Reproducible and replicable CFD: it’s harder than you think

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Completing a full replication study of our previously published findings on bluff-body aerodynamics was harder than we thought. Despite the fact that we have good reproducible-research practices, sharing our code and data openly. Here’s what we learned from three years, four CFD codes and hundreds of runs.

Our research group prides itself for having adopted Reproducible Research practices. Barba (2012) made a public pledge titled “Reproducibility PI Manifesto” (PI: Principal Investigator), which at the core is a promise to make all research materials and methods open access and discoverable: releasing code, data and analysis/visualization scripts.

In 2014, we published a study on Physics of Fluids titled “Lift and wakes of flying snakes”. It is a study that used our in-house code for solving the equations of fluid motion in two dimensions (2D), with a solution approach called the “immersed boundary method.” The key of such a method for solving the equations is that it exchanges complexity in the mesh generation step for complexity in the application of boundary conditions. It makes it possible to use a simple mesh for discretization (structured Cartesian), but at the cost of an elaborate process that interpolates values of fluid velocity at the boundary points to ensure the no-slip boundary condition (that fluid sticks to a wall). The main finding of our study on wakes of flying snakes was that the 2D section with anatomically correct geometry for the snake’s body experiences lift enhancement at a given angle of attack. A previous experimental study had already shown that the lift coefficient of a snake cross section in a wind tunnel gets an extra oomph of lift at 35 degrees angle-of-attack. Our simulations showed the same feature in the plot of lift coefficient. Many detailed observations of the wake (visualized from the fluid-flow solution in terms of the vorticity field in space and time) allowed us to give an explanation of the mechanism providing extra lift. It arises from a vortex on the dorsal side of the body remaining closer to the surface under the effects of interactions with secondary vorticity. The flow around the snake’s body cross section adopts a pattern known as a von Karman vortex street. It is a particularly complex flow, because it involves three shear layers: the boundary layer, a separating free shear layer, and the wake. Physically, each of these shear layers is subject to instabilities. The free shear layer can experience 2D Kelvin-Helmholtz instability, while the wake experiences both 2D and 3D instabilities and can show chaotic behavior. Such flows are particularly challenging for computational fluid dynamics (CFD).

When a computational research group produces this kind of study with an in-house code, it can take one, two or even three years to write a full research software from scratch, and complete verification and validation. Often, one gets the question: why not use a commercial CFD package? Why not use another research group’s open-source code? Doesn’t it take much longer to write yet another CFD solver than to use existing code? Beyond reasons that have to do with inventing new methods, it’s a good question. To explore using an existing CFD solver for future research, we decided to first complete a full replication of our previous results with these alternatives. Our commitment to open-source software for research is unwavering, which rules out commercial packages. Perhaps the most well known open-source fluid-flow software is OpenFOAM, so we set out to replicate our published results with this code. A more specialist open-source code is IBAMR, a project born at New York University that has continued development for a decade. And finally,
our own group developed a new code, implementing the same solution method we had before, but providing parallel computing via the renowned PETSc library. We embarked on a full replication study of our previous work, using three new fluid-flow codes.

This is the story of what happened next: three years of dedicated work that encountered a dozen ways that things can go wrong, conquered one after another, to arrive finally at (approximately) the same findings and a whole new understanding of what it means to do “reproducible research” in computational fluid dynamics.

**Story 1: Meshing and boundary conditions can ruin everything**

Generating good meshes for discretization is probably the most vexing chore of computational fluid dynamics. And stipulating boundary conditions on the edge of a mesh takes some nerve, too. An early example of how frustrating it can be to investigate different outflow boundary conditions is reported in Sani et al. (1994). Our first attempts at a full replication study of the 2D snake aerodynamics with IcoFOAM, the incompressible laminar Navier-Stokes solver of OpenFOAM, showed us just how vexing and unnerving these issues can be.

