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An Encounter with Lattice Boltzmann for Biomedical Applications: interactive simulation to support clinical and design decisions

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ABSTRACT

Medical device design for personalised medicine requires sophisticated tools for optimisation of biomechanical and biofluidic devices. This paper investigates a new real-time tool for simulating structural and fluid scenarios - ANSYS Discovery Live – and we evaluate its capability in the fluid domain through benchmark flows that all involve steady state flow at the inlet and zero pressure at the outlet. Three scenarios are reported:

i. *Laminar flow in a straight pipe*
ii. *Vortex shedding from the Karman Vortex*
iii. *Nozzle flows as characterised by an FDA benchmark geometry*

The solver uses a Lattice Boltzmann method requiring a high performance GPU (nVidiaGTX1080, 8GB RAM). Results in each case were compared with the literature and demonstrated credible solutions, all delivered in near real-time:

i. *The straight pipe delivered parabolic flow after an appropriate entrance length (plug flow inlet conditions).*
ii. *The Karman Vortex demonstrated appropriate vortex shedding as a function of Reynolds number, characterised by Strouhal number in both the free field and within a pipe.*
iii. *The FDA benchmark geometry generated results consistent with the literature in terms of variation of velocity along the centreline and in the radial direction, although deviation from experimental validation was evident in the sudden expansion section of the geometry. This behaviour is similar to previous reported results from Navier-Stokes solvers.*

A cardiovascular stenosis example is also considered, to provide a more direct biomedical context. The current software framework imposes constraints on inlet/outlet boundary conditions, and only supports limited control of solver discretization without providing full field vector flow data outputs. Nonetheless, numerous benefits result from the interactive interface and almost-real-time solution, providing a tool that may help to accelerate the arrival of improved patient-specific medical devices.

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INTRODUCTION

Arguably, the 21st century will be seen as a turning point in the history of medicine, when widespread patient specific modelling became achievable and was integrated within clinical best practice. Although examples of patient specific solutions for pharma and device design are on the increase – supported by broader initiatives to encourage adoption (eg. FDA, Avicenna Alliance[2]) – in today's climate it is equally clear that there is still a long way to go before 'patient specific medicine' becomes standard practice. This paper considers a patient specific simulation technology - computational fluid dynamics (CFD) - and tools for its adoption as part of best practice in medical device design. A particular target for biomedical CFD is cardiovascular interventions where two specific simulation challenges are commonly acknowledged, namely the overhead of long solution times and the reluctance to adopt simulation due to software complexity, requiring considerable experience to ensure that adequate solutions are obtained.

In this context, we report results obtained using a new accelerated flow solver (ANSYS Discovery Live (ANSYS®, Canonsburg, PA, US)) that exploits Lattice Boltzmann methods to produce near real-time transient solutions for a wide range of flow problems, based around an accessible interface. This has significant implications for medical application as it has potential to deliver patient-specific simulation outcomes in clinically pertinent/relevant timescales. In this paper the capability of this solver is evaluated with respect to several flow conditions, relevant to medical device design, for which well documented benchmark solutions exist. We suggest

[2] https://avicenna-alliance.com/files/user_upload/PDF/in-silico-medicine-research.pdf

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that the performance of this new solution technology in these areas is an indication of its capability for more general device-related and physiological simulation, and by way of example a clinical cardiology application is also discussed.

In respect of validating solutions against reference flows, this paper explores the capability of Discovery Live to accurately report flow conditions covering a range of complexity, namely:

i. laminar parabolic flow in a straight pipe - steady state boundary conditions, and resulting steady state velocity/pressure distribution [1]

ii. periodic flow (Karman Vortex) in both an unconstrained domain and a straight pipe - steady state boundary conditions, unsteady output [2,3]

iii. The FDA CFD Nozzle benchmark challenge[3] – steady state boundary conditions, with community validated experimental and CFD-computed velocity/pressure distributions [4]

Each case (i, ii, iii) represents a well-studied and well-described flow allowing the results from ANSYS Discovery Live to be evaluated in each instance. Of particular interest is the description of the flow field (velocity, pressure etc.) as well as the capability of the solver to report the flow field (solution time, robustness etc.). Consequently, the Method section outlines the process of obtaining fluid flow

[3] https://nciphub.org/wiki/FDA_CFD

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solutions, with the Results section both reporting outcomes using ANSYS Discovery Live but also comparing these with published results using alternative methods. The Discussion critiques the performance of this new technology and considers its implications for medical device design and patient specific clinical decision making. As noted above, we also consider its application to a cardiovascular stenotic vessel problem and the insights it offers.

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METHOD

A Discovery Live simulation begins with definition of the fluid domain and this is most easily achieved by importing a CAD representation of the geometry of interest. Internal or external flows can be specified. Details of the geometries and boundary conditions are provided with each of the cases (straight pipe, Karman vortex shedding, FDA benchmark) described below. In all examples, steady state boundary conditions only were considered, with physiologically relevant Reynolds numbers used to explore the flow behaviour. Both water and blood (modelled as Newtonian) can be used as the fluid within the domain with fluid properties specified prior to the simulation. Unlike other computational fluid dynamics approaches, the software requires relatively little input from the user in terms of discretization of the domain through a meshing process as this is handled automatically. The user is provided with an option to select the 'Fidelity' of the simulation through a slider on the interface. The 'Fidelity' setting influences solution speed and the accuracy of the solver output. In these examples moderate fidelity was chosen, with the slider placed 2/3 of the way towards the high 'Fidelity' position. The simulation starts when the 'Simulate (start/pause simulation)' button in the software is pressed (Fig 1). Following this a full 3D solution is displayed dynamically, evolving in real time, with an incrementing time counter visible at the side of the screen. The evolving display is interactive, allowing alternative visualisation modes to be selected in real-time (eg. pressure, velocity, particles, streamlines, contours etc.) and the geometry to be altered as the solution progresses. The solver can even be paused to change boundary condition values, so that these changes influence the subsequent flow field when the simulation is restarted. The facility to report results at fixed points within the flow

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field (through the use of manually placed point probes and data exported as a csv file) was used in this study to record parameters of interest. This data was also presented as a live plot during the simulation, updating in real-time on the screen. The version of Discovery Live used in this exercise was bundled as part of ANSYS release 19.24 and ran on a Win10 platform, hosted on a PC equipped with an nVidia GTX1080 graphics card with 8GB RAM.

(i) Laminar Flow in a Straight Pipe

Steady state flow in a long cylindrical pipe of constant diameter is a simple, but well described and validated flow [1, 5], providing a suitable reference for comparison with the ANSYS Discovery Live solution. The CAD representation of the geometry is shown (internal radius 32mm, length 2m), with boundary conditions that impose a plug flow inlet velocity and zero pressure at the outlet (Fig 2). A summary of salient parameters is provided in Table 1. Along the pipe, the boundary layer originating from the interior wall steadily expands with distance to eventually fill the entire width. After this position the flow is fully developed, i.e. flow characteristics no longer change with increasing distance along the pipe.

The distance over which the flow becomes fully developed is known as the entrance length (L_E) and is a function of the Reynolds number (Re). In the case of laminar flow it is known to be [5]

$$L_E \approx 0.05 \cdot D \cdot Re \tag{1}$$

[4] https://www.ansys.com/ See also … https://www.youtube.com/watch?v=H1jySucPHWk

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With non-slip boundary conditions at the pipe wall and axisymmetry about the centre-line, the fully developed steady state velocity profile (u) is given by [1,5]

$$u(r) = 2U \cdot \frac{R^2 - r^2}{R^2} \quad (2)$$

where U is the average flow velocity, R represents pipe radius (<< length L), and r is the radial coordinate (distance from the pipe centreline). To characterise entrance length, Reynolds number was varied by changing the inlet velocity ($100 \leq Re \leq 1000$, in steps of 100). Probes were placed along the pipe centreline to report flow velocity. This is a maximum under fully developed flow (ie. once the entrance length is exceeded), and equates to $2U$. In order to reconstruct the cross-sectional velocity profile, the numerical solution was probed radially at 9 points, located at distances of $0.5L_E$, $0.8L_E$ and L_E from the pipe entrance. The velocity profile – $u(r)$ - obtained at steady state (determined visually, supported by probe data) was compared to the expected parabolic profile given by Equation 1. The parameters reported from Discovery Live were plotted and compared with analytical descriptions given by Eq. 1 and Eq 2.

(ii) Karman Vortex

The Karman Vortex refers to periodic shedding of vortices from a cylindrical bluff body in an unconstrained free field flow [2]. The resulting flow is typically unsteady and provides a much more challenging scenario for the ANSYS Discovery Live solver, whilst still allowing comparison with well documented behaviour. This study was performed with a 5mm diameter cylindrical pin, in both the free field (for comparison with [2]) and with the pin bisecting a cylindrical pipe (32mm diameter,

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fully developed flow at the pin). The latter relates to direct comparison with a physical and numerical example of the same described in the literature [3]. A sketch depicting both setups is shown in Fig 3, and further details are provided in Table 2. Although the dimensionless Strouhal number (*St*) can be used to characterise the periodicity of the shedding flow [2], we also report the shedding frequency as a function of *Re*. As reported in the literature [1,2], the Strouhal number is a function of the flow characteristics according to:

$$St = \frac{fD}{U} \tag{3}$$

where *f* refers to the shedding frequency, *D* is the diameter of the cylindrical pin, and *U* is the free field flow velocity. Reynolds number was varied by changing the inlet velocity, from 100 ≤ Re ≤ 1000 in steps of 100. In both cases (ie. free field and pipe flow), the shedding frequency was obtained from a probe located at a distance 10D downstream and 1.6D off-axis from the cylindrical pin centre (see Fig 3). By plotting the periodic oscillations of the y-velocity flow component, the shedding frequency could be determined once steady oscillations were visibly established. The Re-dependent shedding behaviour from ANSYS Discovery Live was compared to results (eg. *St*, shedding frequency) reported in the literature.

