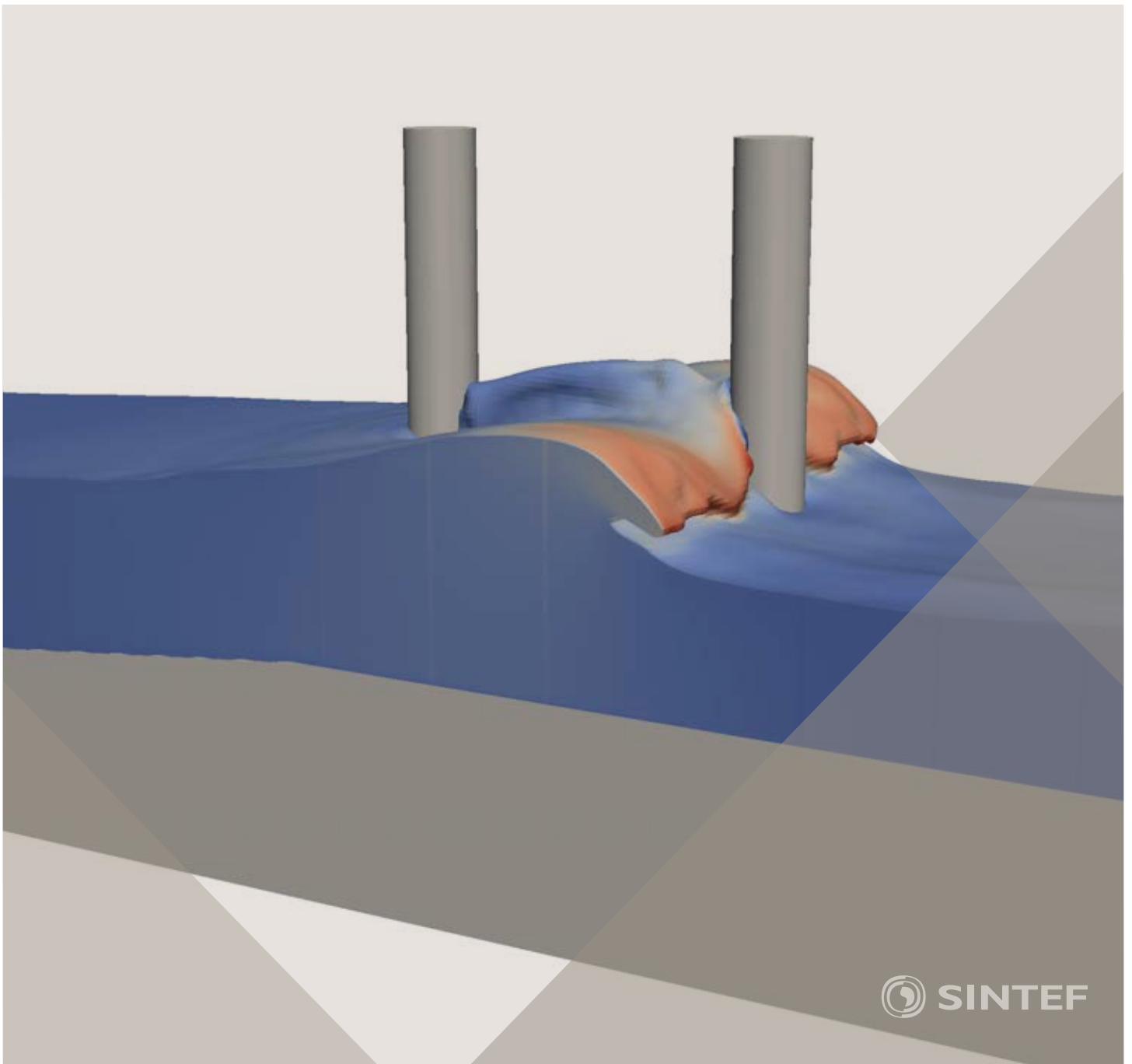


Proceedings of the 12th International Conference on
Computational Fluid Dynamics in the Oil & Gas,
Metallurgical and Process Industries

Progress in Applied CFD – CFD2017



SINTEF Proceedings

Editors:

Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

Proceedings of the 12th International Conference on Computational Fluid Dynamics
in the Oil & Gas, Metallurgical and Process Industries

SINTEF Academic Press

SINTEF Proceedings no 2

Editors: Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

Selected papers from 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Key words:

CFD, Flow, Modelling

Cover, illustration: Arun Kamath

ISSN 2387-4295 (online)

ISBN 978-82-536-1544-8 (pdf)

© Copyright SINTEF Academic Press 2017

The material in this publication is covered by the provisions of the Norwegian Copyright Act. Without any special agreement with SINTEF Academic Press, any copying and making available of the material is only allowed to the extent that this is permitted by law or allowed through an agreement with Kopinor, the Reproduction Rights Organisation for Norway. Any use contrary to legislation or an agreement may lead to a liability for damages and confiscation, and may be punished by fines or imprisonment

SINTEF Academic Press

Address: Forskningsveien 3 B
 PO Box 124 Blindern
 N-0314 OSLO

Tel: +47 73 59 30 00

Fax: +47 22 96 55 08

www.sintef.no/byggforsk

www.sintefbok.no

SINTEF Proceedings

SINTEF Proceedings is a serial publication for peer-reviewed conference proceedings on a variety of scientific topics.

The processes of peer-reviewing of papers published in SINTEF Proceedings are administered by the conference organizers and proceedings editors. Detailed procedures will vary according to custom and practice in each scientific community.

PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen



Organizing committee:

Conference chairman: Prof. Stein Tore Johansen

Conference coordinator: Dr. Jan Erik Olsen

Dr. Bernhard Müller

Dr. Sigrid Karstad Dahl

Dr. Shahriar Amini

Dr. Ernst Meese

Dr. Josip Zoric

Dr. Jannike Solsvik

Dr. Peter Witt

Scientific committee:

Stein Tore Johansen, SINTEF/NTNU

Bernhard Müller, NTNU

Phil Schwarz, CSIRO

Akio Tomiyama, Kobe University

Hans Kuipers, Eindhoven University of Technology

Jinghai Li, Chinese Academy of Science

Markus Braun, Ansys

Simon Lo, CD-adapco

Patrick Segers, Universiteit Gent

Jiyuan Tu, RMIT

Jos Derksen, University of Aberdeen

Dmitry Eskin, Schlumberger-Doll Research

Pär Jönsson, KTH

Stefan Pirker, Johannes Kepler University

Josip Zoric, SINTEF

CONTENTS

PRAGMATIC MODELLING	9
On pragmatism in industrial modeling. Part III: Application to operational drilling	11
CFD modeling of dynamic emulsion stability	23
Modelling of interaction between turbines and terrain wakes using pragmatic approach	29
FLUIDIZED BED	37
Simulation of chemical looping combustion process in a double looping fluidized bed reactor with cu-based oxygen carriers.....	39
Extremely fast simulations of heat transfer in fluidized beds.....	47
Mass transfer phenomena in fluidized beds with horizontally immersed membranes	53
A Two-Fluid model study of hydrogen production via water gas shift in fluidized bed membrane reactors	63
Effect of lift force on dense gas-fluidized beds of non-spherical particles	71
Experimental and numerical investigation of a bubbling dense gas-solid fluidized bed	81
Direct numerical simulation of the effective drag in gas-liquid-solid systems	89
A Lagrangian-Eulerian hybrid model for the simulation of direct reduction of iron ore in fluidized beds.....	97
High temperature fluidization - influence of inter-particle forces on fluidization behavior	107
Verification of filtered two fluid models for reactive gas-solid flows	115
BIOMECHANICS.....	123
A computational framework involving CFD and data mining tools for analyzing disease in carotid artery	125
Investigating the numerical parameter space for a stenosed patient-specific internal carotid artery model.....	133
Velocity profiles in a 2D model of the left ventricular outflow tract, pathological case study using PIV and CFD modeling.....	139
Oscillatory flow and mass transport in a coronary artery.....	147
Patient specific numerical simulation of flow in the human upper airways for assessing the effect of nasal surgery.....	153
CFD simulations of turbulent flow in the human upper airways	163
OIL & GAS APPLICATIONS	169
Estimation of flow rates and parameters in two-phase stratified and slug flow by an ensemble Kalman filter	171
Direct numerical simulation of proppant transport in a narrow channel for hydraulic fracturing application	179
Multiphase direct numerical simulations (DNS) of oil-water flows through homogeneous porous rocks	185
CFD erosion modelling of blind tees	191
Shape factors inclusion in a one-dimensional, transient two-fluid model for stratified and slug flow simulations in pipes	201
Gas-liquid two-phase flow behavior in terrain-inclined pipelines for wet natural gas transportation	207

NUMERICS, METHODS & CODE DEVELOPMENT	213
Innovative computing for industrially-relevant multiphase flows	215
Development of GPU parallel multiphase flow solver for turbulent slurry flows in cyclone.....	223
Immersed boundary method for the compressible Navier–Stokes equations using high order summation-by-parts difference operators	233
Direct numerical simulation of coupled heat and mass transfer in fluid-solid systems	243
A simulation concept for generic simulation of multi-material flow, using staggered Cartesian grids.....	253
A cartesian cut-cell method, based on formal volume averaging of mass, momentum equations.....	265
SOFT: a framework for semantic interoperability of scientific software	273
 POPULATION BALANCE	 279
Combined multifluid-population balance method for polydisperse multiphase flows	281
A multifluid-PBE model for a slurry bubble column with bubble size dependent velocity, weight fractions and temperature.....	285
CFD simulation of the droplet size distribution of liquid-liquid emulsions in stirred tank reactors	295
Towards a CFD model for boiling flows: validation of QMOM predictions with TOPFLOW experiments	301
Numerical simulations of turbulent liquid-liquid dispersions with quadrature-based moment methods.....	309
Simulation of dispersion of immiscible fluids in a turbulent couette flow	317
Simulation of gas-liquid flows in separators - a Lagrangian approach.....	325
CFD modelling to predict mass transfer in pulsed sieve plate extraction columns	335
 BREAKUP & COALESCENCE	 343
Experimental and numerical study on single droplet breakage in turbulent flow	345
Improved collision modelling for liquid metal droplets in a copper slag cleaning process	355
Modelling of bubble dynamics in slag during its hot stage engineering.....	365
Controlled coalescence with local front reconstruction method	373
 BUBBLY FLOWS	 381
Modelling of fluid dynamics, mass transfer and chemical reaction in bubbly flows	383
Stochastic DSMC model for large scale dense bubbly flows.....	391
On the surfacing mechanism of bubble plumes from subsea gas release.....	399
Bubble generated turbulence in two fluid simulation of bubbly flow	405
 HEAT TRANSFER	 413
CFD-simulation of boiling in a heated pipe including flow pattern transitions using a multi-field concept	415
The pear-shaped fate of an ice melting front	423
Flow dynamics studies for flexible operation of continuous casters (flow flex cc).....	431
An Euler-Euler model for gas-liquid flows in a coil wound heat exchanger.....	441
 NON-NEWTONIAN FLOWS.....	 449
Viscoelastic flow simulations in disordered porous media	451
Tire rubber extrudate swell simulation and verification with experiments	459
Front-tracking simulations of bubbles rising in non-Newtonian fluids.....	469
A 2D sediment bed morphodynamics model for turbulent, non-Newtonian, particle-loaded flows.....	479

