Nektar1D Reference Manual

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1 Introduction

Nektar1D is our in-house computer code designed to solve the nonlinear, one-dimensional (1-D) equations of blood flow in a given network of compliant vessels subject to specified boundary and initial conditions. Nektar1D computes blood pressure, blood flow and luminal area waveforms at any point within the arterial network. It plays a crucial role in our research activities, which are detailed on our group's website: `www.haemod.uk`.

This document explains how to compile Nektar1D (Section 2), create a text file containing the input data for a specific simulation (Section 3), run the input file (Section 4), and interpret the output files containing the simulation results (Section 5). It also provides examples of Nektar1D simulations used in our peer-reviewed publications (Section 6) and includes a brief overview of the source code structure (Section 7).

For a review of arterial pulse wave haemodynamics and an explanation of the 1-D equations, we refer to [1]. The numerical scheme used in Nektar1D to solve these equations is detailed in [2]. We have verified the accuracy of the 1-D formulation by comparing it with (i) experimental data from a 1:1 scale cardiovascular simulator rig of the aorta and its major branches, made from silicone tubes [3], (ii) *in vivo* data from humans [4, 5] and rabbits [6], and (iii) numerical data obtained by solving the full 3-D equations of blood flow in compliant vessels [7, 4, 8, 9, 10] (see here for further details). In addition, we have developed pulse wave analysis tools for calibrating pulse wave models (see here for details) and understanding the physical mechanisms underlying the simulated pulse waveforms (see here for details).

We have used Nektar1D to generate populations of thousands of virtual subjects for *in silico* evaluation of pulse wave indices and algorithms [11, 12, 13, 14] (see here for further details). Nektar1D has also been applied in several clinically relevant studies, as described here.

Recently, Nektar1D was coupled to a 3-D cardiac electromechanics model, enabling the study of the effects of pulse wave propagation on cardiac function [15].

We welcome any comments or suggestions for improvements to both this document and Nektar1D. Please send feedback to `jordi.alastruey-arimon@kcl.ac.uk` .

2 Compiling Nektar1D

The easiest way to compile Nektar1D is on Ubuntu 20.04.5 (https://releases.ubuntu.com/20.04.5/). To compile the code, the `g++` and `gfortran` compilers should be installed (they typically come pre-installed with the Linux distribution). Otherwise, they can be installed by entering the following commands:

```
sudo apt-get install g++
sudo apt-get install gfortran
```

The code requires the compilation of two libraries located in `/Hlib` and `/Veclib`, as well as the source code in `1DBio/src`. All makefiles assume that the `make` utility is available and that the following symbolic links have been created:

```
ln -s ../Makefile Makefile       in nektar/Hlib/Linux
ln -s ../MakeHybrid MakeHybrid   in nektar/Hlib/Linux
ln -s GCC.inc Linux.inc          in nektar/Flags
```

The following tools also need to be installed:

- The Yacc compiler: `sudo apt-get install byacc`
- LAPACK and BLAS libraries for linear algebra operations:

```
sudo apt-get install liblapack-dev
```

Veclib can then be built using the following commands:

```
cd ~/nektar/Veclib
make
```

The file `libvec.a` should have been generated in the `/Veclib` directory. Hlib can be built from the `Hlib/Linux` directory using:

```
cd ../Hlib/Linux
make dbx
make opt
```

The files `libhybridg.a` and `libhybridopt.a` should have been generated in `/Hlib/Linux`. Next, the Veclib library should be copied into the Hlib/Linux directory:

```
cd ../..
cp Veclib/libvec.a Hlib/Linux/.
```

Now Nektar1D can be compiled using:

```
cd ~/nektar/1DBio/Linux
make clean
make dbx
```

Once the compilation is complete, the Nektar1D executable file, called `oneDbio`, will be located in the `nektar/1DBio/Linux` folder. The file can be executed with the command `./oneDbio` .

2.1 Making Nektar1D Accessible from Any Directory

To access `./oneDbio` from any directory, you can add its path to your `.bashrc` file, which contains initialisation commands for the shell, such as alias definition, environment variables, and directory additions to the `PATH` variable. First, open the `.bashrc` file in a text editor:

```
vim ~/.bashrc
```

Second, at the end of the file, insert the following line:

```
export PATH=$PATH:/home/username/nektar/1DBio/Linux
```

Replace `username` with your actual username. You can use the `whoami` command to find your username if needed.

Lastly, refresh the environment variables by running

```
source ~/.bashrc
```

Your executable `oneDbio` should now be accessible from any directory.

3 Creating An Input File

This section describes how to create a text input file containing all the parameters for a specific simulation. Examples of input files can be found in the `nektar/examples` folder. At the bottom of each file, you will find the command line required to execute it, which is described in Section 6. A detailed guide on how to run an input file is provided in Section 4.

The input file must have a `.in` extension (*e.g.* `input_file_name.in`) and should contain the following five sections in the specified order:

1. Parameter list
2. Mesh definition
3. Boundary conditions
4. Initial conditions
5. History points

Each section is described below with examples. Comments can be added to any line of the input file and must be preceded by the `#` character.

3.1 Parameter List

The parameter list contains several general parameters of the simulation. The first line of the list must contain an integer indicating the total number of parameters, followed by the list of parameters, with each one written on a separate line. The value of the parameter must come before its identifier. The order of the parameters is not important, but their values must always precede their identifiers. For any simulation, the following parameters must be included:

`EQTYPE`	Integer with the value 0 for the nonlinear formulation and 1 for the linear formulation. Note that the linear formulation is NOT as developed as the nonlinear formulation
`DT`	Time step (in seconds)
`NSTEPS`	Number of time steps
`HISSTEP`	Number of time steps until the next step solution is written to the output file `input_file_name.his`
`Rho`	Blood density (in Kg m^{-3})
`Viscosity`	Blood viscosity (in Pa s)
`Alpha`	Velocity profile parameter α in the frictional force per unit length of the momentum equation, as defined in [2] (after Eq. (1). The velocity profile is given by Eq. (3)). `Alpha` = 4/3 for Poiseuille flow; `Alpha` = 1 for inviscid flow

The following parameters are optional:

`INTTYPE`	Time integration order (1, 2 or 3) of the numerical scheme. By default, `INTTYPE` = 2
`IOSTEP`	Number of time steps until the next step solution is dumped in the output file `input_file_name.out`. By default `IOSTEP` = 0 and .out files are not generated.
`Beta`	Constant stiffness parameter $\beta = 4/3\sqrt{\pi}Eh/A_{\mathrm{d}}$ (in Pa m^{-1}) applied to all the arterial segments of the model, where E is the Young's modulus of the arterial wall, h is the wall thickness, and A_{d} is the luminal area at the reference pressure (usually the diastolic pressure) (see Section 3.2.1)
`Gamma`	Constant wall visco-elasticity parameter $\Gamma = 2/3\sqrt{\pi}\varphi h/A_{\mathrm{d}}$ (in Pa s m^{-1}) applied to all the arterial segments of the model, where φ is the wall viscosity, h is the wall thickness, and A_{d} is the luminal area at the reference pressure (usually the diastolic pressure) (see Section 3.2.1). Note that wall visco-elasticity is only available for the nonlinear solution (`EQTYPE` = 0)
`GammaII`	Constant wall visco-elasticity parameter related to Γ by $\Gamma = 1/2\beta$`GammaII` (in seconds), where Γ and β are defined in Section 3.2.1). This parameter is applied to all the arterial segments of the model and is only available for the nonlinear solution (`EQTYPE` = 0). It is used in `nektar/examples/Experimental/exp37.in` (see Section 6)
`Ao`	Constant luminal cross-sectional area A_{d} (in m^2) applied to all the arterial segments of the model
`pinf`	Pressure (in Pa) at the outflow of each lumped parameter model. By default `pinf` = 0
`Pext`	External pressure P_{ext} (in Pa) to the vessel wall (see Eq. (3.2)). By default `Pext` = 0
`Junc_losses`	1: Switch on energy losses at junctions; 0: no energy losses at junctions. By default `Junc_losses` = 0
`Bifurc_losses`	1: Switch on energy losses at bifurcations; 0: no energy losses at bifurcations. By default `Bifurc_losses` = 0
`Ischemic_Loss`	Pressure drop in Pa due to an ischemic attack. It is used in `nektar/examples/CoW/CoW_autoreg.in` to simulate a ischemic attack [16] and in `nektar/examples/FMD/FMD.in` to simulate inflation and deflation of the cuff in the upper forearm [17]
`Ischemic_TCompres`	Time it takes to reduce the pressure when `Ischemic_Loss` is activated
`NO_STN_DOM`	Domain number with the stenosis model. It is used in `nektar/examples/CCA_Stn/CCA_Stn.in` [7]
`ELM_SIZE`	Element size in the domain with the stenosis model. It is used in `nektar/examples/CCA_Stn/CCA_Stn.in` [7]
`STR_STN_ELM`	Domain number where the stenosis model starts. It cannot be the first element of the domain. It is used in `nektar/examples/CCA_Stn/CCA_Stn.in` [7]
`END_STN_ELM`	Domain number where the stenosis model ends. It cannot be the last element of the domain. It is used in `nektar/examples/CCA_Stn/CCA_Stn.in` [7]

