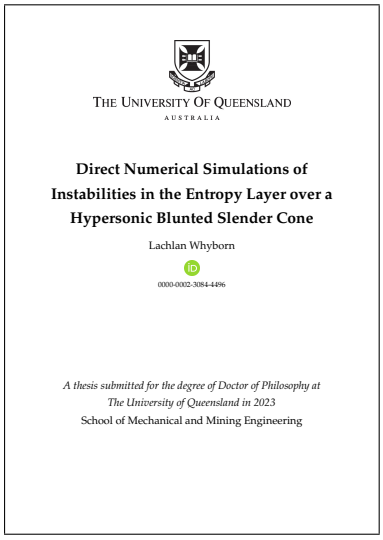
GDTk CHANGELOG 2023-q[2,3,4]

A newsletter for the GDTk Community

11 December 2023

A big year and little time to write the newsletter, so we've packed three quarters of the year into this newsletter: the second and final for 2023.

Congratulations Doctor Whyborn!


THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

Direct Numerical Simulations of Instabilities in the Entropy Layer over a Hypersonic Blunted Slender Cone

Lachlan Whyborn

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A thesis submitted for the degree of Doctor of Philosophy at The University of Queensland in 2023
School of Mechanical and Mining Engineering

Lachlan Whyborn was conferred with his Doctor of Philosophy from The University of Queensland on the 11th of September, 2023. Congratulations Lachlan!

Lachlan used very high fidelity numerical simulations to study instabilities that may lead to transition in the entropy layers of blunted cones in a hypersonic stream. His simulations led to the observation that the entropy layer is receptive to far field disturbances and that the mechanism for instability is one of transient growth. No doubt Lachlan can give you a more nuanced interpretation of his results, and I'm sure he would be pleased to do so.

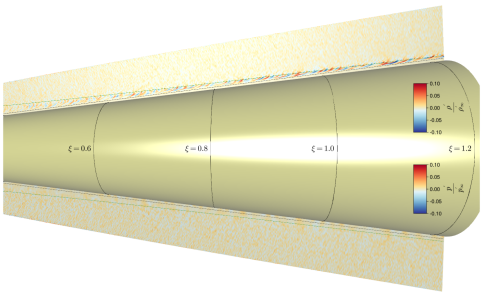
I recall giving a brief introduction at Lachlan's PhD confirmation seminar. At the time, I said an exciting part of Lachlan's project, for me, was that we would be attempting direct numerical simulations with Eilmer for the first time[1] and this would require high-order low-dissipation numerics to get there. It would also require a very close attention to detail at boundaries and block connections so that numerical noise did not pollute the simulation of the flow physics. I am pleased and proud to say we got there, and by we, I mean the heavy lifting was Lachlan's efforts. Peter and I provided character-building arguments with Lachlan along the way.[2] One highlight during Lachlan's project was setting the record for largest Eilmer simulation ever, in terms of cell count. (See last newsletter `2023.q1`).

Lachlan began his PhD study in April of 2019. Let that sink in a moment and try to recall how the world was then! In June of 2019, Lachlan and I travelled to Munich for a kick-off meeting with our project partners, led by Christian Stemmer, at the Technical University of Munich. We had a week of idea exchange and enthusiastically mapped out a 3-year plan that involved student and academic visits in Australia and Germany. Our 3-year plan evaporated in the early part of 2020 and was replaced with zoom meetings; the COVID-19 pandemic had effectively ground international travel to a halt. Nevertheless, in 2022, the PhD students honoured their commitment to the project and did their study exchanges as soon as things were reasonably safe to travel (even if the world mood was still uncertain). Lachlan headed to Germany for a 3-month visit to our TUM partners in June of 2022. Lachlan told me that this was an extremely valuable experience in the early part of his academic career.

The GDTk team is proud of Lachlan's accomplishment and we're pleased that Lachlan is still writing code and challenging the rest of the development team on their assumptions. Lachlan also likes to provoke us on occasion by declaring that `Julia` is the one programming language to the rule them all (for scientific computing). I'm pretty sure that provocation will continue too.

[1] The academic in me needs to qualify this claim. What I mean here by DNS is a deliberate attempt to control grid point spacing so that all temporal frequencies of interest are resolved.

[2] During these robust discussions, it was never entirely clear whose character was being built.

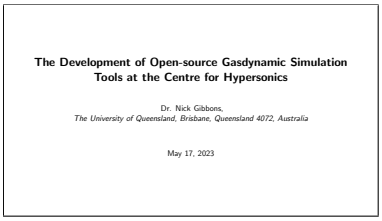


Snapshot of of density and pressure fluctuations, showing that coherent structures in the density field form withing the entropy layer. Entropy layer edege in green; boundary layer edge in black.

