1 Post-processing in VaMPy

This part of the Vascular Modeling Pypeline is dedicated to post-processing. The main purpose of the script compute_hemodynamic_indices.py is to compute hemodynamic indices such as the wall shear stress and oscillatory shear index, and can be executed by entering the following command:

```
$ python automatedPostProcessing/compute_hemodynamic_indices.py --case [PATH TO RESULTS]/Solutions
```

The main purpose of the script compute_flow_and_simulation_metrics.py is to compute simulation specific parameters, and common metrics within fluid dynamics, and can be executed by entering the following command:

2 Mathematical definitions of computed quantities

Table 1: Quantities of compute_hemodynamic_indices.py

Quantity	Abbreviation/Symbol	Definition	Unit
Wall shear stress	WSS, τ	$\mu \frac{\partial u}{\partial n}$	[Pa]
Time averaged wall shear stress	TAWSS	$\frac{1}{T} \int_0^T \tau \ dt$	[Pa]
Temporal wall shear stress gradient	TWSSG	$\frac{1}{T} \int_0^T \left \frac{\partial \tau}{\partial t} \right dt$	[Pa/s]
Oscillatory shear index	OSI	$\frac{1}{2} \left(1 - \frac{\left \int_0^T \tau dt \right }{\int_0^T \tau dt} \right)$	[-]
Relative residence time	RRT	$\frac{1}{(1-2\cdot \mathrm{OSI})\cdot \mathrm{TAWSS}}$	[1/Pa]
Endothelial cell activation potential	ECAP	$\frac{\mathrm{OSI}}{\mathrm{TAWSS}}$	[1/Pa]

 $Table\ 2:\ Quantities\ of\ {\tt compute_flow_and_simulation_metrics.py}$

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Quantity	Abbreviation/Symbol	Definition	Unit
Turbulent velocity u' $u - \bar{u}$ $[m/s]$ Kinematic viscosity ν ν $\frac{\mu}{\rho}$ $[m^2/s]$ Time interval T User defined $[s]$ Time interval Δt $\frac{T}{N}$ $[s]$ Characteristic edge length $\Delta x, h$ CellDiameter (mesh) $[m]$ Courant–Friedrichs–Lewy condition CFL $[ul\frac{\Delta t}{\Delta x}$ $[-]$ Rate of strain S_{ij} $\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ $[1/s]$ Turbulent rate of strain S_{ij} $\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ $[1/s]$ Absolute rate of strain Strain $V(S_{ij}, S_{ij})$ $[1/s]$ Dissipation \mathcal{E} $2\nu(S_{ij}, S_{ij})$ $[m^2/s^3]$ Kinetic energy KE, E_k $\frac{1}{2}\left(u_x^2 + u_y^2 + u_z^2\right)$ $[m^2/s^3]$ Turbulent kinetic energy TKE, k $\frac{1}{2}\left(u_x^2 + u_y^2 + u_z^2\right)$ $[m^2/s^2]$ Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ $[m/s]$ Generalized length scale ℓ^+ $\frac{u^*\Delta x}{\nu}$ $[-]$ Generalized time scale ℓ^+ $\frac{u^*\Delta x}{\nu}$ $[-]$ Kolmogorov length scale η $\left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}}$ $[m]$ Kolmogorov time scale τ_η $\left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{2}}$ $[s]$	Velocity	u	$u(x, y, z, t) = (u_x, u_y, u_z)$	[m/s]
