Geometrical Multiscale Models for the Cardiovascular System - I
Reduced Models for the Circulation
Defective Boundary Data Problems (I)
Outline

• Why do we need (Geometrical) Multiscale Models?
  - Data Driven motivations
  - Physical motivations

• Basic Ingredients of “Multiscale” The Navier-Stokes Equations
  - 1D Models (Euler)
    • Numerical treatment
    • Modeling of curved pipes, bifurcation, etc.
  - Lumped Parameters Models
    • The single compartment
    • The heart
    • Networks

• Defective Boundary Data Problems (I)
Main References


Why do we need Multiscale Models?

Data Driven - between Theory and Practice

A patient-specific quantitative analysis requires
- Geometry
- Boundary conditions

Geometry: many techniques

Boundary conditions:

In practice, we never have all the data required by math theory and most of the time measures are accessible far from the region of interest
Why do we need Multiscale Models?

Physical Motivations: Vascular network is a robust system

Local blood dynamics is influenced by systemic factors
Systemic behavior is influenced by local features

Occlusions and stenoses (local scale) can change significantly the global circulation (upstream and downstream)

LOCAL AND SYSTEMIC DYNAMICS STRONGLY INTERACTING
Residual flow to brain in presence of a carotid occlusion

Residual flow for different occlusion degrees of the Communicating Arteries.

A vascular district is not a stand-alone system

In a patient-specific setting:

**for the Theory we need:**
many data (3 conditions in each fluid point + 3 conditions in each structure point at each instant)
Located at the boundary of the district of interest
Patient-specific

**for the Practice we have:**
Integral/average data
Not necessarily located at the boundary
Generally incomplete

Any filling of the lack of data must be
- Mathematically/Numerically consistent (=mitigate the impact of arbitrariness)
- Physically consistent (=include the systemic dynamics relevant to the local one)
Standard Pressure Conditions

Multiscale Model

Comparison

Standard vs. 1D-2D
The Vascular Multiscale Framework

Numerical modelling of the entire circulation as a full 3D model is not viable

✓ Prohibitive CPU costs
✓ Huge amount of data

Multiscale framework (Lect 1 & 2)
Surrogate Models
Couple Full and Surrogate Models

Surrogate Models: How?
Hierarchy of Models
Trade-off between simplicity and reliability

Coupling: from empirical to rigorous methods
filling the gap between two models
perform the numerical coupling (Tutorial 1)

Data Assimilation (Lect 3): How to complete the patient-specific picture
The Vascular Multiscale Framework (cont)

1D

0D

(Lumped Parameter Models)

2D/3D

A.V.
Models Hierarchy: 3D
(just for the sake of notation)

**BLOOD:**
Models for 3D(2D) domains are based on the incompressible (laminar) Navier-Stokes equations possibly with a non-Newton rheology

\[
\begin{align*}
\rho \frac{\partial \mathbf{u}}{\partial t} - \nabla \cdot \left( \mu \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \right) + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p &= \mathbf{f}, \\
\nabla \cdot \mathbf{u} &= 0
\end{align*}
\]

\[\mathbf{u}=\text{blood velocity, } p=\text{pressure, } \rho=\text{density, } \mu=\text{viscosity}\]

Equations must be completed with suitable matching conditions (green) between fluid and wall models, and boundary/initial conditions (magenta).

**WALL:**
Arterial wall is a complex multilayer structure
Different models can be considered:
from algebraic models (independent rings: radius linearly proportional to the pressure) up to differential viscoelastic ones

Data Driven Computations in the Life Sciences
A. Veneziani - Lecture 1: RM for Circulation
The complete FSI model (e.g. Fernandez)

\[ T_f(u, p) = -pI + \mu (\nabla u + \nabla u^T) \]

\[
\begin{align*}
T_f(u, p) &= k_1 F F^T + k_2 (I - 1)e^{\gamma(I-1)^2} (Fm) \otimes (Fm) \\
m &\equiv \text{unit vector of collagen direction} \\
I &\equiv m^T F^T F m \\
\tilde{T} &= T \text{ mapped to the reference domain} \\
F &\equiv \nabla \xi \text{ deformation tensor}
\end{align*}
\]

\[
\begin{align*}
\rho_f \frac{\partial u}{\partial t} + \rho_f (u \cdot \nabla) u - \nabla \cdot T_f(u, p) &= f_f \\
\nabla \cdot u &= 0 \\
u &= \frac{\partial \eta}{\partial t} \\
T_s(\eta) n - T_f(u, p) n &= 0 \\
\rho_s \frac{\partial^2 \tilde{\eta}}{\partial t^2} - \nabla \cdot \tilde{T}_s(\tilde{\eta}) &= f_s
\end{align*}
\]

in \( \Omega_f \),

in \( \Omega_f \),

on \( \Sigma \),

on \( \Sigma \),

in \( \tilde{\Omega}_s \).
Remarks

1. **Membrane models for the structure**
   In some cases it is reasonable to approximate the structure with a membrane (constant thickness) and include only radial displacements

