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Hossein Sadeghi Khatibani

**Large eddy simulations of
phonatory aerodynamics in
a 3D-FVM larynx model**

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Large eddy simulations of phonatory aerodynamics in a 3D-FVM larynx model

Large-Eddy-Simulation der Aerodynamik bei der Phonation
in einem 3D-FVM-Kehlkopfmodell

Der Technischen Fakultät
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Hossein Sadeghi Khatibani

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Abstract

Human phonation is a complex multiphysical process within the human larynx based on the interaction between the laryngeal airflow, tissues and acoustics. The restricted accessibility to this area challenges the in-vivo investigation of phonatory process, especially when aerodynamics of phonation is matter of interest. Numerical models of the larynx enable us to study more details of this process by providing deep insight into all the three participating physical fields. On the other hand, considering clinical application, for instance as decision-making in pre- and post-surgical processes and medical diagnostics of voice disorders, less progress on employing these tools has been announced till now. A numerical model should be able to provide reliable results in a short computational time with low hardware requirements to be applicable in clinical environment. Accordingly, the high computational costs of a simulation involving all aspects of phonation process have limited the numerical larynx models mostly to the phonation research. One strategy is to reduce the computationally expensive laryngeal fluid-structure interaction (FSI) to a pure flow simulation with moving boundaries of the computational domain. Following this approach in this study, a model of the laryngeal aerodynamics has been developed to evaluate the potentials of the computational fluid dynamics (CFD) both in voice research and clinical operation.

This three-dimensional (3D) CFD model was based on a synthetic larynx model with silicon vocal folds. The experimentally measured flow-induced oscillation of vocal folds was imposed on the boundaries of the numerical model to simulate the vocal folds motion. This motion was modeled through some steps with increasing modeling degree of realism. These models involved static vocal folds, one degree of freedom translational motion of vocal folds with convergent glottal duct, two degree of freedom motion with convergent-divergent shape change imitating the mucosal wave-like motion of synthetic vocal folds and finally this motion with an elliptical glottis shape similar to the experimental model. Finite volume method (FVM), as a common approach in CFD, along with large eddy simulation (LES) for the turbulence modeling was used to simulate the flow dynamics. After performing mesh convergence study and validation with the experimental results, the laryngeal aerodynamic features which may be reproduced with each model and the relevant computational costs were evaluated. In the next step, ventricular folds were added to the larynx model to investigate their aerodynamic effects on phonatory process. At the end, a potential clinical application of the model was evaluated regarding the computational time and resources.

Results showed that increasing modeling complexity enable us to capture more phonatory key features. These characteristic features involve:

- the well-known glottal jet deflection reproduced in all the models with rectangular glottis shape,
- flow separation and creation of intraglottal vortices by improving the motion of vocal folds to the mucosal wave propagation,
- the axis-switching effect and more symmetry of the flow in elliptical glottis models.

Furthermore, the computational costs of the simulations increased by improving the modeling degree of realism and adding more aerodynamic complexities to the model. At this stage, the high computational costs, in the order of some weeks, required by the models to produce the highly accurate results are far above the required short time-to-solution for daily clinical routines. However, the potentials of the numerical model in providing a better understanding of laryngeal aerodynamics are proved.

Regarding the effects of ventricular folds, straightening and elongation of glottal jet and reduction of pressure level in the laryngeal ventricles were detected. Consequently, the flow rate through glottis and the transglottal pressure difference increased. This led to a lower laryngeal flow resistance by considering the entire larynx, which can be interpreted as a higher amount of kinetic energy in the glottal flow. Simultaneously, it led to a higher glottal flow resistance, considering only the glottal area, and accordingly to a higher rate of energy transfer from the glottal flow to the vocal folds. This higher energy transfer can enhance the oscillation of vocal folds. All the mentioned effects were more pronounced in the rectangular glottis models and can vary by changing the subglottal pressure and ventricular gap size. In conclusion, the ventricular folds support the phonation process by reducing the effort for producing the vocal folds oscillations, which can be minimized by an optimal combination of ventricular gap diameter, glottal gap diameter and subglottal pressure.