(iii) FDA Nozzle Model

The FDA CFD benchmark flows [6] were specifically designed to exercise flow solvers and compare their outputs with experimentally obtained reference measurements. These are flows with characteristics that are considered to be representative of

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those found in medical devices. Two benchmark problems [4,6] have been proposed for CFD validation

- flow through connected nozzles of various diameters
- flow in a simplified centrifugal blood pump

This paper considers the Nozzle Benchmark. The geometry consists of an inlet cylinder, coupled to a converging nozzle that connects to a sudden expansion through a short cylindrical pipe section. The CAD representation of the geometry is shown (Fig 4), with boundary conditions that impose steady flow at the inlet (plug velocity profile converted to parabolic by long entrance length) and zero gauge pressure at the outlet; table 3 provides details. Specifically, the model geometry consists of:

- an inlet pipe of radius 6mm and length L_E sufficient to ensure fully developed flow
- a converging section (α=20°, 22.685mm)
- a throat region of radius 2mm and length 40mm, ending with sudden expansion into…
- …a pipe of radius 6mm and length 180mm, chosen to ensure a negligible influence of the outlet boundary condition on the reattachment point.

The pressure/flow output from Discovery Live was compared to the FDA nozzle benchmark data.

An Idealised Clinical Scenario

For clinical context, we consider an idealised vessel based on a coronary artery with two stenoses of different severity. The geometry consists of a 3mm diameter lumen

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constricted by a 75% occlusion (4mm long) and a 45% occlusion (9mm long) as illustrated in figure 1. The boundary conditions impose a physiologically appropriate flowrate by ensuring adequate flow to the downstream vasculature, achieved with a 11.5kPa (87mmHg) pressure drop across the remaining microvascular resistance downstream of the stenotic vessel section. Probes placed either side of each stenosis report centreline pressure as the simulation proceeds. The challenge facing the clinician is whether just one lesion or both lesions should be stented in order to provide the optimal physiological /clinical outcome (maximise flow) for the least amount of stent inserted (to minimise stent-related complications). What strategy should be adopted? Discovery Live was used to evaluate different interventional strategies in real time to interactively ascertain the impact on flows/pressures when any of the occlusions are removed by virtually stenting the them.

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RESULTS

The results reported below relate to solution data from the straight pipe, Karman Vortex and FDA models. The idealised clinical example is also presented, but it cannot benefit from direct comparison with solutions in the literature and therefore its analysis is more qualitative. In all benchmark cases the 3D simulation was allowed to run until steady state or cyclically reproducible flow behaviour was obtained – this is the data reported here. The Discovery Live solver instantly produces a visible, evolving full field solution once initiated, and accordingly, the rate at which simulation time evolved in comparison to wall clock time is also reported.

(i) Laminar flow in a straight pipe

For the laminar flow straight pipe example, once the solver is initiated the plug flow at the inlet is seen to develop into a steady state flow over a period of about 20 simulation secs (*Re* dependent), with parabolic profile apparent at the development length and beyond (Fig 5). Each second of simulation time for the 2m pipe took ~15 secs of wall clock time using our hardware. Radial velocity profiles at distances of $0.5L_E$, $0.8L_E$ and L_E from the pipe entrance are presented in figure 6. The velocity along the central axis in the steady state is reported over a range of Re values in figure 7 with parabolic flow established when the peak velocity reaches twice the (mean) velocity at the inlet. For added detail, the evolving central axis velocity distribution at L_E is shown as a function of simulation time for *Re* 500 in Fig 8. Expected values for the flow according to Eq1 and Eq2 provide context by which to judge the accuracy of the numerical solutions. In all cases solution accuracy was correct to better than 1%.

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(ii) Karman vortex

The shedding of vortices from a 5mm diameter pin was simulated in both the free field and within a 32mm diameter pipe. The free field condition has been examined extensively in the literature, we refer the reader to the collated information presented in the review by Williamson [2] as an established reference. In the case of the pipe flow, the near wall conditions of the straight pipe influences the shedding, and for this case the ANSYS Discovery Live solution is compared with the paper by Fenner et al. [3].

Free field

The Strouhal number derived from the Discovery Live simulation has a tendency to be slightly below that reported in the literature. The frequency of shedding in the free field (as a function of *Re*) is reported in Table 4, supported by figures 9, 10. For real physical flows, at *Re*<100 the flow has a tendency to be steady and not shed, and although the threshold for shedding is notionally about *Re* 50, this can be quite dependent on subtleties of the experimental conditions (eg. stability of the incident flow, smoothness of the pin etc.). ANSYS Discovery Live did not demonstrate vortex shedding at *Re*<90. At higher *Re*, shedding within the simulation does occur, but not immediately, since the flow typically requires a transition period of many seconds (simulation time) at these *Re* before it reaches a steady shedding rhythm. This reproduces behaviour observed under experimental conditions. The rate at which shedding occurs is effectively reported by the periodic behaviour of the y-velocity as

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revealed by the off-axis simulation probe. For this simulation 10sec wall clock time is required for about 1 second of simulation time.

Blevins (1990) [7] reports that the Strouhal number is close to 0.2 over a large range of Reynolds numbers. In the range 250<*Re*<200,000 the empirical formula of equation 4 is known to hold true.

$$St = 0.198(1 - \frac{19.7}{Re}) \quad (4)$$

This results in a value of St=0.19 at Re=500 which – except for Re 200 - compares well (<5% difference) with the value obtained with Discovery Live.

Karman vortex in the straight pipe (near wall case)

The straight pipe demonstrates similar behavior to the free field case, but the closeness of the cylindrical walls of the pipe to the pin influences the shedding behavior, and there are no standard references for shedding under these conditions. This is discussed in the paper by Fenner et al. [3], which provides the context for the Discovery Live simulation described here (see table 5). Shedding reported by Fenner at al. at Re100 does not occur in Discovery Live, but extrapolation from higher Re indicates that the simulation might be at variance with that obtained by experiment by approximately 20%. A summary is presented in fig. 11.

(iii) **FDA Nozzle Model**

The FDA geometry has proven challenging to a wide range of solvers attempting to describe the flow under steady state inlet conditions [4]. The flow is largely transitional and approaches turbulence in regions of the flow domain (particularly,

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downstream of the sudden expansion). Experimental results help to confirm the plug-like velocity profile associated with acceleration through the converging nozzle, and the regions of recirculation downstream of the sudden expansion orifice. The literature reports velocities along the central axis, as well as radial velocity profiles at specified locations for Re 2000 and 3500, and these are used for comparison with this simulation (see figures 12-15). The Discovery Live simulation makes a credible attempt (typically within 10% of reference values) to capture the essence of the flow throughout the domain, including expected recirculation several diameters downstream of the sudden expansion (Fig 16). One second of simulation time took approximately 500 seconds of wall clock time.

Example Clinical Scenario (idealised)

For the clinical scenario, the 11.5kPa (87mmHg) boundary condition is associated with a mean flow velocity of approximately 0.5ms^{-1} in the unrestricted pipe, with peak flows achieving almost 3ms^{-1} in the tightest stenosis. Recirculation is evident behind both occlusions. Severity of occlusion is characterised by the clinically relevant parameter Fractional Flow Reserve (FFR) which is the ratio of pressures distal and proximal to an occlusion (Fig 17). The threshold for intervening (stenting) is ≤0.80. The simulation demonstrates that despite the significant length of the longer lesion (45% occlusion by area), it contributes little to the overall restriction of flow that is present. It is the shorter, narrower stenosis that dominates and it is clearly the preferred candidate for removal (by stenting). According to the results of this simulation there is little justification for stenting both stenoses.

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DISCUSSION

This paper has described application of a new commercial solver to a range of fluid problems from a simple straight pipe to vortex shedding to an FDA-defined nozzle geometry. In respect of flow in a straight pipe, the ANSYS Discovery Live solver proved very capable, accounting for the attachment length and the parabolic profiles at different Re as expected. Since this represents the most fundamental and simplest of flows, it is important that the solver should demonstrate excellent description in this case, for purposes of credibility.

The Karman Vortex is much more demanding as indicated by the work of Lienhard (1966) [8] which reports that the vortex street is laminar for $Re<150$, with periodicity governed either by wake instability ($40<Re<90$) or by vortex shedding ($90<Re<150$). Transition to turbulence occurs for $150<Re<300$ in which the wake is characterized by periodic irregular disturbances. For Re>300 ($300<Re<300{,}000$) the vortex street is fully turbulent. Nonetheless, reproducible shedding behavior in the free field can be obtained experimentally, and is reported in the review by Williamson [2]. Under free field conditions simulated shedding frequency was slightly underestimated, and at particular Re was discrepant by almost 20% compared with experimental data.

Away from free field behaviour, the focus for comparison is Fenner et al. [3] who explored shedding behaviour in the cylindrical pipe (a niche case relevant to quantitative flow imaging [9]). Replacement of the free-field conditions with near-wall constraints imposed by the pipe modifies the flow and shedding behaviour. It was noted at the time of writing (2008) that an IBM SP3 supercomputer used to compute the shedding flow, required weeks of solution time. In contrast, Discovery Live computes a solution in seconds and reports overall features of the shedding behaviour, although this solution is less accurate than the SP3 solution, which was able to describe the shedding frequency to within 10% of that determined by experimental measurement. However, the feasibility of almost-real-time feedback with interactive visualisation has significant implications for the design phases of medical devices, even though some compromise in accuracy might have to be accepted.

Similar outcomes were observed when analysing results from the FDA benchmark geometry in this study. The original context of this problem involved numerous centres submitting numerical solutions during the initial call of the FDA Challenge over a decade ago; these were compared with experiment. Stewart et al. [10] reported that a significant fraction of the submitted numerical solutions were so far removed from the experimental data that they were not selected for consideration in the final analysis. Selection involved a self-consistency check (based on incompressibility assumptions and mass flow conservation) that was used as a quality metric for the numerics, and only solutions demonstrating adequate consistency were considered for further analysis, as reported by Stewart et al.[10]. In this paper, despite the use of a single 'Fidelity' setting for all analyses presented, ANSYS Discovery Live produced a credible solution (compliant with the FDA mass flow metric) that visibly falls within the range of the acceptable solutions reported by Stewart et al. To obtain these results little expertise was necessary, Discovery Live produced a solution using only the bounding geometry for the flow and inlet and outlet conditions, providing results within minutes. Unsurprisingly the results were less convincing downstream of the sudden expansion, where turbulent effects are

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more significant, which was addressed by some centres using turbulence models in the original 2009 analyses [10].