Kinematic viscosity $\nu \qquad \frac{\mu}{\rho} \qquad [\text{m}^2/\text{s}]$ Time interval $T \qquad \text{User defined} \qquad [s]$ Time step $\Delta t \qquad \frac{T}{N} \qquad [s]$ Characteristic edge length $\Delta x, h \qquad \text{CellDiameter (mesh)} \qquad [m]$ Courant–Friedrichs–Lewy condition $\text{CFL} \qquad u \frac{\Delta t}{\Delta x} \qquad [\cdot]$ Rate of strain $S_{ij} \qquad \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \qquad [1/s]$ Turbulent rate of strain $S_{ij} \qquad \frac{1}{2} \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right) \qquad [1/s]$ Absolute rate of strain $S_{train} \qquad \nabla \langle S_{ij}, S_{ij} \rangle \qquad [1/s]$ Dissipation $\mathcal{E} \qquad 2\nu \langle S_{ij}, S_{ij} \rangle \qquad [m^2/s^3]$ Turbulent dissipation $\mathcal{E} \qquad 2\nu \langle S_{ij}, S_{ij} \rangle \qquad [m^2/s^3]$ Kinetic energy $\text{KE}, E_k \qquad \frac{1}{2} \left(u_x^2 + u_y^2 + u_z^2 \right) \qquad [m^2/s^2]$ Turbulent kinetic energy $\text{TKE}, k \qquad \frac{1}{2} \left(u_x^2 + u_y^2 + u_z^2 \right) \qquad [m^2/s^2]$ Friction velocity $u^*, u_\tau \qquad \sqrt{\nu S_{ij}} \qquad [m]s$ Generalized length scale $\ell^+ \qquad \frac{u^* \Delta x}{\nu} \qquad [\cdot]$ Generalized time scale $\ell^+ \qquad \frac{u^* \Delta x}{\nu} \qquad [\cdot]$ Kolmogorov length scale $\eta \qquad \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{2}} \qquad [m]$ Kolmogorov time scale $\tau_\eta \qquad \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{2}} \qquad [m]$	Mean velocity	$ar{u}, u_{ ext{mean}}$	$\frac{1}{T} \int_0^T u dt$	[m/s]
Time interval T User defined [s] Time step Δt $\frac{T}{N}$ [s] Characteristic edge length $\Delta x, h$ CellDiameter (mesh) [m] Courant–Friedrichs–Lewy condition CFL $ u \frac{\Delta t}{\Delta x}$ [-] Rate of strain S_{ij} $\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ [1/s] Turbulent rate of strain S_{ij} $\frac{1}{2}\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)$ [1/s] Absolute rate of strain S_{ij} $\frac{1}{2}\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)$ [1/s] Dissipation \mathcal{E} $2\nu\langle S_{ij}, S_{ij}\rangle$ [m²/s³] Turbulent dissipation \mathcal{E} $2\nu\langle S_{ij}, S_{ij}\rangle$ [m²/s³] Kinetic energy KE, E_k $\frac{1}{2}\left(u_x^2 + u_y^2 + u_z^2\right)$ [m²/s²] Turbulent kinetic energy TKE, k $\frac{1}{2}\left(u_x^2 + u_y^2 + u_z^2\right)$ [m²/s²] Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ [m/s] Generalized length scale ℓ^+ $\frac{u^*\Delta x}{\nu}$ [-] Generalized time scale ℓ^+ $\frac{u^*\Delta x}{\nu}$ [-] Kolmogorov length scale η $\left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}}$ [m] Kolmogorov time scale τ_η $\left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}}$ [m]	Turbulent velocity	u'	$u - \bar{u}$	[m/s]
Time step $\Delta t \qquad \frac{T}{N} \qquad [s]$ Characteristic edge length $\Delta x, h \qquad \text{CellDiameter (mesh)} \qquad [m]$ Courant–Friedrichs–Lewy condition CFL $ u \frac{\Delta t}{\Delta x} \qquad [-]$ Rate of strain $S_{ij} \qquad \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \qquad [1/s]$ Turbulent rate of strain $S_{ij} \qquad \frac{1}{2} \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right) \qquad [1/s]$ Absolute rate of strain $S_{train} \qquad S_{train} \qquad \sqrt{\langle S_{ij}, S_{ij} \rangle} \qquad [n]^2/s^3]$ Dissipation $\mathcal{E} \qquad 2\nu \langle S_{ij}, S_{ij} \rangle \qquad [m^2/s^3]$ Turbulent dissipation $\mathcal{E} \qquad 2\nu \langle S_{ij}, S_{ij} \rangle \qquad [m^2/s^3]$ Kinetic energy $KE, E_k \qquad \frac{1}{2} \left(u_x'^2 + u_y'^2 + u_z'^2 \right) \qquad [m^2/s^2]$ Turbulent kinetic energy $TKE, k \qquad \frac{1}{2} \left(u_x'^2 + u_y'^2 + u_z'^2 \right) \qquad [m^2/s^2]$ Friction velocity $u^*, u_\tau \qquad \sqrt{\nu S_{ij}} \qquad [m/s]$ Generalized length scale $\ell^+ \qquad \frac{u^* \Delta x}{\nu} \qquad [-]$ Generalized time scale $\ell^+ \qquad \frac{u^* \Delta x}{\nu} \qquad [-]$ Kolmogorov length scale $\eta \qquad \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}} \qquad [m]$ Kolmogorov time scale $\tau_\eta \qquad \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{2}} \qquad [s]$	Kinematic viscosity	ν	$rac{\mu}{ ho}$	$[\mathrm{m}^2/\mathrm{s}]$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Time interval	T	User defined	[s]
Courant–Friedrichs–Lewy condition CFL $ u \frac{\Delta t}{\Delta x}$ [-] Rate of strain S_{ij} $\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$ [1/s] Turbulent rate of strain s_{ij} $\frac{1}{2}\left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i}\right)$ [1/s] Absolute rate of strain Strain $\sqrt{\langle S_{ij}, S_{ij}\rangle}$ [1/s] Dissipation ε $2\nu\langle S_{ij}, S_{ij}\rangle$ [m²/s³] Turbulent dissipation ε $2\nu\langle s_{ij}, s_{ij}\rangle$ [m²/s³] Kinetic energy KE, E_k $\frac{1}{2}\left(u_x^2 + u_y^2 + u_z^2\right)$ [m²/s²] Turbulent kinetic energy TKE, k $\frac{1}{2}\left(u_x'^2 + u_y'^2 + u_z'^2\right)$ [m²/s²] Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ [m/s] Generalized length scale ℓ^+ $\frac{u^*\Delta x}{\nu}$ [-] Generalized time scale τ^+ $\frac{u^*\Delta x}{\nu}$ [-] Kolmogorov length scale $\tau^ \frac{(\nu^3)^{\frac{1}{4}}}{\varepsilon}$ [n] Kolmogorov time scale $\tau^ \frac{(\nu^3)^{\frac{1}{4}}}{\varepsilon}$ [s]	Time step	Δt	$rac{T}{N}$	[s]
Rate of strain S_{ij} $\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ [1/s] Turbulent rate of strain s_{ij} $\frac{1}{2} \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right)$ [1/s] Absolute rate of strain S_{train} $\sqrt{\langle S_{ij}, S_{ij} \rangle}$ [1/s] Dissipation ε $2\nu \langle S_{ij}, S_{ij} \rangle$ [m²/s³] Turbulent dissipation ε $2\nu \langle S_{ij}, S_{ij} \rangle$ [m²/s³] Kinetic energy KE, E_k $\frac{1}{2} \left(u_x^2 + u_y^2 + u_z^2 \right)$ [m²/s²] Turbulent kinetic energy TKE, k $\frac{1}{2} \left(u_x'^2 + u_y'^2 + u_z'^2 \right)$ [m²/s²] Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ [m/s] Generalized length scale ℓ^+ $\frac{u^* \Delta x}{\nu}$ [-] Kolmogorov length scale η $\left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}}$ [m] Kolmogorov time scale τ_η $\left(\frac{\nu}{\varepsilon} \right)^{\frac{1}{2}}$ [s]	Characteristic edge length	$\Delta x, h$	CellDiameter(mesh)	[m]
