>
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<tbody>
<tr>
<td>+ Visualizations</td>
<td>+ Simplicity</td>
</tr>
<tr>
<td>+ Three dimensionality/ Four dimensionality (i.e., space and time)</td>
<td>+ Picture of the entire flow</td>
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<tr>
<td>+ Highlight of the recirculation zones</td>
<td>+ Timing</td>
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<tr>
<td>+ Characterization of unsteady flow patterns</td>
<td>+ Real time analysis</td>
</tr>
<tr>
<td>+ More immediate understanding of the fluid motion</td>
<td>+ Its immediateness is attractive for clinicians</td>
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<tr>
<td>+ Path dependent quantities</td>
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<td>+ Dynamical path history</td>
<td></td>
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<td>+ Division of particles into groups regardless of position</td>
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<td></td>
<td></td>
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<tr>
<td>- Convectiveness: less control over the zone of investigation</td>
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<tr>
<td>- Computational cost</td>
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<tr>
<td>- Timing: it is difficult to picture the flow at a specific time instant</td>
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[Gallo et al., 2013]
How to reduce flow complexity?

Helicity influences evolution and stability of both turbulent and laminar flows [Moffatt and Tsinober, 1992]. Helical flow patterns in arteries originate to limit flow instabilities potentially leading to atherogenesis/atherosclerosis.

An arrangement of the bulk flow in complex helical/vortical patterns might play a role in the tuning of the cells mechano-transduction pathways, due to the relationship between flow patterns and transport phenomena affecting blood-vessel wall interaction, like residence time of atherogenic particles.

Helicity – Lagrangian Metric

Starting from the definition of helicity density

$$H_k(s; t) = V \cdot (\nabla \times V) = V(s; t) \cdot \omega(s; t)$$

The Local Normalized Helicity (LNH) is defined as:

$$\text{LNH}(s; t) = \frac{V(s; t) \cdot \omega(s; t)}{|V(s; t)| |\omega(s; t)|} = \cos \varphi(s;t)$$

The helical structure of blood flow was measured calculating the Helical Flow Index (HFI) over the trajectories of the Np particles present within the domain:

$$h_{fi_k} = \frac{1}{(T_{k \text{end}} - T_{k \text{start}})} \int_{T_{k \text{start}}}^{T_{k \text{end}}} |\text{LNH}_k(\zeta)| \, d\zeta$$

$$\text{HFI} = \frac{1}{N_p} \sum_{k=1}^{N_p} h_{fi_k} \quad 0 \leq \text{HFI} \leq 1$$

where Np is the number of points j (j = 1:Np) along the k-th trajectory. [Grigioni et al. 2005, Morbiducci et al. 2007]
Selected Publications


Implementation in Ansys Fluent: CFD model setup

1. Part A: definitions
2. Part B: the Fluent menu (hands-on: Poiseuille and Womersley flow)
3. Part C: user defined functions implementation
Contents Part A

- What is a BC
- Inlet and outlet boundaries
  - Velocity
  - Pressure boundaries
  - Mass-Flow-Inlet
- Wall
- Material properties
Initial conditions and Boundary conditions

- Boundary conditions are a necessary part of the mathematical model.
- In fact Navier-Stokes equations and continuity equation in order to be solved need:
  - initial conditions (starting point for the iterative process)
  - boundary conditions (define the flow regimen problem)
Neumann and Dirichlet boundary conditions

Dirichlet boundary condition:
*Value of velocity at a boundary*
\[ u(x) = \text{constant} \]

Neumann boundary condition:
*Gradient normal to the boundary of a velocity at the boundary,]*
\[ \partial n u(x) = \text{constant} \]
Flow inlets and outlets

- A wide range of boundary conditions types permit the flow to enter and exit the solution domain:
  - General: pressure inlet, pressure outlet.
  - Incompressible flow: velocity inlet, outflow, mass-flow-inlet
- Boundary data required depends on physical models selected.
Pressure BC convention

Pressure boundary conditions require static gauge pressure inputs:

\[ P_{\text{absolute}} = P_{\text{static}} + P_{\text{operating}} \]

An operating pressure input is necessary to define the pressure (the default is given by the sw). Used in hemodynamics since in most outlets:

- Flow rate is not known
- The velocity distribution is not known
Pressure outlet boundary

- Pressure outlet BC can be used in presence of velocity BC at the inlet
- Usually in hemodynamics a zero-stress condition is applied over multiple exits
- The geometry is driving the pressure distribution and the flow repartition
- The static pressure is assumed to be constant over the outlet

Pressure outlet must always be used when model is set up with a pressure inlet
Velocity inlets

- A flat profile is selected by default.
- Other velocity distributions can be set using tables or udf (space/time).
- In hemodynamics is very often used as BC to set a known flow-rate waveform along the heart cycle.
- Thanks to PC MRI instrumentation is possible to obtain spatial and temporal distribution.
Mass-Flow-Inlet

- Specify the mass-flow-rate into the boundary face
- Useful for flow split repartition in multiple IN/OUT geometries
Wall boundaries