2. **Boundary Conditions**
   We did not specify b.c. for
   - Inflow
   - Outflow
   - External surface of the structure
   A typical stand-alone choice:
     - Inflow: Dirichlet (velocity, displacement)
     - Outflow: Neumann (tractions)
   For the external surface we should include the surrounding tissues

3. **Parameter Estimation**
   All the parameters need to be estimated (Lect 3)
Models Hierarchy: 1D

Exploiting the **cylindrical geometry of arterial segments**, suitable **averages of the axial momentum equation and of the mass conservation** can be carried out over the axial section, yielding the following equations (Euler, 1775) for each segment:

\[
\begin{align*}
\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial z} &= 0 \\
\frac{\partial Q}{\partial t} + \alpha \frac{\partial}{\partial z} \left( \frac{Q^2}{A} \right) + A \frac{\partial P}{\partial z} + K_R \frac{Q}{A} &= 0 \\
P - P_0 &= \Psi(A)
\end{align*}
\]

- **\( Q \)** = flow rate, **\( A \)** = section area
- **\( P \)** = section average of the pressure
- **\( K_R \)** = friction coefficient
- **\( \Psi \)** = vessel wall law
- **\( \beta \)** = wall parameters
- **\( A_0 \)** = rest area
- **\( \alpha \)** = Coriolis coefficient

Simple example: \( \psi(A; A_0, \beta_0) = \beta_0 \frac{\sqrt{A} - \sqrt{A_0}}{A_0} \)

See e.g. Peiro’, Veneziani 2009
Single Segment

Assumptions
- Fixed rectilinear axis
- Circular centerline
- Only radial displacement
- No dependence on circumferential coordinate
- Viscous resistance proportional to the flow rate (Poiseuille)
- Constant pressure over each section
- Structure is a membrane with constant thickness
- Axial velocity is dominant

\[
\begin{align*}
\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial z} &= 0 \\
\frac{\partial Q}{\partial t} + \alpha \frac{\partial}{\partial z} \left( \frac{Q^2}{A} \right) + \frac{A}{\rho} \frac{\partial P}{\partial z} + K_R \frac{Q}{A} &= 0 \\
P - P_0 &= \Psi(A)
\end{align*}
\]

\[
\begin{align*}
Q(t, z) &\equiv \rho_f \int_S u_z ds \\
A(t, z) &\equiv |S(t, z)| = \int_S ds \\
P &\equiv A^{-1} \int_S p ds \\
\tilde{u} &\equiv A^{-1} \int_S u_z ds \\
\Rightarrow Q &= \rho_f A \tilde{u}
\end{align*}
\]
The final 1D model (two possible formulations)

**Quasi-Linear form:**
\[
\frac{\partial}{\partial t} \mathbf{U} + H(\mathbf{U}) \frac{\partial \mathbf{U}}{\partial z} + B(\mathbf{U}) = 0, \\
\mathbf{U} = \begin{bmatrix} A \\ Q \end{bmatrix}
\]

where

\[
H(\mathbf{U}) = \begin{bmatrix} 0 & 1 \\ \frac{A}{\rho} \frac{\partial \psi}{\partial A} - \alpha \bar{u}^2 & 2\alpha \bar{u} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ c_1^2 - \alpha \left( \frac{Q}{A} \right)^2 & 2\alpha \frac{Q}{A} \end{bmatrix}
\]

\[
B(\mathbf{U}) = \begin{bmatrix} 0 \\ K_R \left( \frac{Q}{A} \right) + \frac{A}{\rho} \frac{\partial \psi}{\partial A} \frac{dA_0}{dz} + \frac{A}{\rho} \frac{\partial \psi}{\partial \beta} \frac{d\beta}{dz} \end{bmatrix}
\]

\[
e_1 = \sqrt{\frac{A \frac{\partial \psi}{\rho_f \partial A}}}
\]

**Conservative form:**
\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial}{\partial z} F(\mathbf{U}) + S(\mathbf{U}) = 0
\]

\[
F(\mathbf{U}) = \begin{bmatrix} Q \\ \alpha \frac{Q^2}{A} + C_1 \end{bmatrix}
\]
Analysis of the Model

Eigenvalues of $H$: $\lambda_{1,2} = \alpha \bar{u} \pm c_\alpha$ with $c_\alpha = \sqrt{c_1^2 + \bar{u}^2 \alpha (\alpha - 1)}$

The Coriolis coefficient $\alpha$ is $\geq 1$ and depends on the “average” velocity profile postulated.