Turbulent rate of strain $s_{ij} = \frac{1}{2} \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right) \qquad [1/s]$ Absolute rate of strain $Strain = \sqrt{\langle S_{ij}, S_{ij} \rangle} \qquad [1/s]$ Dissipation $\mathcal{E} = 2\nu \langle S_{ij}, S_{ij} \rangle \qquad [m^2/s^3]$ Turbulent dissipation $\mathcal{E} = 2\nu \langle S_{ij}, S_{ij} \rangle \qquad [m^2/s^3]$ Kinetic energy $KE, E_k = \frac{1}{2} \left(u_x^2 + u_y^2 + u_z^2 \right) \qquad [m^2/s^2]$ Turbulent kinetic energy $TKE, k = \frac{1}{2} \left(u_x'^2 + u_y'^2 + u_z'^2 \right) \qquad [m^2/s^2]$ Friction velocity $u^*, u_\tau = \sqrt{\nu S_{ij}} \qquad [m/s]$ Generalized length scale $\ell^+ = \frac{u^* \Delta x}{\nu} \qquad [-]$ Generalized time scale $\ell^+ = \frac{u^* \Delta x}{\nu} \qquad [-]$ Kolmogorov length scale $\eta = \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}} \qquad [m]$ Kolmogorov time scale $\tau_\eta = \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{2}} \qquad [s]$	Courant–Friedrichs–Lewy condition	CFL	$ u rac{\Delta t}{\Delta x}$	[-]
Absolute rate of strain Strain	Rate of strain	S_{ij}	$\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$	[1/s]
Dissipation \mathcal{E} $2\nu\langle S_{ij}, S_{ij}\rangle$ $[\mathrm{m}^2/\mathrm{s}^3]$ Turbulent dissipation ε $2\nu\langle s_{ij}, s_{ij}\rangle$ $[\mathrm{m}^2/\mathrm{s}^3]$ Kinetic energy KE , E_k $\frac{1}{2}\left(u_x^2+u_y^2+u_z^2\right)$ $[\mathrm{m}^2/\mathrm{s}^2]$ Turbulent kinetic energy TKE , k $\frac{1}{2}\left(u_x'^2+u_y'^2+u_z'^2\right)$ $[\mathrm{m}^2/\mathrm{s}^2]$ Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ $[\mathrm{m}/\mathrm{s}]$ Generalized length scale ℓ^+ $\frac{u^*\Delta x}{\nu}$ $[\cdot]$ Generalized time scale t^+ $\frac{u^*2\Delta t}{\nu}$ $[\cdot]$ Kolmogorov length scale η $\left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}}$ $[\mathrm{m}]$ Kolmogorov time scale τ_η $\left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}}$ $[\mathrm{s}]$	Turbulent rate of strain	s_{ij}	$\frac{1}{2} \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right)$	[1/s]
Turbulent dissipation ε $2\nu \langle s_{ij}, s_{ij} \rangle$ $[\text{m}^2/\text{s}^3]$ Kinetic energy KE, E_k $\frac{1}{2} \left(u_x^2 + u_y^2 + u_z^2 \right)$ $[\text{m}^2/\text{s}^2]$ Turbulent kinetic energy TKE, k $\frac{1}{2} \left(u_x'^2 + u_y'^2 + u_z'^2 \right)$ $[\text{m}^2/\text{s}^2]$ Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ $[\text{m/s}]$ Generalized length scale ℓ^+ $\frac{u^* \Delta x}{\nu}$ $[-]$ Generalized time scale t^+ $\frac{u^{*2} \Delta t}{\nu}$ $[-]$ Kolmogorov length scale η $\left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}}$ $[\text{m}]$ Kolmogorov time scale τ_η $\left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}}$ $[\text{s}]$	Absolute rate of strain	Strain	$\sqrt{\langle S_{ij}, S_{ij} angle}$	[1/s]
Kinetic energy KE, E_k $\frac{1}{2} \left(u_x^2 + u_y^2 + u_z^2 \right)$ $[\text{m}^2/\text{s}^2]$ Turbulent kinetic energy TKE, k $\frac{1}{2} \left(u_x'^2 + u_y'^2 + u_z'^2 \right)$ $[\text{m}^2/\text{s}^2]$ Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ $[\text{m/s}]$ Generalized length scale ℓ^+ $\frac{u^* \Delta x}{\nu}$ $[\cdot]$ Generalized time scale t^+ $\frac{u^{*2} \Delta t}{\nu}$ $[\cdot]$ Kolmogorov length scale η $\left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}}$ $[\text{m}]$ Kolmogorov time scale τ_η $\left(\frac{\nu}{\varepsilon} \right)^{\frac{1}{2}}$ $[\text{s}]$	Dissipation	${\cal E}$	$2\nu\langle S_{ij}, S_{ij}\rangle$	$[\mathrm{m}^2/\mathrm{s}^3]$