Last but not least, the high computational costs of the simulations were reduced by decreasing the spatial and temporal resolutions of the numerical model while still obtaining the results with sufficiently good accuracy. Furthermore, the use of high performance computing resources (HPC) was optimized to prevent the waste of the computational power. Consequently, a significantly shorter time-to-solution, in the order of some days, was achieved by using less computational resources. Although the computational costs of the simulations are still higher than the clinical requirements, it can show the potentials of the numerical models to be used in clinical environments by further efforts in the near future.

Zusammenfassung

Die menschliche Phonation basiert auf einem komplexen multiphysikalischen Prozess der Fluid-Struktur-Akustik-Interaktion (FSAI) welche im menschlichen Kehlkopf stattfindet. Diese Interaktion resultiert aus einer Luftströmung durch die Glottis, einer oszillierenden Bewegung der Stimmbänder und einer resultierenden Akustik. Der stark eingeschränkte Zugang zu den innerhalb des Kehlkopfes liegenden Stimmbändern lässt eine in-vivo Untersuchung der Aerodynamik während des Phonationsprozesses nicht zu. Numerische Modelle des Kehlkopfes zur Berechnung von Strömungsvorgängen ermöglichen einen detaillierteren und tieferen Einblick in den Phonationsprozess. In Bezug auf einen Einsatz von numerischen Modellen für die klinische Anwendung bei der medizinischen Diagnostik von Stimmstörungen wurden jedoch bisher wenig Fortschritte erzielt. Für den Einsatz in einem klinischen Umfeld müssen numerische Modelle zuverlässige Ergebnisse innerhalb einer kurzen Rechenzeit (computational costs) in Kombination mit einer geringen Hardware-Anforderung erzielen. Die hohe Rechenzeit, die eine Simulation unter Einbezug aller Aspekte einer Phonation besitzt, beschränkt die numerischen Kehlkopfmodelle hauptsächlich auf die Phonationsforschung. Eine Strategie, die zur Untersuchung der Aerodynamik und Aeroakustik der Phonation verfolgt werden kann, besteht darin, die rechenintensive Fluid-Struktur-Interaktion (FSI) auf eine Strömungssimulation zu reduzieren und die oszillierende Bewegung der Stimmlippen extern vorzugeben. Um das Potenzial von numerischen Modellen sowohl für die Phonationsforschung, als auch für den klinischen Betrieb bewerten zu können, wird in der vorliegenden Arbeit ein numerisches, rein fluiddynamisches Kehlkopfmodell mittels Computational Fluid Dynamics (CFD) entwickelt.

Dieses dreidimensionale (3D) numerische Kehlkopfmodell basiert auf einem synthetischen Kehlkopfmodell mit Silikonstimmlippen. Die experimentell gemessenen, strömungsinduzierten Schwingungen der Stimmlippen wurden im numerischen Modell schrittweise mit zunehmendem Realitätsgrad modelliert. Begonnen wurde mit einem Modell, das eine Stimmlippenbewegung mit einem Freiheitsgrad der Translation und einer geraden Glottisöffnung enthält. Darauf aufbauend wurde ein Modell mit je einem Freiheitsgrad der Translation und der Rotation entwickelt. Abschließend entstand ein Modell mit dieser Stimmlippenbewegung und einer elliptischen Glottisöffnung auf Basis des künstlichen Modells. Für das numerische CFD Modell wurde die Finite-Volumen-Methode (FVM) in Kombination mit einer Large Eddy Simulation (LES) für die Turbulenzmodellierung verwendet. Nach Durchführung einer Gitterstudie und einer Validierung mit experimentellen Ergebnissen wurden die aerodynamischen Merkmale des Kehlkopfmodells und die Rechenzeit des Simulationsmodells bewertet. In einem näch-

sten Schritt wurden die falschen Stimmlippen in das Kehlkopfmodell integriert, um die Auswirkungen der falschen Stimmlippen auf den Phonationsprozess zu untersuchen. Abschließend wurde eine mögliche klinische Anwendung des Modells hinsichtlich seiner Rechenzeit und der Hardwareanforderungen überprüft.

