The Openpipeflow Navier–Stokes Solver

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Abstract

Pipelines appear in a huge range of industrial processes involving fluids, and the ability to accurately predict properties of the flow through a pipe is of fundamental engineering importance. Armed with parallel MPI, Arnoldi and Newton–Krylov solvers, the Openpipeflow code may be used in a range of settings, from large-scale simulation of highly turbulent flow, to the detailed analysis of nonlinear invariant solutions (equilibria and periodic orbits) and their influence on the dynamics of the flow.

1 Motivation and significance

The flow of fluid through a straight pipe of circular cross-section is a canonical setting for the study of stability, transition and properties of turbulent flow. At low flow rates, the flow everywhere is in the direction parallel to the axis of the pipe, a simple 'laminar' flow. At larger flow rates it typically undergoes a transition to a complex 'turbulent' flow, characterised by an abundance of swirling 'eddies'. As early as 1883, Reynolds observed that the transition from laminar to turbulent flow is highly dependent on perturbations of finite amplitude to the initial flow [1].[1] Nevertheless, he also noticed that the appearance of turbulence is consistent with respect to the value of the non-dimensional combination DU/ν, at around 2000, where U is the mean axial speed, D the diameter of the pipe, and ν the kinematic viscosity. This combination is the now famous Reynolds Number, $Re = DU/\nu$, used in a huge range of systems involving fluids, where D and U are typical length and velocity scales for the system.

It has been known for some time that the Navier–Stokes equations together with the no-slip boundary conditions accurately predict the evolution of the flow pattern, e.g. the landmark prediction of supercritical transition to a roll pattern for the flow of water between rotating cylinders by G. I. Taylor [2] (transition due to linear instability beyond a critical rotation rate). Despite this development and the legacy of the work of Reynolds, the nature of subcritical transition (transition in the absence a linear instability) and the dynamics of pipe flow has largely remained a mystery. But much has changed following the discovery finite-amplitude solutions to the Navier–Stokes equations, for pipe flow as recently as 2003 [3]. These solutions, often referred to as 'exact coherent states' [4] are believed to embody the processes that sustain turbulence to and form a 'skeleton' for the dynamic paths taken by the evolving flow patterns. Comprehension of the nonlinear dynamics, particularly of transition in pipes, and likewise in Couette and channel flows, has progressed in leaps and bounds over the last decade, based on the study of these solutions. New more general families of solutions continue to be discovered, and their unstable manifolds are just beginning to be calculated [5, 6, 7, 8].

The code that has evolved into Openpipeflow has played a significant role in the realisation of this odyssey. The core code has recently received upgrades, including a substantially improved parallelization, and continues to be augmented with new utilites for extentions and new methods. With the rapid expansion of computational resources that has occurred over this time, pipe flow is a prime example of a 'high-dimensional' system that is receiving examination with methods previously limited to systems with only a few degrees of freedom, such as the Lorenz attractor or the Kuramoto–Sivashinsky equation; see e.g. [9, 10]. In the other direction, observations from large-scale simulations of pipe flow have inspired low-order models [11, 12]. Pipe flow also provides a simple setting for the development of computationally intensive new methods, such as adjoint optimisation techniques, e.g. [13].

2 Software description

Openpipeflow implements a second-order predictor-corrector scheme, with automatic time-step control, for simulation of flow on the cylindrical domain $(r, \theta, z) \in [0, 1] \times [0, 2\pi/m_p) \times [0, 2\pi/\alpha)$,

[1] Reynolds referred to what we now call 'laminar' and 'turbulent' flows by 'direct' and 'sinuous' flow, respectively.

with the discretisation

$$A(r_n, \theta, z) = \sum_{k<|K|} \sum_{m<|M|} A_{nkm} \, \mathrm{e}^{\mathrm{i}(\alpha k z + m_p m \theta)} \, . \tag{1}$$

The dimension θ is naturally periodic ($m_p = 1$), and periodicity in z is a commonplace approximation. Rotational symmetry ($m_p = 2, 3, ...$) is often applied for the study of small-scale structures. The set of finite-difference points r_n, $n = 1..N$ may be arbitrarily distributed on $[0, 1]$, but by default are located at the roots of a Chebyshev polynomial, bunched towards the boundaries to resolve large gradients that occur in the boundary layer. Following the $\frac{3}{2}$ dealiasing rule, the sums are evaluated on $3K \times 3M$ grids in z and θ respectively.

A pressure-Poisson equation (PPE) formulation is employed and an influence-matrix technique applied for the enforcement of boundary conditions [14]. Let $\boldsymbol{g}$ be a vector of boundary conditions, written such that $\boldsymbol{g} = \boldsymbol{0}$ when they are satisfied. The influence-matrix technique has several nice features.:

- Alternative boundary conditions, e.g. slip or oscillations, are easily introduced by changing the single function that evaluates $\boldsymbol{g}$.
- The usual no-slip and divergence conditions at the boundary are satisfied such that $\|\boldsymbol{g}\|$ is typically at the level of the machine epsilon for the given floating-point precision.
- Computational overhead is negligible compared to evaluation of non-linear terms.
- No stability issues have been observed.

