DOCUMENTATION

Time-averaged simulations results for bi-phasic blood flow simulations in realistic microvascular networks for various single- and multi-capillary occlusion scenarios.

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Related references:

The data set is published in context with the manuscript: [1] *The severity of microstrokes depends on local vascular topology and baseline perfusion*. F Schmid, G Conti, P Jenny and B Weber. eLife. 2021. Doi: 10.7554/eLife.60208

The bi-phasic blood flow simulations have been performed in realistic microvascular networks (MVNs) from the mouse somatosensory cortex first published in:

[2] *The cortical angiome: an interconnected vascular network with noncolumnar patterns of blood flow.* P Blinder, PS Tsai, JP Kaufhold, PM Knutsen, H Suhl and D Kleinfeld. Nature Neuroscience. 2013. Doi: 10.1038/nn.3426

The bi-phasic blood flow model for realistic MVNs has first been published in: [3] *Depth-dependent flow and pressure characteristics in cortical microvascular networks*. F Schmid, PS Tsai, D Kleinfeld, P Jenny and B Weber. PLoS Computational Biology. 2017. Doi: 10.1371/journal.pcbi.1005392

For further information on how to perform bi-phasic blood flow simulation, please contact the corresponding authors of [1] or [3].

Requirements (software):

All simulations and analyses have been performed in Python 2.7. To execute the analysis script the following python libraries need to be installed: cPickle, python-igraph, pandas, seaborn, scipy. The individual analyses script can then be executed by in Python (e.g. "python plot_Figure3.py").

Content:

All folders are stored as compressed archives (*.tar.bz2). On unix-based system the folders can be unpacked by: tar -jxf ARCHIVE_NAME

Time-averaged simulation results (python dictionaries stored as python 2.7 pickle files):

SimulationResults_Baseline.tar.bz2: Folders: MVN1, MVN2

Content: verticesDict_baseline.pkl, edgesDict_baseline.pkl, pathsDict_allPaths_from_DA_to_AV_mainBranch.pkl (generated from prepare_Figure4.py), data_spatial_distribution_AVfactor.pkl (generated from plot_Figure4.py)

SimulationResults_SingleCapillaryOcclusions.tar.bz2:

Folders: 1-in-1-out, 1-in-2-out, 2-in-1-out, 2-in-2-out, 2-in-2-out_high, 2-in-2-out_AL1, 2-in-2-out_AL2, 2-in-2-out_AL3, 2-in-2-out_AL4, 2-in-2-out_AL5, 2-in-2-out_closeToDA, 2-in-2-out_farFromDA Content: verticesDict_baseline.pkl, edgesDict_baseline.pkl, pathsDict_allPaths_from_DA_to_AV_mainBranch_vertexBased.pkl (only folders: 1-in-1-out, 1-in-2-out, 2-in-1-out, 2-in-2-out)

 $Simulation Results_MultiCapillaryOcclusions.tar.bz 2:$

Folders: vesselsOccluded_1, vesselsOccluded_3, vesselsOccluded_5, vesselsOccluded_7, vesselsOccluded_9 Content: verticesDict_baseline.pkl, edgesDict_baseline.pkl, pathsDict_allPaths_from_DA_to_AV_mainBranch_vertexBased.pkl Analysis scripts (python 2.7 scripts in folder Analyses_Scripts):

For details on the figure content see [1]. The verticesDict* and the edgesDict* are converted into graph structure (python-igraph) for all analyses. The functionality of python-igraph is used heavily throughout the various analyses.

helperFunctions.py: various functions used by the other analysis scripts plot_Figure1_and_Figure1-supplement_1_a-d.py:

Input: SimulationResults_Baseline/MVN1/edgesDict_baseline.pkl, SimulationResults_Baseline/MVN1/verticesDict_baseline.pkl, SimulationResults SingleCapillarvOcclusion/2-in-2-out/edgesDict.pkl. SimulationResults SingleCapillaryOcclusion/2-in-2-out/verticesDict.pkl, SimulationResults_SingleCapillaryOcclusion/2-in-1-out/edgesDict.pkl, SimulationResults_SingleCapillaryOcclusion/2-in-1-out/verticesDict.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-2-out/edgesDict.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-2-out/verticesDict.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-1-out/edgesDict.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-1-out/verticesDict.pkl Output: Figures/Figure_1/*, Supplementary_Figures/Figure_1-supplement_1_a-d/* plot_Figure2_and_Figure2_supplement_1_a-d.py: Input: SimulationResults_Baseline/MVN1/edgesDict_baseline.pkl, SimulationResults_Baseline/MVN1/verticesDict_baseline.pkl, SimulationResults_SingleCapillaryOcclusion/2-in-2-out/edgesDict.pkl, SimulationResults_SingleCapillaryOcclusion/2-in-2-out/verticesDict.pkl, SimulationResults_SingleCapillaryOcclusion/2-in-1-out/edgesDict.pkl, SimulationResults SingleCapillaryOcclusion/2-in-1-out/verticesDict.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-2-out/edgesDict.pkl, SimulationResults SingleCapillaryOcclusion/1-in-2-out/verticesDict.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-1-out/edgesDict.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-1-out/verticesDict.pkl **Output**: Figures/Figure_2/*, Supplementary_Figures/Figure_2-supplement_1_a-d/* plot_Figure3.py: Input: SimulationResults_Baseline/MVN1/edgesDict_baseline.pkl, SimulationResults_Baseline/MVN1/verticesDict_baseline.pkl,

SimulationResults_MultiCapillaryOcclusion/*/edgesDict.pkl, SimulationResults_MultiCapillaryOcclusion/*/verticesDict.pkl, **Output:** Figures/Figure_3/*

prepare_Figure4.py (long execution time!):

Input: SimulationResults Baseline/MVN*/edgesDict baseline.pkl,

SimulationResults_Baseline/MVN*/verticesDict_baseline.pkl,

Output: SimulationResults_Baseline/MVN*/pathsDict_allPaths_from_DA_to_AV_mainBranch.pkl plot_Figure4.py (long execution time!):

Input: SimulationResults_Baseline/MVN*/*

Output: SimulationResults_Baseline/MVN*/edgesDict_baseline.pkl (attribute Lfactor_median added), SimulationResults_Baseline/MVN*/data_spatial_distribution_AVfactor.pkl, Figures/Figure_4/*

plot_Figure5.py:

Input: SimulationResults_Baseline/MVN*/*

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Output: Figures/Figure_5/*
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plot_Figure6.py:

Input: SimulationResults_Baseline/MVN1/*, SimulationResults_SingleCapillaryOcclusion/2-in-2out/pathsDict_allPaths_from_DA_to_AV_mainBranch_vertexBased.pkl, SimulationResults_SingleCapillaryOcclusion/2-in-1out/pathsDict_allPaths_from_DA_to_AV_mainBranch_vertexBased.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-2out/pathsDict allPaths from DA to AV mainBranch vertexBased.pkl, SimulationResults_SingleCapillaryOcclusion/1-in-1out/pathsDict_allPaths_from_DA_to_AV_mainBranch_vertexBased.pkl **Output:** Figures/Figure_6/*

Attributes stored in python dictionaries:

Baseline:

verticesDict: contains all relevant information and data stored at vertices.

- index: index of vertex
 - pressure: time averaged pressure at vertex [mmHg]
 - inflowE: list of edges delivering blood to the vertex (inflows of the vertex)
- outflowE: list of edges removing blood from the vertex (outflows of the vertex)
- coords: coordinates of the vertex $[\mu m]$
- pBC: pressure boundary conditions [mmHg], None for internal vertices
- corticalDepth: depth from cortical surface [µm]
- nkind: identifier for the vessel type. 0: pial artery, 1: pial vein, 2: descending arteriole,
 3: ascending vein, 4: capillary

edgesDict: contains all relevant information and data stored at edges.