Hardware

In the context of hardware, Discovery Live relies on GPU acceleration to deliver fast, fluid dynamic simulations. It is only very recently that the marriage of Lattice Boltzmann code with commodity GPU platforms has become effective for real problems. The solver used in Discovery Live exploits a Lattice Boltzmann method in which the discretised space involves transport of 'particles' between interconnected nodes and resolution of collisions at nodes. Each stage is dealt with separately/alternately in accordance with simulation time which is also discretised. With suitable choice of collision operators, the Lattice Boltzmann solution is known to approach (in the limit) a Navier-Stokes description of the flow. The solution process is amenable to parallel computation and therefore the method can benefit greatly from implementation on a GPU platform. A key limitation here is GPU memory (which limits the number of nodes) and only recently have commodity graphics cards become available with sufficient RAM to address realistic problems of the kind described in this paper. A recommended specification is the nVidia GTX 1080 series with 8GB of onboard RAM. The specification of the host PC should be designed to run the graphics card optimally, but the key factor influencing solver performance relates to the GPU specifications. The examples cited in this paper ran on both a desktop equipped with a GTX1080 (8GB) and separately, a laptop equipped with an onboard GTX1070 (8GB). In general the latter ran approximately 20% slower than the former.

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LB Limitations

Although Lattice Boltzmann has several advantages over more traditional Navier-Stokes approaches (including efficient exploitation of massively parallel architectures, effective for complex geometries, porous media etc.) it also suffers from some important limitations. For instance, the density of the LB lattice is typically dictated by the speed of sound in the material, and under certain circumstances this can lead to unacceptably short time steps. This has implications for higher speed flows. Fundamentally, the method struggles to capture the full energetics of a flow and thus is ill suited to compressibility. There are also challenges with incompressible flows, again because of the speed of sound consideration. This often becomes relevant at particular Re, resulting in fine time-steps and consequent slow running of the simulation clock (compared with wall clock) to suitably capture detailed flow structures. This is compounded by the uniform mesh spacing throughout the domain, which can result in poor description of thin layers/gradients. More refined meshes (as influenced by the ‘fidelity’ slider) result in improved description but at the cost of greater compute time. Optimisations are widely present to accelerate computation, but these may rely on constants for fluid parameters like viscosity. Therefore the method is poorly suited to scenarios in which such parameters might be a variable throughout the domain. In spite of such limitations, an LB solver can be very effective in the right circumstances - as demonstrated by this paper - with the real-time interactivity offering genuine insight that can inform design decisions.

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Software interface

The most striking feature of the solver is its immediate presentation of an evolving solution, developing at a smooth frame rate with a 'simulation clock' that advances at a rate comparable with the 'real world clock'. At higher fidelity settings, simulation time increments more slowly, but the solution remains dynamic and the facilities for flow visualisation and probing the flow are informative to the user. The interface is straightforward, enabling exploration of the flow field through views from different perspectives (by dragging the mouse) and/or imposing a different flow visualisation mode. This includes cut planes through the field (oriented via mouse) to display velocity, pressure, etc. as contours and streamlines. A particle representation is also available, but the lack of full vector field data is a notable omission. This adversely impacts Discovery Live's capacity to act as a quantitative tool, since detailed quantitative flow field data is not available. Arguably, this can be obtained to some extent through the use of point probes, but these are placed individually and manually to provide point-like measurements and do not replicate the full field data available from traditional Navier-Stokes CFD solutions or experimental methods such as PIV. Consequently, ANSYS Discovery Live offers a semi-quantitative tool for 'getting a feel' for the flow, and particularly the influence of changes that might be introduced through altering parameters such as flow rate, geometry, fluid properties etc. The interactive nature of the interface and the ease with which changes to the flow simulation can be introduced make this an environment for exploration, and this is the strongest aspect of the Discovery Live software, providing the user with an innate feel for the dynamics of the flow and its sensitivities which can then be applied to design problems. In this capacity, Discovery Live acts as an exploratory

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tool, providing useful real time feedback that can inform design at an appropriate level of 'Fidelity' for this process. This can then be examined at higher 'Fidelity' within Discovery Live and tested more rigorously via established CFD methods and/or experimentation. Use of the software provides insight to the nature of the flow, whilst limiting access to full field characterisation which requires alternative methods - this 'two stage' approach is helpfully promoted by the lack of available vector flow field data.

Constraints

A weakness of the software in its current form is that only a restricted set of flow inlet/outlet boundary conditions can be prescribed. For instance, in our case there was no facility to impose parabolic developed flow at the inlet, all inlet flows used a plug profile. A long pipe was used at the inlet to allow flow development if parabolic inlet profiles were required, with associated increase in solution overhead. Additionally, transient inlet flows are not supported, motivating the use of steady state conditions for this paper. The flexibility of the interface allows the user to pause the simulation, specify a new inlet velocity and then restart it, but this is a crude and unreliable method that is impractical for anything but the simplest of transient inlet conditions.

Potential future applications of such simulation tools include flow phantom design for medical imaging quality assurance applications. We have reported development of an experimental system that produces ring vortex flows from an orifice [11]. This requires an inlet fluid impulse that propels a slug of fluid through the orifice with resultant production of a propagating ring vortex. To explore such flows within

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Discovery Live the impulse can be simulated by pausing the simulation at predefined time points to manually modify the inlet flow velocity. Although this does produce a ring vortex of sorts it is outside the intended application of the solver and is prone to error. As a result the vortex flow is far removed from the ring vortices observed under experimental conditions or those produced by computation from established fully transient Navier-Stokes solvers.

The qualitative nature of ANSYS Discovery Live encourages its solutions to be interpreted with caution, but in truth, this has always been the case for numerical simulation. The best simulations typically require tuning of the solver to the problem in hand, whereas Discovery Live is a versatile tool whose strength is its flexibility. This comes with a cost, namely compromise of solution accuracy, although the software does attempt to address this through the use of the 'Fidelity' slider. The slider offers a trade-off between simulation speed and the accuracy of the solution. In the free field Karman Vortex example, moving the slider to the ‘Speed’ setting (ie. minimum fidelity) delivered 2 secs of simulation time for 1 second of wall clock time, with noticeably coarser spatial solutions. In contrast, at the maximum fidelity setting, the solution required almost 60 secs of wall clock time to achieve 1 sec of simulation time. The user must make a judgement about the trade-offs they are willing to accept in respect of fidelity vs speed.

Finally, because of the design philosophy behind Discovery Live, all problems are innately 3D and time dependent. Therefore, it is not always easy to judge what constitutes the 'steady state' solution (working with Discovery Live is very similar to working with an experiment in this respect). The visual nature of the interface

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encourages visual assessment of what is a representative outcome, and the ability to probe the flow at discreet points can provide evidence to support that decision.

Clinical Implications

The presented clinical use-case concerns patients with suspected coronary artery disease (CAD) who undergo coronary angiography to delineate coronary anatomy. Our idealised example portrays a clinically realistic scenario with two serial stenoses (Figs 1, 17). The priority of the cardiologist is to intervene upon (ie. stent) stenoses capable of limiting coronary blood flow and causing symptoms of myocardial ischaemia but leave alone lesions which are physiologically non-significant. A pressure-sensitive wire is used to measure the pressure drop across a stenosis, with the translesional pressure ratio (FFR) used to determine whether a stent or stents should be deployed to revascularise the heart. Threshold for intervening is FFR≤0.80. This is a relatively straightforward decision in the context of a single, focal narrowing with an FFR ≤0.80. Unfortunately, most patients have serial or diffuse disease with complex inter- and intra-lesion haemodynamic interactions which make it challenging to provide accurate predictions regarding the physiological impact of alternative treatment strategies. Consequently, cardiologists tend towards over-stenting. In the case of our idealised simulation the results indicate that stenting is appropriate for the narrowest occlusion. Intervention upon the less severe stenosis is not warranted because (i) it would have no significant impact on the flow, and (ii) the placing of a stent carries a risk of acute and chronic complications (e.g. vessel dissection or restenosis).

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CFD modelling is increasingly being used to help cardiologists [12] plan interventional procedures by the use of virtual stenting [13,14]. Typically, these simulations have to be prepared, run and interpreted offline. This is acceptable for non-invasive outpatient imaging modalities such as CT coronary angiography (CTCA), but not for those patients undergoing invasive catheterisation who require treatment decision guidance in real time. For these patients, having to prepare, run and interpret CFD simulation would require that they have to be taken off the cath lab table, only to return when analysis is completed. This is unattractive to clinicians, patients and healthcare services. The alternative is that the computation is performed 'live'. The implications of real-time/live computation are considerable. It would enable advanced, CFD-driven haemodynamic simulation and treatment planning for the many patients undergoing cardiac catheterisation across the world. Real-time computation offers many advantages, but it is important to recognise that many additional elements would be needed before it can directly impact the clinical pathway. Components that would need to be addressed include streamlined vessel image capture and segmentation, 3D interpretation, effective boundary definition, a seamless processing pipeline, comprehensible user interface etc., all contributing harmoniously to a clinically integrated system. It is beyond the scope of this paper to discuss these factors in detail, but the availability of a tool like ANSYS Discovery Live makes a significant contribution to such an aspirational clinical workflow.

Design implications

The medical device engineer operates with an array of tools to achieve optimal design and Discovery Live is a useful addition to the designer's toolkit. It should not

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be considered a precision tool, but it does offer many properties that can contribute to the design workflow. For instance, the limited options for setting up the simulation is both a strength and a weakness. Unlike a finite element/volume solver, the user has no control over element type, meshing strategy, density, etc. which is all handled automatically by the software. Mesh sensitivity testing is not a feature of Discovery Live and again this emphasises the semi-quantitative nature of the software, yet it performs remarkably competently with the examples that we investigated.

In design, the original specification pertaining to a medical device might be contemplated as an inverse problem, in which an effective design process might be interpreted as the solution – delivering a device consistent with that specification. A common strategy for solving any inverse problem is iterative solution of many forward problems to identify the best candidate, and the majority of real life design solutions could be characterised this way. Discovery Live actively facilitates this process through its interactive, near-real-time capabilities, thereby informing and potentially accelerating design decisions. This contraction of the early design phase can lead to more fruitful use of time in respect of experimentation and more rigorous numerical methods to determine the optimal configurations.

Final considerations

Discovery Live is better equipped to offer insights than it is to offer high fidelity simulation results, but medicine has always been a combination of art and science, and Discovery Live provides a tool which bridges that gap. The insights afforded come through an accessible and responsive interface that encourages exploration of

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the flow and is capable of informing clinical decision making to help deliver improved outcomes. Even outside the clinic it may have a teaching role, educating clinicians about the impact of their clinical decisions on the resulting haemodynamics. If the limitations described above are appropriately considered, the software has something significant to offer which may help to accelerate the arrival of improved application and patient specific medical devices.