Utilities and templates for runtime- and post-processing are included, including a Newton–Rhapson solver for the calculation and continuation of invariant solutions. The Newton solver for the pipe flow, which has a multiple-shooting option (orbits may be split into multiple sections), calls a utility that implements a combined Krylov- Trust-region approach [15]. This Newton–Krylov–Trust-region utility is designed to be integrable with any simulation code.

Openpipeflow is written in standard Fortran90, using basic modules and derived types. Esoteric extensions to the programming language have been deliberately avoided. The code makes use of FFTW, LAPACK and NetCDF libraries. Optionally, for parallel use an MPI library is required.

2.1 Software Architecture and Functionality

See Fig. 1 for a schematic of the code structure and program interaction. Once parameters are set and

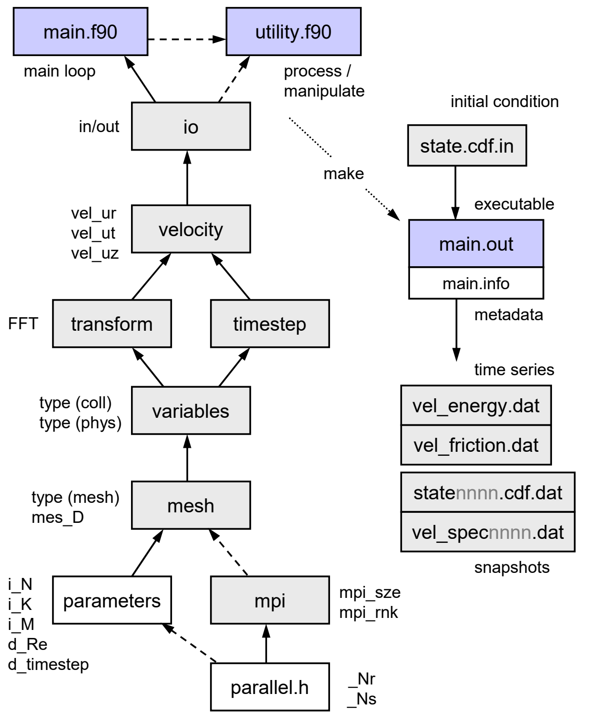

Figure 1: Code structure and program interaction. The MPI library is not required if `_Nr` = `_Ns` = 1. To post-process data it is suffcient for a utility to inherit the io module. To process at run time, it is possible to inherit the whole main loop.

the code built, most jobs begin with a single initial condition, state.cdf.in. Outputs from another job, statennnn.cdf.dat, usually make the best initial conditions (nnnn is a 4-digit numeric label). A variety of potential initial conditions are provided in the database at openpipeflow.org. Truncation or interpolation of initial conditions with another resolution is automatic.

A selection of utilities, plus templates for post-processing or runtime-processing, are described at the online manual.

2.2 Implementation details

Linear systems that originate from the implicit solution of the viscous terms in the Navier–Stokes equations are solved using banded matrices and LU-decomposition for each Fourier mode. By default seven points are involved in the finite-difference stencils.

Parallelisation is acheived via a split into `_Nr` radial and `_Ns` axial sections (#-defined symbols in parallel.h). Due to the form of the data transposes involved in the transforms between 'collocated' (Fourier) and physical space (`type (coll)` and `type (phys)`), the number of cores is limited to $N \times M$. This has been a distant limitation to date.

The recent upgrade to the two-dimensional split from the more obvious one-dimensional 'wall-normal' split (independent 2D-FFTs) extends the maximum number of cores from N to $N \times M$, but also reduces the number of messages that must be sent. The transform involves two stages of FFTs and transposes, but each transpose involves only _Nr or _Ns cores. For _Np = _Nr × _Ns cores, choosing _Nr ≈ _Ns, the number of messages is $O(\sqrt{\_Np})$ versus $O(\_Np)$. This can substantially reduce time lost in latency, the time setting up communications – there are few large messages versus many small ones.

3 Illustrative Examples

3.1 Modelling a Coriolis force

Does the Coriolis force, an extra force term due to rotation of Earth, affect the flow in experiments?

The main loop of the core code calls an empty function several times, var_null(flag), where the flag may be used to detect the current stage of the step. A simple way to model the Coriolis force is then to replace the empty function with a new one in our utility 'Coriolis.f90'. For this example, flag==2 indicates that nonlinear terms have just been evaluated, at which point Coriolis forces may be added to the nonlinear terms. (No changes to the core files, including main.f90, are necessary.)