METALLURGICAL APPLICATIONS.....	491
Experimental modelling of metallurgical processes	493
State of the art: macroscopic modelling approaches for the description of multiphysics phenomena within the electroslag remelting process	499
LES-VOF simulation of turbulent interfacial flow in the continuous casting mold	507
CFD-DEM modelling of blast furnace tapping	515
Multiphase flow modelling of furnace tapholes	521
Numerical predictions of the shape and size of the raceway zone in a blast furnace.....	531
Modelling and measurements in the aluminium industry - Where are the obstacles?	541
Modelling of chemical reactions in metallurgical processes.....	549
Using CFD analysis to optimise top submerged lance furnace geometries	555
Numerical analysis of the temperature distribution in a martensic stainless steel strip during hardening.....	565
Validation of a rapid slag viscosity measurement by CFD.....	575
Solidification modeling with user defined function in ANSYS Fluent.....	583
Cleaning of polycyclic aromatic hydrocarbons (PAH) obtained from ferroalloys plant.....	587
Granular flow described by fictitious fluids: a suitable methodology for process simulations	593
A multiscale numerical approach of the dripping slag in the coke bed zone of a pilot scale Si-Mn furnace.....	599
 INDUSTRIAL APPLICATIONS	 605
Use of CFD as a design tool for a phosphoric acid plant cooling pond	607
Numerical evaluation of co-firing solid recovered fuel with petroleum coke in a cement rotary kiln: Influence of fuel moisture	613
Experimental and CFD investigation of fractal distributor on a novel plate and frame ion-exchanger	621
 COMBUSTION	 631
CFD modeling of a commercial-size circle-draft biomass gasifier.....	633
Numerical study of coal particle gasification up to Reynolds numbers of 1000.....	641
Modelling combustion of pulverized coal and alternative carbon materials in the blast furnace raceway	647
Combustion chamber scaling for energy recovery from furnace process gas: waste to value	657
 PACKED BED.....	 665
Comparison of particle-resolved direct numerical simulation and 1D modelling of catalytic reactions in a packed bed	667
Numerical investigation of particle types influence on packed bed adsorber behaviour	675
CFD based study of dense medium drum separation processes	683
A multi-domain 1D particle-reactor model for packed bed reactor applications.....	689
 SPECIES TRANSPORT & INTERFACES	 699
Modelling and numerical simulation of surface active species transport - reaction in welding processes	701
Multiscale approach to fully resolved boundary layers using adaptive grids.....	709
Implementation, demonstration and validation of a user-defined wall function for direct precipitation fouling in Ansys Fluent.....	717

FREE SURFACE FLOW & WAVES	727
Unresolved CFD-DEM in environmental engineering: submarine slope stability and other applications.....	729
Influence of the upstream cylinder and wave breaking point on the breaking wave forces on the downstream cylinder	735
Recent developments for the computation of the necessary submergence of pump intakes with free surfaces	743
Parallel multiphase flow software for solving the Navier-Stokes equations	752
PARTICLE METHODS	759
A numerical approach to model aggregate restructuring in shear flow using DEM in Lattice-Boltzmann simulations	761
Adaptive coarse-graining for large-scale DEM simulations.....	773
Novel efficient hybrid-DEM collision integration scheme.....	779
Implementing the kinetic theory of granular flows into the Lagrangian dense discrete phase model.....	785
Importance of the different fluid forces on particle dispersion in fluid phase resonance mixers	791
Large scale modelling of bubble formation and growth in a supersaturated liquid.....	798
FUNDAMENTAL FLUID DYNAMICS	807
Flow past a yawed cylinder of finite length using a fictitious domain method	809
A numerical evaluation of the effect of the electro-magnetic force on bubble flow in aluminium smelting process.....	819
A DNS study of droplet spreading and penetration on a porous medium.....	825
From linear to nonlinear: Transient growth in confined magnetohydrodynamic flows.....	831

INVESTIGATING THE NUMERICAL PARAMETER SPACE FOR A STENOSED PATIENT-SPECIFIC INTERNAL CAROTID ARTERY MODEL

Viviana MANCINI¹ & Aslak BERGERSEN², Patrick SEGERS¹, Kristian VALEN-SENDSTAD^{2*}

¹ Ghent University, IBiTech-bioMMeda, 9000 Ghent, BELGIUM

² Simula Research Laboratory, Computational Cardiac Modelling, 1325 Lysaker, NORWAY

* E-mail: kvs@simula.com

ABSTRACT

Systemic risk factors are known to correlate with cardiovascular diseases, but e.g., atherosclerotic plaques are focally distributed and highlight the role of hemodynamically induced forces on vascular remodeling. Computational fluid dynamics (CFD) shows great promise for revealing mechanisms of atherosclerotic plaque progression, but the utility of CFD depends on the robustness of the numerical methods. The aim of the study was to investigate the parameter space of the numerical solutions to understand the resulting flow effects in a stenosed patient-specific internal carotid artery model. Simulations were performed on meshes consisting of 2 to 50M-elements meshes with a kinetic energy-preserving and minimally-dissipative solver, and time step size ranging from $1 \cdot 10^{-4}$ to $5 \cdot 10^{-6}$ seconds. The spatial refinement study revealed large differences in the instantaneous velocity fields, and the coarsest simulation did not provide any meaningful insight into the flow. That being said, the time-averaged results were in acceptable agreement for all spatial and temporal refinement levels. The variations in temporal resolution had minor effects, and the coarsest resolution was found to suffice. In conclusion, even for a highly accurate solver, a relatively high spatial resolution was needed to sufficiently resolve the flow, and we found the 22M-element mesh to offer an optimal balance between computational cost and time-averaged quantities.

Keywords: Stenosis, Computational Fluid Dynamics, Turbulence, Atherosclerotic plaque, Direct Numerical Simulation.

NOMENCLATURE

Latin Symbols

M Million, [-]
 PSD Power spectral density, [m^2/s].

TKE Turbulent kinetic energy, [m^2/s^2]
 $\mathbf{u}(\mathbf{x}, t)$ Instantaneous velocity, [m/s].

Greek Symbols

ν Kinematic viscosity, [m^2/s].
 Δt Time steps size, [s].
 τ Kolmogorov time scale, [s].
 Δx Mesh node spacing, [m].
 η Kolmogorov length scale, [m].
 ε Dissipation rate of TKE, [m^2/s^3].

Sub/superscripts

$\bar{\mathbf{u}}$ Mean velocity component, [m/s].
 \mathbf{u}' Fluctuating velocity component, [m/s].
 $|\mathbf{u}'|$ Magnitude of \mathbf{u}' , [m/s].