GDTk team attends 2023 Queensland Research Software Developers Forum

On 18 May 2023, the GDTk team attended the first ever gathering of Queensland research software engineers and developers. The event was hosted at The University of Queensland and brought together researchers and developers involved in software to support research from around South-east Queensland.

The various groups were invited to introduce themselves to the community via a 10-minute talk. Nick Gibbons presented on behalf of the GDTk group.


The Development of Open-source Gasdynamic Simulation Tools at the Centre for Hypersonics

Dr. Nick Gibbons,
The University of Queensland, Brisbane, Queensland 4072, Australia

May 17, 2023

Welcome Volker Hannemann!

Dr Volker Hannemann from the Deutsches Zentrum für Luft- und Raumfahrt (DLR), Göttingen, joined us in Brisbane for an academic visit commencing on August 2, 2023. As part of welcoming Volker and as a chance to be introduced to everyone, we held an afternoon of Lightning Talks on August 4, 2023 (more on that in the next item). Volker is a scientist in the Spacecraft department and works as a developer of DLR's CFD code, TAU. Volker will be with us as an academic visitor for approximately 6 months. Volker arrived in Australia just in time for some Women's World Cup action, so we took an evening off from CFD to watch Germany play South Korea in the local Brisbane stadium.

In terms of technical activities, Volker has been getting to know our hypersonic code, `Eilmer`, and getting to know the code at the source level. Volker has been working on an implementation of a shock sensor that relies on a transport equation, an idea put forward by Rathi and Sinha.[3] Additionally, Volker regularly joins us at the Eilmer developers' meeting, the Eilmer Users Catch-up, CFTeaTime and the School's fortnightly Computer & Fluids discussion.

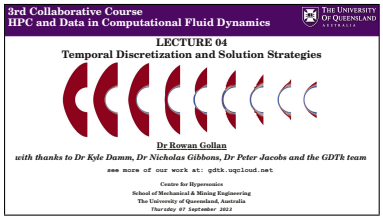
[3] Rathi and Sinha (2023), AIAA J. 61(8), `https://doi.org/10.2514/1.J062810`

Lightning Talks in August 2023

If you spot one of these coffee cups around the Mansergh Shaw Building, you can assume that a speaker at the Winter Lightning Talks is nearby. (The postdocs convinced me that we needed SWAG at the lightning talk events.) On Friday 4 August 2023, we had an afternoon of lightning talks (10-minute presentations) as a way for Volker Hannemann to get to know everyone in the group. As we've come to expect, there was a wide variety of topics packed into 3.5 hours. Here's the list of presenters and talk titles.

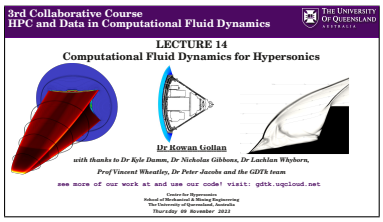
Lachlan Whyborn	An Introduction to Quantum Computing
Alex Muirhead	Rockets!
Carrie Xie	Control Point Form Grid Generation
Rowan Gollan	Brain Chemistry (using neural nets for chemical kinetics)
Rob Watt	Onsager's conjecture: Energy Dissipation in the Euler Equations
Peter Jacobs	Alien Technology for Extracting Cube Roots
Nick Gibbons	Thermodynamics and Dungeons and Dragons
Christine Mittler	The History of Chip Development, or: How a Law became a Trap
Volker Hannemann	Personal Wishlist to Santa CFD
Jamie Border	Simulating heat transfer using Walk-on-Spheres
Daisy Liu	Vacuum Ultraviolet and Visible Spectral Measurements for Simulated Saturn Entry
Kyle Damm	Lord of the Fluxes: One Gradient Approximation to Rule Them All

GDTk contribution to HPCD-CFD lecture series



Around the middle of the year, I had the opportunity to represent the activities of compressible flow CFD in Australia as a member of the organising committee for the High-Performance Computing and Data in Computational Fluid Dynamics (HPCD-CFD) graduate-level course. The course ran from 29 August 2023 to 23 November 2023. It was coordinated by Intersect and supported by National Compute Infrastructure Australia. More details at: `https://intersect.org.au/education/collaborative-graduate-courses/3rd-collaborative-course`

As part of the course, I delivered two lectures in the series. The first (Lecture 4) was quite fundamental in nature and dealt with temporal discretisation. I did get a chance to sneak in some of our cutting-edge algorithm development work by talking about the super time-stepping for solid domains and the Jacobian-free Newton-Krylov solver for accelerating steady-state convergence. The second lecture dealt with the role of CFD for hypersonics. It was a challenge to give coverage to that topic in just 60 minutes, so I made a selective and quite locally biased sampling of the hypersonic CFD activities.