K_T	Empirical constant of the stenosis model. It is used in nektar/examples/CCA_Stn/CCA_Stn.in [7]
Periodic	The inflow boundary condition is periodic. The value of the period is the number given in front of Periodic in seconds
T_initial	Initial time (in s) for the time-average calculations in input_file_name_periodic.tex. By default T_initial = 0
T_final	Final time (in s) for the time-average calculations in input_file_name_periodic.tex. By default T_final = NSTEPS * DT
SkipDomain	Number of domains (starting from domain 1) to be skipped when producing the Latex files input_file_name.tex and input_file_name_periodic.tex. By default SkipDomain = 0
SCAL_F	Scaling factor for the inflow waveform (see Section 3.3.1)
Pulse_Centre	Time of the peak (in s) for the Gaussian function/s used as inflow boundary condition/s (see Eq. (3.8)). By default Pulse_Centre = 1
Pulse_Width	Parameter controlling the width (in s^{-2}) of the Gaussian function/s used as inflow boundary condition/s (see Eq. (3.8)). By default Pulse_Width = 100
FMDHL	Half-life of cumulative shear exposure of the flow-mediated dilation (FMD) model described in [17]
FMDCd	Parameter controlling the time delay in the change in Young's modulus of the FMD model described in [17]
FMDalp	Parameter controlling the magnitude in the change in Young's modulus of the FMD model described in [17]
RVar1	Parameter controlling the variation in magnitude of the time-varying peripheral resistances of all the terminal Windkessels models coupled to the right arm 1-D model arterial segments of the FMD model. The nomenclature α_1 was used for this parameter in Eq. (6) of [17].
RVar2	Parameter controlling the variation in magnitude of the time-varying peripheral resistances of all the terminal Windkessels models coupled to the right arm 1-D model arterial segments of the FMD model. The nomenclature α_2 was used for this parameter in Eq. (6) of [17].
RefT	Time when the reference values were calculated in the FMD model described in [17].
CarCyc	Length of one cardiac cycle in the FMD model described in [17].

The following parameters must be included to simulate a closed-loop 1-D/0-D model of the Fontan circulation [5]:

L_EFFA	Effective length of aortic valve (AoV) (in m)
A_ANNA	Annulus area of AoV (in m^2)
K_VOA	AoV opening rate coefficient (in $mmHg^{-1}s^{-1}$)
K_VCA	AoV closing rate coefficient (in $mmHg^{-1}s^{-1}$)
K_SA	Source resistance coefficient for the flow through the AoV (in s mL^{-1})
E_MINV	Minimum ventricular elastance (in mmHg mL^{-1})
E_MAXV	Maximum ventricular elastance (in mmHg mL^{-1})
V_0V	Reference volume for the ventricle (in mL)
M_1V	Ventricular contraction rate constant (dimensionless)

M_2V	Ventricular relaxation rate constant (dimensionless)
TAU_1V	Ventricular systolic time constant (in s)
TAU_2V	Ventricular diastolic time constant (in s)
K_VENT	Scaling factor used in the time-varying ventricular elastance function to ensure that maximum elastance corresponds to E_MAXV (dimensionless)
L_EFFM	Effective length of atrioventricular valve (AVV) (in m)
A_ANNM	Annulus area of AVV (in m^2)
K_VOM	AVV opening rate coefficient (in $mmHg^{-1}s^{-1}$)
K_VCM	AVV closing rate coefficient (in $mmHg^{-1}s^{-1}$)
K_SM	Source resistance coefficient for the flow through the AVV (in s mL^{-1})
E_MINA	Minimum atrial elastance (in mmHg mL^{-1})
E_MAXA	Maximum atrial elastance (in mmHg mL^{-1})
V_OA	Reference volume for the atrium (in mL)
M_1A	Atrial contraction rate constant (dimensionless)
M_2A	Atrial relaxation rate constant (dimensionless)
TAU_1A	Atrial systolic time constant (in s)
TAU_2A	Atrial diastolic time constant (in s)
K_ATRIUM	Scaling factor used in the time-varying atrial elastance function to ensure that maximum elastance corresponds to E_MAXA (dimensionless)
T_OFFSET	Onset of atrial contraction (in s)
T_PERIOD	Period of the cardiac cycle (in s)
Q_AVG	Mean aortic flow (in mL s^{-1})
V_INITIALV	Initial ventricular volume (in mL)
V_INITIALA	Initial atrial volume (in mL)
V_VESSELS	Volume of the 1-D vessels of the Fontan circulation model (in mL)
V_TOTAL	Total blood volume in the Fontan circulation model (mL)

Additional parameters can be defined by the user; *e.g.* `ELASTIC` is used in `nektar/examples/Experimental/exp37.in` to define a constant Young's modulus for all arterial segments. (This model generates the results for the purely elastic case described in [3].) Note that the number π is defined as `PI` by default throughout any input file.

3.2 Mesh Definition

The geometrical and mechanical properties of all arterial segments, referred to as 'domains' in Nektar1D, are defined in this section. The first line of the section must contain the string `Mesh` followed by `Ndomains =` *integer*, where the integer specifies the number of domains. If there is only one domain, then `Ndomains =` *integer* is not required.

Each domain definition begins with an opening line specifying the number of finite elements (Nel) that make up the domain. For each element, a line is required with four values indicating the following: (i) lower spatial coordinate x; (ii) upper spatial coordinate x; (iii) polynomial order of the element, p; and (iv) quadrature order of the element, q. For example, a domain with a starting point of $x = -0.075$ m and an ending point of $x = 0.075$ m, divided into three equispaced elements with a quadrature and polynomial order of 6, is defined as:

```
Mesh
3       # Nel
-0.075  -0.025  6  6  # x_lower x_upper p q
-0.025  0.025   6  6  # x_lower x_upper p q
0.025   0.075   6  6  # x_lower x_upper p q
```

Material and geometrical properties can be specified for each element of each domain in *Mesh Definition*, as described below for purely elastic (Section 3.2.2) and viscoelastic (Section 3.2.3) arterial walls. If all domains have the same properties, these values can be defined in *Parameter List* (see Section 3.1 for more details). First, we present the most generic tube law – relating changes in blood pressure to changes in cross-sectional area – currently available in Nektar1D (Section 3.2.1).