INTRODUCTION

Atherosclerotic plaque is a leading cause of death in the western world, and causes a local narrowing of the arterial lumen also known as stenosis. The stenosis severity may increase over time to the point where it completely obstructs the blood flow. It is also known that blood clots can form downstream of the stenoses or that unstable plaques can loosen; both of which can result in ischemic stroke or heart attacks.

Computational fluid dynamics (CFD) shows great potential for revealing mechanisms of atherosclerotic plaque progression, e.g., in the carotid bifurcation by modeling patient-specific local hemodynamic forces (Steinman, 2002). However, the efficacy of CFD depends on the robustness of the methods and ability of reproduce results. This has shown to be challenging, especially for transitional biomedical flows, as demonstrated by Steinmann *et al.* (2012) who reported a large variability of jet penetration and complexity of patient-specific internal carotid artery aneurysm. In particular, it is not uncommon in the biomechanics literature to see the use of first order accurate and stabilized numerical schemes, which are well known to

be far too dissipative (Roache *et al.*, 1986). Such schemes have been argued applicable because of the relatively low Reynolds numbers of cardiovascular flows (Stewart *et al.*, 2012), relative to the transition point for steady flow in an infinitely long pipe (Reynolds, 1883). However, we have previously argued that Reynolds experiments might not be the best point of reference and showed that the use of “black-box” CFD solvers using default settings may be misleading us about the nature of the flow in the cardiovascular system (Valen-Sendstad and Steinman, 2014).

The aim of the current study was to use a verified and validated solver for laminar, transitional, and turbulent flows to find an adequate (under-resolved) direct numerical simulation reference solution from a spatial and temporal refinement study, with respect to point of transition and resolution of the flow instabilities through rigorous analysis, but also to determine the required resolution from a pragmatic biomedical point of view.

MODEL DESCRIPTION

Medical images of a common carotid bifurcation with severe stenosis (82% by area) located in the ICA of a 75 years old man were obtained from computed tomography angiography. The medical image was segmented using 3D Slicer (Iannaccone *et al.*, 2014), to obtain a plausible model of the vasculature. The Vascular Modelling Toolkit (Piccinelli *et al.*, 2009) was used to create meshes with a local refinement in the stenotic- and downstream region, but a constant global refinement between each mesh, resulting in four meshes with mean cell length (Δx) of $3.19 \cdot 10^{-4}$, $2.14 \cdot 10^{-4}$, $1.38 \cdot 10^{-4}$, and $1.05 \cdot 10^{-4}$ m. The meshes consists of 2, 6, 22, and 50 million (M) linear tetrahedral cells, and is referred to as the 2, 6, 22, and 50M-element mesh, respectively.

Simulations were performed using the open-source finite element CFD solver *Oasis* (Mortensen and Valen-Sendstad, 2015), where special care was taken to ensure a kinetic energy-preserving and minimally-dissipative numerical solution. We used continuous Lagrange elements with polynomial degree one for both the velocity, and pressure. The fluid properties were set to mimic water, with kinematic viscosity of $\nu = 1 \cdot 10^{-6}$ m²/s to allow for direct comparison with *in-vitro* experiments. The inlet flow rate was set to be peak systolic, 585.52 ml/min, which corresponds to a Reynolds number of 1550 at the inlet. This deliberate choice was made to enable rigorous assessment of the temporal and spatial resolution with respect to the smallest scales present in the flow, however at the cost of a physiological artificial flow condition. A parabolic velocity profile was prescribed as inlet condition and no-slip condition was set along the walls. Figure 1 shows a curve fit based on work from Groen *et al.* (2010) that measured the flow split between the common and internal carotid artery as a function of degree of stenosis using MRI in 33 patients. The shape of the curve shows that most of the flow resistance occurs in the micro-vasculature for stenosis severity less than 65%, whereas the pressure drop across the stenosis dominates the resistance above this threshold. Using this

model, the flow split between the internal and external carotid artery was set as to 31.8% and 68.2%, respectively.

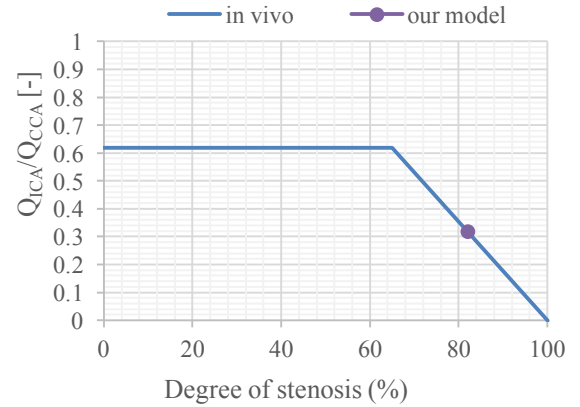


Figure 1: Outflow boundary conditions were set in order to match *in-vivo* values. The model is taken from the work of Groen *et al.* (2010) [10], who measured flow split as a function of degree of stenosis using MRI.

The flow was computed for 2 physical seconds on the coarsest mesh in order to cheaply washout initial transients associated with the artificial initial conditions. This simulation time was then the equivalent of 2 flow-throughs as the length of the model was 0.2 m, and the mean flow at the inlet was 0.1954 m/s. This flow field was then projected onto the 6, 22, and 50M-element meshes as initial conditions. To obtain a velocity field that was statistically converged, the mean velocities were based on simulations from 0.1 to 2.0 seconds. However, due to limitations on CPU hours, the 50M-element simulation was only simulated for 0.7 seconds, and the 22M-element simulation for 1.4 s.

We first performed a spatial refinement study at a fixed time step (Δt) of $2 \cdot 10^{-5}$ seconds. Using the least computationally expensive mesh that gave adequate results, a temporal refinement study was performed, with Δt ranging from $1 \cdot 10^{-4}$ to $5 \cdot 10^{-6}$ seconds.