CONCLUSION

This paper describes application of novel near-real-time fluids solution - through ANSYS Discovery Live - to three incrementally demanding fluid dynamics scenarios (straight pipe, Karman Vortex shedding, FDA nozzle benchmark) and an idealised clinical example. Solutions are displayed and updated at smooth frame rates on screen and encourage exploration of the evolving simulation through interactive visualisation. Results were compared with the literature and demonstrated credible solutions in every case. Despite limitations relating to inlet/outlet boundary conditions, meshing and access to full field vector flow data, the real-time nature of the solver brings numerous benefits to the design cycle and appreciation of flow sensitivities, which may help to accelerate the arrival of improved patient specific medical devices.

ACKNOWLEDGEMENTS

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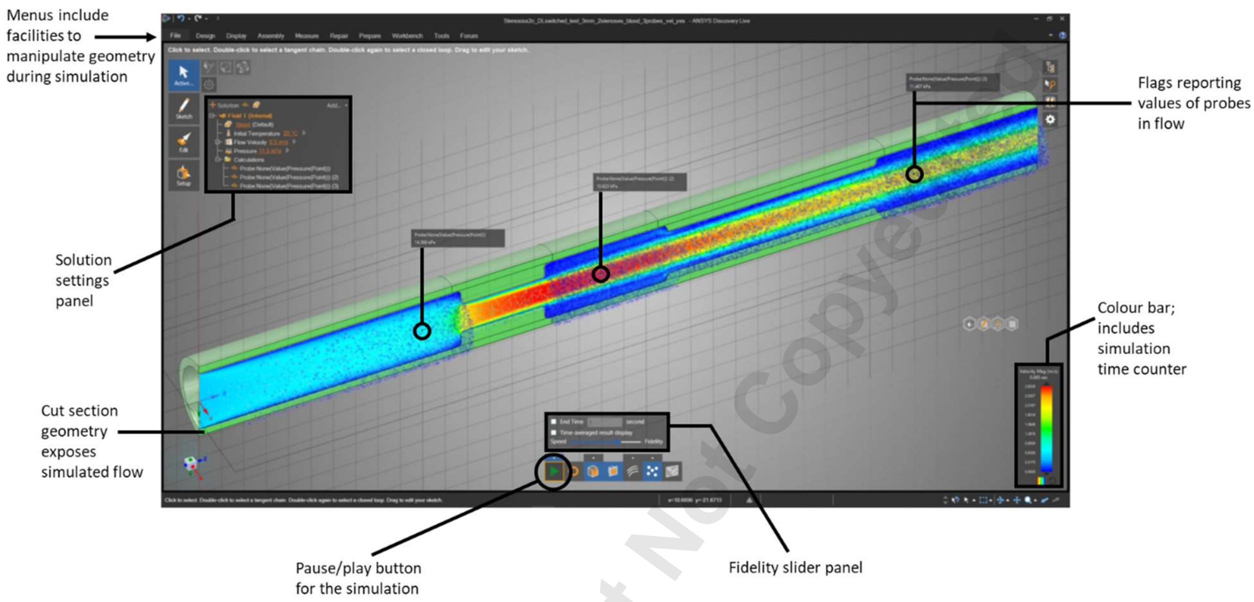
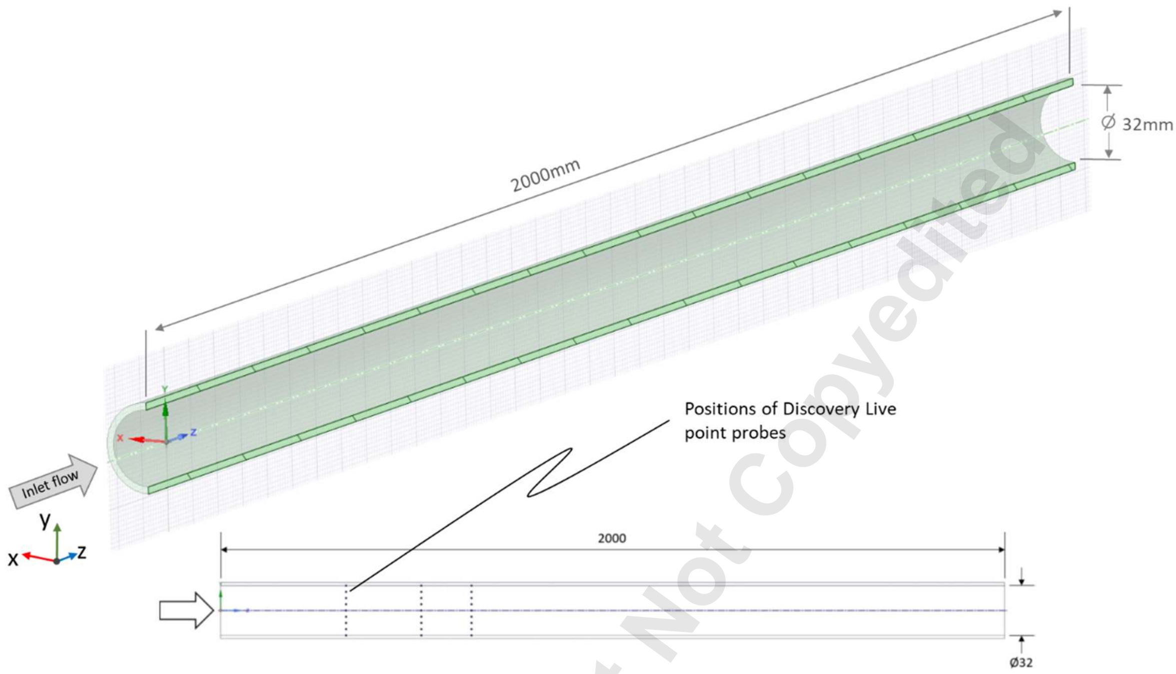
Figures with Captions

Figure 1



Legend: A screenshot of the ANSYS Discovery Live interface. Flow through a 3mm diameter pipe model with two stenoses is being simulated in this example. In addition to interactive manipulation of geometry that affects the simulation (eg. removing stenoses), the interface also offers numerous visualization options. Velocity magnitude along the central plane combined with particle tracking throughout the volume are shown; these update continuously.

Figure 2



Legend: Schematic of the cylindrical straight pipe with plug inlet flow and zero pressure at the outlet

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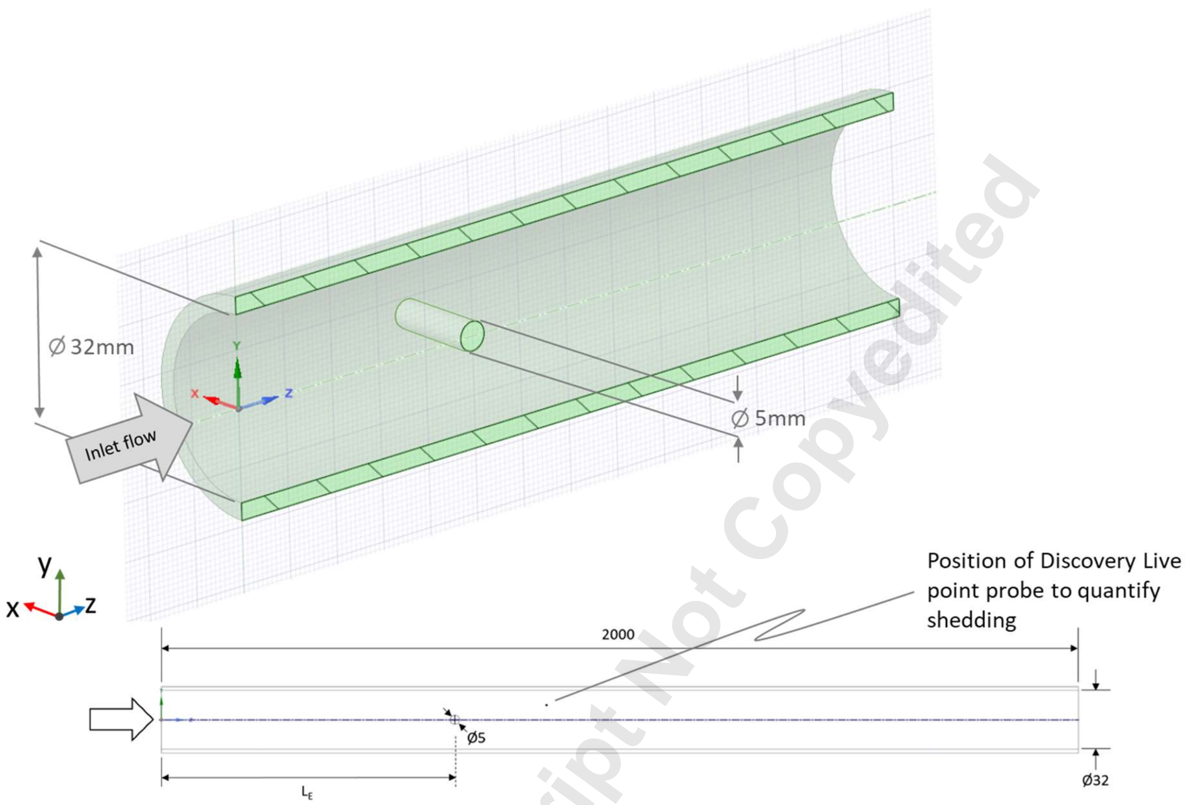
Figure 3



Legend: schematic of the Karman vortex pipe, illustrating parabolic inlet flow at the pin and zero pressure at the outlet. The free field scenario is illustrated in fig 9, and consists of a pin only, relying on external flow, bounded by a box-like domain.