3.2.1 Tube Law

The most generic relationship between changes in blood pressure and changes in cross-sectional area implemented in Nektar1D is a Voigt-type visco-elastic tube law given by

$$P = P_{\mathrm{e}}(A;x) + \frac{\Gamma}{\sqrt{A}}\frac{\partial A}{\partial t}, \tag{3.1}$$

with

$$P_{\mathrm{e}}(A,x) = P_{\mathrm{ext}} + \beta\left(\sqrt{A} - \sqrt{A_{\mathrm{d}}}\right), \tag{3.2}$$

$$\beta(x) = \frac{4}{3}\frac{\sqrt{\pi}\,Eh}{A_{\mathrm{d}}}, \tag{3.3}$$

$$\Gamma(x) = \frac{2}{3}\frac{\sqrt{\pi}\,\varphi h}{A_{\mathrm{d}}} = \frac{4}{3}\frac{\varphi h}{D_{\mathrm{d}}\sqrt{A_{\mathrm{d}}}}, \tag{3.4}$$

where $P(x,t)$ is blood pressure, $P_{\mathrm{e}}(x,t)$ is the elastic component of pressure, P_{ext} is the external pressure, $A(x,t)$ is the luminal cross-sectional area, $h(x)$ is the wall thickness, $E(x)$ is the Young's modulus, and $\varphi(x)$ is the wall viscosity. The reference area $A_{\mathrm{d}}(x)$ and diameter $D_{\mathrm{d}}(x)$ are the area and diameter, respectively, at $P = P_{\mathrm{ext}}$ and $\frac{\partial A}{\partial t} = 0$, with P_{ext} usually taken as the diastolic pressure. Note that the parameter $\beta(x)$ is related to the elasticity of the wall and $\Gamma(x)$ to the viscosity of the wall. Moreover, both $\beta(x)$ and $\Gamma(x)$ are independent of the transmural pressure $P - P_{\mathrm{ext}}$.

3.2.2 Purely-Elastic Simulations

By default, $\Gamma = 0$, meaning all domains have a purely-elastic arterial wall (see Eq. (3.1)). The mechanical properties for a purely-elastic arterial wall can be specified in three different ways:

- Using the stiffness parameter β;
- Using the product of wall's Young's modulus and wall thickness, Eh;
- Using an empirical law that relates the pulse wave velocity c and the reference diameter D_{d}.

The stiffness parameter β
For each domain, the opening line must contain the strings `Beta` and `Area`, as shown in the example below. For each element, β and $A_{\rm d}$ are defined in two different lines, starting with '`Beta =`' and '`Area =`' (or `Ao =`), respectively. The order is important; `Beta` must come before `Area`. Elements can have either constant β and $A_{\rm d}$, or β and $A_{\rm d}$ may vary as a function of the axial coordinate x along the domain. For example,

```
2  # Nel domain 5  Beta Area
0.0  0.0175  6  6  # x_lower x_upper p q
Beta = 404.063553/(3.2000e-03 + -2.8571e-02*x)/(2.7628e-03 + -2.1984e-02*x)
Area = 4.7022e-06 + -6.7010e-05*x + 2.3874e-04*x*x
0.0175  0.035  6  6  # x_lower x_upper p q
Beta = 404.063553/(3.2000e-03 + -2.8571e-02*x)/(2.7628e-03 + -2.1984e-02*x)
Area = 4.7022e-06 + -6.7010e-05*x + 2.3874e-04*x*x
```

This example is taken from `nektar/examples/Rabbit/Rabbit.in`, which models the rabbit systemic circulation used in [6].

Note that it is possible to define a constant β in *Parameter List* and a variable $A_{\rm d}$ in *Mesh Definition*, and vice versa.

Wall Young's modulus times wall thickness, Eh
You can also prescribe the quantity Eh, where $E(x)$ is the Young's modulus of the arterial wall and $h(x)$ is the wall thickness. Nektar1D will compute $\beta(x)$ using Eq. (3.3). For each domain, the opening line must contain the strings `Eh` and `Area`. For each element, Eh is defined in a new line starting with '`Eh =`'. Note that $A_{\rm d}$ must be defined before Eh. For example:

```
2  nel  Eh Area
0.0  0.120685834705770  5  5  # x_lower x_upper p q
Area = 4.5239e-04
Eh = 480
0.120685834705770  0.241371669411541  5  5  # x_lower x_upper p q
Area = 4.5239e-04
Eh = 480
```

This example is taken from `nektar/examples/Aorta/Ao_Eh.in`, which is the single-vessel model of the upper thoracic aorta used in [8, 10]. The material properties in this model can also be prescribed using the stiffness parameter β, as shown in `nektar/examples/Aorta/Ao.in`. Another example where Eh is specified is `nektar/examples/Experimental/exp37.in`. In this case, a constant Young's modulus (defined in *Parameter List* as `ELASTIC`) is used for all arterial segments [3].

Empirical law
Material properties can also be specified through the local pulse wave velocity, $c(x,t)$, which is directly related to $\beta(x)$ through $A(x,t)$,

$$\beta = \frac{2\,\rho\,c^2}{\sqrt{A}}. \tag{3.5}$$

Pulse wave velocities can be calculated using the empirical relationship [18],

$$c = \frac{a}{(D_\mathrm{d})^b}, \tag{3.6}$$

where D_d is the luminal diameter (in mm) at the reference pressure, and a and $b = 0.3$ are empirical coefficients. Nektar1D computes the value of β using

$$\beta = \frac{2\,\rho}{\sqrt{A_\mathrm{d}}}\,\frac{a^2}{(D_\mathrm{d})^{2b}} \tag{3.7}$$

where $D_\mathrm{d} = \sqrt{\frac{4A_\mathrm{d}}{\pi}}$, expressed in mm.

For each domain, the opening line must contain the strings `Empirical_I` and `Area`. For each element, a is defined in a line starting with '`a =`'. Note that the reference area A_d must be defined before a. For example:

```
1  nel domain 3  Empirical_I Area
0.0  0.023  3  3  # x_lower x_upper p q
Area = (4.94808594E-04 - 1.88563815E-03*x + 1.79646802E-03*x*x)
a = CSCAL_a*11.0
```

This example was taken from `nektar/examples/55art/55art_elas.in`, which models the 55 largest systemic arteries [2]. In this example, `CSCAL_a` is defined by the user in *Parameter List*.

3.2.3 Visco-Elastic Simulations

To define a domain with a viscoelastic arterial wall, you must specify the viscoelastic parameter, Γ, using the string `Gamma` in the opening line of the domain definition. Γ can then be defined as a function of the axial coordinate x along the domain. If the stiffness parameter β is used for the purely-elastic part, then `Gamma =` must be placed after the line `Beta =` . For example:

```
1  nel  Beta Area Gamma
0.0  0.126  5  5  # x_lower x_upper p q
Beta = 1.7553E+07
Gamma = 1.8806E+05
Ao = 2.8274e-05
```

This example is taken from `nektar/examples/CCA/CCA_Beta_vw_mesh.in`, which corresponds to a single-vessel model of the common carotid artery [8, 10].

If the wall Young's modulus times wall thickness, Eh, is used for the purely-elastic part, then `Gamma =` must be placed after the lines `Area =` and `Eh =` . For example:

```
1  nel  Eh Area Gamma
0.0  0.126  5  5  # x_lower x_upper p q
Ao = 2.8274e-05
Eh = 3E-4*700E3
Gamma = 1.8806E+05
```

This example is taken from `nektar/examples/CCA/CCA_vw_mesh.in`, which corresponds to the same single-vessel model of the common carotid artery [8, 10].

If the empirical law is used for the purely-elastic part, then `Gamma =` must be placed after the lines `Area =` and `a =` . For example:

```
1  nel domain 3  Empirical_I Area Gamma
0.0  0.023  3  3  # x_lower x_upper p q
Area = (4.94808594E-04 - 1.88563815E-03*x + 1.79646802E-03*x*x)
a = CSCAL_a*11.0
Gamma = 4/3*Varphi4*hD/(CSCAL_Ao*(4.94808594E-04 - 1.88563815E-03*x
    + 1.79646802E-03*x*x))^0.5
```

This example is taken from `nektar/examples/55art/55art.in` which corresponds to a model of the 55 largest systemic arteries [2]. In this example, `CSCAL_a` (a scaling factor for a in Eq. (3.7)), `Varphi4` (the value of φ in Eq. (3.4)), and `hD` (the value of the ratio h/D_{d} in Eq. (3.4)) are defined by the user in *Parameter List*.