Figure 2 shows the region of interest with four lines (A to D) and a point *P*, located 1.7 cm (2.2 diameters) downstream of the center of the stenosis, where instantaneous velocity $\mathbf{u}(\mathbf{x}, t)$, was sampled. Reynolds decomposition was used to separate the instantaneous velocity from the time averaged, $\bar{\mathbf{u}}(\mathbf{x})$, and fluctuating, $\mathbf{u}'(\mathbf{x}, t)$, components, i.e., $\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}'$. Taking the fluctuating velocity magnitude signal, $|\mathbf{u}'|$, as input we computed the power spectral density (PSD) using Welch’s method (Welch, 1967) with 32 segments, and a Hanning windowing function with 50 % overlap.

The coherent vortical structures were identified by the Q-criterion, which is a spatial region where the Euclidean norm of the vorticity tensor $\vec{\omega}$ dominates the strain rate tensor \vec{S} (Equation 1) (Hunt *et al.*, 1988).

$$Q = \frac{1}{2} \left[|\vec{\omega}|^2 - |\vec{S}|^2 \right] > 0$$

Equation 1: The comparison between the vorticity and strain rate tensors obtained through decomposition of the velocity gradient can be used as three-dimensional vortex identification criterion.



Figure 2: Region of interest of the model with lines A to D and point *P*. Flow is going from bottom and up, or alternatively, the common carotid artery is branching into the external carotid (left), and internal carotid artery (right), respectively. The center of stenosis is defined as the midpoint of line B, and is based on the minimum area.

RESULTS

We first focus on basic flow features obtained on the 22M-element mesh shown in Figure 3, which depicts the volumetric velocity magnitude within the common carotid artery and ICA. The top of Figure 3 shows that the flow in the common artery is stable up until the carotid bifurcation, as the flow is uniform and there are no visible minor flow structures. At the bifurcation, the flow develops into a skewed profile towards the external wall of the ICA. Moreover, because of the pronounced curvature of the ICA the flow becomes unstable upstream of the stenosis, as observed in the left most bottom part of Figure 3. The stenosis causes the disturbed flow to accelerate into the stenosis, before the jet breaks down into an unstable flow downstream of the stenosis. However, the flow instabilities quickly dissipate further downstream, and the flow relaminarizes.

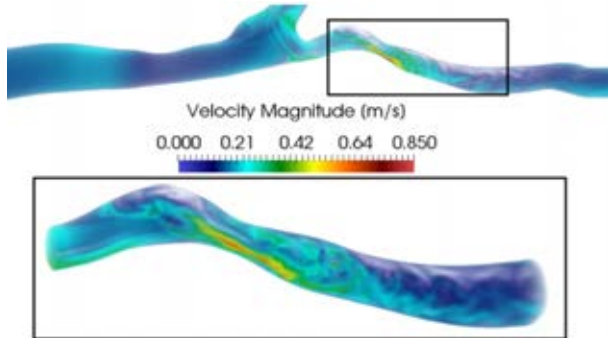


Figure 3: The top shows the volumetric rendering of the instantaneous velocity magnitude in the common and internal carotid arteries, and the bottom part is an enlargement of the box in the top part, showing the stenosis and downstream region.

Firstly, the Q-criterion was used to perform a quantitative comparison of the instantaneous velocity fields as shown in Figure 4. Moving from 2M through 50M there was a consistent increase in the number of vortices. In particular, upstream of the stenosis, the 22 and 50M-element simulations were phenotypically different from the 2 and 6M-element simulations, as there were smaller and more complex structures. In the

downstream region in the 50M-element simulation the vortices were visually easier to see than in the 22M, however we can observe the same type and number of vortices. Visually there are large differences between mesh resolutions based on instantaneous flow fields. Moreover, the 2 and 6M-element simulations does not provide any physical insight into the flow.

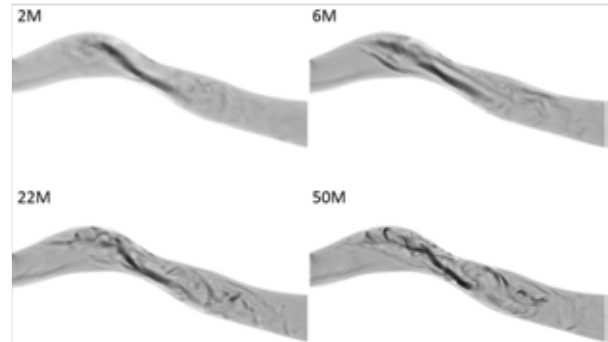


Figure 4: Volumetric rendering of coherent vortical structures at identical times within ICA identified by the Q-criterion.

To further assess the results from the spatial refinement study, we first consider the time-averaged velocities across the lines A to D, shown in Figure 5. In line A, upstream of the stenosis, we observe that the 2 and 6M-element simulations were similar, however relatively different from the 20 and 50M-element simulations which were phenotypically similar.

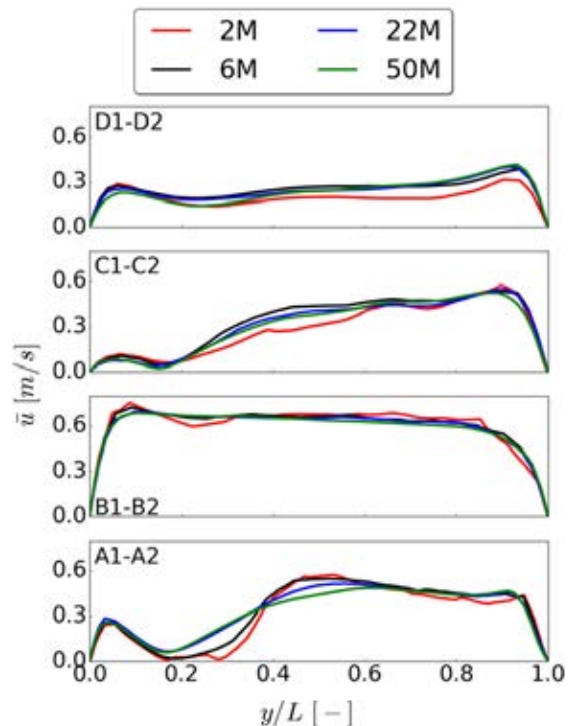


Figure 5: Time-averaged velocity along the four lines of interest for the spatial refinement study.