OpenFOAM can take various types of mesh as input. One popular mesh generator is called GMSH: it produces triangles that are as fine as you want them near the body, while getting coarser as the mesh points are farther away. Already, we encounter a problem: how to create a mesh of triangles that gives a comparable resolution to that obtained with our original structured Cartesian mesh? After dedicated effort, we produced the best mesh we could that matches our previous study in the finest cell width near the body. But when using this mesh to solve the fluid flow around the snake geometry, we got spurious specks of high vorticity in places where there shouldn’t be any (Figure 1). Even though the meshes passed the OpenFOAM quality checks, these unphysical vortices appeared for any flow Reynolds number or body angle of attack we tried—although they were not responsible for the simulations to blow up (fail due to rapid error growth). Finally, we gave up with the (popular) GMSH and tried another mesh generator: SnappyHexMesh (details and plots of the meshes are included in the supplementary materials). Success! No unphysical patches in the vorticity field this time. But another problem persisted: after the wake vortices hit the edge of the computational domain in the downstream side, a nasty back pressure appeared there and started propagating to the inside of the domain (Figure 2). This situation is also unphysical, and we were certain there was a problem with the chosen outflow boundary condition in OpenFOAM, but did not find any way to stipulate another, more appropriate boundary condition. We used a zero-gradient condition for the pressure at the outlet (and tried several other possibilities), which we found was a widespread choice in the examples and documentation of OpenFOAM. After months, one typing mistake when launching a run from the command line made OpenFOAM print out the set of available boundary conditions, and we found that an **advective** condition was available that could solve our problem. All this time, we were looking for a **convective** condition, which is just another name for the same thing: satisfying a linear convection equation at the boundary points. Finally, simulations with OpenFOAM were looking correct—and happily, the main feature of the aerodynamics was replicated: an enhanced lift coefficient at 35 degrees angle-of-attack (Figure 3). But not all is perfect. The time signatures of lift and drag coefficient do show differences between our IcoFOAM calculation and the original published ones (Figure 4). The key finding uses an **average** lift coefficient, calculated with data in a time range that is reasonable but arbitrary. Refining the mesh or reducing the exit criterion of the iterative solvers made a difference of less than 0.5% in this quantity. The average force coefficients match (within <3%) our previous results, despite the differences seen on the time series. Are these the same solutions? Is it acceptable as a replication study? We think yes, but this is a judgement call.

**Postmortem.** IcoFOAM solves the fluid equations using a finite-volume method in an unstructured grid, while our published study used an immersed boundary method in a stretched Cartesian grid. Comparing results obtained under such different conditions is a delicate operation. We made our best attempt at creating a fluid mesh for OpenFOAM that was of similar resolution near the body as we had used before. But unstructured grids are complex geometrical objects. Two unstructured meshes built with the same parameters will not be exactly the same, even. The
Fluid-flow solvers we used:

**cuIBM** — Used for our original study (Krishan et al., 2014), this code is written in C CUDA to exploit GPU hardware, but is serial on CPU. It uses the NVIDIA Cusp library for solving sparse linear systems on GPU. https://github.com/barbagroup/cuIBM

**OpenFOAM** — A free and open-source CFD package that includes a suite of numerical solvers. The core discretization scheme is a finite-volume method applied on mesh cells of arbitrary shape. http://www.openfoam.org

**IBAMR** — A parallel code using the immersed boundary method on Cartesian meshes, with adaptive mesh refinement. https://github.com/ibamr/ibamr

**PetIBM** — Our own re-implementation of cuIBM, but for distributed-memory parallel systems. It uses the PETSc library for solving sparse linear systems in parallel. https://github.com/barbagroup/PetIBM

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**Figure 1:** Vorticity field after 52 time-units of flow-simulation with IcoFOAM for a snake’s section with angle-of-attack 35 degrees and Reynolds number 2000. We created a triangular mesh (about 700k triangles) with the free software GMSH. The box insert at the bottom-right shows a zoom-in to the portion of the mesh with spurious vorticity (seen bottom-center of the main plot).

**Figure 2:** Pressure field after 52 (top) and 53 (bottom) time-units of flow-simulation with IcoFOAM for snake section with angle-of-attack 35 degrees and Reynolds number 2000. The simulation crashed after about 62 time-units because of the back pressure at the outlet boundary.

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mesh-generation procedures are not necessarily deterministic, and regularly produce bad triangles that need to be repaired. The complications of building a **good quality** mesh is one of the reasons some prefer immersed boundary methods!

**Story 2: You can hit snags with other researchers’ codes**

Open-source research software can often be poorly documented and unsupported, and on occasion it can even be an unreadable mess. But in this case, we are in luck. IBAMR is a solid piece of software, the code is documented, and you can even get swift response from the authors via the topical online forum. The developers don’t provide a user’s manual, but they have plenty of examples within the code repository. Still, mastering other researchers’ code is challenging and we hit a couple of snags that complicated the journey.