The slides for those lectures are hosted on our Presentations page. There are many who contributed content to the slides and thanks goes to all of those members of the GDTk community. A special mention is noted on the title slides to the contributions of Kyle, Nick, Lachlan, Peter and Vince.

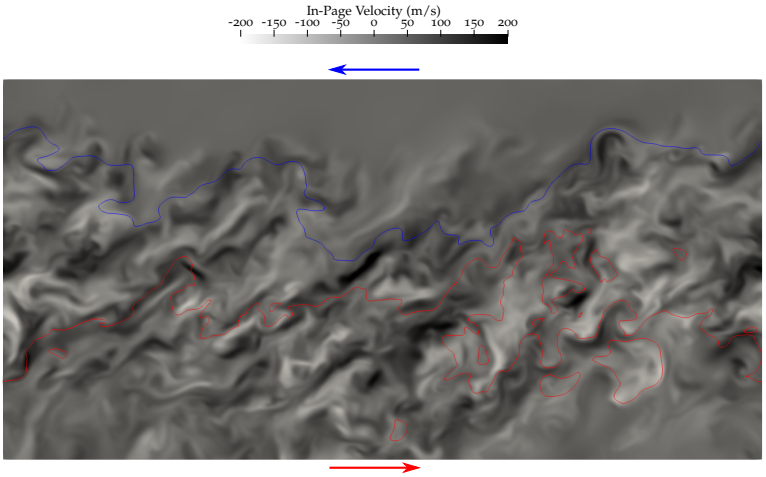
Dev team talks in Centre for Hypersonics seminar series

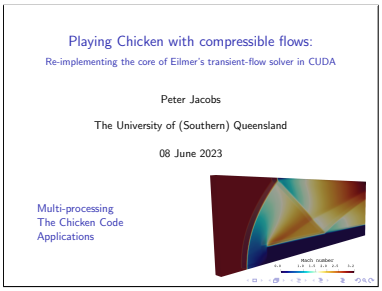
In 2023, three of the core developers gave talks as part of the Centre for Hypersonics seminar series.

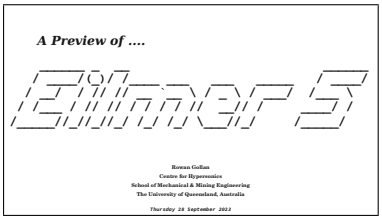
Peter Jacobs, on June 8, spoke about his work on the `Chicken` flow solver. This included some history of modern computer architecture (CPUs) and how that compares and contrasts to GPUs. The talk finished with a demonstration of `Chicken` for some three-dimensional simulations of compressible flow.

On September 28, I gave a preview of Eilmer 5 to the Hypersonics group. I covered the motivation for a version bump from 4 to 5, some recent history and successes in Eilmer development, status of Eilmer 5 development, and a plan for roll-out within the group.

Nick Gibbons presented his recent efforts on optimising the performance of Eilmer to the hypersonics group on November 16. Specifically, Nick has been working on our choice and use of data structures, and how we can code to give favourable access to the data in memory. His talk covers some investigations at small scale and then some practical results at large scale. Nick showed speed-up of 2.25x on a 20-million cell turbulent reacting DNS of a mixing/reacting layer (below). The simulation used 640 cores on one of the Australian supercomputers, Setonix. Before the performance optimisation work, this simulation required 30+ hours of wall-clock time. After: the same simulation ran in 13.4 hours.







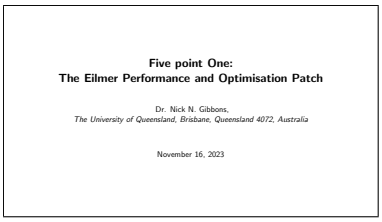


Figure 1: Direct numerical simulation of a reacting mixing layer of ethylene and air. Arrows show initial flow direction. Below the red contour is predominantly fuel; above the blue contour is predominantly air; in between the two is the mixing and burning region.

What's coming up

Here are some things to watch for in the early part of 2024:

- Eilmer 5 to go prime time! The plan is to grow the user base from core team to wider members of the Centre for Hypersonics, and then further. We are staging the roll-out so that we can manage the support to users.
- Peter and Rowan to present an invited Eilmer workshop at the von Karman Institute for Fluid Dynamics in the lecture series on Advanced Computational Fluid Dynamics Methods for Hypersonic Flows from March 25–29 2024.

A request to readers: I would welcome content from our larger community of users. Please send in your news and I'll try to include it in an upcoming newsletter. (It might help me get the newsletter written more frequently also!)