- For a flat profile $\alpha = 1$
- For a parabolic profile $\alpha = 4/3$

If $A \geq 0$ we have two real eigenvalues (hyperbolic system)
If $A > 0$ the two eigenvalues are distinct (strictly hyperbolic system)
If $c_1 \gg \alpha \bar{u}$ then $\lambda_1 \lambda_2 < 0$

It is reasonable to assume $\alpha = 1$.
For the simplest pressure-area law, $c_1$ reads

$$c_1 = \sqrt{\frac{\beta_0 \sqrt{A}}{2 \rho_f A_0}}$$

The system admits two characteristic variables
Characteristic Variables (I)

Denote by $l$ and $r$ the left and right eigenvectors of $H$ respectively, s.t.

$$H = R \Lambda L$$

$$L = \begin{bmatrix} l_1^T \\ l_2^T \end{bmatrix}, \quad R = \begin{bmatrix} r_1 & r_2 \end{bmatrix}, \quad \Lambda = \text{diag}(\lambda_1, \lambda_2) = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}.$$  

Suppose now that the differential forms

$$\partial W_1 = l_{1,1} \partial A + l_{1,2} \partial Q \quad \partial W_2 = l_{2,1} \partial A + l_{2,2} \partial Q$$

are exact, so that

$$\frac{\partial W_1}{\partial U} = l_1, \quad \frac{\partial W_2}{\partial U} = l_2.$$
By multiplying the system by $L$, we reformulate a system in $W_i$, where the dependence on the transport term is diagonalized:

\[
\begin{aligned}
\frac{\partial W_1}{\partial t} + \lambda_1 \frac{\partial W_1}{\partial z} + G_1 &= 0 \\
\frac{\partial W_2}{\partial t} + \lambda_2 \frac{\partial W_2}{\partial z} + G_2 &= 0
\end{aligned}
\]

\[G_i = G_i(W_1, W_2)\]

If we introduce the characteristic lines as the solution of the equations

\[\frac{dz_i}{dt} = \lambda_i(U(t, z_i)), \quad z_i(0) = \bar{z}_i, \quad t > 0 \quad i = 1, 2\]

for a generic initial condition.

Along these lines, we can write:

\[\partial_t W_i + \lambda_i \partial_z W_i = \frac{dW_i}{dt}\bigg|_{z=z_i(t)}\]
Along these lines, the original system becomes ODEs and it reads

\[
\frac{dW_i(t, z_i(t))}{dt} + G_i(W_1, W_2) = 0, \quad i = 1, 2
\]

Notice that the sign of \( \lambda_i \) is governing the direction of propagation of \( W_i \)

\( \lambda_1 > 0 \) \( \Rightarrow \) \( W_1 \) propagates forward \( W_1 \)

\( \lambda_2 < 0 \) \( \Rightarrow \) \( W_2 \) propagates backward \( W_2 \)

\( W_i \) are called characteristic variables

If \( G_i = 0 \), then the characteristic variables are constant along the characteristic lines

In this case the system is decoupled

(However the bc still couple the two characteristic variables)

Along the characteristic the system can be solved as ODE
Characteristic Variables (II)

If $\alpha = 1$, for the algebraic linear pressure-radius relationship the characteristics read

\[
W_1 = \bar{u} + 4 (c_1 - c_{1,0}) \\
W_2 = \bar{u} - 4 (c_1 - c_{1,0})
\]

These can be rewritten as:

\[
W_1 = \bar{u} + \frac{2(P - P_{ext})}{\rho_f (c_1 + c_{1,0})}, \quad W_2 = \bar{u} - \frac{2(P - P_{ext})}{\rho_f (c_1 + c_{1,0})}
\]

and expliciting the physical variables:

\[
A = \left( \frac{2\rho_f A_0}{\beta} \left( \frac{W_1 - W_2}{8} + c_{1,0} \right) \right), \quad Q = A \frac{W_1 + W_2}{2}
\]

$c_{1,0}$ is the speed of sound $c_1$ for the reference area $A_0$ (function of $z$)
Boundary Conditions

As for first order hyperbolic systems, we have to impose exactly one boundary condition at both $z = 0$ and $z = L$. The main types of boundary conditions for our problem are the following.

Non-reflecting Conditions (distal ends)

Non reflecting boundary conditions prescribe only what enters the segment

$$W_1(z = 0) = \text{data}, \quad W_2(z = L) = \text{data}.$$

For a distal end with no reflections (semi-infinite pipe), we prescribe

$$W_2(L) = 0$$

Problem: the characteristic is not a physical quantity – you do not measure it!

To prescribe this condition we need infos from both the physical variables
Reflecting Conditions

A physical reflection is generally function of the outgoing characteristic. A reasonable approach is to introduce a reflection factor $R_t$ such that $0 \leq R_t \leq 1$ with the (distal) condition

$$W_2 = -R_t W_1 + (1 - R_t)W_{2,0} \text{ at } z = L$$

For $R_t = 1$ we have a complete reflection.
For $R_t = 0$ we have the non-reflecting condition $W_2 = \text{const} = W_{2,0}$.

Physical Conditions

Quite often at the proximal end one would prescribe physical variables (pressure or flow rate).