3.3 Boundary Conditions

This section defines the boundary conditions (BCs) for all the domains (arterial segments) that can be prescribed in Nektar1D. The first line of this section must contain the string `Boundary`. Then, for each domain, at least four lines of BC information must be included: two lines with information on the BC at the inlet of the domain, and two lines with information at the outlet. Each line must start with a letter defining the type of BC. There are four types of BCs that can be prescribed at the inlet and outlet of each domain:

1. *Prescribed waveform* (usually at the inlet of the arterial network);
2. *Lumped parameter (0-D) model* (usually at the outlets of terminal branches);
3. *Connection with other domains*;
4. *Fontan circulation* (*i.e.* a closed-loop 1-D/0-D model of the Fontan circulation).

3.3.1 Prescribed Waveform

A blood flow, blood velocity, or blood pressure waveform can be prescribed as BC. Incoming waves can be treated in two different ways: they can either be reflected back into the domain (*reflective BC*) or fully absorbed by the BC (*absorbing BC*). Moreover, a pulse waveform can be defined in a text file by either (i) providing the amplitude and phase angle of all its Fourier harmonics (for flow rate waves only) or (ii) specifying the magnitude of the flow, velocity or pressure for each time step. The file must be named `input_file_name_IN.bcs` if there is only one domain, or `input_file_name_IN_1.bcs` if there are multiple domains.

If the harmonics definition is used, the first line in the `.bcs` file must contain the following three values separated by spaces: number of harmonics, cardiac cycle duration (in seconds), and mean blood flow rate (in m^3/s). This must be followed by a line for each harmonic containing the values of its amplitude and phase angle, separated by a

space. Alternatively, a waveform can be defined as an algebraic function of time in the input file `input_file_name.in`, using `t` to denote time. `AorticFlowWave` can be used to create aortic inflow waveforms under a range of conditions. The source code for this Matlab script is available from here.

The table below lists the Nektar1D commands for imposing a flow, velocity or pressure waveform as a BC, either reflectively or absorbingly, using either a text file .bcs or an algebraic equation in the input file.

		Reflective BC	Absorbing BC
Flow, q	File .bcs (time - flow rate)	`q 2`	`q 3`
	File .bcs (harmonics)	`F 0`	`F 8`
	Algebraic function	`q 0`	`q 1`
Velocity, u	File .bcs (time - velocity)	`u 2`	`u 3`
	Algebraic function	`u 0`	`u 1`
Pressure, p	File .bcs (time - pressure)	`p 2`	`p 3`
	Algebraic function	`p 0`	`p 1`

For example, to prescribe an *in vivo* flow waveform expressed as a sum of harmonics in a reflective manner, the commands at the inlet (or outlet) of the domain are

```
F 0
F 0
```

This type of inflow boundary condition must be accompanied by a text file called `input_file_name_IN.bcs` or `input_file_name_IN_1.bcs`, which contains the harmonics information described above. If the BC is prescribed at the outlet of the domain, the file should be named `input_file_name_OUT.bcs` or `input_file_name_OUT_1.bcs`. See `nektar/examples/AoBif/AoBif.in` for an example of a model using this type of reflective BC, and `nektar/examples/AoBif/AoBif_abs.in` for the equivalent model with an absorbent BC.

For and example of a flow waveform expressed as a time–flow rate text file (.bcs), refer to `nektar/examples/Adan56/adan77.in` .

To prescribe a cosine pressure wave at the inlet of a domain in a reflective manner using an algebraic function, the following commands should be included in the *Boundary conditions* section of the input file:

```
p 0
p = cos(PI*t)
p 0
p = 0
```

This example is taken from `nektar/examples/Sine/Sine.in` . For an example with a prescribed velocity waveform in a reflective manner using an algebraic function, see `nektar/examples/Sine/Sine_vw.in` .

A Gaussian inflow waveform described as

$$Q = ae^{-(t-b)^2/c} \tag{3.8}$$

can be prescribed using `F 7`. The constant parameters a, b and c must be specified in the parameter list using the identifiers `SCAL_F`, `Pulse_Centre` and `Pulse_Width`, respectively. Examples are provided in the folder `nektar/examples/Pulse/` .

Lastly, the following inflow waveforms have been hard-coded in Nektar1D as reflective BCs:

`F 1` – Flow waveform at the aortic root of the *in vitro* model described in [3] and used in `nektar/examples/Experimental/exp37.in` ;

`F 2` – Flow waveform at the rabbit aortic root as described in [6] and used in `nektar/examples/Rabbit/Rabbit.in` ;

`F 3` – Flow waveform at the human aortic root as described in [2] and used in `nektar/examples/55art/55art.in` ;

`F 4` – Flow waveform at the human aortic root as described in [19] and used in `nektar/examples/CoW/CoW.in` ;

`F 6` – Flow waveform at the human common carotid artery as described in [8, 10] and used in `nektar/examples/CCA/CCA.in` .

3.3.2 Lumped Parameter Model

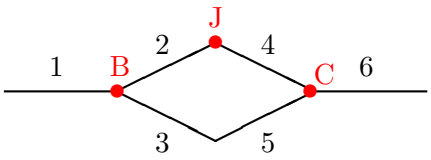
The main types of outlet BCs in Nektar1D are summarised below, along with the two lines of commands required in the *Boundary condition* section of the input file. Further details on these types of BCs can be found in [20].

Reflection coefficient	`T` #	if # = 0, complete absorption of the incoming wave
	`T` #	if # = 1, complete reflection of the incoming wave
Single resistance (R)	`R` #	# is the vascular resistance value in [Pa s m^{-3}]
	`R` #	
2-element windkessel (C-R)	`w` $\#_C$	$\#_C$ is the vascular compliance value in [m^3 Pa^{-1}]
	`w` $\#_R$	$\#_R$ is the vascular resistance value in [Pa s m^{-3}]
3-element windkessel (R_1-C-R_2)	`W` $\#_C$	$\#_C$ is the vascular compliance value
	`W` $\#_R$	$\#_R$ equals the sum of vascular resistances $R_1 + R_2$
4-element windkessel (R_1-C-L-R_2)	`Z` $\#_C$	$\#_C$ is the vascular compliance value
	`Z` $\#_R$	$\#_R$ equals the sum of vascular resistances $R_1 + R_2$
		The inductance value is specified in *Parameter List* as `inductance`

For the three-element Windkessel BC, the value of the first resistance (R_1) is, by default, computed as the characteristic impedance of the end point of the domain (Z_0). If a numeric value is specified after the total resistance value (*i.e.* `W` $\#_R$ $\#_r$), the value of the first resistance R_1 will be multiplied by the absolute value of this factor: $R_1 = |r| * Z_0$. By default, $r = 1$.

3.3.3 Connection with Other Domains

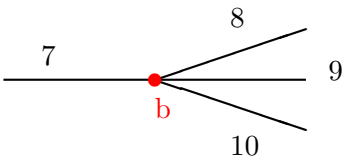
Several types of domain connections can be defined in Nektar1D. The commands for each type are described below and illustrated using examples from arterial networks.