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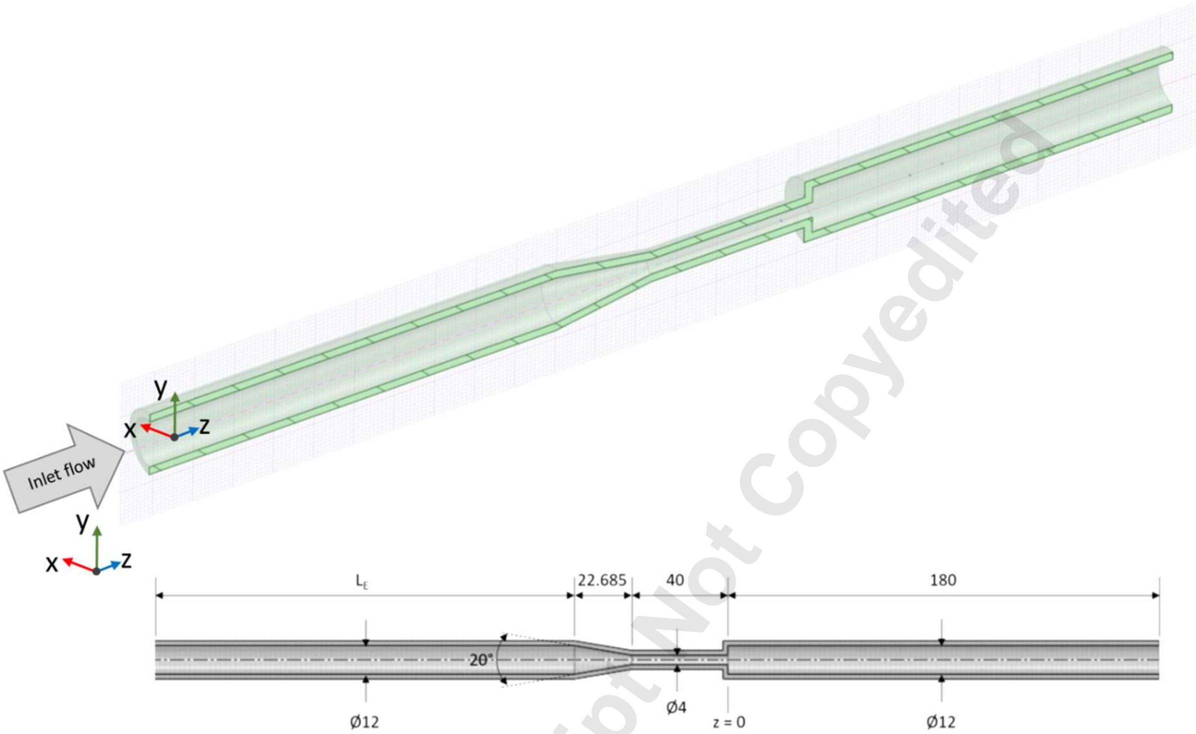
Figure 4



Legend: A schematic of the FDA nozzle model; all units in mm. An extended inlet pipe is designed to deliver parabolic inlet flows to the nozzle with zero pressure at the outlet. Dimensions are in mm.

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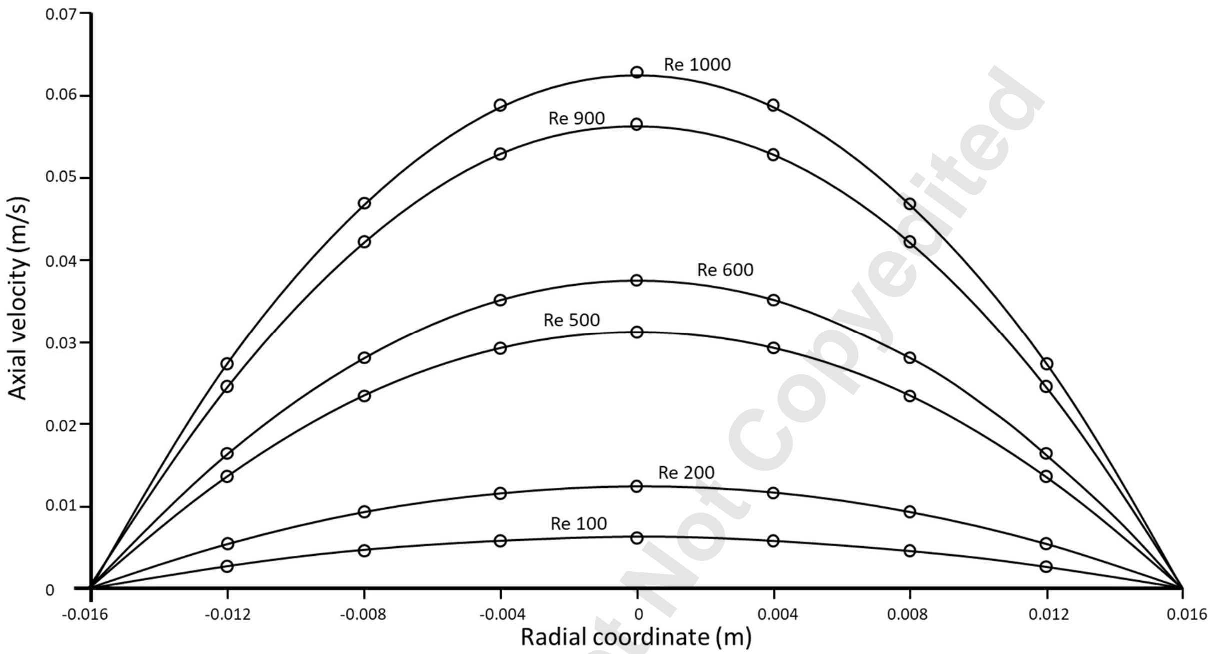
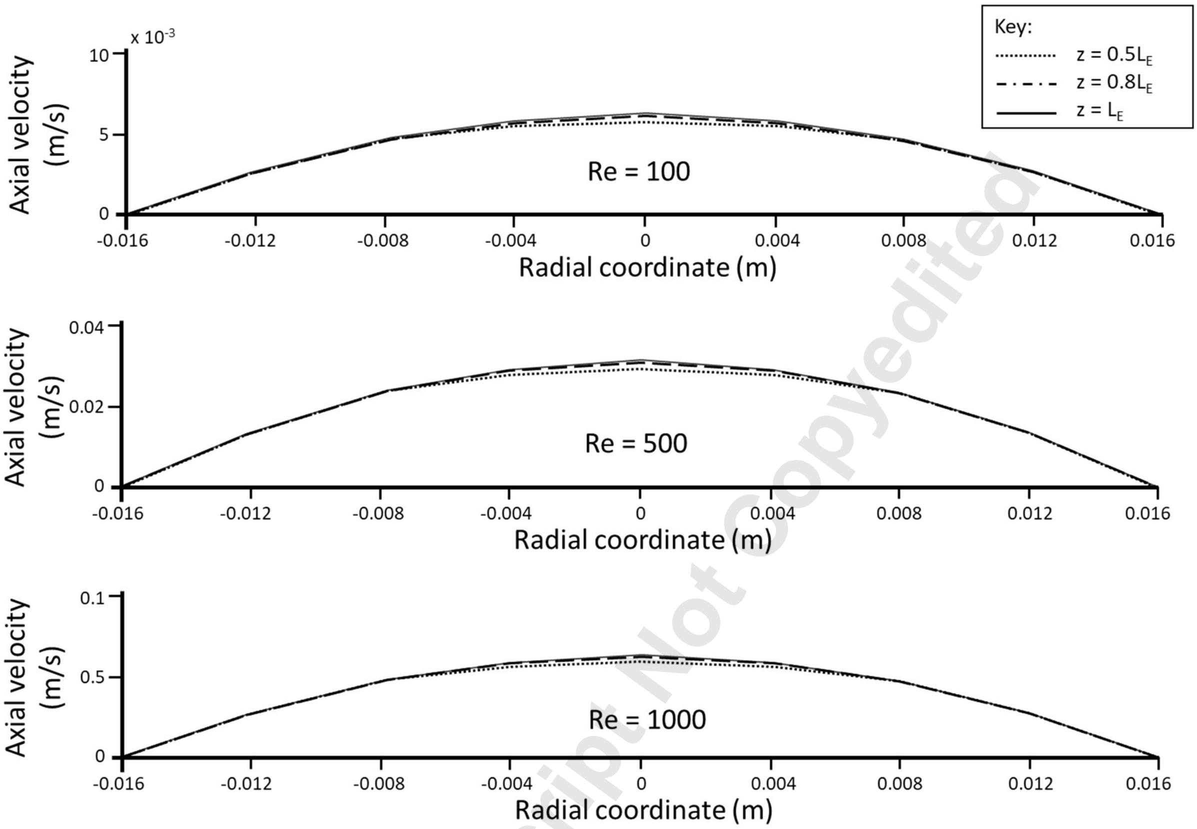
Figure 5



Legend: Comparison between numerically obtained (markers) and expected (solid line) axial velocity profile at a distance L_E from the pipe entrance for Re from 100-1000

Figure 6



Legend: Profile of the axial velocity at distances $0.5L_E$ (dotted line), $0.8L_E$ (dashed line), and L_E (solid line) from the pipe entrance for Re from 100-1000

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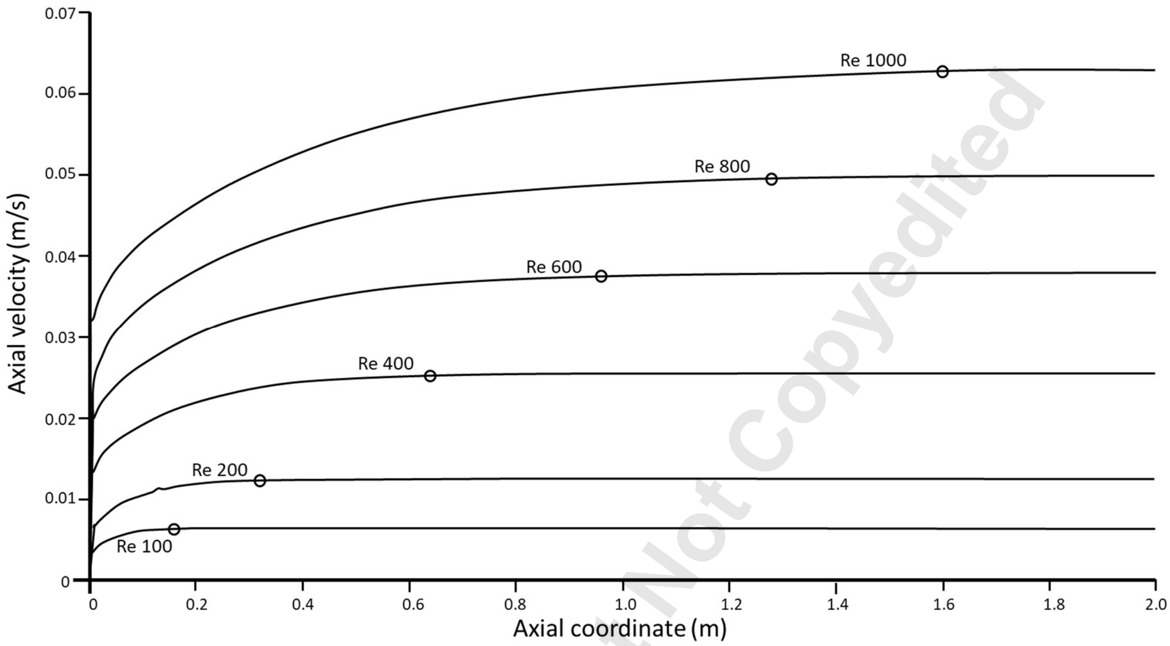
Figure 7



Legend: Axial velocity along the centreline at steady state for Re from 100-1000. The circled points indicate the expected development/entrance length at each Re.