IBAMR is described as “an adaptive and distributed-memory parallel implementation of the immersed boundary method.” The essence of the immersed boundary method is that the fluid is represented by a structured mesh, while the solid boundary is represented by its own, separate mesh that moves with the body. We speak of an Eulerian mesh for the fluid, and a Lagrangian mesh for the solid. The forces exerted by the fluid on the body, and vice versa, appear as an additional integral equation and interpolation schemes between the two meshes. The role of these is to make the fluid “stick” to the wall (no-slip boundary condition) and allow the body to feel aerodynamic forces (lift and drag). Our cuIBM code uses a variant called the immersed-boundary projection method. IBAMR is a library that provides different methods, but despite the variations, we assumed it would work similarly.
We already know that boundary conditions at the outlet of the computational domain can be problematic. This is no different with immersed boundary methods. Our first attempt with IBAMR used a boundary condition at the outlet following their example for flow around a circular cylinder (this turned out to be a traction-free boundary condition). Unfortunately, it resulted in a spurious blockage of the wake vortices when they reach the domain boundary: strong vorticity rebounded from the artificial boundary and propagated back to the domain (Figure 5, top). Of course, this is unphysical and the result is unacceptable.

In a conversation with the main developers on the online forum, they suggested a work-around: using “boundary stabilization,” which adds a forcing to push the vortices out. (IBAMR does not yet provide a convective/advective boundary condition.) With this new configuration, the simulations of the snake profile resulted in a wake that looked physical (Figure 5, bottom), but a computed lift coefficient that was considerably different from our published study (Figure 6). Another dive into Bhalla et al. (2015) led us to notice that the benchmark examples were set up in a way unexpected to us: the no-slip condition is forced inside the body, and not just on the boundary. Immersed boundary methods normally apply the no-slip constraint on boundary points only. When we followed their examples, our simulations with IBAMR were able to replicate the lift enhancement at 35 degrees angle-of-attack, although with a slightly different value of average lift (< 5% off). If we look at the time signature of the lift and drag coefficients, there is excellent agreement with our previous results for 30 degrees angle-of-attack (Re=2000). But at 35 degrees, the time signatures drift apart after about 40 time units (more than 150 thousand time steps). There is a marked drop in the (time varying) lift coefficient (Figure 7), but because the average is calculated over a time range between 32 and 64 time units (a reasonable but arbitrary choice), the final numeric result is not far off our published study. To start, we matched the mesh resolution in the vicinity of the body. Refining the mesh further, reducing the exit criterion of the iterative solver, or enlarging the computational domain did not improve things. Reducing the time
increment, however, did. In Figure 7, we show the time-varying lift coefficients obtained with the parameter CFL set to 0.3 and 0.1—the CFL, or Courant-Friedrichs-Lewy number, constrains the ratio of time increment to grid spacing. Like in the previous case, using OpenFOAM, we make a judgement call that our result with IBAMR does indeed pass muster as a replication of our previous study.

**Postmortem.** Even the best open-source research code can have unexpected attributes that only the original authors know in depth. We still don’t understand why IBAMR requires interior body points to be constrained, despite insistent reading of the literature. One issue that affects our community is that we don’t expect authors to provide in their papers all the details, nor do we require papers to be accompanied by code and data. We learned from this experience that using an open research code and getting correct results with it could involve a long investigative period, potentially requiring communication with the original authors and many failed attempts. If the code is not documented and the original authors not responsive to questions, then building your own code from scratch could be more sensible!
Story 3: All linear algebra libraries are not created equal

Our previous study used culIBM, running on a single GPU device. The largest problem that we can fit in the memory of a high-end GPU has just a few million mesh points, which is not enough to solve three-dimensional flows. We developed PetIBM, a code that uses the same mathematical formulation as culIBM, to allow solving larger problems on distributed CPU systems. Since PetIBM and culIBM implement exactly the same numerical method, you'd expect that giving the two codes the same mesh with the same initial conditions will result in the same solution (within floating-point error). Not so fast! We rely on external libraries to solve sparse linear systems of equations: Cusp for GPU devices and PETSc for distributed CPU systems. It turns out, the iterative solvers may have differences that affect the final solution.