Figure 2 shows the mean axial profile for laminar and turbulent flow for a pipe oriented east-west at an Ekman number $E = \nu/(2\Omega D^2) = 1$. For a pipe filled with water at 20 °C, this corresponds to a diameter D of approximately 8.3cm; $Re = 5300$ in all cases. For this Re, laminar flow shows a substantial response, whereas turbulent flow shows no asymmetry. The turbulent mean profile is indiscernible from the documented test case [16].

3.2 Unstable manifold of a travelling wave solution

A travelling wave solution is an equilibrium when considered in a frame moving at its phase speed. For a given nearby state, the Newton–Krylov utility (newton.f90) can find such solutions and output their leading unstable eigenvectors. In this case we consider the 'upper branch' solution known as N2_ML, which in its symmetry subclass has a single unstable complex eigenvalue. $Re = 2400$, $\alpha = 1.25$, $m_p = 2$. See [17] for further details. To visualise the unstable manifold, we use the addstates.f90 utility to add small multiples of the eigenvector to the solution. These we use as initial conditions

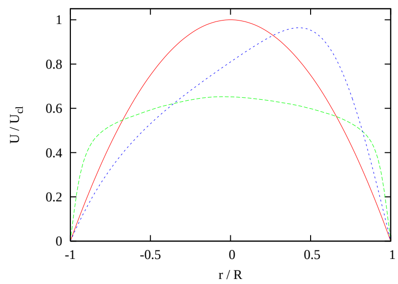

Figure 2: Response of flow at $Re = 5300$ to a Coriolis force. U_{cl} is the centreline speed for laminar flow at this mean flow rate, and $R = D/2$ is the pipe radius. Solid: Laminar flow, $E \to \infty$ (no rotation). Short-dash: Laminar flow, $E = 1$. Long-dash: Turbulent flow, $E = 1$.

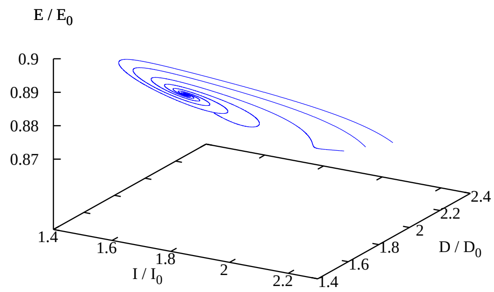

Figure 3: Projection of the unstable manifold of the N2_ML travelling wave solution.

(state.cdf.in), and calculate kinetic energy E, energy input from the applied pressure gradient I, and energy dissipation D, each normalised by their respective value for laminar flow. Figure 3 shows a projection of the unstable manifold of N2_ML, as an outward spiral, and its deformation at larger amplitudes due to nonlinearity.

4 Impact and conclusions

The Openpipeflow solver aims to provide a fast but flexible code, that can be use for state-of-the art research in the study of turbulent flows and transition.

Pipe flow is a classical setting for the development of methods for modelling and analysing dynamical systems, and Openpipeflow has been used by several groups around the world to make an important contribution to notable developments in our understanding of subcritical transition, e.g. [7, 8, 11, 12, 5, 18].

From these developments have arisen many new opportunities. From the theoretical viewpoint, open issues relate to comprehension of the role of newly discovered equilibria and periodic orbits. Such states are believed to provide a skeleton for the dynamics, but describing the topology of the state space for turbulence remains a challenging and active area. Pipe flow, and the study of shear flows in general, draw interest from a range of branches of mathematics and theoretical physics, e.g. pattern formation, control theory, statistical physics, experimental physics. It is an active area of cross-fertilization for the development of mathematical and numerical methods.

From a more practical viewpoint, the dynamical systems approach is being applied in the modelling of other important flows, e.g. flows of fluids of complex rheology, e.g. stress-dependent viscosity, particulate flows and multiphase flows. The study of 'high Reynolds number' flows is also being influenced via application of dynamical systems techniques in large-eddy simulations.

Openpipeflow stands well placed to make an increasingly valuable contribution to this effort. Alongside the application of methods drawn from chaos theory, extensions to Openpipeflow have just been implemented for shear-thinning fluids and LES, for example. From a research perspective, plenty of exciting new developments are in the pipeline.

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Metadata

Nr.	**Code metadata description**	
C1	Current code version	1.11c
C2	Permanent link to code/repository used for this code version	$http://www.openpipeflow.org = index.php?title = File : Openpipeflow - 1.11c.tgz$
C3	Legal Code License	GNU General Public License
C4	Code versioning system used	none
C5	Software code languages, tools, and services used	Fortran90, MPI(optional)
C6	Compilation requirements, operating environments & dependencies	Fortran90, NetCDF, LAPACK, FFTW3
C7	If available Link to developer documentation/manual	$http://www.openpipeflow.org = index.php?title = Manual$
C8	Support email for questions	$ashleypwillis@gmail.com$

Table 1: Code metadata