Die Ergebnisse zeigen, dass ein zunehmender Realitätsgrad in der Modellierung des Kehlkopfmodells eine exaktere Abbildung des Phonationsprozesses ermöglicht. Das Modell mit rechteckiger Glottis beinhaltet die bekannte Ablenkung des Glottal Jets. Im Stimmlippenmodell mit elliptischer Glottis und einer verbesserten Bewegung der Mucosal Wave entstehen eine bessere Unterbrechung der Strömung, intraglottale Wirbel und ein insgesamt symmetrischeres Strömungsfeld. Darüber hinaus erhöhte sich die Rechenzeit der Simulationen mit steigendem Realitätsgrad. Bis jetzt liegen die Rechenzeiten in der Größenordnung von einigen Wochen und damit weit über den Anforderungen des Einsatzes in der klinischen Arbeit. Jedoch wurde das Potential von numerischen Modellen für ein besseres Verständnis des Phonationsprozesses gezeigt.

Mit dem Implementieren der falschen Stimmlippen in das Stimmlippenmodell wurde eine Begradigung und Verlängerung des Glottal Jets sowie eine Verringerung des Druckniveaus in den Kehlkopftaschen festgestellt. Infolgedessen nahmen der durch die Glottis strömende Volumenstrom und die transglottale Druckdifferenz zu. Desweiteren konnten ein Anstieg des Strömungswiderstands der Glottis und eine gleichzeitige Abnahme des Strömungswiderstands des gesamten Kehlkopfbereiches beobachtet werden. Ein weiterer Effekt, der bei vorhandenen falschen Stimmlippen beobachtet wird, ist eine höhere Übertragungsrate der Energie von der Luftströmung auf die Stimmlippen. Dieser Anstieg der Energieübertragungsrate kann zu einer verstärkten strömungsinduzierten Schwingung der Stimmlippen führen. Alle erwähnten Effekte waren bei den rechteckigen Glottismodellen ausgeprägter und können durch das Ändern des subglottalen Drucks und des Abstandes zwischen den falschen Stimmlippen variieren. Zusammenfassend kann eine unterstützende Rolle der falschen Stimmlippen bei der Phonation durch einen verringerten phonatorischen Aufwand beobachtet werden.

Abschließend konnte durch eine Gitter- und Zeitschrittstudie und der damit verbundenen geringeren räumlich-zeitlichen Auflösung des numerischen Modells die Rechenzeit der einzelnen Simulationen unter Berücksichtigung der Reproduzierbarkeit von Phonationseigenschaften reduziert werden. Durch den Einsatz von Hochleistungsrechnern (HPC) konnte die Rechenzeit weiter optimiert werden. Infolgedessen wurde eine erheblich kürzere Laufzeit (in der Größenordnung von wenigen Tagen) erreicht. Obwohl die Rechenzeiten für eine klinische Anwendung immer noch zu hoch sind, zeigt das numerische Modell großes Potential in naher Zukunft im klinischen Umfeld eingesetzt werden zu können.

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Hossein Sadeghi

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Nomenclature

| | |
|--------------------------------|--|
| u | Velocity of the flow parallel to the wall |
| y | Distance to the wall |
| α | Interpolation weighting factor |
| β | Geometric Gauss-LSQ gradient blending factor |
| ϕ | Vector of a general flow parameter for all the cells |
| $\Delta\phi$ | Deviation in the solution between two meshes |
| ΔP_g | Glottal pressure drop |
| ΔP_l | Laryngeal pressure drop |
| ΔP | Pressure drop across a definite part of the larynx |
| Δt | Time step size |
| $\Delta x, \Delta y, \Delta z$ | Mesh size in x, y, z direction |
| δ_ν | Viscous length scale |
| Δ | Length scale of the filter in large eddy simulation |
| \dot{m}^* | Uncorrected mass flux |
| \dot{m}' | Mass flow correction |
| \dot{m} | Mass flow rate |
| \dot{q} | Rate of volumetric heat input per unit mass |
| ϵ | Dissipation rate of turbulent fluctuations |