- Used to bound fluid and solid regions.
- In hemodynamics is usually set at the wall:
  - Tangential fluid velocity equal to wall velocity (usually zero)
  - Normal velocity component is set to be zero.
Material properties

- The physical property of the fluid and solid must be given.
- Fluent DB selection
- UDF definition (we will see that for the rheological models)
- For Newtonian Incompressible fluid we have to provide only density and viscosity.
Part B: The Ansys Fluent menu

Hands-on: POISEUILLE/WOMERSLEY problem

- General menu
- Model menu
- Boundary condition menu (using tables)
- Material menu (blood properties)
- Monitors (blood flow rate, diameter max vel)
- Solver settings (simple, first order)
- Initialization
- Calculation activities (export diameter on outlet section over time)
- Calculation run (dt settings)
Mesh

Inlet (blue)  Wall (grey)  Outlet (red)

Flow direction
Poiseuille flow details

A circular artery with a length of 3 cm and radius of 0.2 cm
Inflow velocity boundary conditions which are uniform in space and time.
The fluid has a kinematic viscosity of 0.04 poise

Schlichting formula:

\[
\frac{E_l}{D} = 0.06 \cdot Re(D)
\]

\(E_l\) is the entrance length

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value [SI units]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\mu) [Kg/ms]</td>
<td>0.004</td>
</tr>
<tr>
<td>(\rho_o) [kg/m³]</td>
<td>1000.</td>
</tr>
</tbody>
</table>
Problem values of interest

\[ V = 0.05, 0.1, 0.2 \text{ [m/s]} \] (steady inlet BC)
Free pressure at the outlet BC
No-slip condition at the wall BC
Newtonian fluid
Incompressible
Laminar flow condition

<table>
<thead>
<tr>
<th>Vin</th>
<th>EI/D</th>
<th>R [m]</th>
<th>Reynolds</th>
<th>DeltaP [Pa]</th>
<th>Q [m³/s]</th>
<th>Vmax [m/s]</th>
<th>L [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05</td>
<td>3.18</td>
<td>0.001996</td>
<td>106.02</td>
<td>11.97</td>
<td>6e-07</td>
<td>0.099</td>
<td>0.03</td>
</tr>
<tr>
<td>0.1</td>
<td>6.36</td>
<td>0.001996</td>
<td>211.36</td>
<td>23.95</td>
<td>1e-06</td>
<td>0.19</td>
<td>0.03</td>
</tr>
<tr>
<td>0.2</td>
<td>12.72</td>
<td>0.001996</td>
<td>409.07</td>
<td>47.91</td>
<td>2e-06</td>
<td>0.39</td>
<td>0.03</td>
</tr>
</tbody>
</table>
El (v = 0.05)
Vmax
Pressure drop
Pressure drop along the pipe
Womersely flow details

A circular artery with a length of 3 cm and radius of 0.2 cm

Inflow velocity boundary conditions which are uniform in space and periodic in time.

The time variation is described by a sinusoidal function

\[ V(t) = V\left(1 + \sin\left(\omega t/T\right)\right) \]

with mean velocity, \( V = 13.5 \text{ cm/s} \), and period, \( T \), of 0.2 s.

The fluid has a kinematic viscosity of 0.04 poise

Resulting in a mean Reynold’s number of 135 and Womersley number of 5.6.
Problem values of interest

- \( V(t) = V(1 + \sin(2\omega t/T)) \) (unsteady inlet BC)
- Free pressure at the outlet BC
- No-slip condition at the wall BC
- Newtonian fluid
- Incompressible
- Laminar flow condition

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Value [SI units]</th>
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</thead>
<tbody>
<tr>
<td>( \mu ) [Kg/ms]</td>
<td>0.004</td>
</tr>
<tr>
<td>( \rho ) [kg/m3]</td>
<td>1000.</td>
</tr>
<tr>
<td>( D ) [m]</td>
<td>0.004</td>
</tr>
<tr>
<td>( T ) [s]</td>
<td>0.2</td>
</tr>
<tr>
<td>( v ) [m/s]</td>
<td>0.135</td>
</tr>
<tr>
<td>Reynolds (mean)</td>
<td>135</td>
</tr>
<tr>
<td>Womersley</td>
<td>5.6</td>
</tr>
<tr>
<td>( L ) [m]</td>
<td>0.03</td>
</tr>
</tbody>
</table>
Results:
Womersley flow

T = 0.02
T = 0.08
T = 0.14
V-profiles at $t=0.02$
V-diam at t=0.02
Pressure drop at t=0.02
Pressure drop at $t=0.02$
t=0.08
t=0.08
t=0.08
t=0.14
t=0.14
t=0.14
Theory vs Ansys
200m cells hexa

3000m cells tetra
3000m tetra
200m hexa
1500m hexa
Vz max:
mean %diff: 0.43
std %diff: 0.06

Vz min:
mean %diff: -3.44
std %diff: 5.70

Vz Averaged:
mean %diff: 3.70
std %diff: 2.17
Comments

• Mesh type&quality do matter
• Avg agreement is good but there are some tricky zones that should be handled with care
• Acceleration and deceleration phases have different level of accuracy
• Solver setup can be considered ok for hemodynamics purposes at similar fluid dynamics conditions
Part C: user defined function implementation