When repeating our previous simulations of the aerodynamics of a snake cross-section with PetIBM, the solutions do not always match those computed with culIBM. At a Reynolds number of 1000, both the time-averaged lift and drag coefficients match. But at Reynolds equal to 2000, average lift and drag match up to 30 degrees angle-of-attack, but not at 35 degrees. That means that we don’t see lift enhancement (Figure 8) and the main finding of our previous study is not fully replicated. Looking at the time evolution of the force coefficients for the simulation with PetIBM at Re=2000 and 35 degrees angle-of-attack, we see a marked drop in lift after 35 time units (top graph in Figure 9). What is different in the two codes? Apart from using different linear algebra libraries, they run on different hardware. Leaving hardware aside for now, let's focus on the iterative solvers. Both Cusp and PETSc use the same convergence criterion. This is not always the case, and needs to be checked! We’re also not using the same iterative solver with each library. The culIBM runs (with Cusp) used an algebraic multigrid preconditioner and conjugate gradient (CG) solver for the modified-Poisson equation. With PETSc, the CG solver crashed because of an indefinite preconditioner (having both positive and negative eigenvalues), and we had to select a different method: we used a bi-CG stabilized algorithm (while still using an algebraic multigrid preconditioner).

Could this difference in linear solvers affect our unsteady fluid-flow solution? The solutions with both codes match at lower angles of attack (and lower Reynolds numbers), so what is going on? Because PetIBM and culIBM use the same method, we don’t need to repeat mesh-convergence analysis. But we did confirm convergence of the solution with respect to the exit criterion of the iterative solvers. We checked everything multiple times. In the process, we did find some small discrepancies. Even a small bug (or two). We found, for example, that the first set of runs with PetIBM created a slightly different problem set-up, compared with our previous study, where the body was shifted by less than one grid-cell width. Rotating the body to achieve different angles of attack was made around a different center, in each case (one used the grid origin at 0,0 while the other used the body center of mass). This tiny difference does result in a different average lift coefficient (bottom graph in Figure 9)! The time signal of lift coefficient shows that the drop we were seeing at around 35 time units now occurs closer to 50 time units, resulting in a different value for the average taken in a range between 32 and 64. Again, this range for computing the average is a choice we made. It covers about ten vortex shedding cycles, which seems enough to calculate the average if the flow is periodic. What is causing the drop in lift? Visualizations of the wake vortices (Figure 10) show that a vortex-merging event occurs in the middle of the wake, changing the near-wake pattern. The previously aligned positive and negative vortices are replaced by a wider wake with a single clockwise vortex on the top side and a vortex dipole on the bottom part. With the change in wake pattern comes a drop in the lift force.

Postmortem. Although PetIBM implements the same immersed-boundary method and was developed by the same research group, we were not able to fully replicate the previous findings. The aerodynamic lift on a snake section at 35 degrees angle-of-attack is a consequence of the near-wake vortices providing extra suction on the upper side of the body. When a vortex merger event changes the wake pattern, lift drops. Vortex merging is a fundamentally two-dimensional instability, so we expect that this problem won’t trouble us in more realistic 3D simulations. But it is surprising that small changes—within the bounds of truncation error, roundoff error and algebraic errors—can trigger this instability, changing the flow appreciably. Even when the only
difference between two equivalent simulations is the linear algebra library used, there can be challenges to reproducibility.

**Story 4: Different versions of your code, external libraries or even compilers may challenge reproducibility**

In the span of about three years, we ran more than 100 simulations with OpenFOAM, IBAMR, and PetIBM, encountering about a dozen things that can go wrong. We replicated our previous scientific finding (enhanced lift at 35 degrees angle-of-attack for sufficiently large Reynolds number) in two out of three campaigns. Ironically, the case that did not replicate our findings was that of our own code re-write. The original code (culIBM) and the re-write (PetIBM) use different linear algebra libraries, and it’s unnerving to think this could change our results. This final story is about what happened when we went back to our original code and tried to reproduce the published findings.

As we mentioned in the opening of this article, we adopted a set of practices years ago to make our research reproducible. The study published as “Lift and wakes of flying snakes” followed the guidance of the “Reproducibility PI Manifesto,” which includes: (1) code developed under version control; (2) completed validation and verification, with report published on Figshare; (3) open data and figures for the main results of the paper on Figshare; (4) pre-print made available on arXiv; (5) code released under MIT License; (6) a Reproducibility statement in the paper. The original work, of course, confirmed grid independence of the solution: Krishnan et al. (2014) report differences in the average lift coefficients in the order of 2% at 35 degrees angle-of-attack and < 0.1% at 30 degrees. Naturally, we expected to be able to reproduce our own results!