- **J: Connection between two domains:** At the outlet of Domain 2 the following two lines of commands must be written to indicate that Domain 2 is connected to Domain 4:
  ```
  J 4 4
  J 4 4
  ```

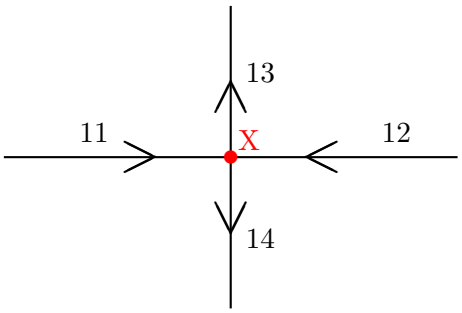
- **B: Splitting Flow Bifurcation:** At the outlet of Domain 1 the following two lines of commands must be written to indicate that Domain 1 is connected to the daughter Domains 2 and 3:
  ```
  B 2 3
  B 2 3
  ```
  Similarly, at the inlet of Domain 3 the following two lines of commands must be written to specify the number of the parent domain (Domain 1) and the other daughter domain (Domain 2):
  ```
  B 1 2
  B 1 2
  ```

- **C: Merging Flow Bifurcation:** At the outlet of Domain 4, the following two lines of commands must be written to indicate that Domain 4 is connected to Domains 5 and 6:
  ```
  C 5 6
  C 5 6
  ```
  Similarly, at the inlet of Domain 6, the commands are:
  ```
  C 4 5
  C 4 5
  ```



- **b: Splitting Flow Trifurcation:** At the outlet of Domain 7, the following two lines of commands must be written to indicate that Domain 7 is connected to Domains 8, 9, and 10:
  ```
  b 8 9 10
  b 8 9 10
  ```
  Similarly, at the inlet of Domain 8, the commands are:
  ```
  b 7 9 10
  b 7 9 10
  ```
  At the inlet of Domain 9 we have:
  ```
  b 7 8 10
  b 7 8 10
  ```
  And at the inlet of Domain 10:

```
b 7 8 9
b 7 8 9
```



- **X: Two-inflow–two-outflow junction:** At the outlet of Domain 11, the following two lines of commands must be written to indicate that Domain 11 is connected to Domains 12, 13, and 14:
  `X 1 12 13 14`
  `X 1 12 13 14`
  Similarly, at the outlet of Domain 12, the commands are:
  `X 0 11 13 14`
  `X 0 11 13 14`
  At the inlet of Domain 13 we have:
  `X 0 11 12 14`
  `X 0 11 12 14`
  And at the inlet of Domain 14:
  `X 0 11 12 13`
  `X 0 11 12 13`
  Another option would be to define the outlet of Domain 11 as '`X 0 12 13 14`' and the outlet of Domain 12 as '`X 1 11 13 14`', but the first number after '`X`' can be '`1`' for only one of the parent domains.

3.3.4 Fontan Circulation Model

The main components of the Fontan circulation model are the aorta, total cavopulmonary connection (TCPC), and the lumped upper body, lower body, lungs, and heart (see Figure 3.1) [5]. The 1-D model aorta is coupled to the 1-D model TCPC through 0-D models of the upper and lower bodies, lungs and heart. The aorta consists of the ascending aorta (AAo), the brachiocephalic artery (BCA), the left common carotid artery (LCCA), the left subclavian artery (LSA), and the descending aorta (DAo). The TCPC includes the superior vena cava (SVC), inferior vena cava (IVC), right pulmonary artery (RPA), and left pulmonary artery (LPA). The heart model consists of the atrium, atrioventricular valve (AVV), ventricle, and aortic valve (AoV). Blood flow is driven by the time-varying elastance of the ventricle (E_{V}) and atrium (E_{A}). The 0-D models of the upper and lower bodies represent the arterial (R_{a}), capillary (R_{c}) and venous (R_{v}) resistances, as well as the arterial (C_{a}) and venous (C_{v}) compliances.

Nektar1D solves the 0-D governing equations using a fourth-order Runge Kutta scheme. The following line must be added to the *Boundary condition* section of the input file:

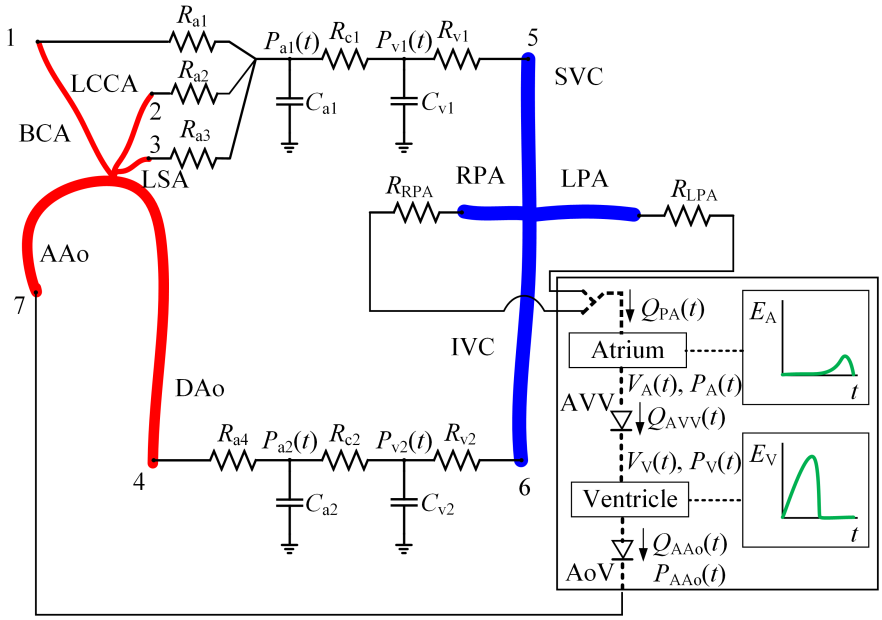


Figure 3.1: Schematic representation of the Fontan circulation 1-D/0-D model. The model consists of 1-D models of the aorta, supra-aortic arteries, left and right pulmonary arteries, and venae cavae, and 0-D models of the upper body, lower body, lungs, and univentricular heart. Each 1-D model boundary (except for the left and right pulmonary arteries) has a numeral code from 1 to 7 (as indicated in the figure), which is used when writing the input file. In addition to 1-D model output results described in Section 5, the Fontan model provides cardiac haemodynamic measures such as atrial volume and pressure, ventricular volume and pressure, and atrio-ventricular flow [5]. AAo: ascending aorta; AoV: aortic valve; AVV: atrioventricular valve; BCA: brachiocephalic artery; DAo: descending aorta; IVC: inferior vena cava; LCCA: left common carotid artery; LSA: left subclavian artery; LPA: left pulmonary artery; RPA: right pulmonary artery; SVC: superior vena cava.

`g code` R_{a1} R_{a2} R_{a3} R_{a4} R_{c1} R_{c2} R_{v1} R_{v2} C_{a1} C_{a2} C_{v1} C_{v2}
`g code` R_{a1} R_{a2} R_{a3} R_{a4} R_{c1} R_{c2} R_{v1} R_{v2} C_{a1} C_{a2} C_{v1} C_{v2}

where the resistances (R) are given in mmHg s mL^{-1}, the compliances (C) are expressed in mL mmHg^{-1}, and `code` is an integer from 1 to 7 corresponding to the number indicated at the boundaries of the 1-D model (see Figure 3.1). Specifically:

- `code = 1` corresponds to the outlet of the brachiocephalic artery,
- `code = 2` to the outlet of the left common carotid artery,
- `code = 3` to the outlet of the left subclavian artery,
- `code = 4` to the descending aorta,
- `code = 5` to the inlet of the superior vena cava,
- `code = 6` to the inlet of the inferior vena cava,

- `code = 7` to the inlet of the ascending aorta.

An example of this type of input file can be found in `nektar/examples/Fontan/Fontan.in`, taken from [5]. The boundary conditions at the outlets of the pulmonary arteries must be specified as single resistances. If a fenestration is to be modelled, it should be added as a short 1-D model vessel with a single resistance outflow boundary condition. The outflows from the pulmonary arteries and the fenestration are then combined and prescribed as inflow to the atrium.