A way of doing that consistently with the hyperbolic nature of the problem at hand is to convert conditions on physical variables into conditions on the characteristic ones.
Numerical Approximation

Taylor-Galerkin scheme (2\textsuperscript{nd} order) \hspace{1cm} Lax-Wendroff FE scheme

\[
(U_{h}^{n+1}, \psi_{h}) = (U_{h}^{n}, \psi_{h}) + \Delta t \left( F_{LW}(U_{h}^{n}), \frac{d\psi_{h}}{dz} \right) - \frac{\Delta t^2}{2} \left( B_{U}(U_{h}^{n}) \frac{\partial F(U_{h}^{n})}{\partial z}, \psi_{h} \right) - \frac{\Delta t^2}{2} \left( H(U_{h}^{n}) \frac{\partial F}{\partial z}(U_{h}^{n}), \frac{d\psi_{h}}{dz} \right) - \Delta t (B_{LW}(U_{h}^{n}), \psi_{h}) \quad \forall \psi_{h} \in V_{h}^{0}
\]

where \( F_{LW}(U) = F(U) - \frac{\Delta t}{2} H(U)B(U) \), \( B_{LW}(U) = B(U) + \frac{\Delta t}{2} B_{U}(U)B(U) \)

Explicit time advancing method.

Stability CFL restriction:

\[
\Delta t \leq \frac{\sqrt{3}}{3} \min_{0 \leq i \leq N} \left[ \frac{h_{i}}{\max_{k=i}^{i+1} (c_{\alpha,k} + |\bar{u}_{k}|)} \right]
\]

The stability requires the introduction of a numerical viscosity, The numerical viscosity actually affects the nature of the problem (hyperbolic→parabolic)
Compatibility Conditions

The given boundary condition is not sufficient to provide all data to close the system at numerical level (2nd order term for stability reasons).

We need find other conditions which have to derive directly from the differential equation at hand.

A possible approach is the so-called characteristic extrapolation technique.

For the sake of simplicity, consider the case \( z = 0 \) and the given condition \( W_1 = g \).

We assume also \( B(U) = 0 \)

At the numerical level, we need another condition, for instance on \( W_2 \). A value for \( W_2 \) can be obtained by moving along the (second) characteristic line:

\[
W_2^{n+1} \approx W_2^n (\lambda_2^n(z = 0)\Delta t)
\]
“Psychologically 1D Models” for Curved Pipes

The set up and the analysis of simple minded (psychologically 1D) models for curved pipes is ongoing. Two possible approaches

**Perturbation theory (after Dean, 1928):**
The model is based on a reference solution. The equations in curved pipes deal with a perturbation of such solution.

**Hierarchical theory (after Green, Naghdii, 1993):**
The solution is regarded as a combination of (polynomial) basis functions (Cosserat direct theory).
Models deal with the coefficients of the expansion of the solution with respect to the selected basis.

**Hierarchical Model Reduction (HiMod - Ern, Perotto, Veneziani, 2009)**
Approach based on diverse numerical discretizations. It can be combined with IsoGeometric Analysis (A. Reali) – see Workshop
A simple example in curved (plane) pipes

Assumptions

\[ u_s = \left( 1 - \frac{x^2 + y^2}{R^2} \right) \left( a(s, t) + b(s, t)x + c(s, t)y \right) \]

\[ u_x = \hat{n}x / R, \quad u_y = \hat{n}y / R, \text{ where } \hat{n} \text{ is the wall velocity.} \]

Convenient set of unknowns:

\[ A \equiv \pi R^2, \quad Q \equiv \frac{\pi}{2} R^2 a, \quad H \equiv \frac{\pi}{12} R^4 b, \quad G \equiv \frac{\pi}{12} R^4 c. \]

The four needed equations are obtained by taking the average of the continuity and axial momentum equations and the weighted averages

\[ P_{11}(\cdot) \equiv \int_S \int \sqrt{g} \cdot d\hat{x}d\hat{y}, \]

\[ P_{21}(\cdot) \equiv \int_S \int \sqrt{g} \cdot \hat{x}d\hat{x}d\hat{y}, \quad P_{22}(\cdot) \equiv \int_S \int \sqrt{g} \cdot \hat{y}d\hat{x}d\hat{y} \]

of the axial momentum equation.

\[ \sqrt{g} = (\hat{y} + R_C) / \hat{y} \]

is the metric tensor invariant.
Resulting equations

\[
\begin{align*}
\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial s} &= 0 \\
\frac{\partial Q}{\partial t} + \frac{1}{R_C} \frac{\partial G}{\partial t} + \frac{4}{3} \frac{\partial}{\partial s} \frac{Q^2}{A} + 6\pi \frac{\partial s}{\partial A} \frac{H^2}{A^2} + \frac{\beta \sqrt{A}}{2\rho A_0} \frac{\partial A}{\partial s} + 8\pi \nu \frac{Q}{A} + \frac{24\pi \nu}{R_C} \frac{G}{A} &= 0 \\
\frac{\partial H}{\partial t} + 2 \frac{\partial}{\partial s} \frac{H Q}{A} + \frac{1}{2} \frac{H}{A} \frac{\partial Q}{\partial s} + 24\pi \nu \frac{H}{A} &= 0 \\
\frac{\partial G}{\partial t} + \frac{1}{6\pi R_C} \frac{\partial Q A}{\partial t} + 2 \frac{\partial}{\partial s} \frac{G Q}{A} + \frac{G}{2A} \frac{\partial Q}{\partial s} + \frac{\hat{\beta}}{A^{3/2}} \frac{\partial A}{\partial s} + 24\pi \nu \frac{G}{A} + \hat{\nu} Q &= 0
\end{align*}
\]

where \( \hat{\beta} := \beta/(8\pi \rho A_0 R_C), \hat{\nu} := 3\nu/R_C. \)

More complex models can be devised, accounting e.g. for a more complex profile for the transversal components of velocity.

