

Advances in Computational Fluid Dynamics

Gregg Walker
Editor

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Preface

In chapter one, we described computational fluid dynamics and its impact on flow measurements using phase-contrast MR-angiography. Computational fluid dynamic (CFD) simulations are discussed with respect to their potential for quality assurance of flow quantification using commercial software for the evaluation of magnetic resonance phase contrast angiography (PCA) data.

The chapter two described the effect of system boundaries on the mean free path for confined gases. The mean free path of rarefied gases is accurately determined using Molecular Dynamics simulations. The simulations are carried out on isothermal argon gas (Lennard-Jones fluid) over a range of rarefaction levels under various confinements (unbounded gas, parallel reflective wall and explicit solid platinum wall bounded gas) in a nanoscale domain..

In chapter three, we described 3D thermo-fluid dynamic simulations of high-speed-extruded starch based products. This chapter aims to investigate a method to perform non-isothermal flow simulations in a complex geometry for generalized Newtonian fluids. For this purpose, 3D numerical simulations of starch based products are performed.

Chapter four is give the detail of numerical analysis of electromagnetic control of the boundary layer flow on a ship hull. In this chapter, electromagnetic control of turbulent boundary layer on a ship hull is numerically investigated. This study is conducted on the geometry of tanker model hull. For this purpose, a combination of electric and magnetic fields is applied to a region of boundary layer on stern so that produce wall parallel Lorentz forces in stream wise direction as body forces in stern flow.

Chapter five explain the wind velocity decreasing effects of wind break fence for snow fall measurement. Freshs now fall is defined as new snow covering an even plane. The depth of snow fall is defined as the increment of the snow layer cover during the time of measurement. The snow depth is generally measured each day and the snow fall is reported in centimeters per day.

In chapter six, we described the Turbulence, Vibrations, Noise and Fluid Instabilities. Practical Approach. Colloquially speaking, turbulence in any language means disorderly, incomprehensible, and of course, unpredictable movement. Consequently, we encounter expressions that employ the word turbulence in social and economic contexts; in aviation whenever there are abnormalities in the air, and even in psychology and the behavioral sciences in reference to turbulent conduct, or a turbulent life, in the sense of a dissolute existence.

In chapter seven, we explain the application of computational fluid dynamics to practical design and performance analysis of turbo machinery. Actually, a CFD-simulator is special-purpose software simulating, in “online” and “real time” modes with a high similarity and in sufficient detail, the physical processes of gas mixture transmission through a particular GTN.

Chapter eight is give the detail of computational fluid dynamics modeling to improve natural flow rate and sweet pepper productivity in greenhouse. Natural flow rate and sweet peppers productivity in tropical greenhouse are improved by CFD simulation is the main objective of this research work. Most of the greenhouse types today are in the arch shape. To develop an improved greenhouse structure for the region, the arch type was built and used as the control model.

In chapter nine, we described an initial investigation of a djoint-based unstructured grid adaptation for vertical flow simulations. A computational fluid dynamics (CFDs) method utilizing unstructured grid technology has been employed to compute vertical flow around a 65° delta wing with sharp leading edge, which is specially known as the geometry of the second international vortex flow experiment (VFE-2). In VFE-2, 65° delta wings with different leading edges had been broadly investigated by experiments, which resulted in a special database for CFDs codes validation.

In chapter ten, we described the combined effects of centrifugal and coriolis instability of the flow through a rotating curved duct with rectangular cross section. Combined effects of centrifugal and coriolis instability of the flow through a rotating curved duct with rectangular cross section have been studied numerically by using a spectral method, and covering a wide range of the Taylor number $0 \leq Tr \leq 2500$ for a constant Dean number $Dn = 2000$. The rotation of the duct about the center of curvature is imposed in the positive direction, and the effects of rotation (Coriolis force) on the flow characteristics are investigated.