3.4 Initial Conditions

This section contains the initial values for the luminal cross-sectional area (A_0) and blood velocity (U_0) in all domains of the simulation. The first line of the section must contain the string `Initial condition`. Next, two lines must be provided for each domain: the first line specifies the value of A_0 and the second line the value of U_0. Both A_0 and U_0 can either be constant values or functions of the spacial coordinate x. For example,

```
Initial condition
a = PI*1E-4          #Initial value of area (in m^2)
u = 0                #Initial value of flow velocity (in m/s)
```

The initial area A_0 can be prescribed to match the area A_d defined in *Mesh Definition* by using `a = Ao`. For example,

```
Initial condition
a = Ao               #Initial value of area equal to the area in Mesh Definition (in m^2)
u = 0                #Initial value of flow velocity (in m/s)
```

However, the initial area is usually computed as the area that yields the prescribed area A_d in *Mesh Definition* at a given pressure P_d. This can be done by setting $P_\mathrm{e} = 0$, $P_\mathrm{ext} = P_\mathrm{d}$, and $A = A_0$ in Eq. (3.2), which results in

$$A_0 = \left(\sqrt{A_\mathrm{d}} - \frac{P_\mathrm{d}}{\beta} \right)^2 . \tag{3.9}$$

Nektar1D can calculate A_0, using Eq. (3.9) if the simulation is initiated using the flag `-i`, followed by a positive real number representing the value of the pressure P_d (in Pa). For example,

```
./oneDbio -i 12666.66 55art.in
```

Using the flag `-i` will overwrite all values of A_0 in *Initial Conditions*. However, note that the *Initial Conditions* section must still be included in the input file. This example is taken from `nektar/examples/55art/55art.in` [2].

3.5 History Points

This section specifies the points in the arterial network, referred to as *history points*, where the computed haemodynamic waveforms are recorded. The first line must contain the string `History`, and the second line must specify the number of domains with history points. Next, for each domain with history points, two lines must be included. The first

line must include an integer indicating the number of history points within the domain, followed by another integer representing the domain number. The second line must specify the x positions of each history point within the domain. Below is an example on how to define history points at the inlet of Domain 1 and at three points in Domain 17. This example is taken from `nektar/examples/Rabbit/Rabbit.in`.

```
History Pts
2                    #Number of domains with history points
1 1                  #Number of points and domain identifier
0.0
3 17                 #Number of points and domain identifier
0.0433 0.065 0.0866
```

4 Running an Input File

To run Nektar1D, open a terminal window, navigate to the directory `nektar/1DBio/Linux`, and type `./oneDbio` followed by the name and extension of the input file; *e.g.*

```
./oneDbio input_file_name.in
```

To run Nektar1D from the directory containing the input file, you can export the path of `./oneDbio` to the shell, as explain in Section 2.1. All output files (see Section 5) will be saved in the directory from which `./oneDbio` is executed.

Please note that input files transferred from a DOS-platform to a Linux-based system may cause execution errors due to differences in character encoding and end-of-line commands. To address this, use the `fromdos` command to convert text files between DOS and UNIX formats. You can install it using the command:

```
sudo apt-get install tofrodos
```

`fromdos` should be used once to convert an input file: `fromdos input_file_name.in` .

The following optional flags can be used with the `./oneDbio` command:

1. `-p #`: Assigns the value given in `#` as the polynomial order for all the elements in the simulation. This flag replaces any values given in the input file.

2. `-q #`: Assigns the value given in `#` as the quadrature order of all the elements in the simulation. This flag replaces any values given in the input file.

3. `-N #`: Divides all domains into the number of equispaced elements given in `#`. This flag replaces the number of elements given in the input file.

4. `-O`: Generates output files (with extension `.out`) containing the variables of the simulation evaluated at the quadrature points of all the domains for different times. See Section 5 for more details.

5. `-L`: Generates output files (with extension `.lum`) containing the variables of the lumped parameter models which change with time. See Section 5 for more details.

6. `-A`: Dumps the luminal cross-sectional area, A – instead of the blood pressure, P – in the output file with extension `.out` .

7. `-B`: Generates output files (with extension `.bcs`) containing time-varying characteristic information (including the Riemann variables) at all the boundaries of the arterial network. See Section 5 for more details.

8. `-a`: Dumps the following additional variables in the history files: (i) forward- and backward-travelling Riemann (or characteristic) variables (in m s^{-1}); (ii) spatial-averaged blood pressure (Pa), blood flow velocity (m s^{-1}), blood flow rate (m s^{-3}), and luminal cross sectional area (m^2) across each domain; (iii) forward and backward-travelling components of pressure (Pa) and velocity (m s^{-1}); and (iv) space derivatives: pressure gradient term (Pa m^{-1}), convective acceleration term (m s^{-2}), flow gradient term ($m^2 s^{-1}$). These additional variables were used for the pulse wave analysis tools described in Willemet *et al.* [14].

   Without this flag, the default variables are: time (s), blood pressure (Pa), blood flow velocity (m s^{-1}), blood flow rate (m s^{-3}), luminal cross sectional area (m^2), and an integer that refers to the point label indicated in the heading (see Section 5).

9. `-d`: Dumps a report file called `input_file_name.txt` containing several parameters of the simulation, including haemodynamic variables at the initial time. The file is generated without running the simulation.

10. `-t`: Dumps a LaTeX report file called `input_file_name.tex` containing several parameters of the simulation, including haemodynamic variables at the initial time. The file is generated without running the simulation.

11. `-R`: Dumps space-averaged variables for the whole arterial network in a file called `input_file_name.avg`. See Section 5 for more details.

12. `-r #`: Scales all peripheral resistances by multiplying them by the value specified in `#`.

13. `-c #`: Scales all peripheral compliances by multiplying them by the value specified in `#`.

14. `-i #`: Sets the initial areas (A_0) in all elements to the values that will produce the areas A_d (specified in *Mesh Definition*) at the pressure given by the value specified in `#`. Equation (3.9) is used to calculate A_0.

The first four flags are used in `nektar/examples/Pulse/.`, and the last four flags are used in `nektar/examples/55art/55art.in` .

5 Output Files

By default, Nektar1D generates the following output text files:

1. *LaTeX report file*: It is called `input_file_name.tex` and, when compiled in LaTeX, displays several tabulated parameters of the simulation and haemodynamic variables at the initial time.

2. *Report file*: It is called `input_file_name.txt` and contains similar information to the previous file in a format that can be read by a normal text editor.

3. *Period LaTeX report file*: It is called `input_file_name_period.tex` and, when compiled in LaTeX, displays several tabulated parameters of the simulation and haemodynamic variables for the time period starting at `T_initial` and ending at `T_final`, with `T_initial` and `T_final` defined in *Parameter List* (Section 3.1).

4. *Property file*: It is called `input_file_name.prp` and contains the following information for each domain: length, inlet radius, outlet radius, inlet wave speed, outlet wave speed, inlet area, outlet area, inlet Γ, and outlet Γ. Radii, wave speeds, and areas are given for the initial time.

5. *Period property file*: It is called `input_file_name_period.prp` and contains the following information for each domain: length, inlet, midpoint and outlet radii, inlet, midpoint and outlet wave speeds, inlet, midpoint and outlet areas, and arterial compliance for the time period starting at `T_initial` and ending at `T_final`, with `T_initial` and `T_final` defined in *Parameter List* (Section 3.1).

6. *Stiffness parameter file*: A single file called `input_file_name.bet` that contains, for each domain, the domain number, the number of history points, and the value of the stiffness parameter β at the x position of each history point (each value in a different line). Domains without a history point are assigned a β value of zero.

7. *History file/s*: They are called `input_file_name.his` if the model consists of a single domain or `input_file_name_#.his` if the model consists of multiple domains, with `#` the number of each domain with history points defined in the *History Points* section of the input file (see Section 3.5). Each history file consists of a header with information on the number of history points in the domain and their x location. After the header there is a matrix of numbers with the following information: time (in s) in the first column; blood pressure (Pa) in the second; blood flow velocity (m s^{-1}) in the third; blood flow rate (m s^{-3}) in the fourth; luminal cross sectional area (m^2) in the fifth; and an integer in the sixth referring to the point label indicated in the heading. For a visco-elastic tube law, the elastic component of pressure, P_e (see Eq. (3.2)), is dumped in the third column (in Pa), followed by flow velocity, flow rate, etc. The temporal spacing of these quantities is defined by `HISSTEP` in *Parameter List* (Section 3.1). History files can be converted into Matlab format, ready for analysis, using `ConvertHistoryFiles` which can be dowloaded from here.