D. Lamponi, PhD Thesis, EPF Lausanne, 2004
**Branching**

A domain decomposition approach:

We prescribe:

- **Flux continuity:** \( Q_1 = Q_2 + Q_3 \)
- **Total pressure continuity:** \( P_{t,1} = P_{t,2} = P_{t,3} \)

Under some additional hypothesis (usually verified in practice) these conditions assure that the coupled problem satisfies a stability condition akin to that of the single artery model.

In principle, it is possible to *account for the bifurcation angle*. In practice, this has a minor impact on numerical results.
The solution is obtained iteratively, looping on the branches
A COMPLEX EXAMPLE: REPRESENTATIONS OF THE WILLIS CIRCLE

*T. Passerini, M.R. De Luca, A.V.
THE SYMMETRIC CASE
THE SYMMETRIC CASE

Time = 0.880000 s
RIGHT CAROTID COMPRESSION TEST
RIGHT CAROTID COMPRESSION TEST

Data Driven Computations in the Life Sciences
A. Veneziani - Lecture 1: RM for Circulation
PCA MISSING (16% PATIENTS)
<table>
<thead>
<tr>
<th></th>
<th>ACA [%]</th>
<th>MCA [%]</th>
<th>PCA [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symmetric</td>
<td>20.77</td>
<td>44.92</td>
<td>34.31</td>
</tr>
<tr>
<td>PCA Missing</td>
<td>20.62</td>
<td>44.57</td>
<td>34.81</td>
</tr>
</tbody>
</table>
CAROTID COMPRESSION ON A PATIENT WITH NO PCA
CAROTID COMPRESSION ON A PATIENT WITH NO PCA

Data Driven Computations in the Life Sciences
A. Veneziani - Lecture 1: RM for Circulation
Fig. 1. Unique vascular anatomy of the ADAN model comprising: 1598 named arteries, 544 perforator vessels, blood supply to 28 specific organs, and to 116 vascular territories.

P.J. Blanco et al. ADAN Network
An Anatomically Detailed Arterial Network Model for One-Dimensional Computational Hemodynamics
IEEE Trans Biomed Eng 2015
Lumped Parameter Models

Subdivide the cardiovascular system in elementary components (compartments) where pressure and flow status is described by a very limited number of parameters. Their evolution is governed by ordinary differential or algebraic equations.

Couple the compartments together by employing basic physical laws. The number of compartments may differ by the detail required.

We will consider 2 examples of compartments

• an artery (by averaging 1D equations)
• the heart

To be coupled together
Lumped Parameter Models for an Arterial Segment

Taking also the **longitudinal average along each arterial segment**, we obtain a LUMPED PARAMETER description

\[
\begin{cases}
\frac{dy}{dt} = A(y, z, t) + b(t) \\
G(y, z, t) = 0.
\end{cases}
\]

An analogy with electrical circuits can be exploited for representing the system:

<table>
<thead>
<tr>
<th>HYDRAULIC</th>
<th>Pressure</th>
<th>Flow rate</th>
<th>Blood viscosity</th>
<th>Blood inertia</th>
<th>Compliance</th>
</tr>
</thead>
<tbody>
<tr>
<td>ELECTRIC</td>
<td>Voltage</td>
<td>Current</td>
<td>Resistance</td>
<td>Inductance</td>
<td>Capacitance</td>
</tr>
</tbody>
</table>
\[ \hat{Q} = \frac{1}{l} \int_{\Gamma} u_z d\nu = \frac{1}{l} \int_{0}^{l} \int_{A(z)} u_z d\sigma dz = \frac{1}{l} \int_{0}^{l} Q dz \]

\[ \hat{p} = \frac{1}{l} \int_{0}^{l} P dz \]

Cylindrical pipe of length \( l \), \( \Gamma_1 \) proximal section, \( \Gamma_2 \) distal section.

\[
\begin{align*}
\frac{C}{L} \frac{d\hat{p}}{dt} + Q_2 - Q_1 &= 0 \\
L \frac{d\hat{Q}}{dt} + R \hat{Q} + P_2 - P_1 &= 0.
\end{align*}
\]

(assuming a parabolic velocity profile)

- \( R := \frac{\rho K_R l}{A_0^2} = \frac{8\pi \rho \nu l}{\pi^2 R_0^4} = \frac{8\mu l}{\pi R_0^4} \)