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Chapter 1

COMPUTATIONAL FLUID DYNAMICS AND ITS IMPACT ON FLOW MEASUREMENTS USING PHASE-CONTRAST MR-ANGIOGRAPHY

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ABSTRACT

Rationale and Objectives: Computational fluid dynamic (CFD) simulations are discussed with respect to their potential for quality assurance of flow quantification using commercial software for the evaluation of magnetic resonance phase contrast angiography (PCA) data. **Materials and Methods:** Magnetic resonance phase contrast angiography data was evaluated with the Nova software. CFD simulations were performed on that part of the vessel system where the flow behavior was unexpected or non-reliable. The CFD simulations were performed with in-house written software. **Results:** The numerical CFD calculations demonstrated that under reasonable boundary conditions, defined by the PCA velocity values, the flow behavior within the critical parts of the vessel system can be correctly reproduced. **Conclusion:** CFD simulations are an important

extension to commercial flow quantification tools with regard to quality assurance.

INTRODUCTION

Magnetic resonance phase contrast angiography meanwhile is an established technique to measure the velocity and the direction of flow [1]. The major drawbacks of this approach are often related to misaligned encoding gradients (venc), a too low SNR or high susceptibility gradients nearby (small) vessels. In each case the relative phase are not unique and the absolute velocity values are wrong. At this point the correct answer to the flow in the critical regions can only be derived on the base of physical models and computational flow dynamics (CFD). Almost all CFD-problems are associated with the solution of the Navier-Stokes equations [2,3], named after Claude-Louis Navier and George Gabriel Stokes, which describe the motion of fluid substances. The calculations were performed on incompressible fluids within human blood vessels. The idea is to selectively model the relevant vessel system and to include the known velocity values from the PCA measurements within the big vessels as boundary conditions. These velocity conditions are sufficient in most cases because the velocities tune in to the given pressure conditions. The intrinsic symmetry of the vessels furthermore can be used to reduce the dimensionality of the problem from three to two, which is necessary to use the software on commercial computers with limited working memory and CPU power—only the relative orientation of the vessels and their diameters (e.g. due to stenoses) have to be considered. The spectrum of potential applications span the simulation of pressure and force distributions near the neck of aneurysms, the velocity and direction of flow within complex vessel systems with or without stenoses and pressure and vorticity distributions near atherosclerotic plaques. In this technical note we will concentrate on a few representative examples in order to demonstrate the importance of quality assurance in addition to commercial flow evaluation software.

METHODS

Flow Measurement

Magnetic resonance phase contrast angiography measurements of flow were performed on a 3 Tesla scanner. The Flash sequence parameters were as follows: Base resolution 256, Phase resolution 60%, Flip angle 25 deg, TR 113.20 ms, TE 4.66 ms, Voxel size: $0.9 \times 0.5 \times 4.0$ mm, TA: 1:06 min, 1st Signal/Mode Pulse/Retro, calculated phases 12, segments 5, slices 1. Each slice was planned on the base of a time-of-flight (TOF) measurement using the Nova software (<http://www.vassolinc.com>), which guarantees the exact orthogonal positioning relative to the course of the vessel. The flow measurements were performed for a number of selected vessels that define a part of the simulated vessel system. Figure 1 shows a typical Nova rendered 3D-presentation of the vessel system of a TOF measurement. The velocities are measured at the positions given by the small slice cartoons perpendicularly oriented to the vessel. The most important aspects which are essential for the choice of these locations are the distance to bifurcations and stenoses because often turbulences may occur in their immediate vicinity. Nova currently provides no option for the separate presentation of systolic and diastolic phases but merely shows the mean volumetric flow rate values on the diagrams (Figure 1(b)). The mean velocity values, necessary for the simulations, are not shown on the Nova diagram, but are stored in a text file.

Preparation of CFD

2D-projections from individual TOF maximum intensity projection maps are co-registered to a template (see e.g. http://commons.wikimedia.org/wiki/Template:Other_versions/Circle_of_Willis, binary mask in Figure 2(a)) while preserving the individual properties (e.g. stenoses, mal- formations, relative orientation). The final mask was used to define the coordinates and nodes essential for the mesh2d Matlab program, which calculates the nodes and elements (Figure 2(b)) necessary for the numerical simulations.