The time-averaged results were for all practical purposes equal at the stenosis (line B). In line C, when the jet from the stenosis breaks down the 22 and 50M-element simulations were similar, while the 2 and 6M-element simulations were under resolved, and under- and overestimated the centerline velocities, respectively. Finally, in line D at the end of the disturbed flow region, the 2M-element simulation under-estimates the time-

averaged velocity, while the other simulations were similar.

The PSD analysis of the fluctuating velocity signal at point P from Figure 2 is illustrated in Figure 6. The 2, 6, and 22M-element simulation seems to converge towards the 50M-element simulation. The 22 and 50M-element simulations were practically identical up until ~ 2000 Hz, however the spectra differs slightly at the higher frequencies. That being said, the analysis was admittedly based on different time-periods, and we would expect even better agreement if simulated for an equal period of time.

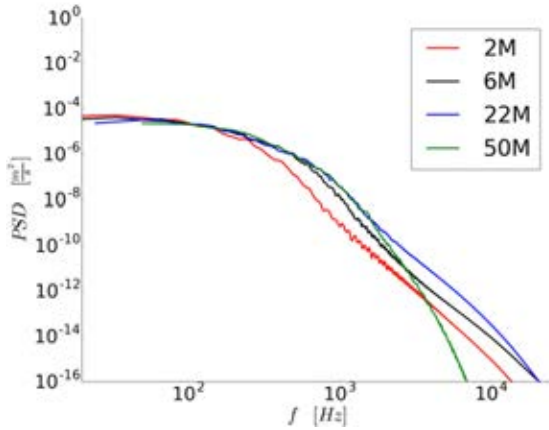


Figure 6: Power spectral density of the velocity field at point P from Figure 2, for the spatial refinement study.

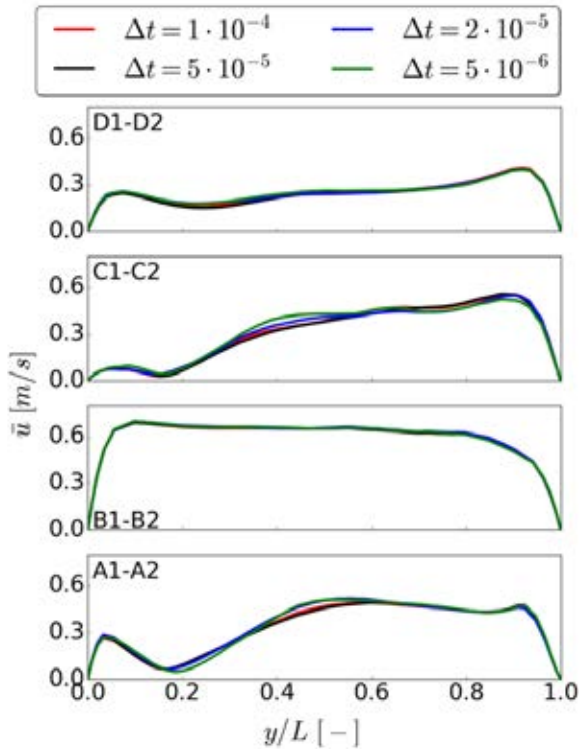


Figure 7: Time-averaged velocity along the four lines of interest for the spatial refinement study.

The temporal refinement study was evaluated similarly to the spatial refinement study. First, we considered the time-averaged velocity in the lines A to D, as shown in Figure 7. In all lines $1 \cdot 10^{-4}$, $5 \cdot 10^{-5}$,

and $2 \cdot 10^{-5}$ were close to indistinguishable. In contrast, the $5 \cdot 10^{-6}$ simulation differed both in line A and C.

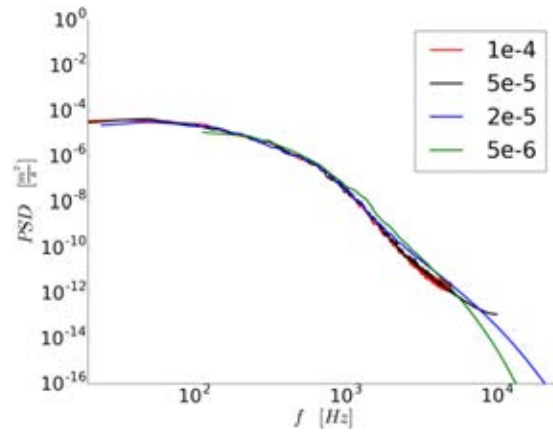


Figure 8: Power spectral density of the velocity field at point P from Figure 2, for the temporal refinement study.

The PSD analyses of the velocity traces recorded in point P are shown in Figure 8. We can observe that all of the different temporal simulations were from a pragmatic point of view equal. However, the temporally coarsest simulations naturally cannot capture the highest frequencies.

DISCUSSION

The aim of this study was to find an adequate (under-) resolved solution relative to the reference solution. From the spatial and temporal refinement study performed, a 22M-element mesh with a time step of $1 \cdot 10^{-4}$ seconds was found to be an optimal choice between computational cost and accuracy. This reference solution will be used in future studies on stenotic carotid bifurcations for comparison with turbulence modeling techniques. That being said, there is admittedly a minor difference between 22 and 50M-element meshes in Figure 5, in addition the simulations were not computed over the same number of physical seconds. To assess if the 50M-element simulation was close enough to a proper direct numerical simulation we compared the spatial (Δx) and temporal (Δt) scales in the numerical simulation to the Kolmogorov length scale (η) and time scale (τ) (Kolmogorov, 1941), respectively, which can be calculated from the dissipation as shown in equation 2.

$$\eta = (v^3/\varepsilon)^{1/4}$$

$$\tau = (v/\varepsilon)^{1/2}$$

Equation 2: Kolmogorov scales depend on the kinematic viscosity (ν) and the rate of dissipation per unit mass of the turbulent kinetic energy (ε).