- \( L := \frac{\rho l}{A_0} = \frac{\rho l}{\pi R_0^2} \)

- \( C := kl = \frac{3\pi R_0^3 l}{2Eh} \)
$P_1$ and the flow rate $Q_2$ prescribed $\implies$ we pose $\hat{p} \approx P_2$, $\hat{Q} \approx Q_1$ $\implies$

\[ \begin{cases} 
C \frac{dP_2}{dt} - Q_1 = Q_2 \\
L \frac{dQ_1}{dt} + RQ_1 + P_2 = P_1
\end{cases} \]

Other networks ($\pi$ and $T$) can be obtained by combining the previous ones.
Lumped Model for the Heart

The heart is a special compartment of the vascular system that needs a specific representation. Exploit some basic mechanics laws like the "Poisson Law" for a spherical container:

\[ V(t) = C(t)(P - P_{ext}) + V_0(t) \]

Heart valves are represented by diodes. Mathematically, their behaviour is described either by a two-state model:

\[ Q = 0 \quad \text{if} \quad \Delta P < 0 \quad \Delta P = 0 \quad \text{if} \quad Q > 0 \]

or by a function of the type:

Time dependent compliance:

\[ Q = Q_0(e^{\beta \Delta P} - 1) \]
Networks of LPM

Branching is handled by imposing continuity of mass flux and pressure, which corresponds to the well known Kirchoff laws for electric circuits.
We have a non-linear **Differential-Algebraic-Equation** (DAE) system

\[
\begin{aligned}
\frac{dy}{dt} &= B(y, z, t) \quad t \in (0, T] \\
G(y, z) &= 0
\end{aligned}
\]

together with the *initial condition vector* \( y_0 \). \( y \) is the vector of the state variables, \( z \) are other variables of the network and \( G \) the algebraic equations that derive from the Kirchhoff laws.

If \( \det \left( \frac{\partial G}{\partial z} \right) \neq 0 \) by the *implicit function theorem* we have

\[
\begin{aligned}
\frac{dy}{dt} &= \Phi(y, t) = A(y, t)y + r(t) \quad t \in (0, T] \\
y(t = t_0) &= y_0.
\end{aligned}
\]
Numerical Treatment of “Defective” Boundary Conditions in 3D Problems

Data (mis)matching:

“Simple Minded” models compute average data over the interface section/compartment.

Navier-Stokes equations require pointwise data.

HOW IS IT POSSIBLE TO FILL THE GAP?
Defective Boundary Data Problems

Navier-Stokes Equations

\[ \frac{\partial}{\partial t} \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p - \nu \Delta \mathbf{u} = \mathbf{f}, \quad t > 0 \]
\[ \text{div}(\mathbf{u}) = 0, \quad t > 0 \]
\[ \mathbf{u} = \mathbf{u}_0, \quad t = 0, \]

supplemented by homogeneous boundary conditions on \( \Gamma_{\text{wall}} \),
(assuming for the sake of simplicity that the walls are rigid),

On \( \Gamma_i \) we will consider:
1. mean pressure problem
2. mean flow rate problem
Mean pressure problem

Boundary data:

$$\frac{1}{\text{meas}(\Gamma_i)} \int_{\Gamma_i} p(t) \, ds = P_i(t), \quad i = 0, \ldots, n,$$

Possible approach (Heywood, Rannacher, Turek, 1996): to find a variational formulation of the problem including the boundary data as natural boundary conditions. The variational formulation will introduce other (natural and homogeneous) conditions that will fill the gap.

Let $V$ be the Sobolev space $H^1_\Gamma(\Omega)$ and $M$ the space $L^2(\Omega)$. 
Variational formulation

Find \( u \in V \) and \( p \in M \) s.t. \( \forall v \in V \) and \( q \in M \)

\[
\begin{cases}
(u_t, v) + c(u, u, v) + a(u, v) + b(p, v) = (f, v) - \sum_{j=1}^{N} P_j \int_{\Gamma_j} v \cdot n \\
b(q, u) = 0
\end{cases}
\]

with the given i.c. and obvious notation. In particular

\[
a(u, v) \equiv \mu \int (\nabla u + \nabla u^T) : \nabla v, \quad b(q, v) \equiv -\int q \nabla \cdot v
\]

Conditions prescribed actually

\[
p - \mu n^T (\nabla u + \nabla u^T) n_{\Gamma_j} = P_j \text{ (constant on } \Gamma_j) \\
(\nabla u + \nabla u^T) n_{\Gamma_j} - [n^T (\nabla u + \nabla u^T) n] n_{\Gamma_j} = 0
\]
The condition is not “perfect” for artificial boundary: it actually assumes an open boundary.
It has been noted by Heywood and Turek that the technical problem is from the transpose of the velocity gradient.

This term is usually discarded in the applications since it disappears in the strong from of the NSE. However, in the weak formulation it should stay.