Numerical Algorithms

The numerical code for the flow simulations is an in-house development, written in Matlab. The program simulates the motion of incompressible fluids via numerical solutions of the 2D, unsteady Navier-Stokes equations. The CFD-program is a vertex centered Finite Volume (FV) code that uses the median dual mesh to form the control volumes about each vertex by connecting the centroids of each cell to their edge midpoints. The time and spatial linearizations are dealt with separately. Fully 2nd order piecewise linear reconstructions are used to develop sparse operators, which approximate the continuous differential terms. These methods can be found in detail in [4, 5] described by terms like Green's theorem and its application to face averaged gradients (Laplacian, un-weighted least squares) or upwind piece-wise linear extrapolation with the HQUICK slope limiter (non-linear part). The time integration of the equations is based on the well-known fractional step method [5,6]. The non-staggered pressure/velocity arrangement was shown to support the common mesh scale pressure oscillation and hence the standard 2nd order incremental pressure correction method [7,8] was modified to incorporate Rhie-Chow stabilization [9]. This reduced the order of the time integration to 1st/2nd. Unlike many other Navier-Stokes solvers the CFD-program makes use of a complete LU factorization for the Poisson pressure equation. Instead of using standard iterative approaches like preconditioned bi-conjugate gradients stabilized method (bicgstab (Matlab)) we decided on including the fill reducing UMFPACK algorithm [10], an approach which was shown to be far more efficient in this case. The momentum equations are solved in a semi-implicit manner. The non-linear terms are evaluated explicitly via a 2nd order TVD Runge-Kutta method [11]. In order to solve the linear systems that arise due to the implicit treatment of the viscous terms, the bicgstab method was favored. Minimization of errors associated with the numerical solution was managed according to the concepts of Roache et al. [12].

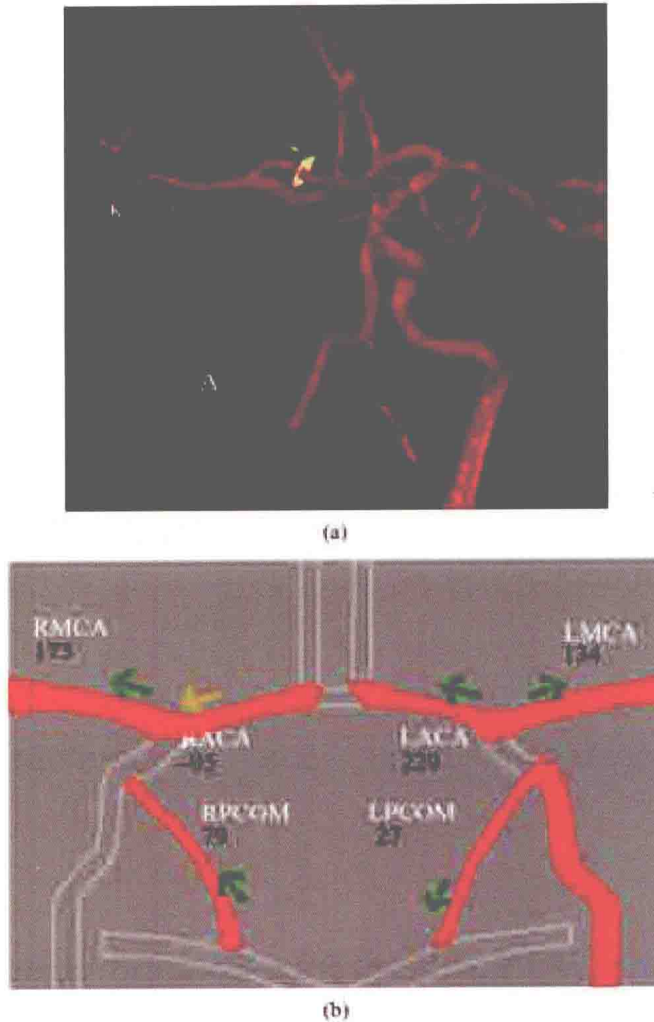


Figure 1. A typical 3D-plot (a) of a NOVA flow planning system, illustrating the rendered vessel system according to the TOF measurement. The velocities are measured at the positions given as small slice cartoons perpendicularly oriented to the vessel (here the right ACA). In (b) one possible schematic Nova diagram of a part of the circle-of-willis system is shown, which contains information about the vessel names, the direction of flow (green arrow) and volumetric flow rate values (ml/min).