| | |
|-------------------|--|
| η | Kolmogorov length scale |
| $\frac{D}{Dt}$ | Substantial derivative |
| Γ | Diffusivity |
| κ | Wavenumber |
| λ_T | Taylor microscale or the turbulence length scale |
| \mathbf{A} | Matrix of the coefficients of the algebraic equations system |
| \mathbf{b} | Vector of the right hand side of the algebraic equations system |
| \mathbf{ds} | Vector of the infinitesimal element of the surface (\mathbf{nds}) |
| \mathbf{e} | Vector of errors of the algebraic equations system |
| \mathbf{f}^ϕ | Convective or diffusive flux through a cell face |
| \mathbf{I} | Identity tensor |
| \mathbf{n} | Unit vector perpendicular to the surface |
| \mathbf{r} | Vector of residuals of the algebraic equations system |
| \mathbf{S}_d | Traceless symmetric part of the square of the velocity gradient tensor |
| \mathbf{s} | Surface area vector (\mathbf{ns}) |
| \mathbf{T}_s | Anisotropic subgrid stress tensor in large eddy simulation |
| \mathbf{T}_t | Total viscous and SGS stress tensor |
| \mathbf{T} | Viscous stress tensor |
| \mathbf{u}_g | Grid velocity vector |
| R | Specific gas constant |
| T | Temperature field |
| μ | Dynamic viscosity |
| ν_t | Eddy-viscosity |
| ν | Kinematic viscosity |

| | |
|----------------------|--|
| ω_k | Orthogonal vorticity field |
| ω_p | Pressure under-relaxation factor |
| ω_u | Velocity under-relaxation factor |
| ϕ | A general flow parameter |
| Ψ | Phase difference |
| τ_w | Wall shear stress |
| \mathbf{f} | External force |
| \mathbf{u} | Velocity vector |
| \mathbf{x} | Cell centroid |
| Υ | Rhie-and-Chow dissipation |
| $\hat{\mathbf{S}}$ | Filtered rate of strain in large eddy simulation |
| $\hat{\mathbf{u}}^*$ | Intermediate velocity field in PISO algorithm |
| $\hat{\mathbf{u}}$ | Filtered or resolved component of the velocity vector in large eddy simulation |
| \hat{P}' | Cell pressure correction field |
| \hat{P} | Modified filtered pressure in large eddy simulation |
| ξ | Normalized variable diagram (NVD) |
| A_i | Amplitude of displacement of vocal folds margins ($i=1,2$) |
| A | Glottal area |
| a | Momentum coefficient |
| B | Wall log-law constant |
| C_κ | Kármán constant |
| C_ω | WALE model constant |
| C_k | Kolmogorov constant |
| C_s | Smagorinsky model constant |

| | |
|-------------------|---|
| C | Courant number |
| c | Sound speed |
| d_g | Glottal gap diameter |
| d_{VeF} | Ventricular folds gap diameter |
| ds | Infinitesimal element of the surface |
| dv | Infinitesimal element of the volume |
| dy_{ELL} | Translational motion of vocal folds for elliptical glottis |
| dy | Translational motion of vocal folds |
| D | Diffusive flux through a cell face |
| $E(\kappa)$ | Turbulent kinetic energy spectrum |
| $Err_{rel}^{L^2}$ | L^2 norm relative errors |
| err | Relative error |
| e | Internal energy |
| f_g | Grid flux |
| F_H | Horizontal component of the aerodynamic forces on the vocal folds surfaces |
| F_V | Vertical component of the aerodynamic forces on the vocal folds surfaces |
| f_0 | Fundamental frequency of vocal folds oscillation |
| GCI | Grid convergence index |
| G | Filter function of large eddy simulation |
| h | Representative cell site for calculation of GCI |
| K_r | Residual kinetic energy in large eddy simulation |
| k | Thermal conductivity |
| l_0 | Size of largest eddies in turbulent flow |
| l_{DI} | The edge between the inertial and dissipation subranges in high Re turbulent flow |