- diameter: effective vessel diameter [µm]. See [3] for details.
- htd: time averaged discharge hematocrit [-].
- connectivity: tuple of vertex indices which are connected by the edge.
- mainAV: identifier for ascending venule (AV) main brain. 1: is AV main brain, 0: no AV main branch
- mainDA: identifier for descending arteriole (DA) main brain. 1: is DA main brain, 0: no DA main branch
- flow: time averaged flow rate [µm³ ms⁻¹]
- length: tortuous vessel length $[\mu m]$ See [1] and [3] for details.
- tissueVolume: topological tissue volume supplied by vessel [µm³]. See [1] for details.
- nkind: identifier for the vessel type. 0: pial artery, 1: pial vein, 2: descending arteriole,
 3: ascending vein, 4: capillary
- edgesFulfillingSelection: identifier if vessels fulfils selection criteria to qualify for analysis. 1: vessel included for analysis, 0: vessel not included for analysis. Details on the selection criteria are provided in [1].
- htt: time averaged tube hematocrit [-]
- RBCflux: time averaged RBC flux [RBC/s] computed from the discharge hematocrit and the flow rate.
- sign: sign describing the flow direction in the vessel. +: flow direction from source (vertex with lower index) to target (vertex with higher index), -: flow direction from target to source vertex. Based on time averaged pressure values.
- points: list of tortuous vessel coordinates of the edge $[\mu m].$ Starting at the source vertex. Ending at the target vertex.
- Lfactor_median: AV-factor of the vessel. None if no AV-factor can be assigned. See [1] for details. Attribute added by plot_Figure4.py
- pathsDict_allPaths_from_DA_to_AV_mainBranch: contains all flow path from DA main brain to AV main branch. For details see [1].
 - startPoint: list of vertex indices of the end point of the DA
 - endPoint: list of vertex indices of the end point of the AV
 - allPaths: list of lists of vertex indices describing all paths between a the associated startPoint and endPoint.

<u>data_spatial_distribution_AVfactor:</u> contains information on the spatial distribution of venule-sided capillaries (AV-factor > 0.5). For details see [1].

- edges_L_mean_50um: list of all edges for which the average AV-factor in an analysis sphere of 50 μm has been computed.
- resulting_L_mean_50um: average AV-factor for an analysis sphere for 50 μm (see Figure4/AV_factor_delta_analysisSphere50_MVN*.pkl)
- shortest_distance_to_closest_vessel: list of shortest distances to any vessel for all discretization points along all venule sided capillaries.
- shortest_distance_to_Lfactor_lt_05: list of shortest distances to an arteriole-sided capillary (AV-factor < 0.5) for all discretization points along all venule sided capillaries.

Occlusion scenarios (both single- and multi-capillary occlusions): verticesDict:

- index: index of vertex
- coords: coordinates of the vertex [µm]
- pressure_strokeIndex_n: time averaged pressure at vertex [mmHg] for the simulation where edge n has been occluded. For details see [1].

edgesDict:

- htd_strokeIndex_n: time averaged discharge hematocrit [-] for the simulation where edge n has been occluded. For details see [1].
- flow: time averaged flow rate $[\mu m^3\,ms^{\text{-}1}]$ for the simulation where edge n has been occluded. For details see [1].
- RBCflux: time averaged RBC flux [RBC/s] computed from the discharge hematocrit and the flow rate for the simulation where edge n has been occluded. For details see [1].
- htt: time averaged tube hematocrit [-] for the simulation where edge n has been occluded. For details see [1].
- connectivity: tuple of vertex indices which are connected by the edge.
- diameter_strokeIndex_n: effective vessel diameter [μm] for the simulation where edge n has been occluded (only given for multi-capillary occlusions).

<u>pathsDict_allPaths_from_DA_to_AV_mainBranch_vertexBased:</u> contains all flow path from DA main brain to AV main branch (unique vertex sequences). For details see helperFunctions.py \rightarrow function convert_pathsDict_to_unique_vertexSequence.

- startPoint_strokeIndex_n: list of vertex indices of the end point of the DA for the simulation where edge n has been occluded.
- endpoint_strokeIndex_n: list of vertex indices of the end point of the AV for the simulation where edge n has been occluded.
- allPaths_strokeIndex_n: list of lists of vertex indices describing all paths between a the associated startPoint and endpoint for the simulation where edge n has been occluded.