8. *History points location*: A single file called `input_file_name.loc` that, for each domain, contains the domain number, the number of history points, and the x position of each history point (each value in a different line).

In addition, the following output text files can be generated using the flags described in Section 4:

1. *Output file/s*: Files containing the variables of the simulation evaluated at the quadrature points of all the domains for different times. They are created using the flag `-O`. They are called `input_file_name.out` if the model consists of a single domain or `input_file_name_#.out` if the model consists of multiple domains, with `#` the number of each domain. Each output file consists of a header with information on the number of elements, points dumped (total and for each element)

and time steps dumped. The number of time steps dumped is defined by `IOSTEP` in *Parameter List* (Section 3.1). For each time step, there is a matrix of numbers with the following information: x location (m) in the first column; blood pressure (Pa) in the second; blood flow velocity (m s^{-1}) in the third; forward characteristic (m s^{-1}) in the fourth; and backward characteristic (m s^{-1}) in the fifth. The flag `-A` (in addition to `-O`) dumps the luminal cross-sectional area (A), instead of blood pressure (P), in the second column.

2. *Lumped parameters file/s*: They are obtained using the flag `-L`. We can have a single file called `input_file_name_out.lum`, if there is only one domain with an outflow boundary condition, or multiple files called `input_file_name_out_#.lum`, if there are multiple domains with outflow boundary conditions, with `#` the number of each terminal domain. Each file contains a matrix of numbers with the following information: time (s) in the first column; blood pressure (Pa) at the inflow of the lumped parameter model in the second; blood flow rate (m s^{-3}) at the inflow of the lumped parameter model in the third; blood pressure (Pa) at the compliance in the fourth; and blood flow rate (m s^{-3}) at the outflow of the lumped parameter model in the fifth.

3. *Inflow characteristic information file/s*: They are obtained using the flag `-B`. We can have a single file called `input_file_name_IN.bcs` in a model with only one domain or multiple files called `input_file_name_IN_#.bcs` in a model with multiple domains, with `#` the number of each domain with an inflow boundary condition. Each file contains a matrix of numbers with the following information calculated at the first point of the domain: time (s) in the first column; $\rho c W_\mathrm{f}$ (Pa) in the second, with ρ blood density, c pulse wave velocity, and W_f the forward characteristic variable; $-\rho c W_\mathrm{b}$ (Pa) in the third, with W_b the backward characteristic variable; $W_\mathrm{f}/2$ (m s^{-1}) in the fourth; $W_\mathrm{b}/2$ (m s^{-1}) in the fifth; and $-W_\mathrm{b}/W_\mathrm{f}$ in the sixth. These information was used in [21] to study the effect of inflow boundary conditions on the shape of the pressure and flow waveforms.

4. *Outflow characteristic information file/s*: They are obtained using the flag `-B`. It is called `input_file_name_OUT.bcs` in a model with only one domain or `input_file_name_OUT_#.bcs` in a model with multiple domains, with `#` the number of each domain with an outflow boundary condition. Each file contains a matrix of numbers with the following information calculated at the last point of the domain: time (s) in the first column; $\rho c W_\mathrm{f}$ (Pa) in the second, with ρ blood density, c pulse wave velocity, and W_f the forward characteristic variable; $-\rho c W_\mathrm{b}$ (Pa) in the third, with W_b the backward characteristic variable; $W_\mathrm{f}/2$ (m s^{-1}) in the fourth; $W_\mathrm{b}/2$ (m s^{-1}) in the fifth; and $-W_\mathrm{b}/W_\mathrm{f}$ in the sixth. These information was used in [21] to study the effect of outflow boundary conditions on the shape of the pressure and flow waveforms.

5. *Average parameters file*: It is a single file obtained using the flag `-R`. It is called `input_file_name.avg` and contains the space-average information described in the header and in [22].

The Fontan model simulation described in Section 3.3.4 produces a `.fo`-type output file with the same name as that of the input file. This file contains the 16 columns described in Table 1.

Table 1: Variables stored in a .fo-type file during the Fontan circulation model simulation.

Column	Variable	Description
1	t (s)	Simulation time
2	P_{a1} (mmHg)	Pressure in the arterioles of the upper body
3	P_{v1} (mmHg)	Pressure in the venules of the upper body
4	P_{a2} (mmHg)	Pressure in the arterioles of the lower body
5	P_{v2} (mmHg)	Pressure in the venules of the lower body
6	V_{V} (mL)	Ventricular volume
7	Q_{AAo} (mL s^{-1})	Flow through the aortic valve (AoV)
8	ζ_{AoV} (–)	AoV opening state (0 = completely closed; 1 = completely open)
9	V_{A} (mL)	Atrial volume
10	Q_{AVV} (mL s^{-1})	Flow through the atrioventricular valve (AVV)
11	ζ_{AVV} (–)	AVV opening state (0 = completely closed; 1 = completely open)
12	V_{blood} (mL)	Blood volume in the model
13	Q_{PA} (mL s^{-1})	Blood flow through the pulmonary arteries
14	P_{AAo} (mmHg)	Aortic pressure (at the ascending aorta)
15	P_{V} (mmHg)	Ventricular pressure
16	P_{A} (mmHg)	Atrial pressure

6 Examples

We provide input files for the following examples of 1-D simulations, as described in our peer-reviewed publications. These can be found in the folder `nektar/examples/`. At the end of each file, you will find the command line needed to execute the simulation.

`55art/` – Model of the 55 larger systemic arteries in the human under normal physiological conditions [2]. Two input files are provided: cd55art_elas.in simulates the arterial wall as a purely-elastic material and `55art.in` as a visco-elastic material.

`116art/` – Models of the 116 larger systemic arteries in the human under normal physiological conditions for the 25 and 65 year-old baseline virtual subjects described in [13]. The input files are called `116art_25yo.in` and `116art_65yo.in`, respectively.

`Adan56/` – Model of the 56 larger systemic arteries in the human described in [8]. The input file is called `adan77.in` (77 indicates the number of domains used in the Nektar1D simulation).

`AoBif/` – Model of the human aortic bifurcation described in [8, 10]. The following cases are provided: `AoBif.in` (reflective boundary condition); `AoBif_abs.in` (absorbent boundary condition); and `AoBif_vw.in` (visco-elastic arterial wall case; reflective boundary condition).

`Aorta/` – Model of the human upper thoracic aorta described in [8, 10]. The following cases are provided: `Ao.in` (mechanical properties described using the stiffness parameter β); `Ao_Eh.in` (mechanical properties described using the stiffness parameter Eh); `Ao_vw.in` (visco-elastic arterial wall case; mechanical properties described using the stiffness parameter Eh); and `Ao_Beta_vw.in` (visco-elastic arterial wall case; mechanical properties described using the stiffness parameter Eh).

`CCA/` – Model of the human common carotid artery described in [8, 10]. The following cases are provided: `CCA.in` (purely-elastic arterial wall case; mechanical properties described using the stiffness parameter Eh); `CCA_Beta.in` (purely-elastic arterial wall case; mechanical properties described using the stiffness parameter β); `CCA_vw.in` (visco-elastic arterial wall case; mechanical properties described using the stiffness parameter β); `CCA_vw_mesh.in` (visco-elastic arterial wall case with Γ described in *Mesh Definition*; mechanical properties described using the stiffness parameter Eh); `CCA_Beta_vw.in` (visco-elastic arterial wall case; mechanical properties described using the stiffness parameter β); and `CCA_Beta_vw_mesh.in` (visco-elastic arterial wall case with Γ described in *Mesh Definition*; mechanical properties described using the stiffness parameter β).

`CCA_Stn/` – Model of the human common carotid artery with a stenosis described in [7].

`CoW/` – Model of the upper thoracic aorta and larger arteries of the upper body, including the circle of Willis. The following cases are provided: `CoW.in` (purely elastic arterial wall model published in [23]); and `CoW_AutoReg.in` (model with cerebral autoregulation described in [16]).