The first hurdle we faced is that, three years after we completed our previous study, we have updated our lab computers: new operating systems, new GPU devices, new external libraries. The code itself has been modified to implement new features. Happily, we have version con-
So, we set out to reproduce our results with cuIBM using (1) the “same” old version of the code and (2) the current version. In both cases, we used identical input parameters (Lagrangian markers to discretize the geometry, grid parameters, flow conditions, and solver parameters). But the three-year-old simulations used a version of Cusp (0.3.1) that is no longer compatible with the oldest CUDA version installed on our machines (5.0). Thus, we adapted “old” cuIBM to be compatible with the oldest version of Cusp (0.4.0) that we can run. The case at angle-of-attack 35 degrees and Reynolds number 2000 now gave an appreciable difference compared with our previous study: the instantaneous force coefficients start to slowly drop after about 60 time units (Figure 11(c)). Now, this is really the same code, with only a difference in the version of the linear algebra library. Repeating the case with the most current version of cuIBM and the same version of Cusp (0.4.0) leads to the same force signals, with a slight drop towards the end (Figure 11(d)). And the same is the case with the current version of cuIBM and a later version of Cusp (0.5.1). The final findings in these cases do not vary from our published work: there is, in fact, lift enhancement at 35 degrees angle-of-attack … but the results match only because we calculate the average lift in a time interval between 32 and 64. Yet, the flow solution was affected by changing the version of a dependent library. (The revision history of Cusp says that they refactored the smooth-aggregation solver between the two versions we are using.) The hardware was also different (a K20 GPU versus a C2070 in our older study), and the operating system, and the compiler. (Note that we always run in double precision.) In an iterative linear solver, any of these things could be related to lack of floating-point reproducibility. And in unsteady fluid dynamics, small floating-point differences can add up over thousands of time steps to eventually trigger a flow instability (like vortex merging).

**Postmortem.** Making research codes open source is not enough for reproducibility: we must be meticulous in documenting every dependency and the versions used. Unfortunately, some of those dependencies will get stale over time, and might cease to be available or usable. Your application code may give the same answer with a different version of an external library, or it may not. In the case of unsteady fluid dynamics, the nonlinear nature of the equations combined with numerical non-reproducibility of iterative linear solvers (in parallel!) can change the results.

**Lessons learned**

Reproducibility and replication of studies are essential for the progress of science, and much of science today advances via computation. We use computer simulations to create new knowledge. How can we certify that this new knowledge is justified, that there is enough evidence to support it? The truth is computational science and engineering lacks an accepted standard of evidence. Some previous efforts in CFD have sought to compare results from multiple codes: e.g., Dimonte et al. (2004) report results for Rayleigh-Taylor instability using seven different
Figure 11: Instantaneous force coefficients on the snake’s section at Reynolds number 1000 and angle 35 degrees (top-left) and Reynolds number 2000 and angle 30 degrees (top-right). Bottom-left: instantaneous force coefficients at Reynolds number 2000 and angle-of-attack 35 degrees running the same version of cuIBM (adapted to CUSP-0.4.0) than the one used for our previous study. Bottom-right: drop of the mean force coefficients observed over the end of the simulation using two versions of cuIBM (“current” and “old”) with different CUSP versions (0.4.0 and 0.5.1).

Definition of reproducible research:

The literature is rife with confused and sometimes contradictory meanings for reproducible research, reproducibility, replicability, repetition, etc. It is thus worth clarifying what we mean by these terms. The phrase “reproducible research” in reference to computational studies that can be reproduced by other scientists was introduced by geophysics professor Jon Claerbout in the 1990s. An early volume of CiSE published an article about the reproducible-research environment they created in his group at Stanford. Their goal was complete documentation of scientific computations, in such a way that a reader can reproduce all the results and figures in a paper using the author-provided computer programs and raw data. This ability requires open data and open-source software, and for this reason the reproducibility movement is closely linked with the open science movement. In following years, the term replication was distinctly adopted to refer to an independent study, re-running experiments to generate new data that, when analyzed, leads to the same findings. We follow this convention, clarified more recently in an article in Science.

Reproducible research—Authors of a study provide their code and data, allowing readers to inspect and re-run the analysis to recreate the figures in the paper. Reproducible research makes replication easier.

Replication—An independent study that generates new data, using similar or different methods, and analyzes it to arrive at the same scientific findings as the original study.