CPU Parameters

The CFD simulations were performed on a personal computer with Intel® Xeon processor, 2.4 GHz, 12 GB RAM, CPUs, NVIDIA Quadro FX 580, Video RAM 512 MB, GPU frequency 450 MHz, Ubuntu 10.04.

Program Features

The mesh2d program of Mat lab was used for the 2D mesh (triangles) generation. This type of mesh allows the automatic treatment of complex geometries. The mesh2d algorithm optimizes the mesh quality which is important to guarantee correct results. The CFD program solves the Navies-Stokes equations for the velocity and pressure fields of incompressible fluids. The time step size and the stability of the integration are adjustable. The velocity values measured by PCA were used as the boundary conditions (at the nodes). The program includes a module that calculates the $[x,y]$ forces applied to a boundary due to pressure and skin friction effects and can be used in this example to calculate the lift and drag forces on an aneurysm neck.

Patient

High grade stenosis of the left ICA and occlusion of the right ICA.

RESULTS

The total time needed for the preparation and simulation is in the range of 3 min which is actually feasible for emergency cases. The computer, however, should at least have 4 GB working memory and processors of the new generation (Pentium IV, Xeon) with at least 2.4 GHz. Figure 2(a) shows a typical bitmap of the circle-of-willis which is then transformed to a 2D-mesh with nodes and elements (Figure 2(b)) using the mesh2d Mat-lab program. As a typical example for the application of the CFD-simulations, the data of a patient before and after stenting of the left ICA was used. The velocity values at the boundaries were given by the PCA measurements. The simulations of the corresponding vessel system before (Figures 3(a)-(c)) and after stenting (Figures 4(a)-(c)) confirm the change in direction within the LPCOM vessel (Figure 4(b)) with respect to the situation before stenting (Figure 3(b)): it is opposite to the flow within the RPCOM (Figures 3(c) and 4(c)). The associated Nova diagrams are shown in Figure 3(d) (before stent) and Figure 4(d) (after stent). The measured mean velocity values are shown in Table 1.

In order to demonstrate the potential of the CFD simulation technique, an example for such an (artificial) aneurysm is given in Figure 5, for which the velocity (Figure 5(a)) and pressure distributions (Figure 5(b))