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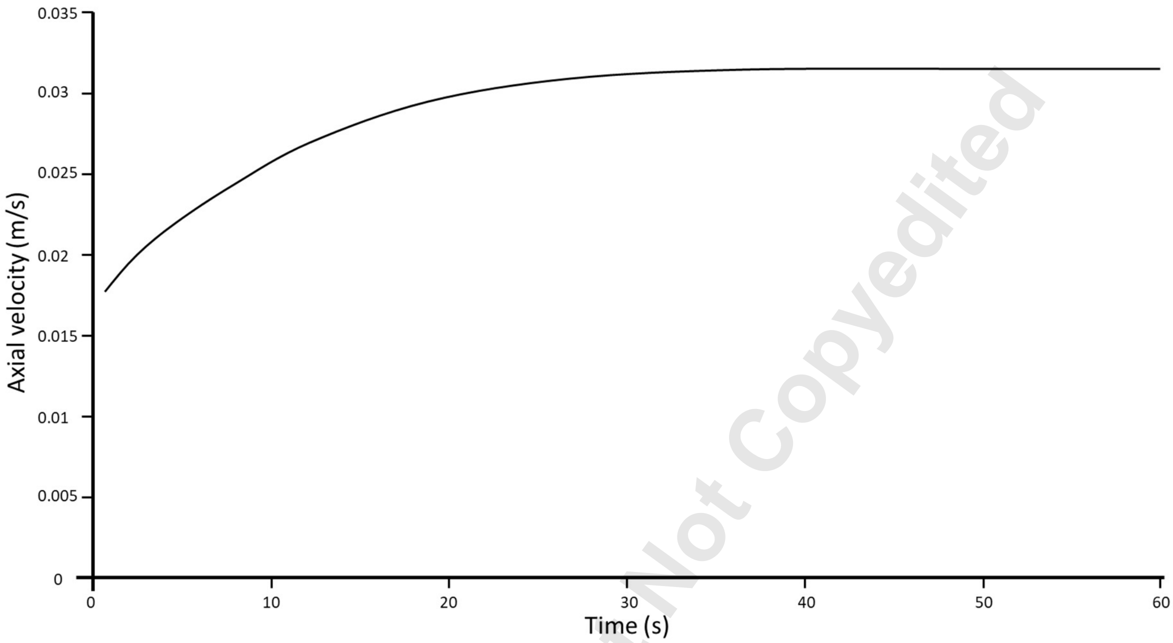
Figure 8



Legend: Axial velocity at L_E as a function of simulation time for Re = 500

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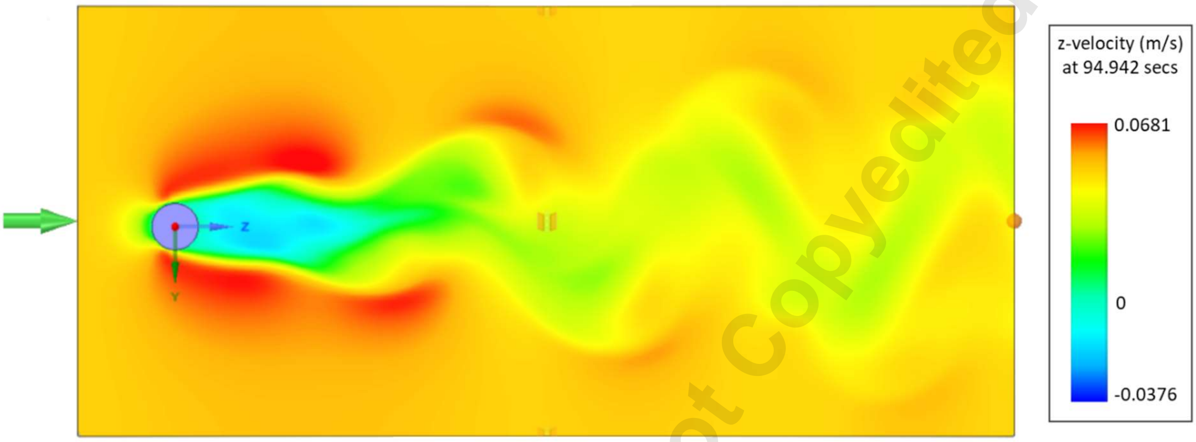
Figure 9



Legend: 95 secs of simulation time with free field periodic shedding from a 5mm diameter bluff body (cylinder) in the free field. The bounding box illustrates the volume of the solution domain, with visualisation of the magnitude of the z-velocity field down the central plane in this example

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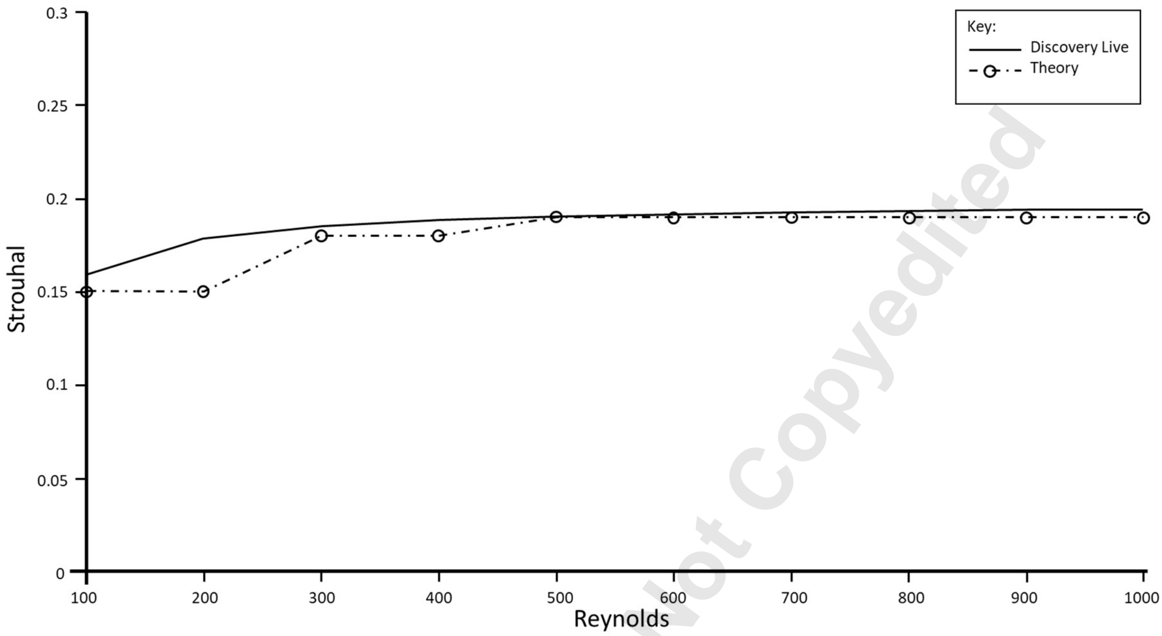
Figure 10



Legend: Strouhal number vs Reynolds number for the free field case

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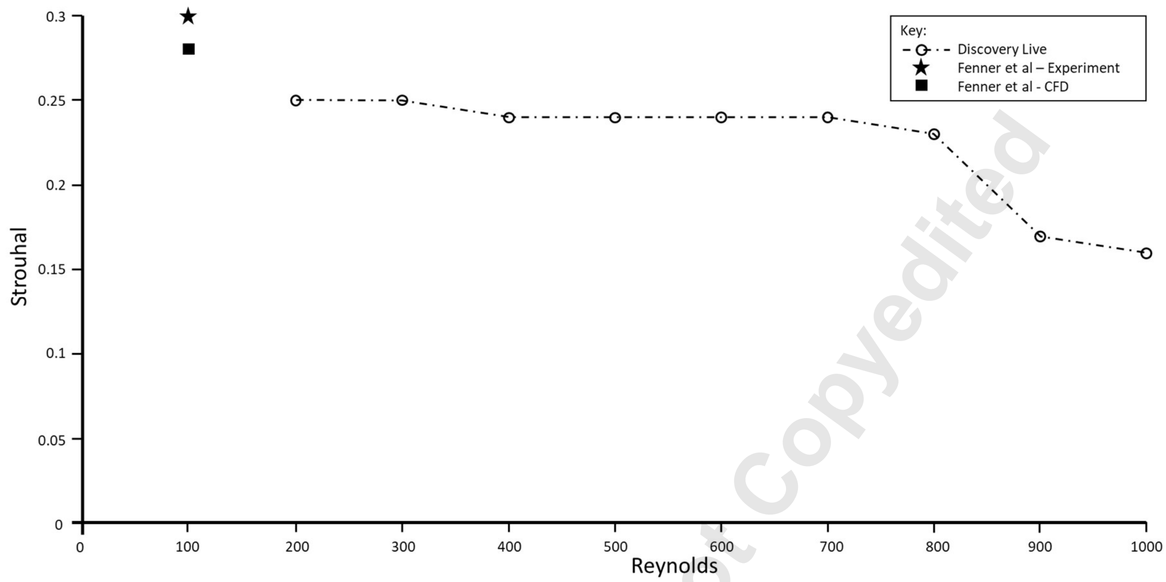
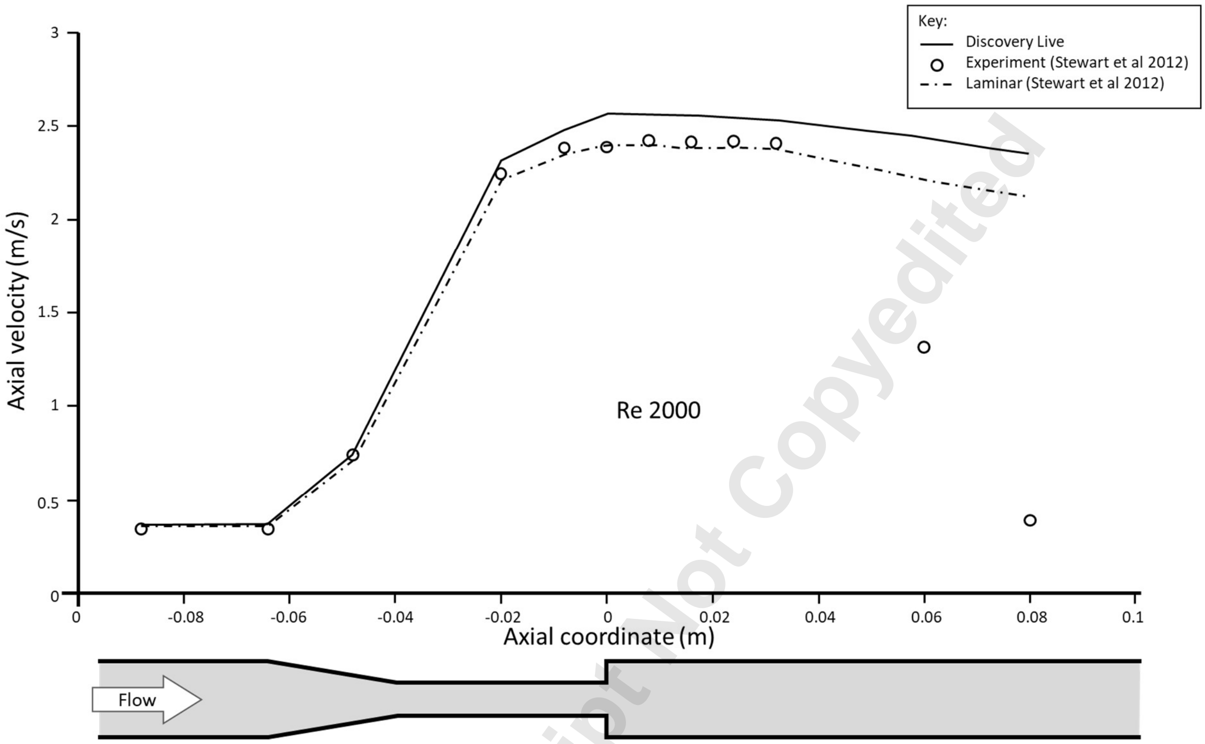
Figure 11