CiSE has dedicated two theme issues to reproducibility: January/February 2009 and July/August 2012.
codes (from five institutions), while the AIAA drag-prediction workshop\textsuperscript{12} and the high-lift-prediction workshop\textsuperscript{13} have been collecting results for years using a variety of commercial and non-commercial (mostly closed) software. However, these efforts don’t have a specific goal of replicating a published finding nor are they concerned with reproducible workflows. We label computational research reproducible when authors provide all the necessary data and the computer code to run the analysis again, re-creating the results. But what data are necessary? We found that open-source code and open data sets are a minimal requirement. Exhaustive documentation during the process of computational research is key. This includes documenting all failures. Current publication custom is biased towards positive results.\textsuperscript{14} The CFD community does not have a habit of communicating negative results; one rare example is the analysis of Godunov methods and its failures by Quirk (1997).\textsuperscript{15} In the case of IBAMR, negative results with points only on the boundary are not among the examples provided: the situation may be obvious to the authors, but not to the users. We learned how important the computational mesh and the boundary conditions can be. A reproducible computational paper should include the actual meshes used in the study (or a deterministic mesh-generation code) and careful reporting of boundary conditions. This is rarely (if ever!) the case. We learned that in addition to developing our code under version control, we need to carefully record the versions used for all dependencies. In practice, such careful documentation is feasible only with a fully automated workflow: launching simulations via running scripts, storing command-line arguments for every run, capturing complete environment settings. Post-processing and visualization ideally should also be scripted, avoiding software GUIs for manipulation of images. New tools have emerged to help reproducible workflows; for example, Docker containers to capture the full state of the operating system, application software, and dependencies.

We learned that highly unsteady fluid dynamics is a particularly tough application for reproducibility. The Navier-Stokes equations are nonlinear and can exhibit chaotic behavior under certain conditions (e.g., geometry, Reynolds number, external forcing). Some flow situations are subject to instabilities, like vortex merging in two dimensions and other vortex instabilities in 3D. In any application that has sufficient complexity, we should repeat simulations checking how robust they are to small variations. And report negative results! Understandably, long 3D simulations that take huge computational resources may not be feasible to repeat. We should continue the conversation about what it means to do reproducible research in high-performance computing (HPC) scenarios. When large simulations run on specific hardware with one-off compute allocations, they are unlikely to be reproduced. In this case, it is even more important that researchers advance towards these HPC applications on a solid progression of fully reproducible research at the smaller scales.

Computational science and engineering makes ubiquitous use of linear algebra libraries like PETSc, Hypre, Trilinos and many others. Rarely do we consider that using different libraries might produce different results. But that is the case. Sparse iterative solvers use various definitions of the tolerance criterion to exit the iterations, for example. The very definition of residual could be different. This means that even when we set the same value of the tolerance, different libraries may declare convergence differently! This poses a challenge to reproducibility, even if the application is not sensitive to algebraic error. The situation is aggravated by parallel execution. Global operations on distributed vectors and matrices are subject to rounding errors that can accumulate to introduce uncertainty in the results.

We are recommending more rigorous standards of evidence for computational science and engineering, but the reality is that most CFD papers are not even accompanied by a release of code and data. The reasons for this are varied: historical, commercial interests, academic incentives, time efficiency, export controls, etc. The origins of CFD in the Los Alamos Laboratory in the 1940s was secret research, and when computer code was stored in large boxes of punched cards or big rolls of magnetic tape, there was hardly a way to “share” it.\textsuperscript{16} The 1970s saw the birth of commercial CFD, when university professors and their students founded companies funded under the US government’s SBIR program. It’s not unreasonable to speculate that the potential for commercial exploitation was a deterrent for open-source release of CFD codes for a long time. It is only in the last 15 years or so that open-source CFD codes have become available. But the CFD literature became entrenched in the habit
of publishing results without making available the code that generated those results. And now, we face the clash between the academic incentive system and the fact that reproducible research takes a substantial amount of time and effort. This campaign to replicate our previous results taught us many lessons on how to improve our reproducibility practices, and we are committed to maintaining this high standard. We will continue to share our experiences.

Supplementary materials

We provide supplementary materials in the GitHub repository for this paper, including: (1) all input files to generate the runs reported in the paper; (2) Jupyter notebooks for all the simulations, detailing every condition (dependencies, compilation, mesh, boundary conditions, solver parameters, command-line options); (3) Python codes needed to recreate all the figures included in the paper. In addition, we separately report our efforts to assess independence of the solution with respect to grid spacing, time increment and iterative tolerance (with each code).

Our codes are available for unrestricted use, under the MIT license; to obtain the codes and run the tests in this paper, the reader may follow instructions on https://github.com/barbagroup/snake-repro.

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