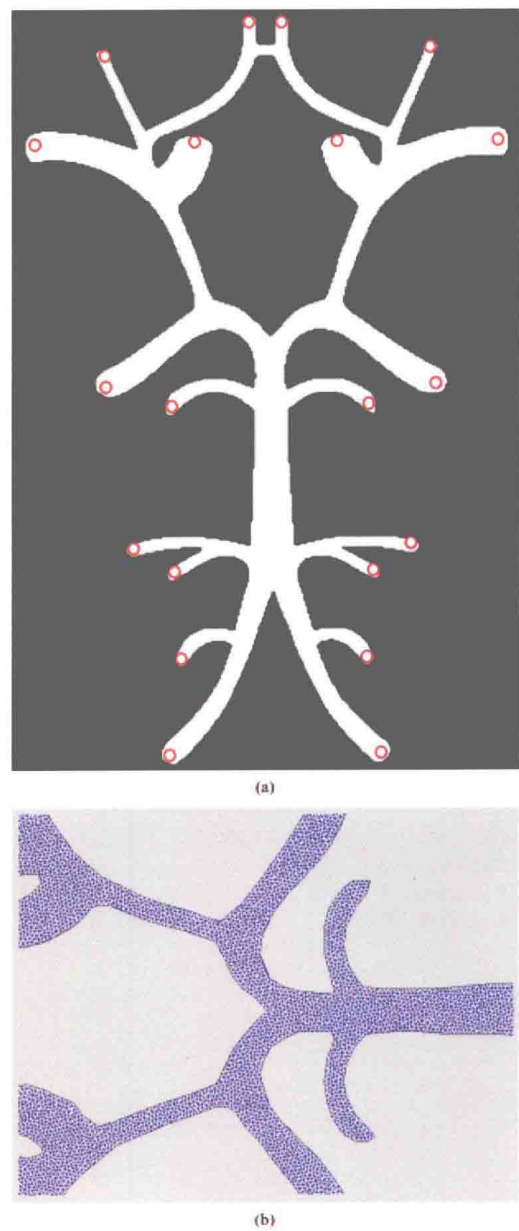
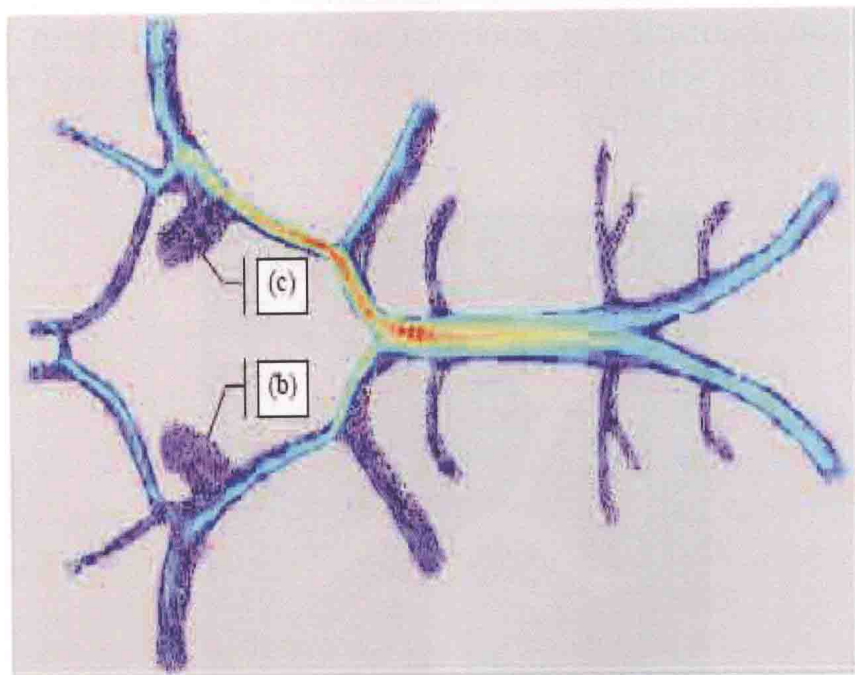
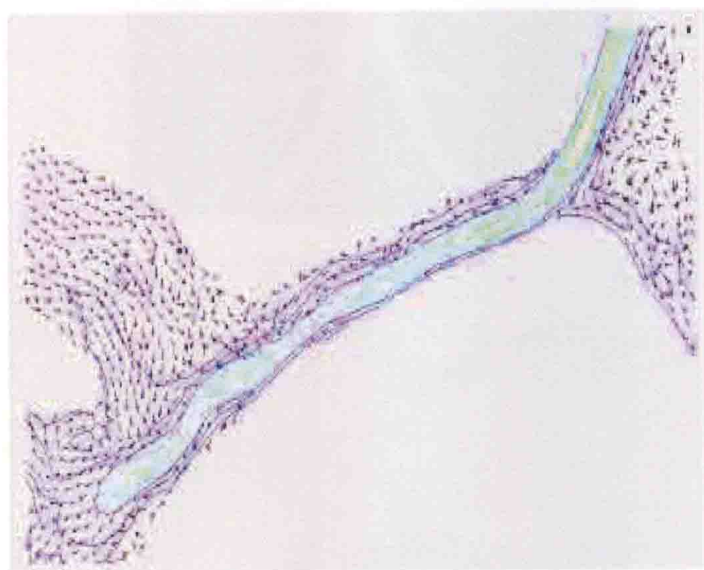


Figure 2 The bitmap of the circle-of-Willis vessel system (a) and the mesh nodes and elements for a part of it (b), calculated by the mesh2d Mat lab program. The mesh serves as the base for the CFD simulations. Potential boundaries which may have non-zero in- or outflow are marked with red cycles.



(a)



(b)