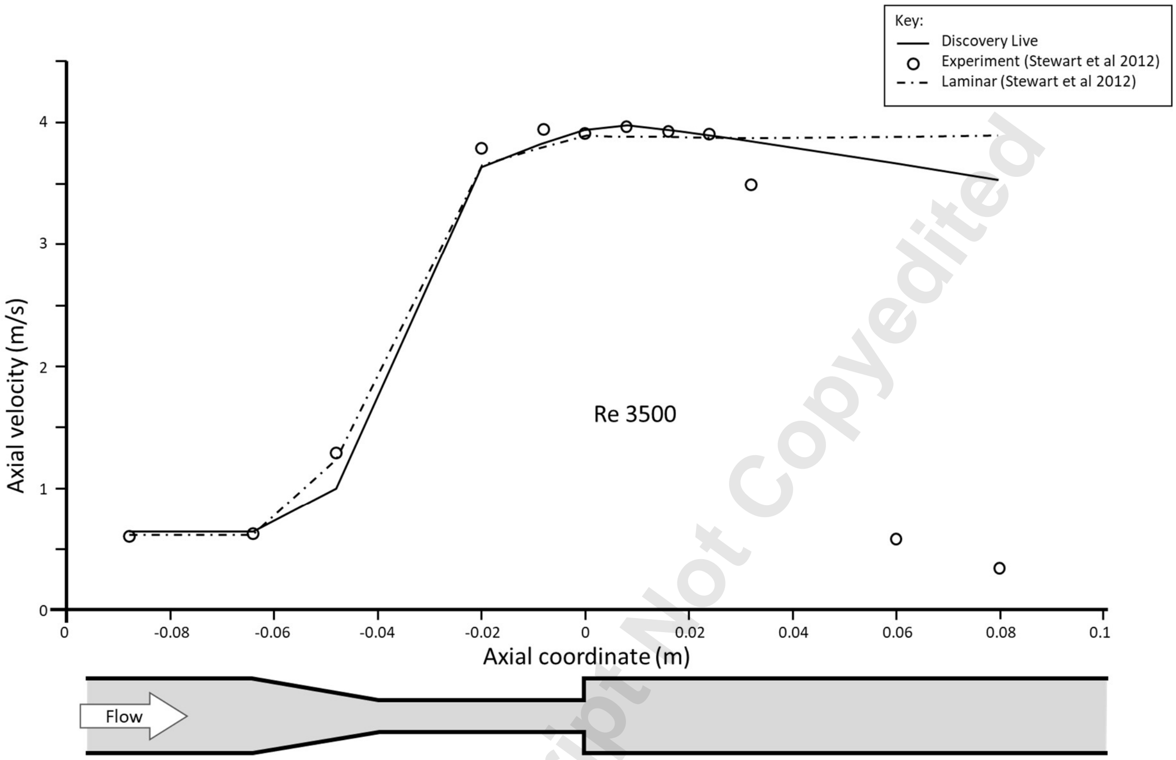
Legend: Strouhal number vs Reynolds number for the Karman Vortex in the cylindrical pipe. The points at Re=100 refer to data from the literature

Figure 12



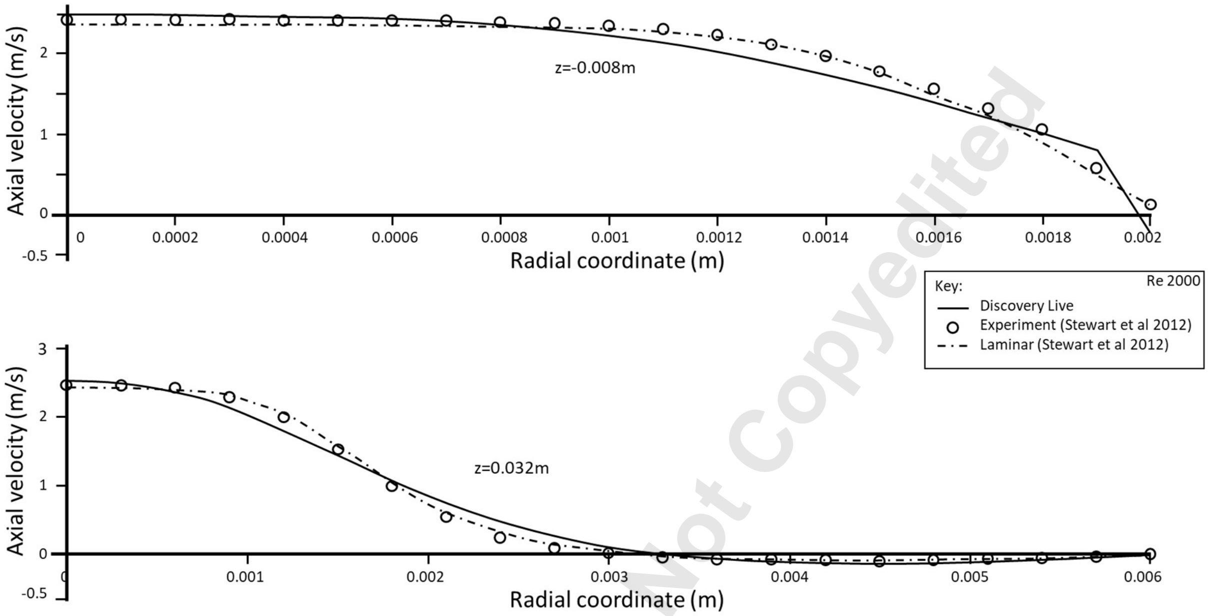
Legend: Distribution of z-velocity along the nozzle centreline at steady state for Re=2000. The position of the sudden expansion occurs at z=0.

Figure 13



Legend: Distribution of z-velocity along the nozzle centreline at steady state for Re=3500. The position of the sudden expansion occurs at z=0.

Figure 14



Legend: Distribution of the z-velocity in the nozzle along the radial direction at z = -0.008m and z = 0.032m at steady state for Re=2000

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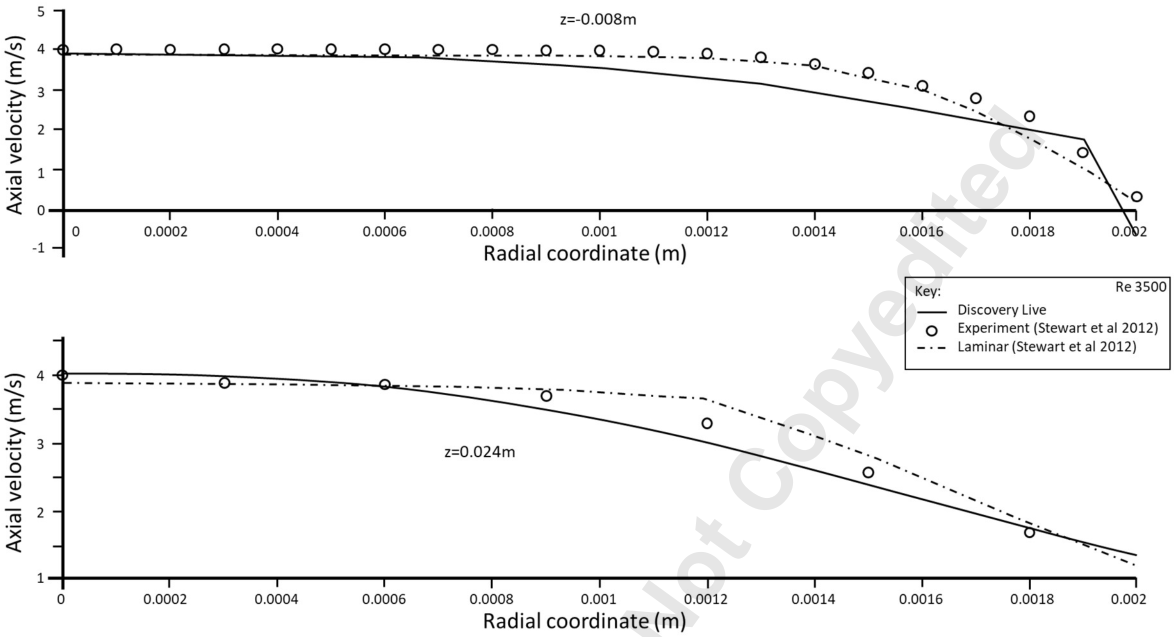
Figure 15



Legend: Distribution of the z-velocity in the nozzle along the radial direction at z = -0.008m and z = 0.024m at steady state for Re=3500