Alternative: if we expect the boundary to feature a fully developed flow one can prescribe zero tangential velocity.
This eliminates the spurious effects also with the correct weak formulation
See Tutorial 1.
Mean flow rate problem

Suppose that the flow rates are prescribed over the artificial (red) sections:

\[ \int_{\Gamma_i} \mathbf{u} \cdot \mathbf{n} d\gamma = Q_i \quad (*) \]

For the rigid case, compatibility condition on the data:

\[ Q_0 = - \sum_{i=1}^{n} Q_i. \]

A first (practical) solution:

1. select a velocity profile (e.g. a parabolic one)
2. Tune up the profile for the fulfillment of (*): Dirichlet conditions.

This is strongly perturbative for the solution: spurious boundary effects reduced by extending the computational domain (FLOW EXTENSIONS).
A Second Approach: HRT

Give a suitable variational formulation to the problem

1. \( V^* = \left\{ \mathbf{v} \in H^1_{\Gamma_D}, \text{s.t.} \int_{\Gamma_i} \mathbf{v} \cdot \mathbf{n} = 0, \ i = 0, 1, \ldots, n \right\} \),

2. \( \mathbf{b}_i \in V, \ i = 1, \ldots, n \) such that:

\[
\nabla \cdot \mathbf{b}_i = 0, \ \int_{\Gamma_0} \mathbf{b}_i \cdot \mathbf{n} \, ds = -1, \ \int_{\Gamma_j} \mathbf{b}_i \cdot \mathbf{n} \, ds = \delta_{ij},
\]

where \( \delta_{ij} \) is the Kroenecker symbol.

\( \mathbf{b}_i \) are called flux-carriers.

3. \( a(\mathbf{v}, \mathbf{w}) = \int_{\Omega} \mu \nabla \mathbf{v} \cdot \nabla \mathbf{w} \, d\omega, \ (\mathbf{v}, \mathbf{w}) = \int_{\Omega} \mathbf{v} \cdot \mathbf{w} \, d\omega. \)
Weak formulation of the flux problem:

**PROBLEM**
Given \( f \in L^2(0, T; L^2(\Omega)) \) and \( u_0 \in V \), find \( u = w + \sum_{i=1}^{n} Q_i b_i \), with \( w \in V^* \) and \( p \in L^2(\Omega) \) such that for all \( v \in V^* \) and \( q \in L^2(\Omega) \)

\[
\begin{cases}
\left( \frac{\partial u}{\partial t} + u \cdot \nabla u, v \right) + a(u, v) - (p, \nabla \cdot v) = (f, v), \\
(q, \nabla \cdot u) = 0,
\end{cases}
\]

for all \( t > 0 \), with \( u = u_0 \) for \( t = 0 \). □

**PROPOSITION (V. 1998)**
The implicit “do-nothing” conditions associated to this formulation are:

\[
(p - \nu \partial_n u_n) |_{\Gamma_i} = C_i, \quad \partial_n u_\tau |_{\Gamma_i} = 0, \quad \text{for } i = 0, \ldots, n,
\]

where \( C_0 \) is an arbitrary function of time and the \( C_i \)’s \( (i = 1, \ldots, n) \) are unknown functions of time (and constant in space).

**Drawback of this approach for the flux problem**: numerical discretization of \( V^* \).
Third Approach: augmented reformulation

(Formaggia, Gerbeau, Nobile, Quarteroni, 2001 for the steady case
Venezianini, Vergara, 2004, 2007 for the unsteady case)

Basic idea: Flux conditions (*) regarded as a constraint on the solution to be forced with a Lagrange multiplier approach.

**Problem**
Given \( f \in L^2(0, T; L^2(\Omega)) \) and \( u_0 \in V \), find \( u \), and \( p \in L^2(\Omega) \) such that for all \( v \in V \) and \( q \in L^2(\Omega) \)

\[
\begin{cases}
\left( \frac{\partial u}{\partial t} + u \cdot \nabla u, v \right) + a(u, v) - \left( p, \nabla \cdot v \right) + \sum_{i=1}^{n} \lambda_i \int_{\Gamma_i} v \cdot n \, ds = (f, v), \\
(q, \nabla \cdot u) = 0, \\
\int_{\Gamma_i} u \cdot n \, ds = Q_i, \quad i = 1, \ldots, n,
\end{cases}
\]

for all \( t > 0 \), with \( u = u_0 \) for \( t = 0 \).

It is possible to prove that this solution is the same as for the HRT approach with \( C_1 = \lambda_i \).
Numerical Treatment of the Augmented Problem

**Major drawbacks of the augmented formulation:**

1. solution of a larger problem (see Tutorial 1);
2. non-standard Navier-Stokes solver required.

**Tasks:**

1. devise a numerical scheme for the separate computation of velocity/pressure and Lagrange multipliers;
2. recast the computation of velocity/pressure computation in the form of a “standard” Navier-Stokes problem (to be solved with standard solvers).

**Two possible schemes:**

1. a “fixed-point” formulation (not needed for steady problems);
2. Schur complement scheme.