One of the assumptions behind the Kolmogorov hypothesis is that the turbulence is homogenous isotropic. It is obvious from Figure 3 that the (turbulent) kinetic energy is not homogenous. To assess whether the post-stenotic flow instabilities were isotropic, we computed the time-averaged mean squared fluctuating

velocities along the centerline between lines A and D in Figure 2. Figure 9 shows that the mean squared fluctuating velocities are at the same order of magnitude, however there are large variations, and thus cannot be called isotropic. Therefore, computing the Kolmogorov scales is a very conservative estimate of the smallest length scales in this mildly unstable flow.

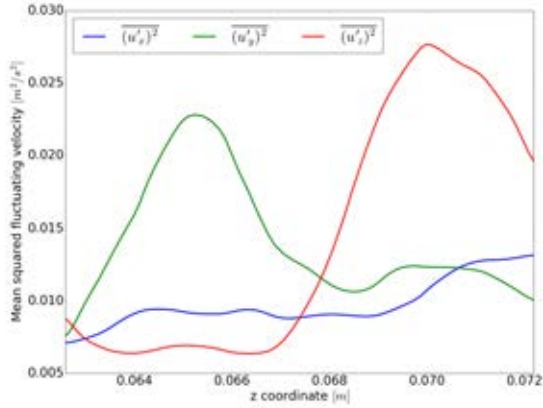


Figure 9: Mean squared fluctuating component of the velocity recorded along the centreline of the internal carotid artery.

The results of spatial assessment can be found in Table 1, displaying the characteristic node spacing Δx_{mean} , the smallest Kolmogorov length scale η_{min} , and the maximum ratio between Δx and η . There are two things to notice, first the Kolmogorov length scale converges, as the mesh is refined. Second, the maximum ratio between Δx and η on the two finest meshes are below 10, which is typically sufficient to capture > 95 % of the dissipation (Pope, 2001). If the simulations, from a numerical point of view, were truly converged, the ratio should be unity. However, the Kolmogorov scales only can be considered a conservative estimate as none of the rigid assumptions behind the hypothesis are met in this weakly unstable flow. Moreover, the differences between the 22, and 50M-element simulations were negligible, and a finer simulation will most likely not provide additional insight. We therefore consider the 50M-element simulation sufficiently refined from a pragmatic point of view, and by extension the 22M-element mesh for biomedical applications, where one is typically interested in a rapid classification once the tools are validated.

Furthermore, the difference in CPU hours is substantial, the 22M simulation with $\Delta t = 1 \cdot 10^{-4}$ seconds used 1420 CPU hours on 96 cores, while the 50M simulation $\Delta t = 2 \cdot 10^{-5}$ seconds would have spent 16 496 CPU hours on 128 cores to simulate 2 physical seconds, thus an order of magnitude difference.

Table 1: Comparison between Kolmogorov length scale η and the spatial scale of the numerical grid Δx .

Number of cells	2M	6M	22M	50M
Δx_{mean} [m]	3.19E-4	2.14E-4	1.38E-4	1.05E-4
η_{min} [m]	9.81E-6	9.30E-6	8.91E-6	8.58E-6
$(\Delta x/\eta)_{max}$ [-]	21.93	14.04	9.31	7.49

The temporal assessment of the flow simulation can be found in Table 2, showing the minimum Kolmogorov time scale τ_{min} and the ratio between the numerical time scale Δt and τ_{min} . The two best resolved simulations were below the Kolmogorov time scale. However, we can observe from the PSD in Figure 8, that there was energy at higher fluctuations than the Nyquist frequency for the suggested Δt . If we are interested in the mean flow features, this cutoff is not important as there are for all practical purposes, no energy in the fluctuating component above 5000 Hz. However, since we are studying the fluctuations in the post-stenotic region, these high frequency fluctuations might be important. If such high frequency fluctuations were of interest, then the mesh itself might be the limiting factor, as the eddies associated with the high frequencies cannot be represented in mesh.

All quantitative analyses shown here were based on time-averaged results. However, there are evidences from the biomedical literature that temporal changes might be play an important role in remodeling of the arteries (Valen-Sendstad *et al.*, 2011, 2013, 2014).

From a numerical point of view, an even larger time step might have been acceptable, but $\Delta t = 1 \cdot 10^{-4}$ seconds is very close to the stability criteria of the numerical scheme used in the solver. The Courant–Friedrichs–Lewy (CFL) number for the 22M-element mesh simulation was 1.3, and the typical limit for this solver is 3-4 CFL.

Table 2: Comparison between Kolmogorov time scale τ and the temporal scale of the simulations Δt .

Δt [s]	1.00E-4	5.00E-5	2.00E-5	5.00E-6
τ_{min} [s]	7.96E-5	7.96E-5	7.93E-5	7.92E-5
$\Delta t/\tau_{min}$ [-]	1.2563	0.6281	0.2522	0.0631

We have admittedly not tested all parameters of the complete solution strategy space, exemplified by numerical schemes, viscosity models, compliant walls, etc.

A limitation of the current study is first of all that the simulations were not run for the same period of time. Secondly, the simulations were performed assuming rigid walls. However, compliant effects are normally considered negligible, and is nevertheless not of any importance in arterial growth and remodeling (Malek *et al.*, 1999). That being said, the effect of a compliant model in combination with turbulent-like flows remains to be assessed. Furthermore, the fluid used for these simulations was water instead of blood to allow for direct comparison against *in-vitro* experiments, which will be the focus of future work. However, non-Newtonian effects have shown to have negligible effects on the hemodynamics of carotid bifurcations and intracranial aneurysms (Lee and Steinman, 2007; Khan *et al.*, 2016).

As part of a larger consortium, the final aim of this line of investigation is to build a non-contact device to diagnose severe stenosis in the carotid arteries through the analysis of neck's skin displacement. We will therefore compute the sensitivity of the flow split and of noise in the inflow pulse through in-silico experiments,

since both factors can be challenging to control in the in-vitro experiments.