| | |
|-----------------|--|
| l_{EI} | The edge between the energy-containing and inertial ranges in high Re turbulent flow |
| $l_{ventricle}$ | Ventricle length |
| l_{VF} | Length of vocal folds |
| L | Characteristic length scale of the flow |
| l | Size of the eddies in turbulent flow |
| M | Mach number |
| N | Total number of the cells |
| OQ | Open quotient |
| P^* | Guess pressure in PISO algorithm |
| P' | Experimental relative pressure to the environmental pressure |
| P_0 | Relative pressure to the environment equal to 0 Pa |
| P'_s | Experimental subglottal pressure relative to the environmental pressure |
| P_s | Subglottal pressure relative to the environmental pressure |
| P'_{60} | Experimental relative pressure to the environmental pressure at 60 mm downstream of the glottis exit |
| P_{in} | Relative pressure to the environmental pressure at the inlet of numerical domain |
| P_{out} | Relative pressure to the environmental pressure at the outlet of numerical domain |
| P_{th} | Threshold pressure relative to the environmental pressure |
| P | Pressure relative to the environmental pressure |
| Q | Flow rate |
| R_g | Glottal flow resistance |
| R_l | Laryngeal flow resistance |
| $Re_\eta = 1$ | Reynolds number of Kolmogorov scales |
| Re_{cr} | Critical Reynolds number for transition from laminar to turbulent flow |

| | |
|-----------------|--|
| Re | Reynolds number |
| rf | Refinement factor between two meshes |
| R | Flow resistance |
| r | Residual |
| SQ | Speed quotient |
| s | Surface area |
| t_η | Kolmogorov time scale |
| T_n | Time interval of the cycle with closing vocal folds |
| T_o | Time interval of the cycle with open glottis |
| T_p | Time interval of the cycle with opening vocal folds |
| T_{DI} | Rate of energy transfer from larger scales between the inertial and dissipation subranges in high Re turbulent flow |
| T_{EI} | Rate of energy transfer from larger scales between the energy-containing and inertial ranges in high Re turbulent flow |
| t_{VF} | Thickness of vocal folds |
| T | Period of vocal folds oscillation |
| t | time |
| u^+ | Dimensionless velocity |
| u' | Residual or subgrid-scale (SGS) component of the velocity field in large eddy simulation |
| u_η | Kolmogorov velocity scale |
| u_τ | Friction (shear) velocity |
| u_x, u_y, u_z | Component of velocity vector in x, y, z direction |
| u | Velocity magnitude |
| v | Volume |
| w_1 | displacement of inferior margin of vocal folds |

w_2 displacement of superior margin of vocal folds
 W_n Net work performed by the flow on the vocal fold over an entire oscillation cycle
 x, y, z Spatial coordinates
 x' Dummy variable of convolution integration
 y^+ Dimensionless wall distance
CPU time Accumulated time for all the processors to perform the simulation
Wall time Overall real time elapsed on the simulation

Subscripts

i Iterator of the cells
 j Iterator of the neighbouring cells
 k Iterator of the cell faces

Superscripts

\bar{m} Time-averaged mass flow rate
CD Central difference scheme
FOU First order upwind scheme
 gv Glottal velocity profile
G Green-Gauss
LSQ Least-squares
 m An iteration step
 $n + 1$ Current time step
 n Previous time step
 p Relative pressure distribution
 sgv Supraglottal velocity profile
SOU Second order upwind scheme