- Udf intro
- Udf resources from Ansys
- C programming intro
- Mesh terminology and udf data types
- Examples
User defined functions

Ansys Fluent is a commercial codes but is programmable according to a C-like syntax and using a set of predefined macros and functions. A program able to interact with the Fluent solver using these macros/functions is called USER DEFINED FUNCTION (udf). Using udf it’s possible to implement several tasks but we will focus our attention only on:

1. Space/time dependent boundary condition
2. non-Newtonian fluid properties
3. Post-processing and reporting
Ansys udf manual

The manual contains all the available MACROS and functions to interact with the Ansys solver.
We will refer to the manual for introducing this topic.
Udf programming is a well-established, stable and powerful tool to customize the Ansys solver and build reusable chunk of software that can be easily applied to a wide range of case study.
Udf-manual contents

• Introduction
• DEFINE macros
• Additional macros
• Interpreted udf
• Compiled udf
• Hooking udf to fluent
• Parallel considerations
• Examples
• Appendix on c programming basic
C programming intro

Statement is every declaration, assignment, operation, initialization,…
Statements are identified with a semicolon:  \textit{statement;}\n
A group of statements is a block
Block are identified with curly brackets:  \{ \textit{statement-1;statement-2;…;} \}\n
Comments can be placed at any point in the program between:  \textit{/* …… */}\n
Variables:
\begin{itemize}
\item Local: defined within the body functions (use as many as you need)
\item Global: defined outside the body functions (limit as much as you can)
\end{itemize}
Mesh hierarchy

- node: mesh point
- node thread: grouping of nodes
- edge: boundary of a face (3D)
- face: boundary of a cell (2D or 3D)
- face thread: grouping of faces
- cell: control volume into which domain is broken up
- cell center: location where cell data is stored
- cell thread: grouping of cells
- domain: a grouping of node, face, and cell threads
Data type

Node
face_t
cell_t
Thread
Domain

Node is a structure data type that stores data associated with a mesh point.
face_t is an integer data type that identifies a particular face within a face thread.
cell_t is an integer data type that identifies a particular cell within a cell thread.
Thread is a structure data type that stores data that is common to the group of cells or faces
Domain is a structure data type that stores data associated with a collection of node, face, and cell threads
Compiled udf

[ponzini@lagrange ~]$ cd summer-casedata/Carotid/
[ponzini@lagrange Carotid]$ ls libudf3/
   lnamd64  Makefile  src
[ponzini@lagrange Carotid]$ ls libudf3/lnamd64/
   3ddp_host  3ddp_node
[ponzini@lagrange Carotid]$ ls libudf3/lnamd64/3ddp_node/
   flux_out.c  flux_out.o  libudf.so  makefile  makelog  udf_names.c  udf_names.o  vin_cca_fourier.c  vin_cca_fourier.o
[ponzini@lagrange Carotid]$ ls libudf3/lnamd64/3ddp_host/
   flux_out.c  flux_out.o  libudf.so  makefile  makelog  udf_names.c  udf_names.o  vin_cca_fourier.c  vin_cca_fourier.o
[ponzini@lagrange Carotid]$ ls libudf3/src/
   flux_out.c  makefile  vin_cca_fourier.c
[ponzini@lagrange Carotid]$ ls libudf3/src/
   flux_out.c  makefile  vin_cca_fourier.c
[ponzini@lagrange Carotid]$ more libudf3/src/makefile
Udf directories tree

- libudf3
  - makefile
  - src
  - lnamd64
    - 3d
    - 3ddp
    - 3ddp_node
Examples

1. Space/time BC via udf
2. Material properties via udf
3. Post-processing via udf
1. space/time boundary condition via udf

- define_profile: space/time dependent velocity
- f_profile: used together with define_profile
define_profile

```c
void define-profile(name,t,i)
```

Symbol `name`: name used to handle the udf into fluent as BC

`Thread *t`: pointer to a thread where the bc is set

`int i`: index to identify the variable to be set

Returning type: void

See `vinlet_cca.c` source file
&
`flux_out.c` source file
f_profile macro

F_PROFILE can be used to store a boundary condition in memory for a given face and thread, and is typically nested within a face loop. See mem.h for the complete macro definition for F_PROFILE

```c
void F_PROFILE( f, t, i)
face_t f
Thread *t
int i
```
2. non-Newtonian fluid properties via udf

\[ real \text{ DEFINE\_PROPERTY}\( (\text{name}, c, t) \) \]

**Symbol name:**

- `cell_t c`: cell index
- `Thread *t`: pointer to the cell thread on which we apply the property

**Returning type:** `real`

See ballyc.c source file
3. Post-processing via udf

User can export via udf values at certain cells for further processing of the data.
Usually used in hemodynamics to compute integral value of the WSS at the wall over the heart cycle or part of it.

See post4osi.c source file
References

• Ansys udf-manual
• “The C Programming Language”, Kernighan & Ritchie, 1988