CONCLUSION

We analyzed the flow field of a patient-specific carotid artery bifurcation with severe stenosis. The flow was found to become unstable already upstream of the stenosis because of flow separation at the bifurcation. The acceleration and deceleration of the flow caused by the stenosis itself led to the occurrence of vortices which propagated downstream of the stenosis until relaminarization started around 4 cm downstream.

We found an adequate under-resolved solution relative to the reference solution. From the spatial and temporal refinement study performed, a 22M mesh with a time step of $\Delta t = 1 \cdot 10^{-4}$ seconds was found to be an optimal choice between computational cost and accuracy.

REFERENCES

- GROEN, H.C., SIMONS, L., VAN DEN BOUWHUIJSEN, Q.J., BOSBOOM, E.M.H., GIJSEN, F.J., VAN DER GIESSEN, A.G., VAN DE VOSSE, F.N., HOFMAN, A., VAN DER STEEN, A.F., WITTEMAN, J.C. *et al.* (2010). “MRI-based quantification of outflow boundary conditions for computational fluid dynamics of stenosed human carotid arteries”. *Journal of Biomechanics*, **43**(12), 2332–2338.
- HUNT, J.C., WRAY, A.A. and MOIN, P. (1988). “Eddies, streams, and convergence zones in turbulent flows”. *Center for Turbulence Research, Report CTR-588*.
- IANNACCONE, F., DE BOCK, S., DE BEULE, M., VERMASSEN, F., VAN HERZEELE, I., VERDONCK, P., SEGERS, P. and VERHEGGHE, B. (2014). “Feasibility of a priori numerical assessment of plaque scaffolding after carotid artery stenting in clinical routine: proof of concept.” *The International Journal of Artificial Organs*, **37**(12), 928–939.
- KHAN, M., STEINMAN, D. and VALEN-SENDSTAD, K. (2016). “Non-Newtonian versus numerical rheology: Practical impact of shear-thinning on the prediction of stable and unstable flows in intracranial aneurysms”. *International Journal for Numerical Methods in Biomedical Engineering*.
- KOLMOGOROV, A.N. (1941). “The local structure of turbulence in incompressible viscous fluid for very large Reynolds numbers”. *Dokl. Akad. Nauk SSSR*, **30**, 301–305.
- LEE, S.W. and STEINMAN, D.A. (2007). “On the relative importance of rheology for image-based CFD models of the carotid bifurcation”. *Journal of Biomechanical Engineering*, **129**(2), 273–278.
- MALEK, A.M., ALPER, S.L. and IZUMO, S. (1999). “Hemodynamic shear stress and its role in atherosclerosis”. *JAMA*, **282**(21), 2035–2042.
- MORTENSEN, M. and VALEN-SENDSTAD, K. (2015). “Oasis: A high-level/high-performance open source Navier–Stokes solver”. *Computer Physics Communications*, **188**, 177–188.
- PICCINELLI, M., VENEZIANI, A., STEINMAN, D.A., REMUZZI, A. and ANTIGA, L. (2009). “A framework for geometric analysis of vascular structures: application to cerebral aneurysms”. *IEEE Transactions on Medical Imaging*, **28**(8), 1141–1155.
- POPE, S.B. (2001). *Turbulent flows*. IOP Publishing.
- REYNOLDS, O. (1883). “An experimental investigation of the circumstances which determine whether the motion of water shall be direct or sinuous, and of the law of resistance in parallel channels.” *Proceedings of the Royal Society of London*, **35**(224–226), 84–99.
- ROACHE, P.J., GHIA, K.N. and WHITE, F.M. (1986). “Editorial policy statement on the control of numerical accuracy”. *Journal of Fluids Engineering*, **108**(1), 2–2.
- STEINMAN, D.A. (2002). “Image-based computational fluid dynamics modeling in realistic arterial geometries”. *Annals of Biomedical Engineering*, **30**(4), 483–497.
- STEINMAN, D.A., HOI, Y., FAHY, P., MORRIS, L., WALSH, M.T., ARISTOKLEOUS, N., ANAYIOTOS, A.S., PAPAHRILAOU, Y., ARZANI, A., SHADDEN, S.C. *et al.* (2013). “Variability of computational fluid dynamics solutions for pressure and flow in a giant aneurysm: the ASME 2012 summer bioengineering conference CFD challenge”. *Journal of Biomechanical Engineering*, **135**(2), 021016.
- STEWART, S.F., PATERSON, E.G., BURGREN, G.W., HARIHARAN, P., GIARRA, M., REDDY, V., DAY, S.W., MANNING, K.B., DEUTSCH, S., BERMAN, M.R. *et al.* (2012). “Assessment of CFD performance in simulations of an idealized medical device: results of FDAs first computational interlaboratory study”. *Cardiovascular Engineering and Technology*, **3**(2), 139–160.
- VALEN-SENDSTAD, K. and STEINMAN, D. (2014). “Mind the gap: impact of computational fluid dynamics solution strategy on prediction of intracranial aneurysm hemodynamics and rupture status indicators”. *American Journal of Neuroradiology*, **35**(3), 536–543.
- VALEN-SENDSTAD, K., MARDAL, K.A., MORTENSEN, M., REIF, B.A.P. and LANGTANGEN, H.P. (2011). “Direct numerical simulation of transitional flow in a patient-specific intracranial aneurysm”. *Journal of Biomechanics*, **44**(16), 2826–2832.
- VALEN-SENDSTAD, K., MARDAL, K.A. and STEINMAN, D.A. (2013). “High-resolution CFD detects high-frequency velocity fluctuations in bifurcation, but not sidewall, aneurysms”. *Journal of Biomechanics*, **46**(2), 402–407.
- VALEN-SENDSTAD, K., PICCINELLI, M. and STEINMAN, D.A. (2014). “High-resolution computational fluid dynamics detects flow instabilities in the carotid siphon: Implications for aneurysm initiation and rupture?” *Journal of Biomechanics*, **47**(12), 3210–3216.
- WELCH, P. (1967). “The use of fast Fourier transform for the estimation of power spectra: a method based on time averaging over short, modified periodograms”. *IEEE Transactions on Audio and Electroacoustics*, **15**(2), 70–73.