Turbulent kinetic energy TKE, k $\frac{1}{2} \left(u_x'^2 + u_y'^2 + u_z'^2 \right) [m^2/s^2]$ Friction velocity u^*, u_τ $\sqrt{\nu S_{ij}}$ $[m/s]$ Generalized length scale ℓ^+ $\frac{u^* \Delta x}{\nu}$ $[-]$ Generalized time scale t^+ $\frac{u^{*2} \Delta t}{\nu}$ $[-]$ Kolmogorov length scale η $\left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}}$ $[m]$ Kolmogorov time scale τ_η $\left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}}$ $[s]$	Turbulent dissipation	arepsilon	$2\nu\langle s_{ij},s_{ij}\rangle$	$[\mathrm{m}^2/\mathrm{s}^3]$
Friction velocity u^{\star}, u_{τ} $\sqrt{\nu S_{ij}}$ $[\text{m/s}]$ Generalized length scale ℓ^{+} $\frac{u^{\star} \Delta x}{\nu}$ $[\cdot]$ Generalized time scale t^{+} $\frac{u^{\star^{2} \Delta t}}{\nu}$ $[\cdot]$ Kolmogorov length scale η $\left(\frac{\nu^{3}}{\varepsilon}\right)^{\frac{1}{4}}$ $[\text{m}]$ Kolmogorov time scale τ_{η} $\left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}}$ $[\text{s}]$	Kinetic energy	KE, E_k	$\frac{1}{2}\left(u_x^2 + u_y^2 + u_z^2\right)$	$[\mathrm{m}^2/\mathrm{s}^2]$
Generalized length scale $\ell^{+} \qquad \frac{u^{\star}\Delta x}{\nu} \qquad [-]$ Generalized time scale $t^{+} \qquad \frac{u^{\star^{2}\Delta t}}{\nu} \qquad [-]$ Kolmogorov length scale $\eta \qquad \left(\frac{\nu^{3}}{\varepsilon}\right)^{\frac{1}{4}} \qquad [m]$ Kolmogorov time scale $\tau_{\eta} \qquad \left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}} \qquad [s]$	Turbulent kinetic energy	TKE, k	$\frac{1}{2} \left({u_x'}^2 + {u_y'}^2 + {u_z'}^2 \right)$	$[\mathrm{m}^2/\mathrm{s}^2]$
Generalized time scale $t^{+} \qquad \frac{u^{\star 2}\Delta t}{\nu} \qquad [-]$ Kolmogorov length scale $\eta \qquad \left(\frac{\nu^{3}}{\varepsilon}\right)^{\frac{1}{4}} \qquad [m]$ Kolmogorov time scale $\tau_{\eta} \qquad \left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}} \qquad [s]$	Friction velocity	$u^{\star}, u_{ au}$	$\sqrt{ u S_{ij}}$	[m/s]
Kolmogorov length scale $\eta \qquad \qquad \left(\frac{\nu^3}{\varepsilon}\right)^{\frac{1}{4}} \qquad \qquad [m]$ Kolmogorov time scale $\tau_{\eta} \qquad \qquad \left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}} \qquad \qquad [s]$	Generalized length scale	ℓ^+	$\frac{u^{\star}\Delta x}{\nu}$	[-]
Kolmogorov time scale $ au_{\eta}$ $\left(\frac{\nu}{\varepsilon}\right)^{\frac{1}{2}}$ [s]	Generalized time scale	t^+	$\frac{u^{\star 2}\Delta t}{\nu}$	[-]
1	Kolmogorov length scale	η	$\left(rac{ u^3}{arepsilon} ight)^{rac{1}{4}}$	[m]
Kolmogorov velocity scale u_{η} $(\varepsilon \nu)^{\frac{1}{4}}$ $[\mathrm{m/s}]$	Kolmogorov time scale	$ au_\eta$	$\left(rac{ u}{arepsilon} ight)^{rac{1}{2}}$	[s]
	Kolmogorov velocity scale	u_{η}	$(arepsilon u)^{rac{1}{4}}$	[m/s]