`Experimental/` – 37-artery network simulating blood flow in the cardiovascular simulator rig described in [3, 8]. The following cases are provided: `exp37.in` (purely elastic arterial wall case) and `exp37_vw.in` (visco-elastic arterial wall case).

`FMD/` – Model of the 116 larger systemic arteries in the human coupled to a flow-mediated dilation model, as described in [17]. The input file is called `FMD.in` .

`Fontan/` – Patient-specific, closed-loop, 1-D/0-D model of the Fontan circulation of a 10-year-old, anesthetized patient with hypoplastic left heart syndrome [5]. The input file is called `Fontan.in` .

`Pulse/` – Single pulse propagation in a straight reflection-free vessel as described in [8, 23]. The following cases are provided: `Pulse.in` (inviscid fluid and inviscid wall); `Pulse_sym.in` (inviscid fluid and inviscid wall, with the pulse wave propagated from the outlet); `Pulse_vf.in` (viscous fluid and inviscid wall); `Pulse_vf_sym.in` (viscous fluid and inviscid wall, with the pulse wave propagated from the outlet); `Pulse_vw.in` (viscous wall and inviscid fluid); `Pulse_vw_Mesh.in` (viscous wall and inviscid fluid, with geometrical and material properties defined in 'Mesh definition'); `Pulse_vw_sym.in` (viscous wall and inviscid fluid, with the pulse wave propagated from the outlet); `Pulses.in` (inviscid fluid and inviscid wall with a pulse prescribed at the inlet and another at the outlet) and `Pulses_vw.in` (inviscid fluid and viscous wall with a pulse prescribed at the inlet and another at the outlet).

`Rabbit/` – Model of the 59 larger systemic arteries in the rabbit described in [6]. The input file is called `Rabbit.in` .

`Sine/` – Propagation of a single frequency, sinusoidal wave in a straight reflection-free vessel for which an analytical solution exists [23]. The following cases are provided: `Sine.in` (inviscid fluid and inviscid wall); `Sine_vf.in` (viscous fluid and inviscid wall); and `Sine_vw.in` (viscous wall and inviscid fluid).

7 Source Code Structure

The main functions of the code are located in `nektar/1DBio/src/main.C`, and the input file is read by functions in `nektar/1DBio/src/setup.C` . The header files are located in `nektar/1DBio/include`, and the external libraries are in `nektar/Hlib` and `nektar/Veclib`.

References

[1] Alastruey J, *et al.* Arterial pulse wave modelling and analysis for vascular age studies: a review from VascAgeNet. *Am. J. Physiol. Heart Circ. Physiol.* 2023; **325**:H1–H29.

[2] Alastruey J, Parker K, Sherwin S. *Arterial pulse wave haemodynamics. In Anderson (Ed.) 11th International Conference on Pressure Surges*, chap. 7. Virtual PiE Led t/a BHR Group (ISBN: 978 1 85598 133 1), 2012; 401–442.

[3] Alastruey J, Khir A, Matthys K, Segers P, Sherwin S, Verdonck P, Parker K, Peiró J. Pulse wave propagation in a model human arterial network: Assessment of 1-D visco-elastic simulations against *in vitro* measurements. *J. Biomech.* 2011; **44**:2250–2258.

[4] Alastruey J, Xiao N, Fok H, Schaeffter T, Figueroa C. On the impact of modelling assumptions in multi-scale, subject-specific models of aortic haemodynamics. *J. R. Soc. Interface* 2016; **13**:1–17.

[5] Aramburu J, Ruijsink B, Chabiniok R, Pushparajah K, Alastruey J. Patient-specific closed-loop model of the Fontan circulation: Calibration and validation. *Heliyon* 2024; **10**:e30 404.

[6] Alastruey J, Nagel S, Nier B, Hunt A, Weinberg P, Peiró J. Modelling pulse wave propagation in the rabbit systemic circulation to assess the effects of altered nitric oxide synthesis. *J. Biomech.* 2009; **42**:2116–2123.

[7] Jin W, Alastruey J. Arterial pulse wave propagation across stenoses and aneurysms: Assessment of 1-D simulations against 3-D simulations and in vitro measurements. *J. R. Soc. Interface* 2021; **18**(20200881):1–17.

[8] Boileau E, Nithiarasu P, Blanco P, Müller L, Fossan F, Hellevik L, Donders W, Huberts W, Willemet M, Alastruey J. A benchmark study of numerical schemes for one-dimensional arterial blood flow modelling. *Int. J. Numer. Meth. Biomed. Eng.* 2015; **31**:1–31, doi:10.1002/cnm.2732.

[9] Flores J, Alastruey J, Poire EC. A novel analytical approach to pulsatile blood flow in the arterial network. *Ann. Biomed. Eng.* 2016; **44**:3047–3068.

[10] Xiao N, Alastruey J, Figueroa C. A systematic comparison between 1-D and 3-D hemodynamics in compliant arterial models. *Int. J. Numer. Meth. Biomed. Eng.* 2014; **30**:204–231.

[11] Hong J, Nandi M, Charlton P, Alastruey J. Noninvasive hemodynamic indices of vascular aging: an in silico assessment. *Am. J. Physiol. Heart Circ. Physiol.* 2023; **325**:H1290–H130.

[12] Wang T, Jin W, Liang F, Alastruey J. Machine learning-based pulse wave analysis for early detection of abdominal aortic aneurysms using in silico pulse waves. *Symmetry* 2021; **13(5)**:804.

[13] Charlton P, Mariscal-Harana J, Vennin S, Li Y, Chowienczyk P, Alastruey J. Modeling arterial pulse waves in healthy aging: a database for in silico evaluation of hemodynamics and pulse wave indexes. *Am. J. Physiol. Heart Circ. Physiol.* 2019; **317**:H1062–H1085.

[14] Willemet M, Alastruey J. Arterial pressure and flow wave analysis using time-domain 1-D hemodynamics. *Ann. Biomed. Eng.* 2015; **43**:190–206.

[15] Caforio F, Augustin C, Alastruey J, Gsell M, Plank G. A coupling strategy for a first 3D-1D model of the cardiovascular system to study the effects of pulse wave propagation on cardiac function. *Comput. Mech.* 2022; **70**:703–722.

[16] Alastruey J, Moore S, Parker K, David T, Peiró J, Sherwin S. Reduced modelling of blood flow in the cerebral circulation: Coupling 1-D, 0-D and cerebral auto-regulation models. *Int. J. Numer. Meth. Fluids* 2008; **56**:1061–1067.

[17] Jin W, Chowienczyk P, Alastruey J. An in silico simulation of flow-mediated dilation reveals that blood pressure and other factors may influence the response independent of endothelial function. *Am. J. Physiol. Heart Circ. Physiol.* 2020; **318**:H1337–H1345.

[18] Reymond P, Merenda F, Perren F, Rüfenacht D, Stergiopulos N. Validation of a one-dimensional model of the systemic arterial tree. *Am. J. Physiol. Heart Circ. Physiol.* 2009; **297**:H208–H222.

[19] Alastruey J, Parker K, Peiró J, Byrd S, Sherwin S. Modelling the circle of Willis to assess the effects of anatomical variations and occlusions on cerebral flows. *J. Biomech.* 2007; **40**:1794–1805.

[20] Alastruey J, Parker K, Peiró J, Sherwin S. Lumped parameter outflow models for 1-D blood flow simulations: effect on pulse waves and parameter estimation. *Commun. Comput. Phys.* 2008; **4**:317–336.

[21] Alastruey J, Parker K, Peiró J, Sherwin S. Analysing the pattern of pulse waves in arterial networks: a time-domain study. *J. Eng. Math.* 2009; **64**:331–351.

[22] Alastruey J. On the mechanics underlying the reservoir–excess separation in systemic arteries and their implications for pulse wave analysis. *Cardiov. Eng.* 2010; **10**:176–189.

[23] Alastruey J, Passerini T, Formaggia L, Peiró J. Physical determining factors of the arterial pulse waveform: theoretical analysis and estimation using the 1-D formulation. *J. Eng. Math.* 2012; **77**:19–37.