Scalars, vectors, tensors and their operators and products

| Denotation | Notation | \in | Production |
|---------------------------------------|--|---------------------------|--|
| Scalar (0th order tensor) | a, B | \mathbb{R} | |
| Vector (1st order tensor) | \mathbf{a}, \mathbf{b} | $\mathbb{R}^{3 \times 1}$ | $[\mathbf{a}]_i, [\mathbf{b}]_i$ |
| Tensor (2nd order tensor) | \mathbf{A}, \mathbf{B} | $\mathbb{R}^{3 \times 3}$ | $[\mathbf{A}]_{ij}, [\mathbf{B}]_{ij}$ |
| Identity Tensor | \mathbf{I} | $\mathbb{R}^{3 \times 3}$ | $[\mathbf{I}]_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$ |
| Nabla operator | ∇ | $\mathbb{R}^{3 \times 1}$ | $[\nabla]_i = \frac{\partial}{\partial x_i}$ |
| Transpose of a vector | \mathbf{a}^T | $\mathbb{R}^{1 \times 3}$ | $[\mathbf{a}^T]_j = [\mathbf{a}]_i$ |
| Transpose of a tensor | \mathbf{A}^T | $\mathbb{R}^{3 \times 3}$ | $[\mathbf{A}^T]_{ij} = [\mathbf{A}]_{ji}$ |
| Gradient of a scalar | ∇a | $\mathbb{R}^{3 \times 1}$ | $[\nabla a]_i = \frac{\partial a}{\partial x_i}$ |
| Gradient of a vector | $\nabla \mathbf{a}$ | $\mathbb{R}^{3 \times 3}$ | $[\nabla \mathbf{a}]_{ij} = \frac{\partial [\mathbf{a}]_i}{\partial x_j}$ |
| Divergence of a vector | $\nabla \cdot \mathbf{a}$ | \mathbb{R} | $= \sum_{i=1}^3 \frac{\partial [\mathbf{a}]_i}{\partial x_i}$ |
| Laplacian of a vector | $\nabla^2 \mathbf{a} = \nabla \cdot (\nabla \mathbf{a})$ | $\mathbb{R}^{3 \times 1}$ | $[\nabla^2 \mathbf{a}]_i = \sum_{j=1}^3 \frac{\partial^2 [\mathbf{a}]_i}{\partial x_j \partial x_j}$ |
| Divergence of a tensor | $\nabla \cdot \mathbf{A}$ | $\mathbb{R}^{3 \times 1}$ | $[\nabla \cdot \mathbf{A}]_i = \sum_{j=1}^3 \frac{\partial [\mathbf{A}]_{ji}}{\partial x_j}$ |
| Vector inner, scalar or dot product | $\mathbf{a} \cdot \mathbf{b}$ | \mathbb{R} | $= \sum_{i=1}^3 [\mathbf{a}]_i [\mathbf{b}]_i$ |
| Vector outer, vector or cross product | $\mathbf{a} \times \mathbf{b} = \mathbf{a} \mathbf{b}^T$ | $\mathbb{R}^{3 \times 3}$ | $[\mathbf{a} \mathbf{b}^T]_{ij} = [\mathbf{a}]_i [\mathbf{b}]_j$ |
| Tensor dot product | $\mathbf{A} \cdot \mathbf{B}$ | $\mathbb{R}^{3 \times 3}$ | $[\mathbf{A} \cdot \mathbf{B}]_{ij} = \sum_{k=1}^3 [\mathbf{A}]_{ik} [\mathbf{B}]_{kj}$ |
| Tensor double dot product | $\mathbf{A} : \mathbf{B}$ | \mathbb{R} | $= \sum_{i=1}^3 \sum_{j=1}^3 [\mathbf{A}]_{ij} [\mathbf{B}]_{ij}$ |
| Trace of a tensor | $\text{tr}(\mathbf{A})$ | \mathbb{R} | $= \sum_{i=1}^3 [\mathbf{A}]_{ii}$ |