Let us focus on the second one
Schur complement scheme

Discretized (and linearized) augmented problem reads:

\[
\begin{bmatrix}
S & \tilde{\Phi}^t \\
\tilde{\Phi} & 0
\end{bmatrix}
\begin{bmatrix}
X^{n+1} \\
\Lambda^{n+1}
\end{bmatrix} =
\begin{bmatrix}
\tilde{F}^{n+1} \\
\mathbf{Q}^{n+1}
\end{bmatrix}
\]

\[S = \begin{bmatrix}
K & C^t \\
C & 0
\end{bmatrix}\]

is the matrix associated to the NS eqns, \(\tilde{F}^{n+1} = [f^{n+1}, 0]^T\) the associated forcing term;

\[\tilde{\Phi} = \begin{bmatrix}
\Phi & 0
\end{bmatrix}\]

is the matrix associated to the terms \(\int_{\Gamma_i} \mathbf{v} \cdot \mathbf{n} d\sigma\).

\(X = [U \quad P]^t\) nodal vectors of velocity/pressure, \(\Lambda\) Lagrange multipliers vector.

If the LBB condition holds, \(S\) is nonsingular and we can reduce the system:

\[\tilde{\Phi}S^{-1}\tilde{\Phi}^t\Lambda^{n+1} = \tilde{\Phi}S^{-1}\tilde{F}^{n+1} - \mathbf{Q}^{n+1}\]

Matrix \(R = \tilde{\Phi}S^{-1}\tilde{\Phi}^t\) is the Schur complement associated to the system.

This matrix can be solved by a GMRes method. At each iteration a NS problem in \(S\) has to be solved.

\[\Rightarrow\] Convergence in (at most) \(n\) iterations (small number), entailing \(n + 1\) NS "standard" solutions.
... even better (Munch, Veneziani, Villa 2015)

Take advantage of the Trilinos multiple right hand side solver

\[
\begin{cases}
SX_b = \tilde{F} \\
-\tilde{\Phi} S^{-1} \tilde{\Phi}^T \Lambda = \tilde{\Phi} X - Q \quad (k \times k) \\
SX = SX_b - \tilde{\Phi}^T \Lambda = \tilde{F} - \tilde{\Phi}^T \Lambda
\end{cases}
\]

“Smart” reformulation:
- do not use iterative solvers for the Schur complement (\(k\) iterations)
- multiple rhs solvers (magic of Trilinos)

\[
S \begin{bmatrix} X_b & Y \end{bmatrix} = \begin{bmatrix} \tilde{F} & \tilde{\Phi}^T \end{bmatrix} \quad (k + 1) \text{ solves}
\]

\[
\Lambda = \left( \tilde{\Phi} Y \right)^{-1} \left( \tilde{\Phi} X_b - Q \right), \quad X = X_b - Y \Lambda
\]

Small system
Numerical Results

Validation of the augmented approach: Poiseuille and Womersley solutions (solid) recovered by solving the augmented problem (dots)

<table>
<thead>
<tr>
<th>Errors (Womersley)</th>
<th>$h = 1/16$</th>
<th>$h = 1/32$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t = 0.001$</td>
<td>$1.043 \cdot 10^{-4}$</td>
<td>$1.211 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$\Delta t = 0.0005$</td>
<td>$4.063 \cdot 10^{-5}$</td>
<td>$3.679 \cdot 10^{-5}$</td>
</tr>
</tbody>
</table>
Data Driven Computations in the Life Sciences
A. Veneziani - Lecture 1: RM for Circulation
Remarks

1. Different formulation for the Navier-Stokes equations can be exploited, yielding different homogeneous natural conditions. For instance, if the viscous term is reformulated in terms of the curl operator, total pressure conditions are naturally associated.

2. Although in principle possible also for mean pressure conditions, the Lagrangian multiplier approach is inaccurate, because the additional conditions imply a constant velocity on the artificial sections.

3. Other approaches can be used - see next Lecture

4. Approximate techniques for the Lagrangian multiplier approach (fixed point for unsteady problems) are available with a (sometimes significant) reduction in computational costs.
Left: pressure in a 2D anastomosis computed with an inexact Lagrangian multiplier approach. Right: Absolute error introduced by the scheme. (V., Vergara, An approximate method for solving the incompressible Navier-Stokes problems with flow rate bc’s, CMAME 2007)

<table>
<thead>
<tr>
<th>Test Case</th>
<th>Exact</th>
<th>Inexact</th>
<th>CPUin/CPUex</th>
</tr>
</thead>
<tbody>
<tr>
<td>Womersley</td>
<td>10 min 31s</td>
<td>5 min 46 s</td>
<td>0.55</td>
</tr>
<tr>
<td>Anastomosis with 1 inlet</td>
<td>7 min 58s</td>
<td>4 min 27 s</td>
<td>0.56</td>
</tr>
<tr>
<td>Anastomosis with 2 inlets</td>
<td>11 min 3 s</td>
<td>4 min 33 s</td>
<td>0.41</td>
</tr>
</tbody>
</table>

CPU times for different test cases of the original and inexact Lagrangian multiplier approaches.