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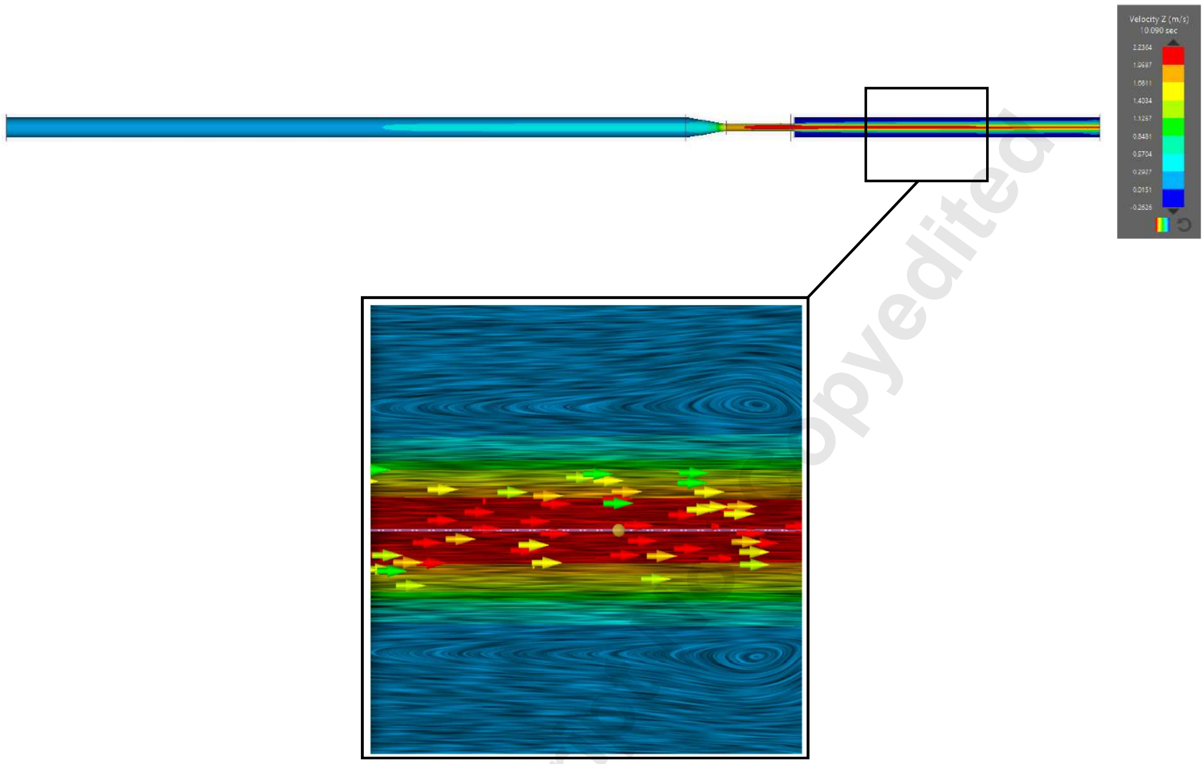
Figure 16



Legend: Colour plots of the magnitude of the velocity field at steady state at Re =2000, with visible recirculating flow downstream of the sudden expansion.

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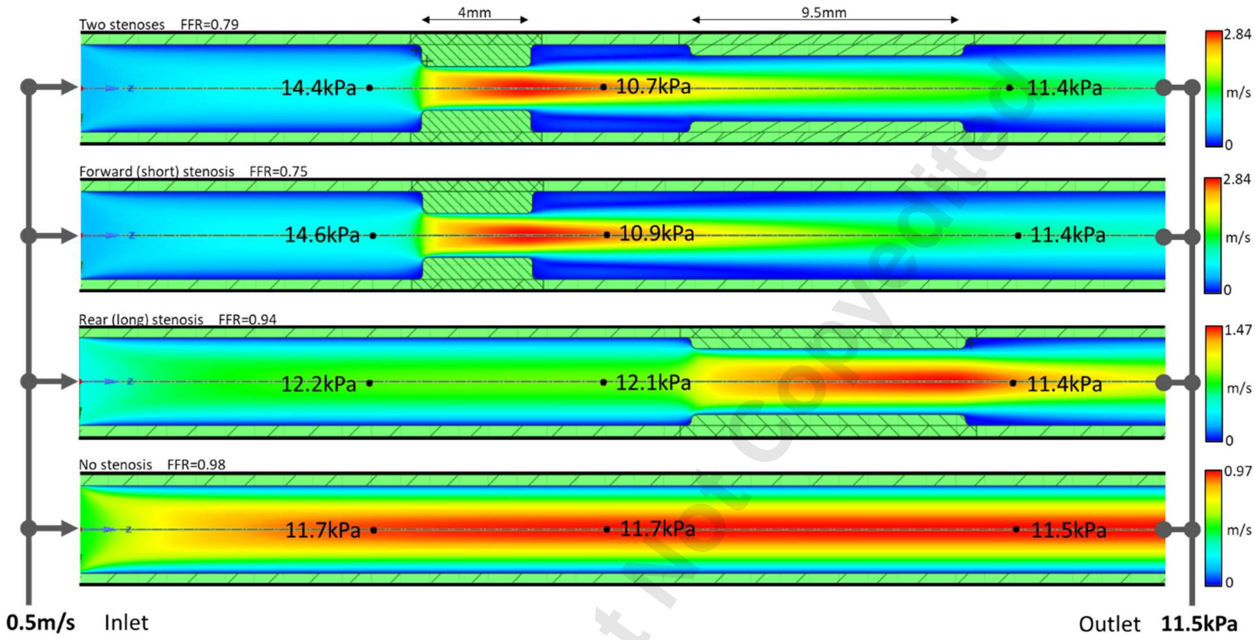
Figure 17



Legend: The idealised clinical example involves a 3mm diameter pipe occluded by two stenoses (75% occlusion and 4mm long; 45% occlusion and 9.5mm long). The flows are computed in near real-time and allow interactive removal of the stenoses. Point probes are used to report centerline pressure, whereas the colour map displays velocity magnitude. Fractional Flow Reserve (FFR) computes the ratio of pressures either side of the lesion.

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Tables with Captions

Table 1

		Steady State Laminar Flow in Cylindrical Pipe
Boundary conditions		Plug flows at the inlet covering a range of velocities corresponding to Reynolds numbers (Re) from 100 - 1000 in steps of 100.
		Zero gauge pressure present at the outlet
		Non-slip conditions on the pipe wall
Metrics of Performance		Accuracy of the fully developed parabolic flow profile, with reference to established, documented behaviour
		Entrance length
Discovery Live settings		Modelled as an internal flow
		Probes placed along the axis and radially to report flow velocity data

Legend: Simulation settings for laminar flow in a straight pipe

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Table 2

		Karman Vortex (free field, 5mm pin)	**Karman Vortex (5mm pin, 32mm pipe)**
Boundary conditions		Steady, free field flow covering a range of velocities corresponding to Reynolds numbers (Re) from 100 -1000 in steps of 100.	Plug flows introduced to extended inlet pipe to deliver parabolic flow at the pin, covering a range of velocities corresponding to Reynolds numbers (Re) from 100 -1000 in steps of 100.
		Slip conditions at the boundary of the free field domain+zero gauge pressure at the downstream boundary	Zero gauge pressure present at the outlet
		Non-slip conditions on the wall of the shedding pin	Non-slip conditions on the pipe wall
Metrics of Performance		Re at the onset of shedding	Re at the onset of shedding
		Shedding frequency as a function of Re	Shedding frequency as a function of Re
Discovery Live settings		Modelled as an external flow	Modelled as an internal flow
		Probes reporting y-velocity, placed 10 pin diameters downstream and 1.6 pin diameters off axis from pin position	Probes reporting y-velocity, placed 10 pin diameters downstream and 1.6 (=R_{pipe}/2) pin diameters off axis from pin position

Legend: Simulation settings for the Karman Vortex – free field and straight pipe

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Table 3

		FDA Challenge Geometry
Boundary conditions		Plug flows at the inlet at Re 2000 and 3500 as reported in the literature
		Zero gauge pressure at the outlet
		Non-slip conditions on the pipe wall
Metrics of Performance		Accuracy of the axial velocity profile at specified locations within the geometry, 8mm ahead of, or 24mm and 32mm downstream of, the sudden expansion
		Distribution of the z-component of flow velocity as a function of position along the central axis of the geometry
Discovery Live settings		Modelled as an internal flow
		Probes reporting z-velocity, placed along the axisymmetric axis and radially

Legend: Simulation settings for the FDA nozzle model

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Table 4

Inlet Velocity (m/s)	Re	Shedding Freq from Discovery Live simulation (Hz)	St	St according to literature	Transition time to steady shedding (simulated secs)	Approximate number of seconds wall clock time per second of simulation time.
0.02	100	0.6	0.15	0.16	40	3
0.04	200	1.2	0.15	0.18	25	5
0.06	300	2.1	0.18	0.18	15	8
0.08	400	2.9	0.18	0.19	10	12
0.1	500	3.8	0.19	0.19	7-8	15
0.12	600	4.5	0.19	0.19	5	18
0.14	700	5.4	0.19	0.19	4	21
0.16	800	6.1	0.19	0.19	4	25
0.18	900	6.7	0.19	0.19	4	28
0.2	1000	7.6	0.19	0.19	2-3	31

Legend: Tabulated characteristics of the free field shedding flow (Karman Vortex) as computed by Discovery Live for a range of Re. Comparison with values from the literature is also shown.

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Table 5

Inlet Velocity (m/s)	Re	Shedding Freq from Discovery Live simulation (Hz)	St	Transition time to steady shedding (simulated secs)	Approximate number of seconds wall clock time per second of simulation time.
0.02	100	-			8
0.04	200	2	0.25	15	11
0.06	300	3	0.25	12-13	10
0.08	400	3.9	0.24	11-12	13
0.1	500	4.85	0.24	10-11	15
0.12	600	5.7	0.24	9-10	18
0.14	700	6.6	0.24	7-8	21
0.16	800	7.4	0.23	7-8	24
0.18	900	6	0.17	6-7	28
0.2	1000	6.5	0.16	5-6	29

Legend: Tabulated characteristics of the shedding flow (Karman Vortex) within the straight pipe as computed by Discovery Live for a range of Re. The geometry containing the flow replicates the work of the literature in which experimental flow and CFD at Re=100 produced St=0.3 and St=0.28 respectively. Discovery Live failed to shed vortices at Re=100.